TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

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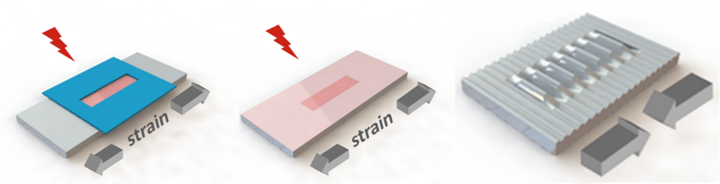
Formation of wrinkles in a bi-layer system using manifold-valued finite elements

GAMM 2023 Dresden, June 2nd, 2023

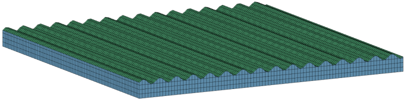
Formation of wrinkles in bi-layer systems

- project with Leibniz-Institute for Polymer Research Dresden
- **goal: creation of wrinkles of different wavelengths ($sub\!-\!\mu m$) with sharp transition areas while controlling the splitting behavior**
- experiments:
  1. stretching of the base material (elastic polymer layer)
  2. creation of a thin structured layer on top through different gas treatments
  3. relaxation of the base layer



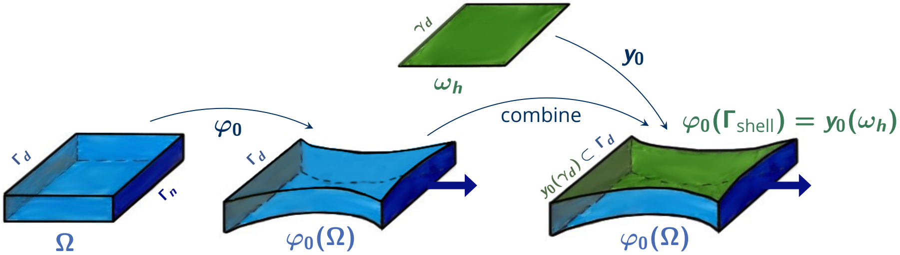
Simulation of the bi-layer system

- modelling the bi-layer system:
  - combination of an elastic 3D-model and an elastic shell model
  - minimization problem of a non-linear and non-convex energy functional
- simulation of the minimization problem:
  - discretization using appropriate finite elements
  - solve the discrete problem numerically
- analytical results: existence of solutions of the continuous and discrete minimization problem



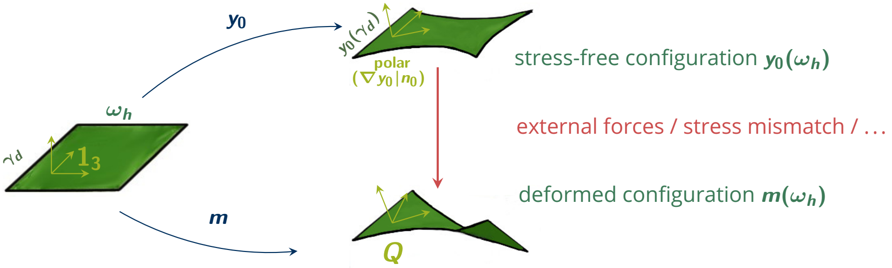
Combination of an elastic 3D-model and an elastic shell model

- elastic 3D-model: Mooney-Rivlin material model
- elastic shell model: Cosserat shell model
- base material in stress-free state is $\Omega \subset \mathbb{R}^3$, stretched state is $\varphi_0(\Omega)$
- shell in stress-free state is the curved manifold $\varphi_0(\Gamma_{\text{shell}}) \subset \partial\varphi_0(\Omega)$
- parameter domain $\omega_h \subset \mathbb{R}^2$ with $y_0(\omega_h) = \varphi_0(\Gamma_{\text{shell}})$, $y_0 \in H^1(\mathbb{R}^2, \mathbb{R}^3)$



Shell model: Cosserat shell model with initial curvature

- shell in stress-free state is the curved manifold $y_0(\omega_h)$
- deformed configuration given through pair (m, Q)
- deformation function $m : \omega_h \to \mathbb{R}^3$, microrotation $Q : \omega_h \to \mathrm{SO}(3)$
- no normality assumptions, in-plane rotations



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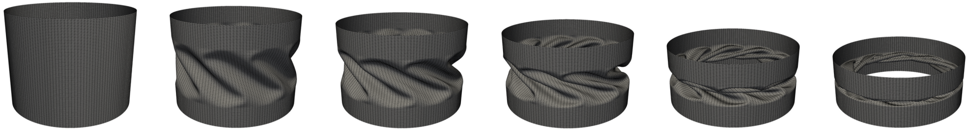

[N., Sander, Neff, Bîrsan. (2023). A geometrically nonlinear Cosserat shell model for orientable and non-orientable surfaces: Discretization with geometric finite elements. Submitted.]

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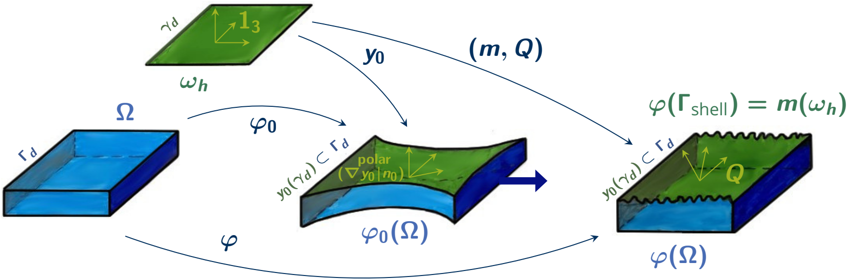
Dirichlet nodes in pink.

[N., Sander, Neff, Bîrsan. (2023). A geometrically nonlinear Cosserat shell model for orientable and non-orientable surfaces: Discretization with geometric finite elements. Submitted.]

