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Numerical treatment of a geometrically nonlinear Cosserat shell model with nonplanar stress-free configuration

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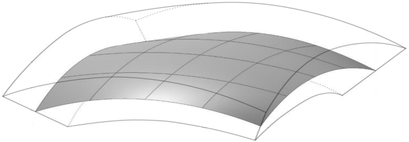
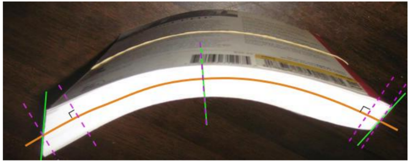
Shell models

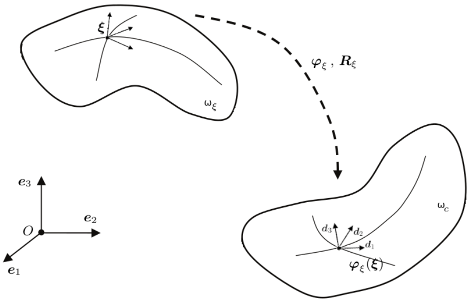
- Goal: Model the deformation of thin bodies under load
- Approach: Use physically reasonable assumptions to reduce a 3D-model to a 2D-model consisting of a midsurface with thickness $h > 0$
- Assumptions of the Cosserat shell model:
  - thickness does not change during deformation
  - straight lines normal to the midsurface remain straight (but not necessarily normal) after deformation
  - complete behavior under load is modeled using a deformation function together with independent local microrotations





The Cosserat shell model with nonplanar stress-free configuration *

- stress-free configuration $\omega_\xi \subset \mathbb{R}^3$
- deformed surface $\omega_c \subset \mathbb{R}^3$
- deformation function of the midsurface $\varphi_\xi : \omega_\xi \to \omega_c$, so $\omega_c := \varphi_\xi(\omega_\xi)$
- microrotation $R_\xi : \omega_\xi \to \mathrm{SO}(3)$, $R_\xi(\xi) = (d_1|d_2|d_3)$



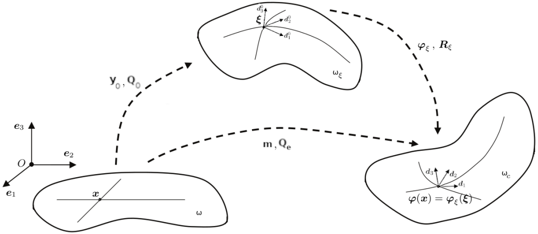
*[Bîrsan, Ghiba, Martin & Neff. (2019). **Refined dimensional reduction for isotropic elastic Cosserat shells with initial curvature.**]

The Cosserat shell model with nonplanar stress-free configuration

- map a planar reference configuration ω to ω_ξ

$$y_0 : \omega \subset \mathbb{R}^2 \to \mathbb{R}^3 \quad \text{, so} \quad y_0(\omega) = \omega_\xi \text{ and } \omega_c = \varphi_\xi \circ y_0(\omega)$$

- initial microrotation: $Q_0(x_1, x_2) := \operatorname{polar}(\nabla y_0 \,|\, \boldsymbol{n_0})$, $\boldsymbol{n_0}$ is the normal vector to ω_ξ
  $Q_0 = (d_1^0 | d_2^0 | d_3^0) \in \mathrm{SO}(3)$, d_i^0 are all orthonormal to each other and $\boldsymbol{n_0} = d_3^0$
- total shell deformation $\quad m(x_1, x_2) := \varphi_\xi \circ y_0(x_1, x_2) : \omega \to \omega_c$
- microrotation of the shell $\quad Q_e(x_1, x_2) := R_\xi \circ y_0(x_1, x_2) : \omega \to \mathrm{SO}(3)$



Terms from differential geometry

The domain ω_ξ is a manifold parametrized by y_0, so for each $\xi \in \omega_\xi$ we have:

- covariant base vectors of the tangent plane to ω_ξ at a point :

$$\boldsymbol{a}_1 := \frac{\partial y_0}{\partial x_1}, \quad \boldsymbol{a}_2 := \frac{\partial y_0}{\partial x_2}$$

  and their contravariant counterparts: $\boldsymbol{a}^1$, $\boldsymbol{a}^2$

- surface gradient for a vector field $\mathbf{f}$

$$\mathrm{Grad}_s\, \mathbf{f} := \sum_{\alpha=1,2} \frac{\partial}{\partial x_\alpha} \mathbf{f} \otimes \boldsymbol{a}^\alpha$$

- the first and second fundamental tensor and the alternator tensor

$$\mathbf{a} := \sum_{\alpha=1,2} \boldsymbol{a}_\alpha \otimes \boldsymbol{a}^\alpha, \qquad \mathbf{b} := -Grad_s \boldsymbol{n}_0, \qquad \mathbf{c} := -n_0 \times \mathbf{a}$$

- Gauss and mean curvature $K := \kappa_1 \cdot \kappa_2$, $H := \frac{\kappa_1+\kappa_2}{2}$,
  where κ_1 and κ_2 are the maximal and the minimal curvature

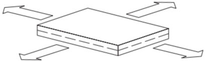
- surface element $a(x_1, x_2) = \sqrt{\det\left((\nabla y_0)^T \nabla y_0\right)}$

Strain and curvature measures

- shell strain tensor, measures displacement from stress-free state:

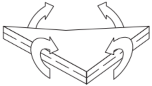
$$E^e := {Q_e}^T \operatorname{Grad}_s m - \mathbf{a} \in \mathbb{R}^{3\times3}$$

as $h \ll 1$, "no" strain in thickness direction, so we can find a coordinate system

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

- shell bending-curvature tensor, measures how much the mid-suface bends away from the mid-surface in stress-free state:

$$K^e := \sum_{\alpha=1,2} {Q_e}^T \left(\operatorname{axl} \left(\frac{\partial Q_e}{\partial x_\alpha} {Q_e}^T \right) \right) \otimes \boldsymbol{a}^\alpha \in \mathbb{R}^{3\times3} \, *$$

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

*For $Q \in \mathbb{R}^{3\times3}$ skew-symmetric: $\operatorname{axl}(Q) = Q_{23} e_1 + Q_{31} e_2 + Q_{12} e_3 \in \mathbb{R}^3$

Resulting minimization problem

- external loads result in the potential $\overline{\Pi}(m, Q_e)$
- Dirichlet boundary conditions on $\gamma_d \subset \partial\omega$ given by $m_{|_{\gamma_d}} = g_d \in H^1(\omega, \mathbb{R}^3)$
- Assumption: the shell consists of an hyperelastic material, so there is an energy density function for the shell
- deformation and microrotation (m, Q_e) minimize the total energy functional for shells:

$$I(m, Q_e) = \int_\omega \left[W_{\text{memb}}(E^e, K^e) + W_{\text{bend}}(K^e) \right] a(x_1, x_2)\, dx_1\, dx_2 - \overline{\Pi}(m, Q_e)$$

Resulting minimization problem

The total energy functional for shells

$$I(m, Q_e) = \int_\omega \Big[W_{\text{memb}}(E^e, K^e) + W_{\text{bend}}(K^e)\Big] a(x_1, x_2)\, dx_1 dx_2 - \overline{\Pi}(m, Q_e)$$

consists of:

- the membrane part

$$W_{\text{memb}}(E^e, K^e) = \left(h - K\frac{h^3}{12}\right) W_m(E^e) + \left(\frac{h^3}{12} - K\frac{h^5}{80}\right) W_m(E^e\mathbf{b} + \mathbf{c}K^e)$$
$$+ \frac{h^3}{6} W_m(E^e, \mathbf{c}K^e\mathbf{b} - 2H\mathbf{c}K^e) + \frac{h^5}{80} W_{mp}((E^e\mathbf{b} + \mathbf{c}K^e)\mathbf{b})$$

- the bending-curvature part

$$W_{\text{bend}}(K^e) = \left(h - K\frac{h^3}{12}\right) W_{curv}(K^e) + \left(\frac{h^3}{12} - K\frac{h^5}{80}\right) W_{curv}(K^e\mathbf{b}) + \frac{h^5}{80} W_{curv}(K^e\mathbf{b}^2)$$

