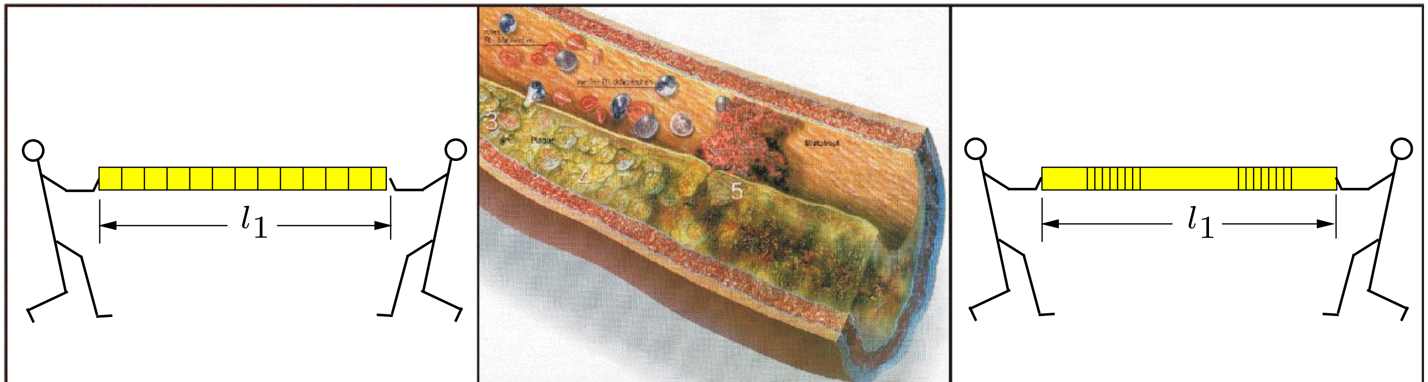
On the Construction of Polyconvex Free Energy Functions

Patrizio Neff



$$\boldsymbol{m} = \boldsymbol{a} \otimes \boldsymbol{a}\ ,\ \ \Psi(\boldsymbol{C}, \boldsymbol{m}) = \hat{\Psi}(\boldsymbol{Q}^T \boldsymbol{C} \boldsymbol{Q}, \boldsymbol{Q}^T \boldsymbol{m} \boldsymbol{Q})\ ,\ \ \boldsymbol{S} = 2\partial_{\boldsymbol{C}} \Psi$$

- Background and Motivation
- Convexity Conditions, Remarks on Invariant Theory
- Construction of Anisotropic Free Energies
- Anisotropic Free Energy for Soft Tissues
- Numerical Examples
- Conclusion

Acknowlegdement J. Schröder & D. Balzani

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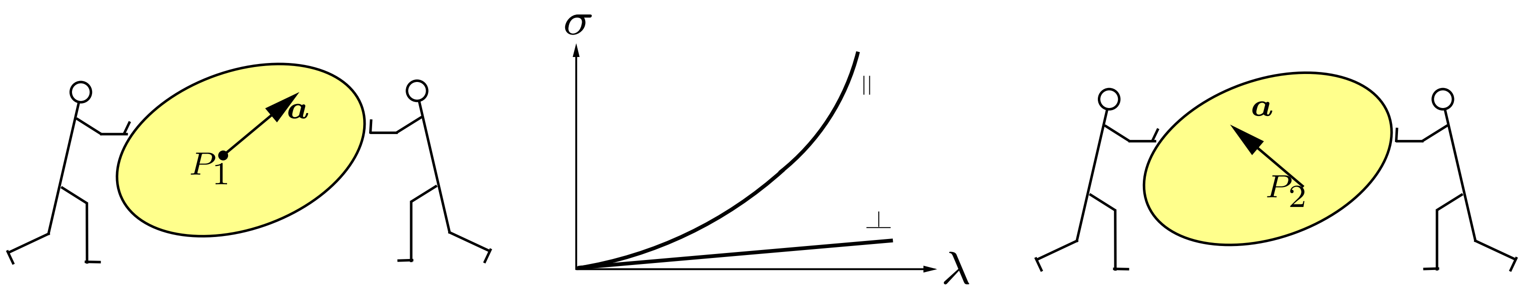
Background and Motivation

- Biological soft tissues are transverse isotropic: Models proposed by Fung et al. [1979], [1993], Weiss, Maker & Govindjee [1996], Holzapfel et al. [1996], Delfino et al. [1997], ...
  For an overview see Holzapfel [2000].