Combination of an elastic 3D-model and an elastic shell model

- mismatch of the stress-free states results in wrinkled configuration
- configuration: deformation and microrotation function pair (φ, Q)
- deformations $\varphi : \Omega \to \mathbb{R}^3$ and $m : \omega_h \to \mathbb{R}^3$
- microrotation $Q : \omega_h \to \mathrm{SO}(3)$



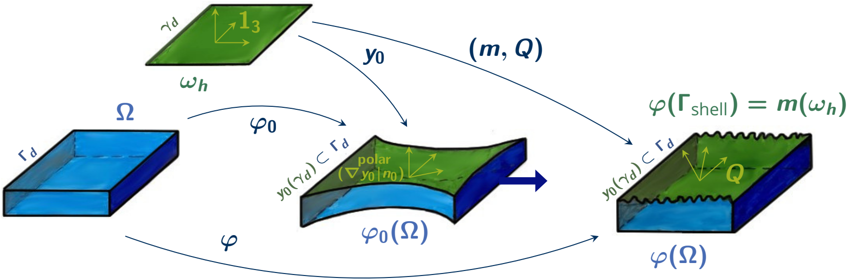
Combination of an elastic 3D-model and an elastic shell model

- wrinkled configuration (φ, Q) is a minimizer of the combined functional

$$J = J_{3D}(\nabla \varphi) + J_{\text{shell}}(\nabla m, Q, \nabla Q) \qquad \text{with } \varphi(\Gamma_{\text{shell}}) = m(\omega_h)$$

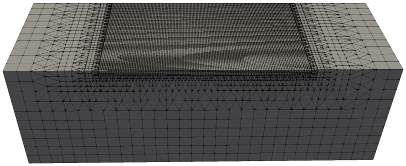
$$\text{on } A = \left\{ (\varphi, Q) \in W^{1,q}(\Omega, \mathbb{R}^3) \times H^1(\omega_h, \mathrm{SO}(3)) \;\middle|\; q > 3,\ \varphi|_{\Gamma_d} = Id,\ \varphi|_{\Gamma_{\text{shell}}} \in H^1 \right\}$$

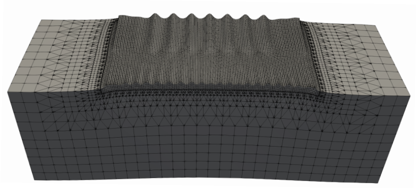
- existence of minimizing function pairs follows with the direct method



Discretization of the continuous model

- discretize Ω using an appropriate triangulation $\mathcal{T}$
- yields matching triangulation τ of ω_h
- Lagrange finite elements of order p_1 for the deformation: $\varphi_h \in V_{p_1}(\mathcal{T}, \mathbb{R}^3)$
- rotation function Q maps to the nonlinear manifold SO(3)
  $\rightarrow$ manifold-valued FE space $V_{p_2}(\tau, \mathrm{SO}(3)) \subset H^1(\tau, \mathrm{SO}(3))$
- generalize Lagrange interpolation to a nonlinear Riemannian manifold $\mathcal{M}$



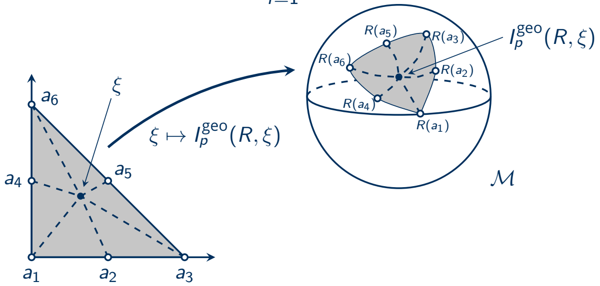


Construction using geodesic distances

- for $T \in \tau$ consider Lagrange nodes $a_1, \dots, a_m$ and polynomials $\lambda_1, \dots, \lambda_m : T \to \mathbb{R}$
- recall p-th order Lagrange polynomial interpolation of a function $f : T \to \mathbb{R}$

$$f_h(\xi) = I_p^{\text{poly}}(f(a_1), \dots, f(a_m), \xi) := \sum_{i=1}^m \lambda_i(\xi) f(a_i) \quad \text{is equivalent to}$$

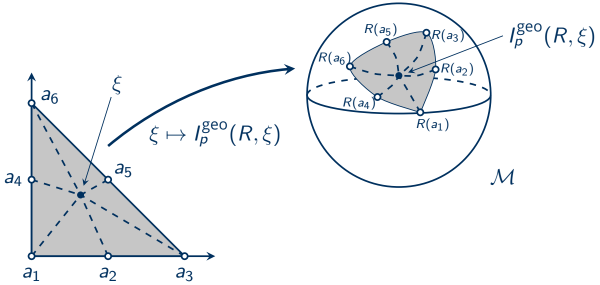
$$f_h(\xi) = \arg\min_{x \in \mathbb{R}} \sum_{i=1}^{m} \lambda_i(\xi) \, |f(a_i) - x|^2$$



Construction using geodesic distances

- Lagrange interpolation

$$f_h(\xi) = \arg\min_{x \in \mathbb{R}} \sum_{i=1}^{m} \lambda_i(\xi)\, |f(a_i) - x|^2$$



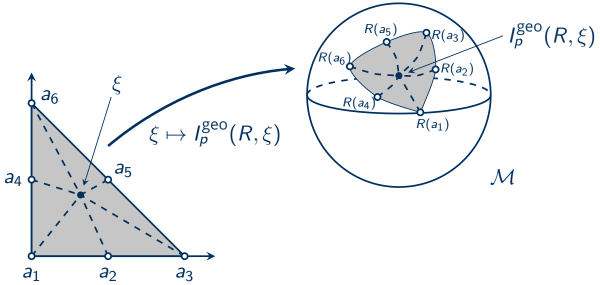
Construction using geodesic distances

- Lagrange interpolation

$$f_h(\xi) = \arg\min_{x \in \mathbb{R}} \sum_{i=1}^{m} \lambda_i(\xi) \, |f(a_i) - x|^2$$