- with the bilinear forms W_m, W_{mp} and W_{curv}
- the thickness $h > 0$, the tensors $\mathbf{a}, \mathbf{b}, \mathbf{c}$, the Gauss curvature K, the mean curvature H, and the surface element $a(x_1, x_2)$ as defined before

Resulting minimization problem: Existence of minimizers

Goal: Find (m, Q_e) minimizing the total energy functional for shells in the admissible set $\mathcal{A} = \left\{(m, Q_e) \in H^1(\omega, \mathbb{R}^3 \times \mathrm{SO}(3)) \;\middle|\; m_{|_{\gamma_d}} = g_d\right\}$:

Theorem (Existence of minimizers*)

The minimization problem admits at least one solution pair $(m, Q_e) \in \mathcal{A}$ if:

- *$h \ll 1$ is small enough such that $\left(h - K\frac{h^3}{12}\right) > 0$ and $\left(\frac{h^3}{12} - K\frac{h^5}{80}\right) > 0$ and therefore $W_{memb}(E^e, K^e)$ and $W_{bend}(K^e)$ are uniformly convex*
- *the potential $\overline{\Pi}(m, Q_e)$ is weakly lower semi-continuous and bounded*
- *the boundary data satisfies $g_d \in H^1(\omega, \mathbb{R}^3)$*
- *y_0 fulfills the requirements in $(^*)$*

Proof: The direct method of variations.

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

Numerical treatment: Discretization

- discretize ω_ξ using an appropriate triangulation $\mathcal{T}$: ω_h
- using the theory from above: transform each triangle $\tau \in \mathcal{T}$ to a reference triangle:

$$\int_\tau ..\, d\tau \text{ to } \int_T ..\, a(x_1, x_2) dx_1 dx_2$$

- deformation m: Lagrangian finite elements of order p_1: $V_{p_1,h}(\omega_h, \mathbb{R}^3)$
- microrotation Q_e: Geodesic Finite Elements (*) of order p_2: $V_{p_2,h}(\omega, \mathrm{SO}(3))$
- discrete function space $\mathcal{S}_h := V_{p_1,h}(\omega_h, \mathbb{R}^3) \times V_{p_2,h}(\omega_h, \mathrm{SO}(3))$
- H^1-conforming discretization:

$$(\varphi_h, R_h) \in \mathcal{S}_h \subset H^1(\omega_h, \mathbb{R}^3 \times \mathrm{SO}(3))$$

*[Sander, Neff & Bîrsan (2016). **Numerical treatment of a geometrically nonlinear planar Cosserat shell model.**]

Numerical treatment: Algebraic formulation

- algebraic formulation of the continuous minimization problem is

$$I(m_h, (Q_e)_h) = \int_{\omega_h} \left[W_{\text{memb}}(E_h^e, K_h^e) + W_{\text{bend}}(K_h^e) \right] d\omega_h - \overline{\Pi}(m_h, (Q_e)_h)$$

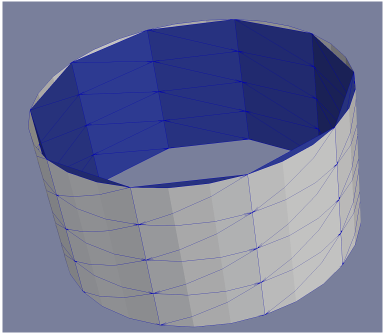
$$(m_h, (Q_e)_h) \in \mathcal{S}_h : \quad I(m_h, Q_{eh}) \leq J(v, U) \qquad \forall (v, U) \in \mathcal{S}_h$$

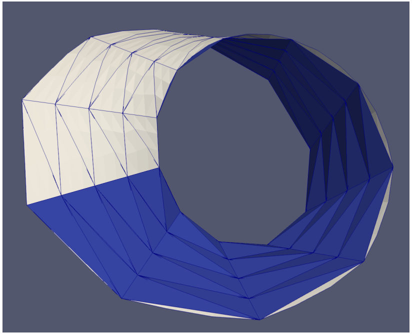
- $(m_h, (Q_e)_h)$ given using values in the Riemannian manifold $\mathbb{R}^{3N} \times \mathrm{SO}(3)^M$, $N, M =$ degrees of freedom in $V_{p_1,h}(\omega, \mathbb{R}^3)$ and $V_{p_2,h}(\omega_h, \mathrm{SO}(3))$
- solve using a Riemannian Trust-Region-Algorithm* with a direct solver for the constraint inner problems
- existence of minimizers can also be shown using the direct method of variations

* [Absil, Mahony, & Sepulchre. (2008). **Optimization Algorithms on Matrix Manifolds .** Princeton, New Jersey: Princeton University Press.

