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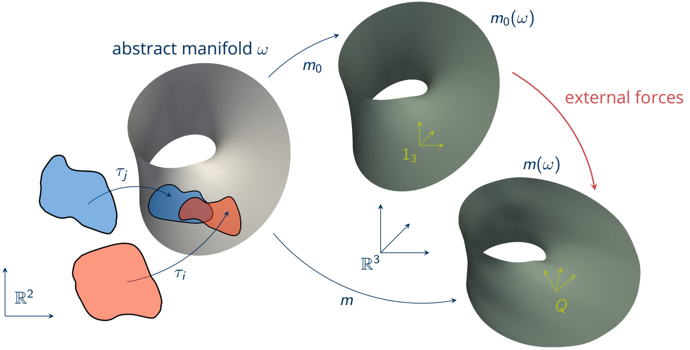
Manifold-valued finite elements: Construction by generalizing Lagrange interpolation and applications

TU Wien, December 7th, 2022

Cosserat shell with initial curvature

- consider external forces on a shell subject to Dirichlet boundary conditions
- stress-free state of the shell is a curved manifold given through an initial configuration $m_0 \in H^1(\omega, \mathbb{R}^3)$ together with coordinate patches $\tau_i : \mathbb{R}^2 \to \omega$
- Cosserat models allow an independent microrotation Q of the particles
- deformed configuration is function pair $m : \omega \to \mathbb{R}^3$ and $Q : \omega \to \mathrm{SO}(3)$



Cosserat shell with initial curvature

- admissible set

$$\mathcal{A} = \Big\{(m, Q) \in H^1(\omega, \mathbb{R}^3) \times H^1(\omega, \mathrm{SO}(3)) \;\Big|\; \text{Dirichlet boundary conditions for } m\Big\}$$

- deformed configuration (m, Q) is a minimizer of the energy functional

$$\operatorname*{arg\,min}_{(m,Q)\in\mathcal{A}} J(m, Q) = J_{\text{shell}}(m, Q) + \text{external forces}(m, Q)$$

- existence of minimizers follows for suitable parameters of J_{shell} and suitable external forces with the direct method

[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.]

Cosserat shell with initial curvature

- hyperelastic material model

$$J_{\text{shell}}(m, Q) = \int_\omega W(E^e, K^e)\,\mathrm{d}\omega$$

- geometry of stress-free state $m_0(\omega)$: first fundamental tensor $\mathbf{a} = \sum_{\alpha=1}^2 a_\alpha \otimes a^\alpha$
- co- and contravariant basis vectors a_1, a_2, a^1, a^2 of $m_0(\omega)$
- elastic shell strain tensor

$$E^e : \omega \to \mathbb{R}^{3\times 3}, \qquad E^e := \sum_{\alpha=1}^{2} Q^T \frac{\partial m}{\partial x_\alpha} \otimes a^\alpha - \mathbf{a}$$

- elastic shell bending–curvature tensor

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

Cosserat shell with initial curvature

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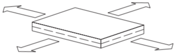
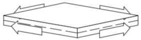
- geometry of stress-free state $m_0(\omega)$: first fundamental tensor $\mathbf{a} = \sum_{\alpha=1}^{2} a_\alpha \otimes a^\alpha$
- co- and contravariant basis vectors a_1, a_2, a^1, a^2 of $m_0(\omega)$
- elastic shell strain tensor, there is a coordinate system (not necessarily orthogonal) in which

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

$\epsilon_{11}, \epsilon_{22}$  $\epsilon_{12}, \epsilon_{21}$ 

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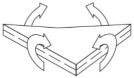
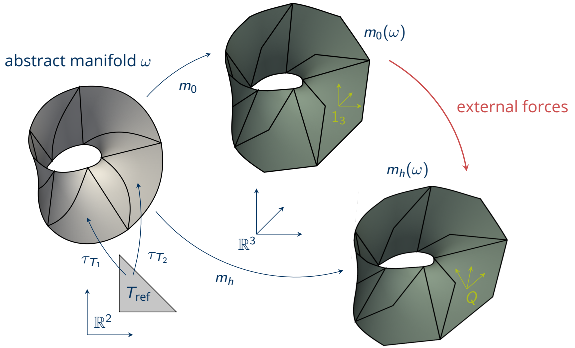
κ_{11}, κ_{22}  κ_{12}, κ_{21} 

Discretization of the minimization problem for the shell

- discretize ω using an appropriate triangulation $\mathcal{T}$
- standard Lagrange FEs of order p_1 for the deformation function: $m_h \in V_{p_1}(\mathcal{T}, \mathbb{R}^3)$
- rotation function Q maps to the nonlinear manifold SO(3)
  $\rightarrow$ standard Lagrange FEs cannot be used for Q_h
  $\rightarrow$ manifold-valued FE space $V_{p_2}(\mathcal{T}, \mathrm{SO}(3)) \subset H^1(\mathcal{T}, \mathrm{SO}(3))$