- Typical behavior of biological soft tissues:



  Exponential type behavior in fiber direction; nearly linear stress-strain characteristic in transverse direction.

- Coordinate free representation of finite anisotropic elasticity within the framework of invariant theory. Gurevich [1964], Weyl [1946], Wang [1969], [1970], [1971], Smith [1965], [1971], Boehler [1979], ...

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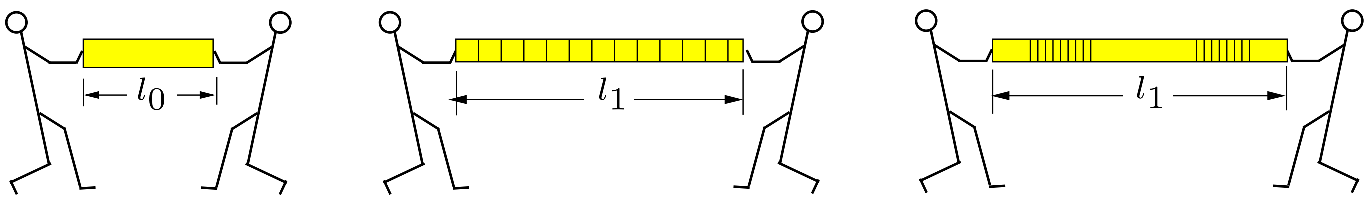
Background and Motivation

- In finite elasticity, the existence of minimizers is based on the direct methods of the calculus of variations (weak convergence). This is based on concepts like quasiconvexity Morrey [1952], and polyconvexity Ball [1977], see also Ciarlet [1989], Dacorgna [1989], Silhavý [1997].

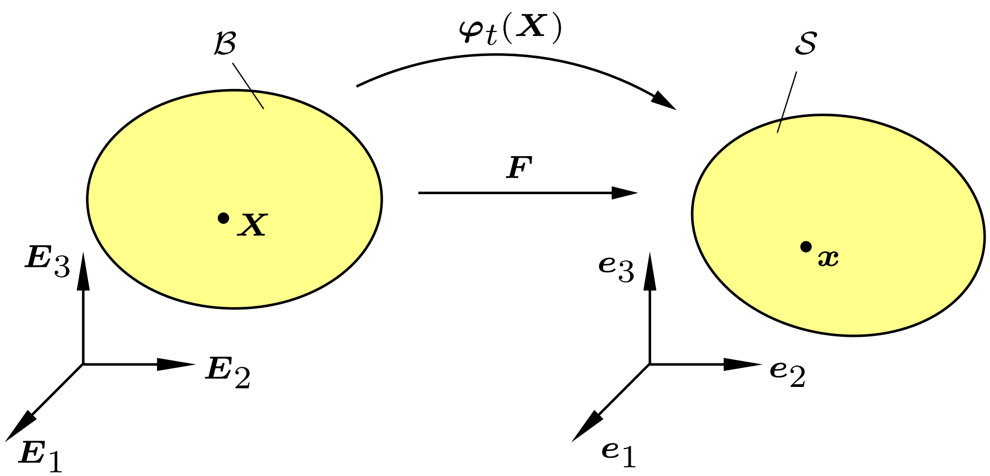


- Finite strain models are often based on direct extensions of small strain formulations, that means replacing of ε by $\boldsymbol{E}$.
- Problem: Simple formulation of the free energy in terms of $\boldsymbol{E}$ do not fulfill the quasiconvexity condition of Morrey [1952], i.e. the existence of a solution (minimizer) is not guaranteed.

Goal of the talk

- Construction of anisotropic, polyconvex free energy functions.
- Coordinate free representation based on the invariant theory.

Basic Kinematics



Deformationgradient

$$\boldsymbol{F}(\boldsymbol{X}) := \mathrm{Grad}\boldsymbol{\varphi}_t(\boldsymbol{X}) = \mathrm{Grad}\boldsymbol{x}(\boldsymbol{X})$$