- define geodesic interpolation of $R : T \to \mathcal{M}$

$$R_h(\xi) = I_p^{\text{geo}}(R(a_1), \dots, R(a_m), \xi) := \arg\min_{M \in \mathcal{M}} \sum_{i=1}^{m} \lambda_i(\xi) \operatorname{dist}(R(a_i), M)^2$$



Construction using geodesic distances

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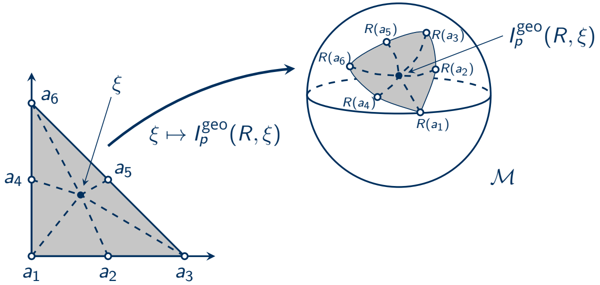
$$R_h(\xi) = I_p^{\text{geo}}(R(a_1), \dots, R(a_m), \xi) := \underset{M \in \mathcal{M}}{\arg\min} \sum_{i=1}^{m} \lambda_i(\xi) \operatorname{dist}(R(a_i), M)^2$$

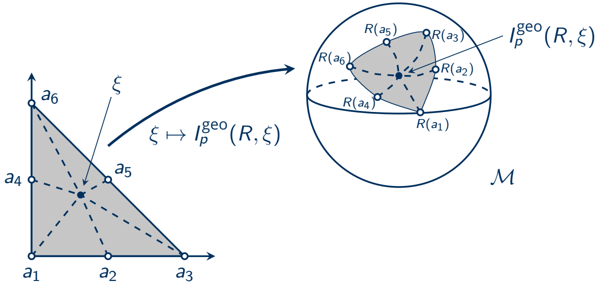


Construction using geodesic distances

- define geodesic interpolation of $R : T \to \mathcal{M}$

$$R_h(\xi) = I_p^{\text{geo}}(R(a_1), \dots, R(a_m), \xi) := \operatorname*{arg\,min}_{M \in \mathcal{M}} \sum_{i=1}^{m} \lambda_i(\xi) \operatorname{dist}(R(a_i), M)^2$$

- minimizer can be found by Newton-type method
- define global finite element space $V_p^{\text{geo}}(\tau, \mathcal{M})$ by demanding continuity on τ



Discrete minimization problem

Problem

Minimize

$$J(\varphi_h, Q_h) = J_{3D}(\nabla \varphi_h) + J_{shell}(\nabla m_h, Q_h, \nabla Q_h) \qquad \text{with } \varphi(\Gamma_{shell}) = m_h(\omega_h)$$

in the admissible set

$$A_h = \left\{ (\varphi_h, Q_h) \in V_{p_1}(\mathcal{T}, \mathbb{R}^3) \times V_{p_2}(\tau, SO(3)) \,\middle|\, (\varphi_h)_{|\Gamma_d} = Id \right\}.$$

Theorem

The above minimization problem has a solution if J fulfills reasonable assumptions.

Proof: Direct method in the calculus of variations:

- *J is bounded from below, weakly lower semi-continuous and coercive.*
- *The limit of a pointwise convergent function sequence in A_h is again in A_h.*

Algebraic minimization problem

Problem

Minimize

$$J(\vec{\varphi}_h, \vec{Q}_h) = J_{\mathrm{MR}}(\vec{\varphi}_h) + J_{\mathrm{shell}}(\vec{m}_h, \vec{Q}_h) \qquad \text{with } \varphi_h(\Gamma_{\mathrm{shell}}) = m_h(\omega_h)$$

in the admissible set

$$\vec{A}_h = \left\{ (\vec{\varphi}_h, \vec{Q}_h) \text{ coefficients for } (\varphi_h, Q_h) \,\middle|\, (\varphi_h)_{|\Gamma_d} = Id \right\}.$$

- $\vec{A}_h \subset \mathbb{R}^{3N_{3D}} \times (\mathrm{SO}(3))^{N_{2D}}$
- N_{3D} and N_{2D}: total number of degrees of freedom in triangulations $\mathcal{T}$ and τ
- **nonlinear, nonconvex minimization problem** on $\mathbb{R}^{3N_{3D}} \times (\mathrm{SO}(3))^{N_{2D}}$
- solve using **Riemannian trust-region method**
  or **Riemannian proximal Newton method**

Riemannian trust-region method for $J : \mathcal{M} \to \mathbb{R}$

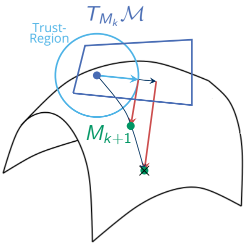
Given an iterate $M_k \in \mathcal{M}$, a retraction $R_{M_k} : T_{M_k}\mathcal{M} \to \mathcal{M}$ and a Trust-Region radius r_k:

1. approximate J around M_k using a quadratic model

$$q_k : T_{M_k}\mathcal{M} \to \mathbb{R}$$

$$q_k(s) = J(M_k) + \left\langle \operatorname{grad}_M J_{|M_k}, s \right\rangle + \frac{1}{2}\left\langle \operatorname{Hess}_M J_{|M_k} \cdot s, s \right\rangle$$

where $\operatorname{grad}_M \in T_M\mathcal{M}$ and $\operatorname{Hess}_M \cdot s \in T_M\mathcal{M}$



2. minimize q_k inside the trust region

$$s_k = \operatorname*{arg\,min}_{s \in T_{M_k}\mathcal{M}, \|s\| \le r_k} q_k(s)$$

i.e. solve $\operatorname{Hess}_M J_{|M_k} s_k = -\operatorname{grad}_M J_{|M_k}, \|s\| \le r_k$

3. if $J(R_{M_k}(s_k)) \ge J(M_k)$ or q_k approximates J badly: decrease r_k and repeat step
   if $J(R_{M_k}(s_k)) < J(M_k)$ and q_k approximates J well: set $M_{k+1} = R_{M_k}(s_k)$, increase r_k according to quality of q_k

4. return M_{k+1} once $\|s_k\| < \text{tol}$

[Absil, Mahony, & Sepulchre. (2008). Optimization Algorithms on Matrix Manifolds. Princeton, New Jersey.]