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Problem

Find minimizing function pair of

$$J(m_h, Q_h) = J_{\text{shell}}(m_h, Q_h) + \textit{external forces}(m_h, Q_h)$$

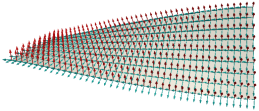
in the admissible set

$$\mathcal{A} = \left\{ (m_h, Q_h) \in V_{p_1}(\mathcal{T}, \mathbb{R}^3) \times V_{p_2}(\mathcal{T}, \mathrm{SO}(3)) \;\middle|\; \text{Dirichlet boundary conditions for } m_h \right\}.$$

Construction of $V(\omega, \mathcal{M}) \subset H^1(\omega, \mathcal{M})$

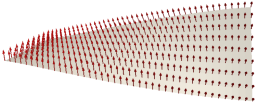
- problems with nonlinear manifolds
  - shell models with microrotation $Q = (d_1 | d_2 | d_3)$, e.g., Cosserat shell

    configuration is $(m, Q) \in (\mathbb{R}^3, \mathrm{SO}(3))$



  - shell models with one director d, e.g., Reissner-Mindlin shell

    configuration is $(m, d) \in (\mathbb{R}^3, S^2)$



  - spin of elementary particles $\in \mathrm{SU}(2)$
  - underlying gauge groups of Yang–Mills equations $\mathrm{SU}(2), \mathrm{SU}(3), \ldots$
- generalize Lagrange interpolation
  - using a projection-based construction
  - or construction using geodesic distances

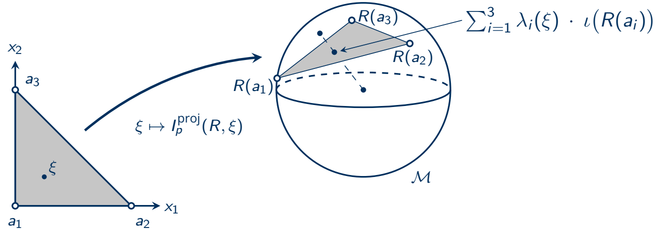
Projection-based construction

- for $T \in \mathcal{T}$ 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 $f : T \to \mathbb{R}$

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

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

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



Projection-based construction

- function evaluation ✓
- evaluate the derivatives $\frac{\partial}{\partial x_\alpha}(R_h)_{|\xi} \in T_{R_h(\xi)}\mathcal{M}$

$$\frac{\partial}{\partial \vec{x}}(R_h)_{|\xi} = \frac{\partial}{\partial \vec{x}} I_p^{\text{proj}}(R(a_1), \dots, R(a_m), \xi)$$
$$= \underbrace{\nabla \mathrm{P}\left(\sum_{i=1}^{m} \lambda_i(\xi) \cdot \iota(R(a_i))\right)}_{\text{“}\in \mathbb{R}^{\dim(\mathcal{M}) \times N}\text{“}} \cdot \underbrace{\left(\sum_{i=1}^{m} \frac{\partial}{\partial \vec{x}} \lambda_i(\xi) \cdot \iota(R(a_i))\right)}_{\in \mathbb{R}^{N \times \dim(T)}}$$

Needed quantities for the projection-based construction:

- embedding $\iota : \mathcal{M} \to \mathbb{R}^N$
- projection $P : \mathbb{R}^N \to \mathcal{M}$ with derivative $\nabla P \in (T\mathcal{M})^N$

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)

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:
  $$X_{i+1} = \frac{1}{2}\left(X_i + X_i^{-T}\right)$$
  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

Projection-based construction for SO(3)

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  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 $X_{i+1} = \operatorname{polar}(A)$, $(\nabla X)_{i+1} = \nabla_A \operatorname{polar}(A)$
- derivative of projection $\nabla_A \operatorname{polar}(A) \in \mathbb{R}^{3\times 3\times 3\times 3}$ iteratively as well

Projection-based construction for SO(3) with quaternions

- evaluation of the function

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

- evaluation of the derivative

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

Projection-based construction for SU(2)

$$\mathrm{SU}(2) := \left\{ A \in \mathbb{C}^{2\times 2} \;\middle|\; A^H = A^{-1},\ \det(A) = 1 \right\}$$

- group of complex rotations in 2D
- three-dimensional, nonlinear manifold
- SU(2) homeomporphic to unit quaternions, $\mathrm{SU}(2) =$

$$\left\{ A = \left(q_1 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + q_2 \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} + q_3 \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + q_4 \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} \right) \;\middle|\; q_i \in \mathbb{R},\ \ q_1^2 + q_2^2 + q_3^2 + q_4^2 = 1 \right\}$$