Right Cauchy-Green tensor

$$\boldsymbol{C} := \boldsymbol{F}^T\boldsymbol{F}$$

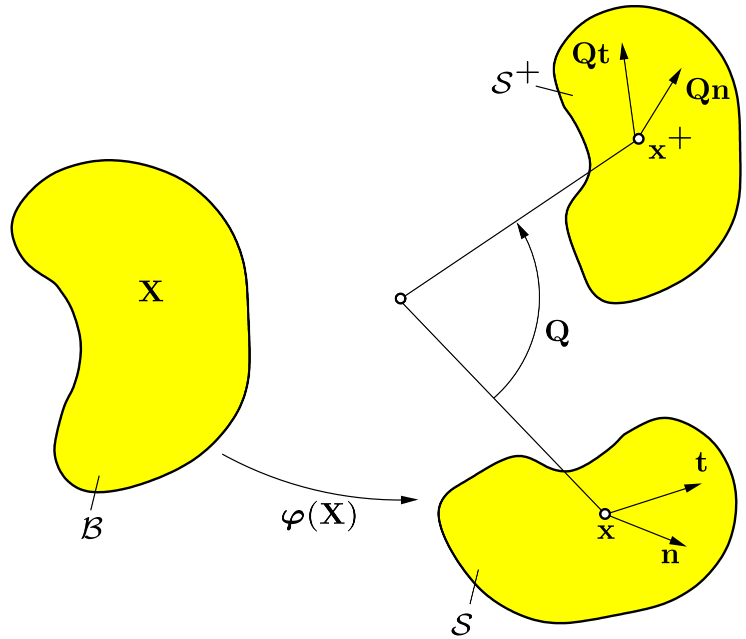
Green-Lagrange strain tensor

$$\boldsymbol{E} := \tfrac{1}{2}(\boldsymbol{C} - \boldsymbol{1})$$

Linearized Green-Lagrange strain tensor

$$Lin[\boldsymbol{E}] =: \boldsymbol{\varepsilon}$$

Material Frame Indifference, Objectivity



Superposed rigid body motions on $\mathcal{S}$

$$\boldsymbol{x} \to \boldsymbol{Q}\boldsymbol{x}\,,\ \boldsymbol{F} = \nabla_{\boldsymbol{X}}\boldsymbol{\varphi}\,,\ \boldsymbol{F}^+ = \boldsymbol{Q}\boldsymbol{F}$$

Invariance of constitutive equation

$$\hat{\psi}(\boldsymbol{F}) = \hat{\psi}(\boldsymbol{Q}\boldsymbol{F})$$

Requirement of objectivity demands

$$\boldsymbol{S}(\boldsymbol{F}) = \boldsymbol{S}(\boldsymbol{Q}\boldsymbol{F});\ \boldsymbol{Q}\boldsymbol{P}(\boldsymbol{F}) = \boldsymbol{P}(\boldsymbol{Q}\boldsymbol{F});\ \boldsymbol{Q}\boldsymbol{\sigma}(\boldsymbol{F})\boldsymbol{Q}^T = \boldsymbol{\sigma}(\boldsymbol{Q}\boldsymbol{F});\ \forall\,\boldsymbol{Q}\ \in \mathrm{SO}(3)$$

Reduced forms in $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$ satisfy a priori objectivity

$$\boldsymbol{S} \quad = \quad 2\partial_C\hat{\psi}(\boldsymbol{C})$$

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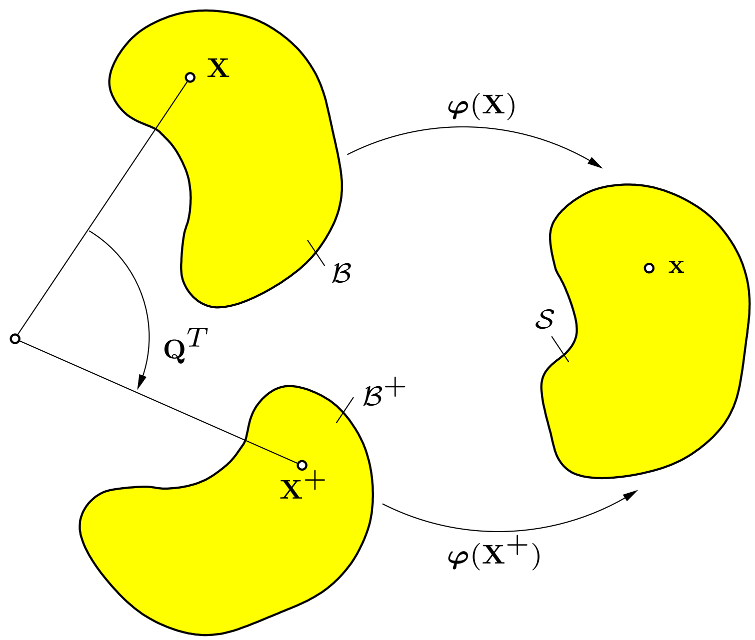
Concept of Material Symmetry