Riemannian Proximal Newton method for $J : \mathcal{M} \to \mathbb{R}$

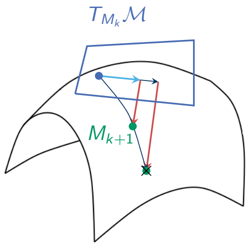
Given $M_k \in \mathcal{M}$, retraction $R_{M_k} : T_{M_k}\mathcal{M} \to \mathcal{M}$ and a regularization parameter p_k:

1. approximate J around M_k using a quadratic model

$$q_k : T_{M_k}\mathcal{M} \to \mathbb{R}$$

$$q_k(s) = J(M_k) + \langle \operatorname{grad}_M J_{|M_k}, s\rangle + \frac{1}{2}\langle [\operatorname{Hess}_M J_{|M_k} + p_k \cdot Id][s], s\rangle$$

where $\operatorname{grad}_M \in T_M\mathcal{M}$ and $\operatorname{Hess}_M[s] \in T_M\mathcal{M}$,
p_k such that $[\operatorname{Hess}_M J_{|M_k} + p_k \cdot Id]$ is positive definite



2. minimize q_k $\qquad s_k = \arg\min_{s \in T_{M_k}\mathcal{M}} q_k(s)$

i.e. solve $\qquad \left[\operatorname{Hess}_M J_{|M_k} + p_k \cdot Id\right] s_k = -\operatorname{grad}_M J_{|M_k}$

3. if $J(R_{M_k}(s_k)) \geq J(M_k)$ or q_k approximates J badly: increase p_k and repeat step
   if $J(R_{M_k}(s_k)) < J(M_k)$ and q_k approximates J well: set $M_{k+1} = R_{M_k}(s_k)$, decrease p_k according to quality of q_k
4. return M_{k+1} once $\|s_k\| < \text{tol}$

[Huang & Wei. (2019). Riemannian proximal gradient methods. Mathematical Programming, Springer, Issue 194.]
[N. Formation of wrinkles in bi-layer systems. Dissertation.]

Algebraic minimization problem

Problem

Minimize

$$J(\vec{\varphi}_h, \vec{Q}_h) = J_{3D}(\vec{\varphi}_h) + J_{shell}(\vec{m}_h, \vec{Q}) \quad \textit{with } \vec{\varphi}_h(\Gamma_{shell}) = \vec{m}_h(\omega_h)$$

in the admissible set $\vec{A}_h \subset \mathbb{R}^{3N_{3D}} \times (\mathrm{SO}(3))^{N_{2D}}$.

One iteration:

1. **Setup** the problem: At $(\vec{\varphi}_h, \vec{Q}_h)_k$, calculate (analytic or automatic differentiation)

$$\mathrm{grad}_{\text{coefficients}} J(\vec{\varphi}_h, \vec{Q}_h)_k, \quad \mathrm{Hess}_{\text{coefficients}} J(\vec{\varphi}_h, \vec{Q}_h)_k$$

2. **Solve** the inner, **constrained or modified** problem

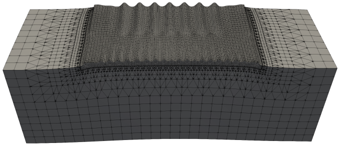
$\rightarrow$ both methods: **global convergence, superlinear local convergence**

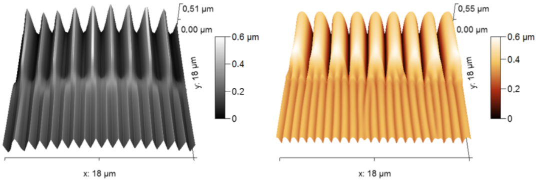
$\rightarrow$ depends on the problem and the infrastructure, which method is better

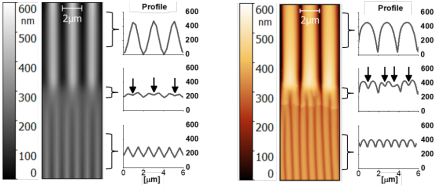
$\rightarrow$ both methods might even find different local minima

Simulations: Wavelength transitions

- all simulations using the `Dune` libraries
- 79.578 second-order nodes in $\mathcal{T}$
- 9.801 second-order nodes in τ





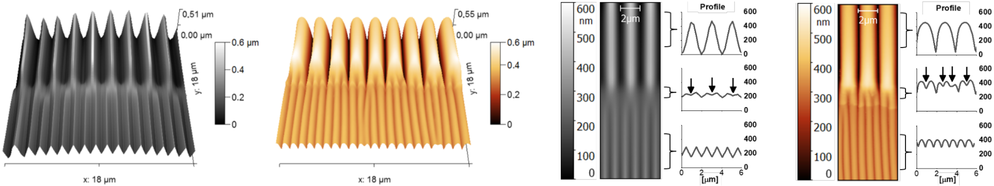


[Knapp, N., Nitschke, Sander, Fery. (2021). Controlling line defects in wrinkling: a pathway towards hierarchical wrinkling structures. Soft Matter, Issue 17.]
[Youett. (2015). Dynamic large deformation contact problems and applications in virtual medicine.]