- embedding $\iota_{\mathrm{SU}(2)\to\mathbb{H}}(A) = (q_1, q_2, q_3, q_4) = \vec{q}$
- projection $P : \mathbb{H} \to \mathrm{SU}(2)$, $P(\vec{q}) = \frac{\vec{q}}{\|\vec{q}\|}$
- derivative of projection $\nabla_{\vec{q}} P(\vec{q}) \in \mathbb{R}^{4\times 4}$

Construction using geodesic distances

- recall p-th order Lagrange polynomial interpolation of a function $f : T \to \mathbb{R}$

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

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

- using an intrinsic distance on $\mathcal{M}$, define geodesic interpolation of $R : T \to \mathcal{M}$

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

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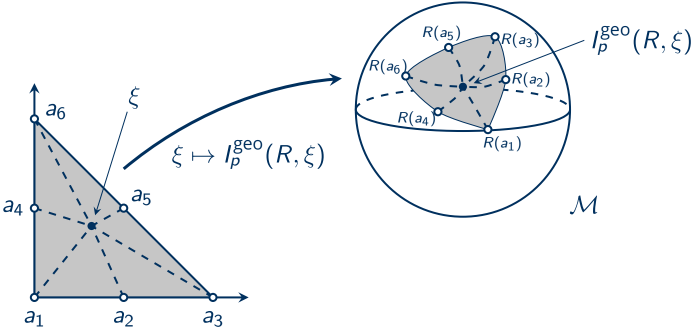
Construction using geodesic distances

- solve
$$R_h(\xi) = \arg\min_{M \in \mathcal{M}} \sum_{i=1}^{m} \lambda_i(v)\, \mathrm{dist}(R(a_i), M)^2 =: \arg\min_{M \in \mathcal{M}} f(M)$$
- $f : \mathcal{M} \to \mathbb{R}$ is convex, can be solved by Newton-type method



Riemannian Newton-type method for $f : \mathcal{M} \to \mathbb{R}$

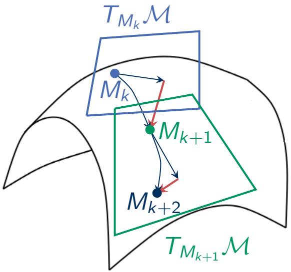
Given an iterate $M_k \in \mathcal{M}$ and a retraction $R_{M_k} : T_{M_k}\mathcal{M} \to \mathcal{M}$

1. approximate f around M_k using a quadratic model

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

$$q_k(s) = f(M_k) + \left\langle \operatorname{grad}_M f_{|M_k}, s \right\rangle + \frac{1}{2}\left\langle \operatorname{Hess}_M f_{|M_k}[s], s \right\rangle$$

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



2. minimize q_k

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

i.e. solve $\quad \operatorname{Hess}_M f_{|M_k} \, s_k = -\operatorname{grad}_M f_{|M_k}$

3. set $M_{k+1} = R_{M_k}(s_k)$
4. return M_{k+1} once $\|s_k\| < \text{tol}$

Here: $\operatorname{grad}_M f = \sum_{i=1}^{m} \lambda_i(v) \frac{\partial}{\partial M} \operatorname{dist}(R(a_i), M)^2$ and $\operatorname{Hess}_M f = \sum_{i=1}^{m} \lambda_i(v) (\frac{\partial}{\partial M})^2 \operatorname{dist}(R(a_i), M)^2$

Evaluation of the derivatives $\frac{\partial}{\partial \vec{x}}(R_h)_{|\xi}$

- denote

$$f_{\vec{R},\vec{w}}(M) = \sum_{i=1}^{m} w_i \operatorname{dist}(R_i, M)^2, \quad f_{\vec{R},\vec{w}} : \mathcal{M} \to \mathbb{R},$$

  where $\vec{R} := (R_1, \dots, R_m)$, $\vec{w} := (w_1, \dots, w_m)$

- then for $\vec{R}_a := (R(a_1), \dots, R(a_m))$, $\vec{\lambda}_\xi := (\lambda_1(\xi), \dots, \lambda_m(\xi))$

$$R_h(\xi) = \operatorname*{arg\,min}_{M \in \mathcal{M}} f_{\vec{R}_a,\vec{\lambda}_\xi}(M), \quad \text{and thus} \quad \frac{\partial}{\partial M} f_{\vec{R}_a,\vec{\lambda}_\xi}(R_h(\xi)) = \vec{0} \in T_M\mathcal{M}$$