Numerical treatment: Experiments

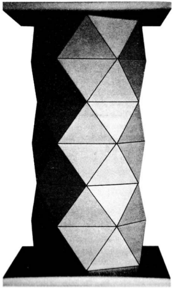
- discretize ω_ξ using an appropriate triangulation $\mathcal{T}$: ω_h
- the moebius strip here is not homeomorphic to a flat domain in $\mathbb{R}^2$!
- use dune-curvedgeometry for a better approximation of the geometry



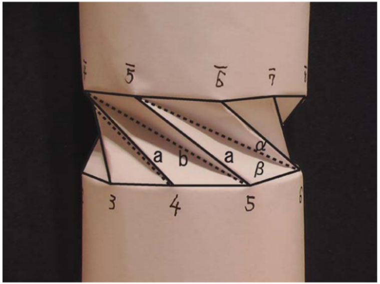


Buckling of a thin cylindrical shell under axial and torsional load *

- fundamental problems of elastic stability
- axial load: highly unstable response, settles into a localized form of the Yoshimura or diamond pattern
- torsional load: forms similar but oblique shapes, which can fold entirely flat



Yoshimura pattern

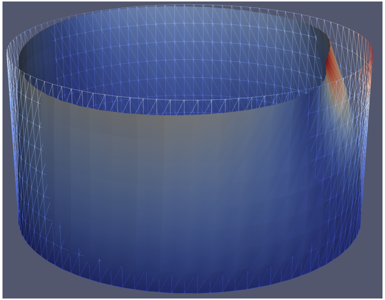


torsional load

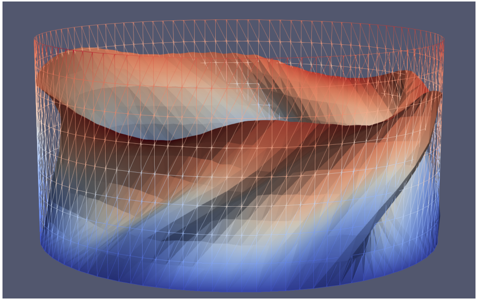
*[Hunt,& Ario (2004). **Twist buckling and the foldable cylinder: an exercise in origami.**]

Buckling of a thin cylindrical shell under axial and torsional load

- radius $= 10$, height $= 10$, 400 elements
- thickness $h = 0.1$
- fixed at $x = 0$



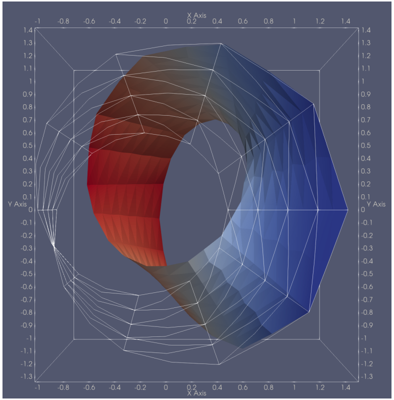
axial load of $2.1 \cdot 10^3$



torsional twist of 45°

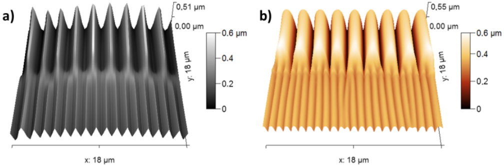
Force on a Moebius strip

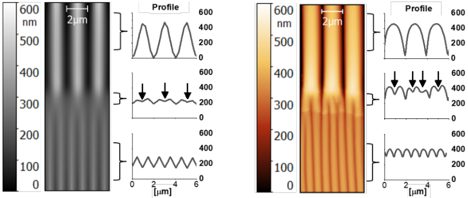
- radius $= 1$, height $= 1$
- 80 elements
- thickness $h = 0.01$
- fixed at $x > 0.8$
- Force of $(2, 0, 0)$
  at $x < 0$