Superimposed rigid body motions on $\mathcal{B}$

$$\boldsymbol{X} \rightarrow \boldsymbol{Q}^T \boldsymbol{X}$$

implies the transformation rules

$$\boldsymbol{Q}^T \boldsymbol{S}(\boldsymbol{F})\boldsymbol{Q} = \boldsymbol{S}(\boldsymbol{F}\boldsymbol{Q});\ \boldsymbol{P}(\boldsymbol{F})\boldsymbol{Q} = \boldsymbol{P}(\boldsymbol{F}\boldsymbol{Q});\ \forall\, \boldsymbol{Q} \in \mathrm{SO}(3)$$

Special rotations with $\boldsymbol{Q} \in \mathcal{G}_k$

$$\hat{\psi}(\boldsymbol{F}\boldsymbol{Q}) = \hat{\psi}(\boldsymbol{F}) \quad \forall\, \boldsymbol{Q} \ \in \ \mathcal{G}_k, \boldsymbol{F}$$

must conform to the same stress response, e.g.

$$\boldsymbol{P}(\boldsymbol{F}\boldsymbol{Q}) = \boldsymbol{P}(\boldsymbol{F}) \quad \forall\, \boldsymbol{Q} \ \in \ \mathcal{G}_k, \boldsymbol{F}$$

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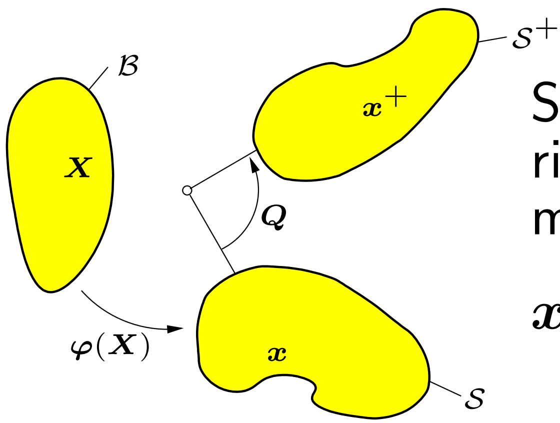
Material Frame Indifference, Objectivity



Superposed rigid body motions on $\mathcal{S}$

$$\boldsymbol{x} \rightarrow \boldsymbol{Q}\boldsymbol{x}$$

Invariance of constitutive equation

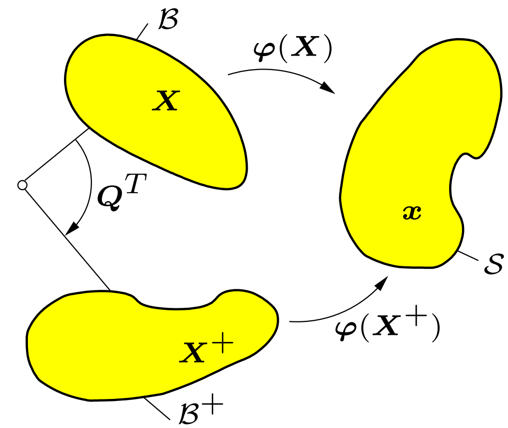
$$\hat{\psi}(\boldsymbol{F}) = \hat{\psi}(\boldsymbol{Q}\boldsymbol{F})$$

demands

$$\boldsymbol{S}(\boldsymbol{F}) = \boldsymbol{S}(\boldsymbol{Q}\boldsymbol{F}) \;\; \forall\, \boldsymbol{Q} \;\in \mathrm{SO}(3)$$

$$\Rightarrow \quad \boldsymbol{S} = 2\partial_C \hat{\psi}(\boldsymbol{C})$$

Material Symmetry, Isotropy of Space



Superimposed rigid body motions on $\mathcal{B}$

$$\boldsymbol{X} \rightarrow \boldsymbol{Q}^T\boldsymbol{X}$$

Implies the transformation rules

$$\boldsymbol{Q}^T\boldsymbol{S}(\boldsymbol{F})\boldsymbol{Q} = \boldsymbol{S}(\boldsymbol{F}\boldsymbol{Q}) \; \forall\, \boldsymbol{Q} \in \mathcal{G}_k, \boldsymbol{F}$$

Goal: Extension of $\mathcal{G}_k$-invariant to $\mathrm{SO}(3)$-invariant functions by using representation theorems of isotropic tensor functions.