- define the function $F : \mathcal{M}^m \times \mathbb{R}^m \times \mathcal{M} \to T\mathcal{M}$ as

$$F(\vec{R}, \vec{w}, M) := \frac{\partial}{\partial M} f_{\vec{R},\vec{w}}(M), \quad \text{so} \quad F(\vec{R}_a, \vec{\lambda}_\xi, R_h(\xi)) = \vec{0} \in T_M\mathcal{M}$$

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

Evaluation of the derivatives $\frac{\partial}{\partial \vec{x}}(R_h)_{|\xi}$

- total derivative $\frac{\mathrm{d}}{\mathrm{d}\vec{x}} F$ is

$$\frac{\mathrm{d}}{\mathrm{d}\vec{x}} F(\vec{R}, \vec{w}, M) = \frac{\partial}{\partial \vec{R}} F(\vec{R}, \vec{w}, M) \cdot \overbrace{\frac{\partial}{\partial \vec{x}} \vec{R}}^{=0} + \frac{\partial}{\partial \vec{w}} F(\vec{R}, \vec{w}, M) \cdot \frac{\partial}{\partial \vec{x}} \vec{w} + \frac{\partial}{\partial M} F(R_i, w_i, M) \cdot \frac{\partial}{\partial \vec{x}} M$$

- $F(\vec{R}_a, \vec{\lambda}_\xi, R_h(\xi)) = \vec{0}$ for all ξ, so

$$\frac{\mathrm{d}}{\mathrm{d}\vec{x}} F_{|(\vec{R}_a, \vec{\lambda}_\xi, R_h(\xi))} = \vec{0} \in \mathbb{R}^{\dim(\mathcal{M}) \times \dim(T)}$$

- $$\Leftrightarrow \underbrace{\frac{\partial}{\partial \vec{w}} F_{|(\vec{R}_a, \vec{\lambda}_\xi, R_h(\xi))}}_{\text{“}\in \mathbb{R}^{\dim(\mathcal{M}) \times m}\text{“}} \cdot \underbrace{\frac{\partial}{\partial \vec{x}} \vec{\lambda}_\xi}_{\in \mathbb{R}^{m \times \dim(T)}} + \underbrace{\frac{\partial}{\partial M} F_{|(\vec{R}_a, \vec{\lambda}_\xi, R_h(\xi))}}_{\text{“}\in \mathbb{R}^{\dim(\mathcal{M}) \times \dim(\mathcal{M})}\text{“, invertible}} \cdot \underbrace{\frac{\partial}{\partial \vec{x}} (R_h)_{|\xi}}_{\text{“}\in \mathbb{R}^{\dim(\mathcal{M}) \times \dim(T)}\text{“}} = \vec{0}$$

- solve this linear system for $\frac{\partial}{\partial \vec{x}}(R_h)_{|\xi}$

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

Evaluation of the derivatives $\frac{\partial}{\partial \vec{x}}(R_h)_{|\xi}$

$$\underbrace{\frac{\partial}{\partial \vec{w}} F_{|(\vec{R}_a,\vec{\lambda}_\xi,R_h(\xi))}}_{\text{“}\in\mathbb{R}^{\dim(\mathcal{M})\times m}\text{“}} \cdot \underbrace{\frac{\partial}{\partial \vec{x}} \vec{\lambda}_\xi}_{\in\mathbb{R}^{m\times\dim(T)}} + \underbrace{\frac{\partial}{\partial M} F_{|(\vec{R}_a,\vec{\lambda}_\xi,R_h(\xi))}}_{\text{“}\in\mathbb{R}^{\dim(\mathcal{M})\times\dim(\mathcal{M})}\text{“, invertible}} \cdot \underbrace{\frac{\partial}{\partial \vec{x}}(R_h)_{|\xi}}_{\text{“}\in\mathbb{R}^{\dim(\mathcal{M})\times\dim(T)}\text{“}} = \vec{0}$$

$$\frac{\partial}{\partial \vec{w}} F_{|(\vec{R}_a,\vec{\lambda}_\xi,R_h(\xi))} = \frac{\partial}{\partial \vec{w}} \frac{\partial}{\partial M} f_{\vec{R}_a,\vec{\lambda}_\xi}(R_h(\xi)) = \left[\frac{\partial}{\partial M} \operatorname{dist}(R(a_i), R_h(\xi))^2\right]_{i=1,\dots,m}$$

$$\frac{\partial}{\partial M} F_{|(\vec{R}_a,\vec{\lambda}_\xi,R_h(\xi))} = \left(\frac{\partial}{\partial M}\right)^2 f_{\vec{R}_a,\vec{\lambda}_\xi}(R_h(\xi)) = \sum_{i=1}^{m} \lambda_i(\xi) \left(\frac{\partial}{\partial M}\right)^2 \operatorname{dist}(R(a_i), R_h(\xi))^2$$