Simulations: Wavelength transitions

- problem setup on 24 tasks, Intel(R) Xeon(R) CPU E5-2680, 2.50 GHz, 2.67 GB RAM
- trust-region: monotone multigrid method for constrained inner problems
- proximal Newton: CHOLMOD direct solver for modified inner problems

	steps	total time	setup	solve
trust-region	56	24.35 h	10.37 h	12.61 h
proximal Newton	120	40.4 h	38.4 h	1.39 h



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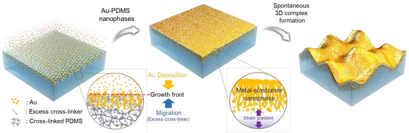
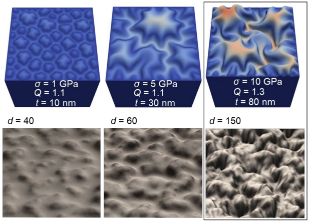
Simulations: **Tri-layer system of polymer + Gold/polymer + Gold**

- goal: create stretchable, flexible conductors
- apply gold layer of different thicknesses on top of a polymer base
- 132.718 second-order nodes in $\mathcal{T}$
- problem setup parallel on 24 tasks

simulation on the right	steps	total time	setup	solve
trust-region	607	115.89 h	35.97 h	73.76 h

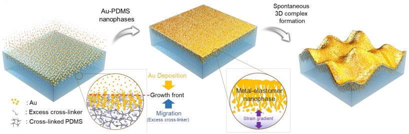


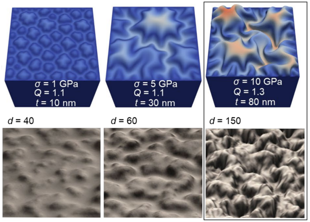


[Chae, Choi, N., Cho, Besford, Knapp, Masushko, Zabila, Pylypovskyi, Avdoshenko, Sander, Makarov, Fery. (2022). Three-dimensional complex of reticular metal–elastomer nanophases. Submitted.]

Summary

- combination of an elastic material model and a Cosserat shell model
- discretization using suitable finite elements
- geodesic FEs: construction using geodesic distances
- Riemannian trust-region method or Riemannian proximal Newton method

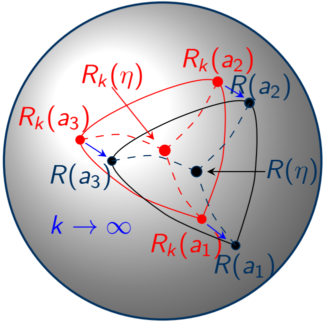




A: Properties of $V^{\text{proj/geo}}(\mathcal{T})$: Complete subset of $H^1(\omega, \mathcal{M})$

Theorem

Let $\mathcal{M}$ be a complete metric space, and let (R_k) be a sequence of geodesic finite element functions with $R_k : T \to \mathcal{M}$ for all $k \in \mathbb{N}$, converging pointwise to some limit function $R : T \to \mathcal{M}$. Then the limit function is also a geodesic finite element function.



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Proof.

- suppose the limit function R^* is **not** a minimizer of the form

$$\underset{R \in SO(3)}{arg\ min} \sum_{i=1}^{m} \lambda_i(v) dist(Q(a_i), R)^2$$

- then there is another minimizer $\tilde{R}$
- take a fraction of the difference $e = R^* - \tilde{R}$
- with this we can create a contradiction

□

B: The Cosserat shell model

$$J_{\text{shell}}(m, Q) = \int_{\omega_h} W_{\text{shell}}(E^e, K^e) \cdot a(x_1, x_2)\ \mathrm{d}x$$

- the only shell model where one can rigorously prove existence of solutions
- deduced from a 3D-Cosserat model
- approximation of the thin 3D-material using the midsurface
- stress-free state of the shell is the curved manifold $y_0(\omega_h)$

B: The Cosserat shell model

$$J_{\text{shell}}(m, Q) = \int_{\omega_h} W_{\text{shell}}(E^e, K^e) \cdot a(x_1, x_2)\ \mathrm{d}x$$

- co- and contravariant base vectors $a_1 = \frac{\partial y_0}{\partial x_1}, a_2 = \frac{\partial y_0}{\partial x_2}, a^1, a^2$
- first fundamental tensor $\mathbf{a} = \sum_{\alpha=1}^{2} a_\alpha \otimes a^\alpha$
- elastic shell strain tensor

$$E^e : \omega_h \to \mathbb{R}^{3\times 3}, \quad E^e := \sum_{\alpha=1}^{2} Q^T \left(\frac{\partial m}{\partial x_\alpha}\right) \otimes a^\alpha - \mathbf{a}$$

- elastic shell bending-curvature tensor

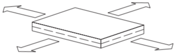
$$K^e : \omega_h \to \mathbb{R}^{3\times 3}, \quad K^e := \sum_{\alpha=1}^{2} \operatorname{axl}\left(Q^T \frac{\partial Q}{\partial x_\alpha}\right) \otimes a^\alpha$$

B: The Cosserat shell model

$$J_{\text{shell}}(m,Q)=\int_{\omega_h} W_{\text{shell}}(E^e,K^e)\cdot a(x_1,x_2)\,\mathrm{d}x$$

- co- and contravariant base vectors $a_1=\frac{\partial y_0}{\partial x_1},\, a_2=\frac{\partial y_0}{\partial x_2},\, a^1,\, a^2$
- first fundamental tensor $\mathbf{a}=\sum_{\alpha=1}^{2} a_\alpha\otimes a^\alpha$
- elastic shell strain tensor, there is a coordinate system in which

$$E^e\approx\begin{pmatrix}\epsilon_{11} & \epsilon_{12} & 0\\ \epsilon_{21} & \epsilon_{22} & 0\\ 0 & 0 & 0\end{pmatrix},\quad \epsilon_{11},\epsilon_{22}$$

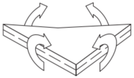


$\epsilon_{12},\epsilon_{21}$

- elastic shell bending-curvature tensor, there is a coordinate system in which

$$K^e\approx\begin{pmatrix}\kappa_{11} & \kappa_{12} & 0\\ \kappa_{21} & \kappa_{22} & 0\\ 0 & 0 & 0\end{pmatrix},\quad \kappa_{11},\kappa_{22}$$