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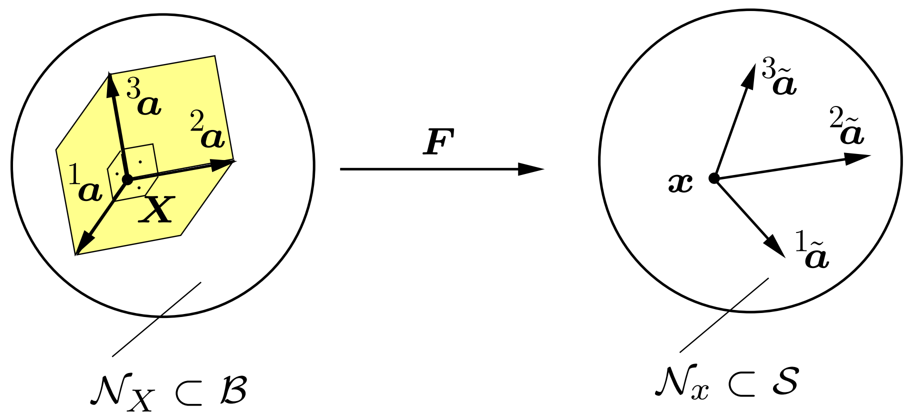
Elements of Invariant Theory

Basic idea: Introduce structural tensors ${}^i\boldsymbol{M} = {}^i\boldsymbol{M}({}^j\boldsymbol{a})$, ${}^j\boldsymbol{a}$ are preferred directions in $\mathcal{B}$



Invariant group of structural tensors is $\mathcal{G}_k$

$$ {}^i\boldsymbol{M}({}^j\boldsymbol{a}) = \boldsymbol{Q}^T\,{}^i\boldsymbol{M}({}^j\boldsymbol{a})\boldsymbol{Q} \quad \forall\, \boldsymbol{Q} \in \mathcal{G}_k $$

Anisotropic tensor function with respect to $\boldsymbol{C}$

$$ \boldsymbol{Q}^T\boldsymbol{S}(\boldsymbol{C}, {}^i\boldsymbol{M})\boldsymbol{Q} = \boldsymbol{S}(\boldsymbol{Q}^T\boldsymbol{C}\boldsymbol{Q}, {}^i\boldsymbol{M}) \;\; \forall\, \boldsymbol{Q} \in \mathcal{G}_k $$

Isotropic tensor function with respect to $\boldsymbol{C}$ and ${}^i\boldsymbol{M}|_{i=1,2,3}$

$$ \boldsymbol{Q}^T\boldsymbol{S}(\boldsymbol{C}, {}^i\boldsymbol{M})\boldsymbol{Q} = \boldsymbol{S}(\boldsymbol{Q}^T\boldsymbol{C}\boldsymbol{Q}, \boldsymbol{Q}^T\,{}^i\boldsymbol{M}\boldsymbol{Q}) \;\; \forall\; \boldsymbol{Q} \in \mathrm{SO}(3) $$

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Transverse Isotropy: Polynomial Basis in $\boldsymbol{C}$ and $\boldsymbol{M}$

Hilbert's Theorem: For a finite system of vectors and tensors, there exists an integrity basis which consists of a finite number of invariants.

Principal invariants of $\boldsymbol{C}$

$I_1 = \text{tr}\,\boldsymbol{C}\,, I_2 = \text{tr}[\text{Cof}\boldsymbol{C}]\,, I_3 = \det\boldsymbol{C}$

Basic invariants of $\boldsymbol{C}$

$J_1 = \text{tr}\boldsymbol{C}\,, J_2 = \text{tr}[\boldsymbol{C}^2]\,, J_3 = \text{tr}[\boldsymbol{C}^3]$

Transverse Isotropy: $\boldsymbol{M} := \boldsymbol{a} \otimes \boldsymbol{a}$ is a rank-one tensor with $||\boldsymbol{M}|| = 1$

$$\bar{I}_M = \mathrm{tr}\,\boldsymbol{M}\ ,\ \text{tr}[\text{Cof}\boldsymbol{M}] = 0\ ,\ \det\boldsymbol{M} = 0$$