Needed quantities for the construction using geodesic distances:

- intrinsic distance function on the manifold $\operatorname{dist}_{\mathcal{M}}(\,\cdot\,,\,\cdot\,)$
- first and second covariant derivative $\frac{\partial}{\partial M}\operatorname{dist}_{\mathcal{M}}(\,\cdot\,, M)^2$, $(\frac{\partial}{\partial M})^2 \operatorname{dist}_{\mathcal{M}}(\,\cdot\,, M)^2$
- retraction $R_M : T_M\mathcal{M} \to \mathcal{M}$

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Geodesic distances for SO(3)

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

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

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

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

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

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

Geodesic distances for SO(3)

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

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

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

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

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

Geodesic distances for SU(2)

- representation using quaternions $\mathbf{q} = q_1 + q_2\hat{\mathbf{i}} + q_3\hat{\mathbf{j}} + q_4\hat{\mathbf{k}}$
- distance of two elements $\mathbf{q}$ and $\mathbf{p}$ is

$$\mathrm{dist}_{\mathrm{SU}(2)}(\mathbf{q},\mathbf{p}) = \mathrm{acos}(\langle \vec{q}, \vec{p}\rangle)$$

- maximal distance is π, realized for two antipodal quaternions, i.e., $\mathbf{q}$ and $-\mathbf{q}$
- covariant derivatives, with $\mathrm{P}_{T_{\vec{p}}\mathrm{SU}(2)} :=$ projection to $T_{\vec{p}}\mathrm{SU}(2)$

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

- second covariant derivative $(\frac{\partial}{\partial \vec{p}})^2 \mathrm{dist}_{\mathrm{SO}(3)}(\mathbf{q},\mathbf{p})^2 \in \mathbb{R}^{4\times 4}$
- retraction = exponential map on S^3
- for $v \in T_{\mathbf{q}}S^3$, given as $\vec{v}$ in quaternion coordinates

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

Global Finite Element Space

- Projection-based construction:

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

- Construction using geodesic distances

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

$\to$ Finite Element space on whole triangulation $\mathcal{T}$ of ω

$$V_p^{\text{proj/geo}}(\mathcal{T},\mathcal{M}) := \Big\{R_h\in C(\omega)\;\Big|\;\forall T\in\mathcal{T}\;\exists(R(a_1),\dots,R(a_m))\in\mathcal{M}^m \text{ such that } \forall\xi\in T:(R_h)_{|T}(\xi) = I_p^{\text{proj/geo}}(R(a_i),\xi)\Big\}$$

Properties of $V_p^{\text{proj/geo}}(\mathcal{T},\mathcal{M})$

Recall properties of the Lagrange finite element space $V_p^{\text{poly}}(\mathcal{T},\mathbb{R})$:

- nestedness: for orders $p_1 \leq p_2$ it holds

$$V_{p_1}^{\text{poly}}(\mathcal{T},\mathbb{R}) \subset V_{p_2}^{\text{poly}}(\mathcal{T},\mathbb{R})$$

- $I_p^{\text{poly}}(f(a_1),\dots f(a_n),\xi)$ is differentiable with respect to all arguments
- $V_p^{\text{poly}}(\mathcal{T},\mathbb{R})$ is a closed subset of $H^1(\omega,\mathbb{R})$
- interpolation error between a function $f \in W^{(p+1),2}(\omega,\mathbb{R})$ and its approximation f_h on a grid $\mathcal{T}$ with grid size h with FEs of order p

$$\|f - f_h\|_{H^k(\omega,\mathbb{R})} \leq c(p,\omega,\mathcal{T})|h|^{p+1-k}|f|_{W^{(p+1),2}(\omega,\mathbb{R})}$$

Properties of $V_p^{\mathrm{proj/geo}}(\mathcal{T}, \mathcal{M})$

- nestedness: for orders $p_1 \leq p_2$ it holds

$$V_{p_1}^{\mathrm{proj}}(\mathcal{T}, \mathcal{M}) \subset V_{p_2}^{\mathrm{proj}}(\mathcal{T}, \mathcal{M})$$

- no nestedness for $V_p^{\mathrm{geo}}(\mathcal{T}, \mathcal{M})$
- $I_p^{\mathrm{proj/geo}}(R(a_1), \dots R(a_n), \xi)$ are differentiable with respect to all arguments
- $V_p^{\mathrm{proj/geo}}(\mathcal{T}, \mathcal{M})$ are both closed subsets of $H^1(\omega, \mathcal{M})$
- interpolation error depends optimally on the grid size as well

[N., Sander, Neff, Bîrsan. A Cosserat shell model with general reference configuration and its discretization with GFE. In preparation.]
[Grohs, Hardering, Sander. (2014). Optimal A Priori Discretization Error Bounds for Geodesic Finite Elements. Found Comput Math 15.]
[Hardering. (2014). L^2–discretization error bounds for maps into Riemannian Manifolds. Numerische Mathematik 139.]