κ_{12},κ_{21}



B: The Cosserat shell model

$$J_{\text{shell}}(m, Q) = \int_{\omega_h} \left(W_{\text{memb}}(E^e, K^e) + W_{\text{bend}}(K^e) \right) \cdot a(x_1, x_2) \; \mathrm{d}x$$

$$\begin{aligned} W_{\text{memb}}(\boldsymbol{E^e}, \boldsymbol{K^e}) :=& \left(h - K\frac{h^3}{12}\right) W_{\text{m}}(\boldsymbol{E^e}) + \left(\frac{h^3}{12} - K\frac{h^5}{80}\right) W_{\text{m}}(\boldsymbol{E^e}\mathbf{b} + \mathbf{c}\boldsymbol{K^e}) \\ &+ \frac{h^3}{6} W_{\text{b}}(\boldsymbol{E^e}, \mathbf{c}\boldsymbol{K^e}\mathbf{b} - 2H\mathbf{c}\boldsymbol{K^e}) + \frac{h^5}{80} W_{\text{mp}}((\boldsymbol{E^e}\mathbf{b} + \mathbf{c}\boldsymbol{K^e})\mathbf{b}) \\ W_{\text{bend}}(\boldsymbol{K^e}) :=& \left(h - K\frac{h^3}{12}\right) W_{\text{curv}}(\boldsymbol{K^e}) + \left(\frac{h^3}{12} - K\frac{h^5}{80}\right) W_{\text{curv}}(\boldsymbol{K^e}\mathbf{b}) + \frac{h^5}{80} W_{\text{curv}}(\boldsymbol{K^e}\mathbf{b}^2) \end{aligned}$$

- W_{m}, W_{mp}, W_{curv} quadratic forms bounding the norms of their arguments
- W_{b} bilinear form, can be absorbed into W_{m}, W_{mp}, W_{curv}
- $\mathbf{b} = -\sum_\alpha \frac{\partial n_0}{\partial x_\alpha} \otimes a^\alpha$ second fundamental tensor, **c** alternating pseudo-tensor
- K, H are Gauss and mean curvature of ω_h
- h is the shell thickness, if h is small enough, all prefactors are positive

B: The Cosserat shell model

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Theorem (J_{shell})

If h is small enough, the parametrization y_0 is smooth enough and $m_{|\gamma_d} = Id$, then

- *J_{shell} is coercive.*
- *J_{shell} is bounded from below on A.*
- *J_{shell} is $H^1(\omega_h, \mathbb{R}^3) \times H^1(\omega_h, \mathrm{SO}(3))$-weakly lower semi-continuous.*

[Ghiba, Bîrsan, Lewintan & Neff. (2020). The isotropic Cosserat shell model including terms up to $O(h^5)$. Part II: Existence of minimizers. J Elast 142.]

B: The Cosserat shell functional in detail

Bilinear and quadratic forms:

- $W_{\mathrm{b}}(S,T) = \mu\langle \mathrm{sym}(S), \mathrm{sym}(T)\rangle + \mu_c\langle \mathrm{skew}(S), \mathrm{skew}(T)\rangle + \frac{\lambda\mu}{\lambda+2\mu}\,\mathrm{tr}(S)\cdot\mathrm{tr}(T)$
- $W_{\mathrm{m}}(S) = W_{\mathrm{b}}(S,S)$
- $W_{\mathrm{mp}}(S) = W_{\mathrm{m}}(S) + \frac{\lambda^2}{2(\lambda+2\mu)}\big[\mathrm{tr}(S)\big]^2$
- $W_{\mathrm{curv}}(S) = \mu L_c^2\Big(b_1\|\mathrm{sym}(S)\|^2 + b_2\|\mathrm{skew}(S)\|^2 + (b_3 - \frac{b_1}{3})\big[\mathrm{tr}(S)\big]^2\Big)$

where

- μ, λ are the Lamé parameters
- $\mu_c \geq 0$ is the Cosserat couple modulus
- $L_c > 0$ represents an internal length which is characteristic for the material
- $b_1, b_2, b_3 > 0$ are dimensionless constitutive coefficients
- **c** alternating pseudo-tensor, $\mathbf{c} := \frac{1}{a(x_1,x_2)}\big(a_1\otimes a_2 - a_2\otimes a_1\big) : \omega_\xi \to \mathbb{R}^{3\times 3}$.
- interesting/critical: $h \to 0$, $\mu_c \to 0$, $L_c \to 0$

[Neff. (2005). A finite-strain elastic–plastic Cosserat theory for polycrystals with grain rotations. Int. Journal of Engineering Science 44.]

C.1: General Trust-Region-Method in $\mathbb{R}^N$

- nonlinear minimization problem with a functional $J : \mathbb{R}^N \to \mathbb{R}$
- given a current iterate $x_k \in \mathbb{R}^N$:
  approximate J in a **neighborhood** around x_k using a model $m_k : \mathbb{R}^N \to \mathbb{R}$

$$m_k(s) = J(x_k) + \partial J(x_k) \cdot s + \frac{1}{2} s^T \cdot \partial^2 J(x_k) \cdot s$$

C.2: General Trust-Region-Method in $\mathbb{R}^N$

One trust region step:

1. setup model m_k in a neighborhood r_k around x_k
2. solve quadratic constraint problem