Further applications for shell models

- cooperation with the Institut für Polymerforschung
- goal: simulate certain wavelengths, hierarchical wrinkle formation (transition between different wavelengths) and even a combination of different shells
- simulation: coupling of the shell-models and classical 3D-elasticity





A.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 $m_k : \mathbb{R}^N \to \mathbb{R}$

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

A.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 $J(x_k + s_k) > J(x_k)$

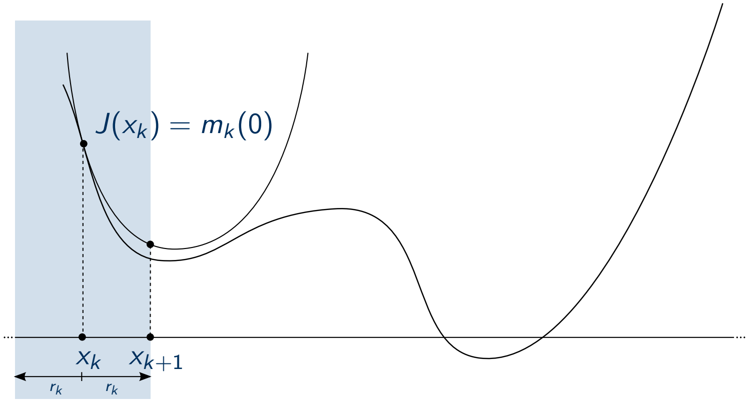
   set $x_{k+1} = x_k$ and decrease radius, e.g. $r_{k+1} = \frac{1}{2} r_k$

else : set $x_{k+1} = x_k + s_k$

   if : $\rho_k \gg 1$: increase radius, e.g. $r_{k+1} = 2 r_k$

   else : keep radius $r_{k+1} = r_k$

A.3 General Trust-Region-Algorithm in R^N



A.4 Riemannian Trust-Region-Algorithm

Trust-Region-Algorithm for the Riemannian manifold $\mathcal{M} := \mathbb{R}^{3N_1} \times SO(3)^{N_2}$

- map the minimization problem for $J : \mathcal{M} \to \mathbb{R}$ to a minimization problem for the pullback of J under R_{x_k} (retraction from $T_{x_k}\mathcal{M}$ to $\mathcal{M}$):

$$\hat{J}_{x_k} : T_{x_k}\mathcal{M} \to \mathbb{R}, \ \hat{J}_{x_k}(s) = J(R_{x_k} s)$$

- model m_k given by:

$$m_k(s) = J(x_k) + \langle \, grad \; J(x_k), s \rangle + \frac{1}{2} \langle Hess(\, J(x_k))[s], s \rangle$$

- minimization problem in tangent plane $T_{x_k}\mathcal{M}$ at the point x_k

$$s_k = \underset{s \in T_{x_k}\mathcal{M}, \, ||s||_\infty \leq r_k}{argmin} \quad m_k(s)$$

- $\rho_k = \frac{J(x_k) - J(R_{x_k}(s_k))}{m_k(0) - m_k(s_k)}, \qquad x_{k+1} = R_{x_k}(s_k)$

A.5 Convergence of the Riemannian Trust-Region-Algorithm

- Riemannian Trust-Region-Algorithm converges to a set of critical points if we achieve a certain energy decrese in each step (*)
- not guaranteed that it converges to a local minimizer
- actually possible to construct problems where this algorithm gets stuck in a saddle point

*[P.-A. Absil, R. Mahony, & R. Sepulchre. (2008). **Optimization Algorithms on Matrix Manifolds .** Princeton, New Jersey: Princeton University Press. p.149, Theorem 7.4.4]

B Geodesic Finite Elements

As the space $H^1(\omega, \mathrm{SO}(3))$ is not linear, we do geodesic interpolation