Cosserat shell: Minimization problem in the FE space

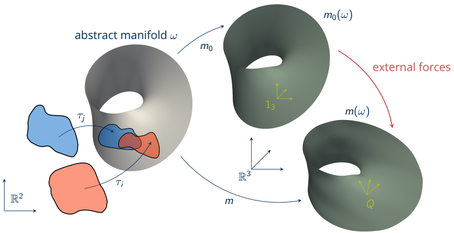
Problem

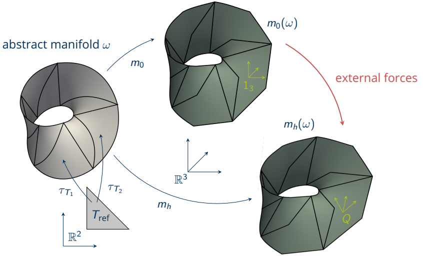
Find minimizing function pair of

$$J(m_h, Q_h) = J_{\text{shell}}(m_h, Q_h) + \textit{external forces}(m_h, Q_h)$$

in the admissible set

$$\mathcal{A} = \left\{ (m_h, Q_h) \in V_{p_1}(\mathcal{T}, \mathbb{R}^3) \times V_{p_2}(\mathcal{T}, \mathrm{SO}(3)) \;\middle|\; \text{Dirichlet boundary conditions for } m_h \right\}.$$





Cosserat shell: Minimization problem in the FE space

Problem

Find minimizing function pair of

$$J(m_h, Q_h) = \int_\omega W(E_h^e, K_h^e)\,\mathrm{d}\omega + \textit{external forces}(m_h, Q_h)$$

in the admissible set

$$\mathcal{A} = \left\{ (m_h, Q_h) \in V_{p_1}(\mathcal{T}, \mathbb{R}^3) \times V_{p_2}(\mathcal{T}, \mathrm{SO}(3)) \;\middle|\; \text{Dirichlet boundary conditions for } m_h \right\}.$$

- elastic shell strain tensor $E_h^e := \sum_{\alpha=1}^2 {Q_h}^T \frac{\partial m_h}{\partial x_\alpha} \otimes a^\alpha - \mathbf{a}$
- elastic shell bending-curvature tensor $K_h^e := \sum_{\alpha=1}^2 \operatorname{axl}\left({Q_h}^T \frac{\partial Q_h}{\partial x_\alpha} \right) \otimes a^\alpha$

Cosserat shell: Minimization problem in the FE space

Problem

Find minimizing function pair of

$$J(m_h, Q_h) = \int_\omega W(E_h^e, K_h^e)\, \mathrm{d}\omega + \textit{external forces}(m_h, Q_h)$$

in the admissible set

$$\mathcal{A} = \left\{ (m_h, Q_h) \in V_{p_1}(\mathcal{T}, \mathbb{R}^3) \times V_{p_2}(\mathcal{T}, \mathrm{SO}(3)) \,\middle|\, \text{Dirichlet boundary conditions for } m_h \right\}.$$

Theorem (Existence of minimizers)

Under reasonable assumptions on the functional W, on the external forces and on the stress-free configuration m_0, this minimization problem has a minimizer in $\mathcal{A}$.

[N., Sander, Neff, Bîrsan. A Cosserat shell model with general reference configuration and its discretization with GFE. In preparation.]

Cosserat shell: Algebraic minimization problem

Problem

Minimize

$$J(\vec{m}_h, \vec{Q}_h) = J(\vec{m}_h, \vec{Q}_h) + \textit{external forces}(m_h, Q_h)$$

in the admissible set

$$\vec{A}_h = \left\{ (\vec{m}_h, \vec{Q}_h) \text{ coefficients for } (m_h, Q_h) \;\middle|\; \text{Dirichlet boundary conditions for } \vec{m}_h \right\}.$$

- $\vec{A}_h \subset \mathbb{R}^{3N} \times (\mathrm{SO}(3))^N$, N total number of degrees of freedom in triangulation $\mathcal{T}$
- $\vec{m}_h$ is represented with $3N$ coefficients
- $\vec{Q}_h$ is represented with $4N$ coefficients (quaternions)

Recall: Riemannian Newton-type method for $f : \mathcal{M} \to \mathbb{R}$

Given an iterate $M_k \in \mathcal{M}$ and a retraction $R_{M_k} : T_{M_k}\mathcal{M} \to \mathcal{M}$