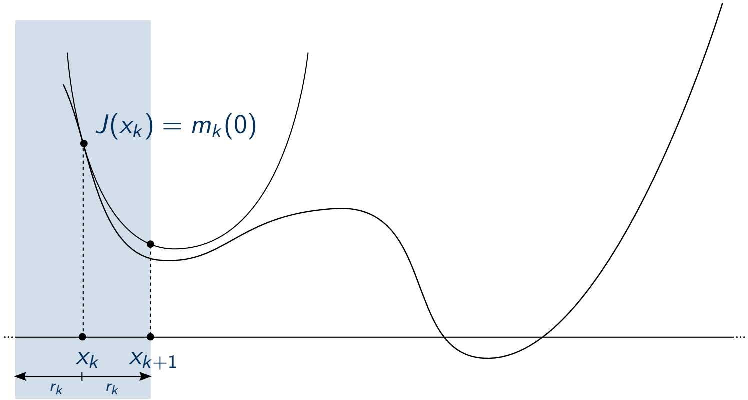
$$s_k = \underset{s\in\mathbb{R}^N,\ ||s||_\infty \leq r_k}{argmin} \quad m_k(s)$$

   in an inner iteration, might be non-convex

3. accept or decline the correction s_k: $\rho_k = \frac{J(x_k) - J(x_k + s_k)}{m_k(0) - m_k(s_k)}$

   if : $\rho_k \ll 1$ or $J(x_k + s_k) > J(x_k)$
   set $x_{k+1} = x_k$ and decrease radius, e.g. $r_{k+1} = \frac{1}{2} r_k$
   else : set $x_{k+1} = x_k + s_k$
   if : $\rho_k \gg 1$: increase radius, e.g. $r_{k+1} = 2r_k$
   else : keep radius $r_{k+1} = r_k$

C.3: General Trust-Region-Algorithm in R^N



D: The space $H^1(\omega_h, \mathrm{SO}(3))$

Defined as

$$H^1(\omega_h, \mathrm{SO}(3)) := \left\{ v \in H^1(\omega_h, \mathbb{R}^{3\times 3}) \;\middle|\; v(x) \in \iota(\mathrm{SO}(3)) \text{ almost everywhere} \right\}.$$

- using the canonical immersion ι of $\mathrm{SO}(3)$ into $\mathbb{R}^{3\times 3}$
- $H^1(\omega_h, \mathrm{SO}(3))$ is complete because it is a closed subset of $H^1(\omega_h, \mathbb{R}^{3\times 3})$.

E: Properties of geodesic FEs: Completeness

Theorem

Let $\mathcal{M}$ be a complete metric space, and let (R_k) be a sequence of geodesic finite element functions with $R_k : T \to \mathcal{M}$ for all $k \in \mathbb{N}$, converging pointwise to some limit function $R : T \to \mathcal{M}$. Then the limit function is also a geodesic finite element function.

Proof.

- suppose the limit function R^* is **not** a minimizer of the form

$$\mathop{arg\ min}_{R \in \mathrm{SO}(3)} \sum_{i=1}^{m} \lambda_i(v) dist(Q(a_i), R)^2$$

- then there is another minimizer $\tilde{R}$
- take a fraction of the difference $e = R^* - \tilde{R}$
- with this we can create a contradiction

□

F: Projection-based construction

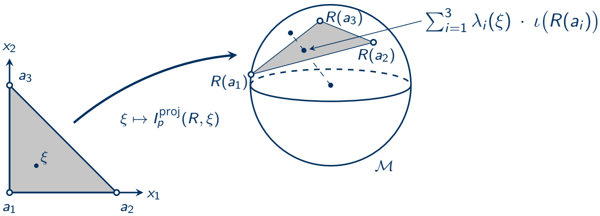
- for $T \in \tau$ consider Lagrange nodes $a_1, \ldots, a_m$ and polynomials $\lambda_1, \ldots, \lambda_m : T \to \mathbb{R}$
- recall p-th order Lagrange polynomial interpolation of a function $f : T \to \mathbb{R}$

$$f_h(\xi) = I_p^{\text{poly}}(f(a_1), \ldots, f(a_m), \xi) := \sum_{i=1}^{m} \lambda_i(\xi) f(a_i)$$

- with the embedding $\iota : \mathcal{M} \to \mathbb{R}^N$ and the closest point projection $P : \mathbb{R}^N \to \mathcal{M}$

$$R_h(\xi) = I_p^{\text{proj}}(R(a_1), \ldots, R(a_m), \xi) := \mathrm{P}\left(\sum_{i=1}^{m} \lambda_i(\xi) \cdot \iota(R(a_i))\right)$$

- evaluation of derivatives with chain rule



F: Projection-based construction for SO(3)

$$\mathrm{SO}(3) := \left\{ Q \in \mathbb{R}^{3\times 3} \;\middle|\; Q^T = Q^{-1},\ \det(Q) = 1 \right\}$$

- group of rotations in 3D
- representation using the coefficients $\vec{q} = (q_1, q_2, q_3, q_4) \in \mathbb{R}^4$ of unit quaternions

$$\mathbb{H} := \left\{ \mathbf{q} = q_1 + q_2\hat{\mathbf{i}} + q_3\hat{\mathbf{j}} + q_4\hat{\mathbf{k}} \;\middle|\; q_i \in \mathbb{R}, \hat{\mathbf{i}}^2 = \hat{\mathbf{j}}^2 = \hat{\mathbf{k}}^2 = \hat{\mathbf{i}}\hat{\mathbf{j}}\hat{\mathbf{k}} = -1 \right\}$$

  with $\|\mathbf{q}\|^2 = q_1^2 + q_2^2 + q_3^2 + q_4^2 = 1$
- unit quaternions are homeomorphic to the unit sphere S^3
- embedding

$$\iota_{\mathrm{SO}(3)\to\mathbb{H}} \begin{pmatrix} q_1^2 + q_2^2 - q_3^2 - q_4^2 & 2q_2q_3 - 2q_1q_4 & 2q_2q_4 + 2q_1q_3 \\ 2q_2q_3 + 2q_1q_4 & q_1^2 - q_2^2 + q_3^2 - q_4^2 & 2q_3q_4 - 2q_1q_2 \\ 2q_2q_4 - 2q_1q_3 & 2q_3q_4 + 2q_1q_2 & q_1^2 - q_2^2 - q_3^2 + q_4^2 \end{pmatrix} = (q_1, q_2, q_3, q_4)$$

- $1:2$ – correspondence, as $\mathbf{q}$ and $-\mathbf{q}$ result in same rotation
- multiplication of quaternions corresponds to the multiplication in SO(3)

F: Projection-based construction for SO(3)

$$\mathrm{SO}(3) := \left\{ Q \in \mathbb{R}^{3\times 3} \,\middle|\, Q^T = Q^{-1},\ \det(Q) = 1 \right\}$$