- Let $T_{ref} \in \omega_h$ with nodes a_j, $j = 1, \dots, m$ and Lagrangian interpolation polynomials $\lambda_i : T_{ref} \to \mathbb{R}$, $\lambda_i(a_j) = \delta_{ij}$ for $i, j = 1, \dots m$ and $\sum_{i=1}^m \lambda_i = 1$
- usual Lagrangian interpolation of a function $f : T_{ref} \to \mathbb{R}$ can be written as a minimization problem

$$v \mapsto \underset{w \in \mathbb{R}}{arg\ min} \sum_{i=1}^{m} \lambda_i(v) |f(a_i) - w|^2$$

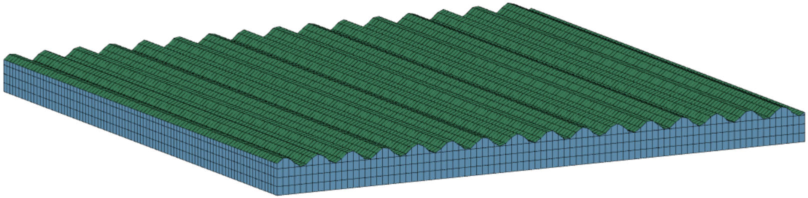
- analogously: interpolation of a function $f : T_{ref} \to \mathrm{SO}(3)$

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

- unique minimizer if the R_i are close enough together (*)

*[Sander, O., Neff, P. & Bîrsan, M. (2016). **Numerical treatment of a geometrically nonlinear planar Cosserat shell model.** Computational Mechanics 57(5): 817-840, p.8, Theorem 5]

C.1 Coupling of the System



- elastic substrate stretched, then coated with a thin, hard film
- Cosserat shell on top
- releasing the stretch results in mechanical instability phenomenon: formation of wrinkles

C.2 Mooney-Rivlin-Model

- material behavior under stress given by

$$J_e(\varphi) = \int_{\Omega} W_e(\nabla\varphi(x))\, dx + \int_{\Gamma_n} \varphi \cdot g \, dS$$

- reference domain $\Omega \subset \mathbb{R}^3$, deformation function $\varphi : \Omega \to \mathbb{R}^3$, $det(\nabla\varphi) > 0$
- force g applied at Neumann boundary Γ_n, Dirichlet boundary on the opposite side

C.3 Elastic Energy Density Function

- general Mooney-Rivlin energy density function:

$$W_e(\nabla\varphi) = \sum_{i,j=0}^{n} c_{ij}(\overline{I_1} - 3)^i(\overline{I_2} - 3)^j + \frac{1}{2}k \cdot log(det(\nabla\varphi))^2$$

- depending on the invariants I_1 and I_2 of the right Cauchy-Green deformation tensor $(\nabla\varphi)^T(\nabla\varphi)$
- $\overline{I_1} = \frac{I_1}{(det(\nabla\varphi))^{\frac{2}{3}}} = \frac{\lambda_1^2+\lambda_2^2+\lambda_3^2}{(det(\nabla\varphi))^{\frac{2}{3}}}$ and $\overline{I_2} = \frac{I_2}{(det(\nabla\varphi))^{\frac{4}{3}}} = \frac{\lambda_1^2\lambda_2^2+\lambda_2^2\lambda_3^2+\lambda_1^2\lambda_3^2}{(det(\nabla\varphi))^{\frac{4}{3}}}$
  with $\lambda_1, \lambda_2, \lambda_3$ eigenvalues of $\nabla\varphi$
- polyconvex density function for suitable parameters c_{ij}
- $\frac{1}{2}k \cdot log(det(\nabla\varphi))^2$ punishes large volume changes

C.4 Coupling of the System

Combine the Cosserat energy and the elastic energy:

$$J(\varphi, R) = \int_{\Omega} W_e(\nabla\varphi)\, dV + \int_{\Gamma_\xi} W_c(\varphi_{|\Gamma_\xi}, R)\, dS$$

$$\varphi = Id \text{ on } \Gamma_d, \quad Q_e = Id \text{ in } \Omega\backslash\Gamma_\xi$$

- reference configuration $\Omega \subset \mathbb{R}^3$
- deformation $\varphi \in H^1(\Omega, \mathbb{R}^3)$
- microrotation $Q_e \in H^1(\Gamma_\xi, \mathrm{SO}(3))$
- Cosserat boundary $\Gamma_\xi \subset \partial\Omega$
- Dirichlet boundary $\Gamma_d \subset \partial\Omega$