1. approximate f around M_k using a quadratic model

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

$$q_k(s) = f(M_k) + \langle \operatorname{grad}_M f_{|M_k}, s\rangle + \frac{1}{2}\langle \operatorname{Hess}_M f_{|M_k}[s], s\rangle$$

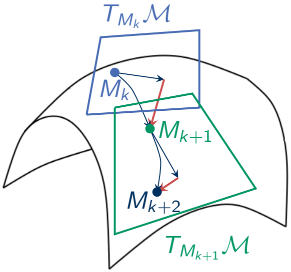
   where $\operatorname{grad}_M \in T_M\mathcal{M}$ and $\operatorname{Hess}_M[s] \in T_M\mathcal{M}$

2. minimize q_k

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

   i.e. solve $\quad \operatorname{Hess}_M f_{|M_k} s_k = -\operatorname{grad}_M f_{|M_k}$

3. set $M_{k+1} = R_{M_k}(s_k)$
4. return M_{k+1} once $\|s_k\| < \text{tol}$



Riemannian Trust-Region method for $f : \mathcal{M} \to \mathbb{R}$

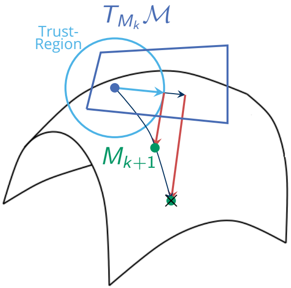
Given an iterate $M_k \in \mathcal{M}$, a retraction $R_{M_k} : T_{M_k}\mathcal{M} \to \mathcal{M}$ and a Trust-Region radius r_k:

1. approximate f around M_k using a quadratic model

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

$$q_k(s) = f(M_k) + \langle \operatorname{grad}_M f_{|M_k}, s \rangle + \frac{1}{2} \langle \operatorname{Hess}_M f_{|M_k}[s], s \rangle$$

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



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 $\operatorname{Hess}_M f_{|M_k} s_k = -\operatorname{grad}_M f_{|M_k}, \|s\| \le r_k$

3. if $f(M_k + s_k) \ge f(M_k)$: repeat using smaller radius r_k
   if $f(M_k + s_k) < f(M_k)$: 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 Trust-Region method for the Cosserat shell

Problem

Minimize

$$J(\vec{m}_h, \vec{Q}_h) = J(\vec{m}_h, \vec{Q}_h) + \textit{external forces}(m_h, Q_h)$$

in the admissible set

$$\vec{A}_h = \left\{ (\vec{m}_h, \vec{Q}_h) \text{ coefficients for } (m_h, Q_h) \;\middle|\; \text{Dirichlet boundary conditions for } \vec{m}_h \right\}.$$

1. at a given iterate $(\vec{m}_h, \vec{Q}_h)_k$, calculate $\text{grad}_{\text{coefficients}} J(\vec{m}_h, \vec{Q}_h)$ and $\text{Hess}_{\text{coefficients}} J(\vec{m}_h, \vec{Q}_h)$ using:
   - algorithmic differentiation
   - automatic differentiation (e.g., ADOL-C or CoDiPack)
2. solve constraint inner problem using e.g., Monotone-Multigrid-Method

$$\text{Hess}\, J(\vec{m}_h, \vec{Q}_h)\, \vec{s}_k = -\,\text{grad}\, J(\vec{m}_h, \vec{Q}_h), \quad \|\vec{s}_k\| \leq r_k$$

[Youett. (2015). Dynamic large deformation contact problems and applications in virtual medicine.]

Simulations: Klein bottle under load

- all simulations implemented in C++, using the `Dune` libraries
- discretization with 3072 triangular elements, FEs of second order
- fix Klein bottle with dirichlet boundary conditions on back side, volume load in direction of handle
- 73 Trust-Region steps

Time for the problem setup	9 h	$\approx$ 7.4 min per step
Time to solve	2 h	$\approx$ 1.7 min per step
Total time	11 h	$\approx$ 9.1 min per step

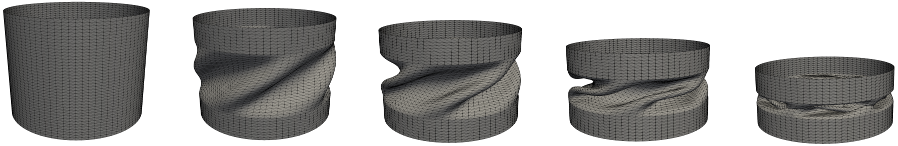
[Sander. (2020). DUNE – The Distributed and Unified Numerics Environment. Springer.]