- projection $P : \mathbb{R}^{3\times 3} \to \mathrm{SO}(3)$, $P(A) = \mathrm{polar}(A)$, evaluate using Heron's method

  1. initial iterate: $X_1 = A$
  2. iterate:
  $$X_{i+1} = \tfrac{1}{2}\left(X_i + X_i^{-T}\right)$$
  3. when $\|X_{i+1} - X_i\|_F <$ tolerance: return $X_{i+1} = \mathrm{polar}(A)$

- derivative of projection $\nabla_A\, \mathrm{polar}(A) \in \mathbb{R}^{3\times 3\times 3\times 3}$ iteratively as well

F: Projection-based construction for SO(3)

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- projection $P : \mathbb{R}^{3\times 3} \to \mathrm{SO}(3)$, $P(A) = \mathrm{polar}(A)$, evaluate using Heron's method
  1. initial iterates: $X_1 = A, (\nabla X)_1 = 1_{3\times 3\times 3\times 3}$, with
  2. iterate:
  $$X_{i+1} = \tfrac{1}{2}\left(X_i + X_i^{-T}\right)$$
  $$(\nabla X)_{i+1} = \tfrac{1}{2}\left((\nabla X)_i - X_i^{-T}(\nabla X^T)_i X_i^{-T}\right)$$
  3. when $\|X_{i+1} - X_i\|_F <$ tolerance: return $X_{i+1} = \mathrm{polar}(A)$, $(\nabla X)_{i+1} = \nabla_A \,\mathrm{polar}(A)$
- derivative of projection $\nabla_A \,\mathrm{polar}(A) \in \mathbb{R}^{3\times 3\times 3\times 3}$ iteratively as well

F: Projection-based construction for SO(3) with quaternions

- evaluation of the function

$$q_h(\xi) = \iota_{\mathrm{SO}(3)\to\mathbb{H}}\left(\operatorname{polar}\left(\sum_{i=1}^{m}\lambda_i(\xi)\;\cdot\;R(a_i)\right)\right)$$

- evaluation of the derivative

$$\frac{\partial}{\partial\vec{x}}(q_h)_{|\xi} = \underbrace{\nabla\iota_{\mathrm{SO}(3)\to\mathbb{H}}\left(R(a_i)\right)}_{\in\mathbb{R}^{4\times(3\times3)}}\cdot\underbrace{\nabla_A\operatorname{polar}\left(\sum_{i=1}^{m}\lambda_i(\xi)\cdot R(a_i)\right)}_{\in\mathbb{R}^{3\times3\times3\times3}}\cdot\underbrace{\left(\sum_{i=1}^{m}\frac{\partial}{\partial\vec{x}}\lambda_i(\xi)\;\cdot\;R(a_i)\right)}_{\in\mathbb{R}^{(3\times3)\times\dim(T)}}$$

G: Geodesic distances for SO(3)

- intrinsic distance $\mathrm{dist}_{\mathrm{SO}(3)}(A, B) = \|\log(A^T B)\|_F$, with matrix logarithm
- using quaternions: distance of two rotations **q** and **p** is

$$\mathrm{dist}_{\mathrm{SO}(3)}(\mathbf{q}, \mathbf{p}) = \begin{cases} 2\,\mathrm{acos}(\langle \vec{q}, \vec{p} \rangle), & \text{if} \quad 0 \leq 2\,\mathrm{acos}(\langle \vec{q}, \vec{p} \rangle) \leq \pi \\ 2\pi - 2\,\mathrm{acos}(\langle \vec{q}, \vec{p} \rangle), & \text{if} \quad \pi < 2\,\mathrm{acos}(\langle \vec{q}, \vec{p} \rangle) \leq 2\pi \end{cases}$$

- maximal distance is π, realized for $\langle \vec{q}, \vec{p} \rangle = 0$, i.e. rotations that are "180° apart"
- covariant derivatives, with $\mathrm{P}_{T_{\vec{p}}\mathrm{SO}(3)} :=$ projection to $T_{\vec{p}}\mathrm{SO}(3)$

$$\frac{\partial}{\partial \vec{p}} \mathrm{dist}_{\mathrm{SO}(3)}(\mathbf{q}, \mathbf{p})^2 = \mathrm{P}_{T_{\vec{p}}\mathrm{SO}(3)} \left(\frac{\mp 8\,\mathrm{acos}(\langle \vec{q}, \vec{p} \rangle)}{\sqrt{1 - (\langle \vec{q}, \vec{p} \rangle)^2}} \cdot \vec{q} \right) = \frac{\mp 8\,\mathrm{acos}(\langle \vec{q}, \vec{p} \rangle)}{\sqrt{1 - (\langle \vec{q}, \vec{p} \rangle)^2}} \cdot (\vec{q} - \langle \vec{q}, \vec{p} \rangle \vec{p}) \in T_{\vec{p}}\mathrm{SO}(3)$$

- second covariant derivative $(\frac{\partial}{\partial \vec{p}})^2\, \mathrm{dist}_{\mathrm{SO}(3)}(\mathbf{q}, \mathbf{p})^2 \in \mathbb{R}^{4 \times 4}$

[Sander. (2012). Geodesic finite elements on simplicial grids. Int. J. Numer. Meth. Engineering 92.]

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- maximal distance is π, realized for $\langle \vec{q}, \vec{p} \rangle = 0$, i.e. rotations that are "180° apart"
- retraction = exponential map on S^3
- for $v \in T_{\mathbf{q}} S^3$, given as $\vec{v}$ in quaternion coordinates

$$R_{\mathbf{q}} v = \text{Exp}_{\mathbf{q}}\, v = \cos(\|\vec{v}\|)\vec{q} + \sin(\|\vec{v}\|)\frac{\vec{v}}{\|\vec{v}\|}$$

[Sander. (2012). Geodesic finite elements on simplicial grids. Int. J. Numer. Meth. Engineering 92.]