[N., Bîrsan, Neff, Sander. Geometric Finite Elements for a geometrically nonlinear Cosserat shell model with nonplanar stress-free configuration. In preparation.]

Simulations: Clamped cylinder with torsional displacement

- discretization with 6400 triangular elements, FEs of second order
- simulation on the very right: 173 Trust-Region steps

Total time for the problem setup	29.84 h	$\approx$ 10.4 min per step
Total time to solve	3.15 h	$\approx$ 1 min per step
Total time	32.99 h	$\approx$ 11.4 min per step



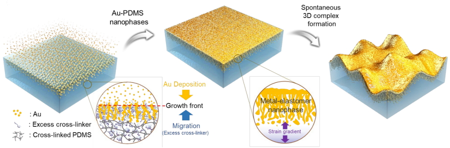
$\alpha = 0$ $\quad$ $\alpha = \frac{2}{32} \cdot 2\pi$ $\quad$ $\alpha = \frac{3}{32} \cdot 2\pi$ $\quad$ $\alpha = \frac{4}{32} \cdot 2\pi$ $\quad$ $\alpha = 0.14 \cdot 2\pi$

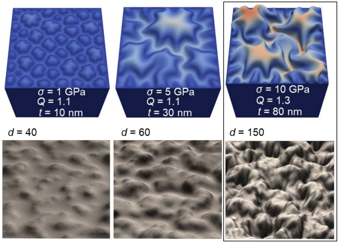
[N., Bîrsan, Neff, Sander. Geometric Finite Elements for a geometrically nonlinear Cosserat shell model with nonplanar stress-free configuration. In preparation.]

Simulations: Cosserat shell coupled with 3D elastic material

- quadratic elements in the shell: $48 \times 48 = 2304$, FEs of second order
- deformation function 389 154 DOFs
- simulation on the very right: 607 Trust-Region steps

Total time for the problem setup (parallel on 24 tasks)	35.97 h	$\approx$ 3.5 min per step	all tasks: 84 min
Total time to solve	73.76 h	$\approx$ 7.3 min per step	
Total time	115.89 h	$\approx$ 11.5 min per step	

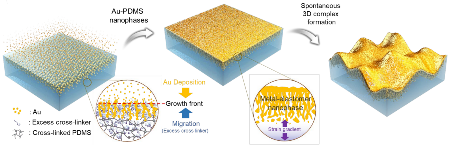


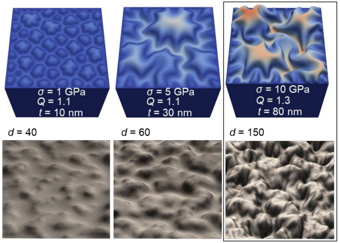


[Chae, Choi, N., Cho, Besford, Knapp, Masushko, Zabila, Pylypovskyi, Avdoshenko, Sander, Makarov, Fery. (2022). Three-dimensional complex of reticular metal-elastomer nanophases. Submitted.]

Summary

- generalization of Lagrange finite elements suitable for manifold-valued functions
- projection-based construction and construction using geodesic distances
- explicit constructions for SO(3) and SU(2)
- resulting finite element spaces have similar properties as Langrange FE spaces

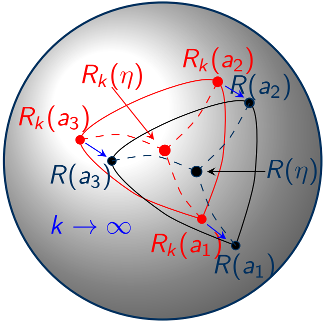




A: Properties of $V^{\text{proj/geo}}(\mathcal{T})$: Complete subset of $H^1(\omega, \mathcal{M})$

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.



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.

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 functional in detail

$$J_{\mathrm{shell}}(m,Q) = \int_\omega \big(W(E^e,K^e)\,\mathrm{d}\omega = \int_\omega \big(W_{\mathrm{memb}}(E^e,K^e) + W_{\mathrm{bend}}(K^e)\big)\,\mathrm{d}\omega$$

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

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

B: The Cosserat shell functional in detail

$$J_{\text{shell}}(m, Q) = \int_\omega \left(W(E^e, K^e\right) \mathrm{d}\omega = \int_\omega \left(W_{\text{memb}}(E^e, K^e) + W_{\text{bend}}(K^e)\right) \mathrm{d}\omega$$

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

Theorem (J_{shell})

If h is small enough, the initial configuration m_0 is smooth enough and m fulfills Dirichlet boundary conditions, then

- *J_{shell} is coercive.*
- *J_{shell} is bounded from below on $\mathcal{A}$.*
- *J_{shell} is $H^1(\omega, \mathbb{R}^3) \times H^1(\omega, \mathrm{SO}(3))$-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
- 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.]