Mixed invariants in $\boldsymbol{C}$ and $\boldsymbol{M}$

$$J_4 = \text{tr}[\boldsymbol{C}\boldsymbol{M}]\,,\ J_5 = \text{tr}[\boldsymbol{C}^2\boldsymbol{M}]\,,\ J_6 = \text{tr}[\boldsymbol{C}\boldsymbol{M}^2]\,,\ J_7 = \text{tr}[\boldsymbol{C}^2\boldsymbol{M}^2]$$

Polynomial basis with $J_4 \equiv J_6$ and $J_5 \equiv J_7$

$$\mathcal{P}_1 := \{I_1, I_2, I_3, J_4, J_5, \bar{I}_M\} \quad \text{or} \quad \mathcal{P}_2 := \{J_1, ...J_5, \bar{I}_M\}$$

$\mathcal{P}_1$, $\mathcal{P}_2$ are two possible **Integrity bases**. ψ, isotropic in $(\boldsymbol{C}, \boldsymbol{M})$, is of the form

$$\psi = \hat{\psi}(I_1, I_2, I_3, J_4, J_5, \bar{I}_M) = \sum_{j=1}^{n} \hat{\psi}_j(I_1, I_2, I_3, J_4, J_5, \bar{I}_M)$$

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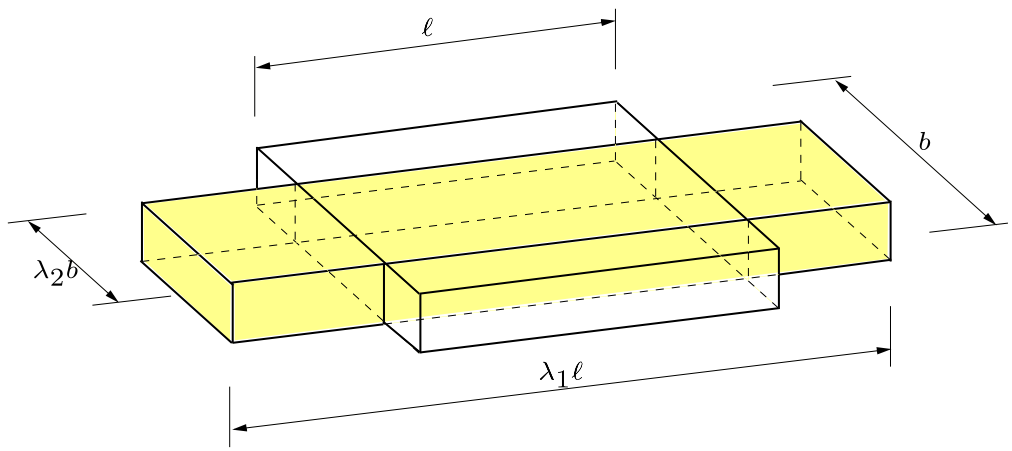
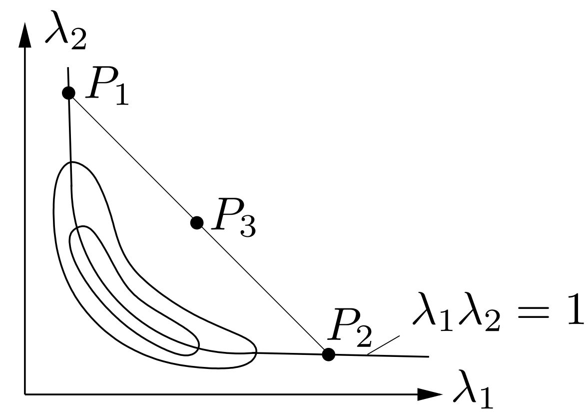
Conflicts with Convexity of $W(\boldsymbol{F})$

$$\Delta\boldsymbol{F} : \hat{\mathbb{C}}(\boldsymbol{F}) : \Delta\boldsymbol{F} > 0 \quad \text{mit} \quad \hat{\mathbb{C}} := \partial^2_{\boldsymbol{F}\boldsymbol{F}} W(\boldsymbol{F})$$

Nearly incompressible rubber sheet





Non-physical implication of convexity

$$W(P_3) \leq W(P_1) = W(P_2)$$

Further problems: Incompatible with objectivity; incompatible with growth condition, i.e. $W(\boldsymbol{F}) \to \infty$ if det$[\boldsymbol{F}] \to 0^+$; excludes instability problems

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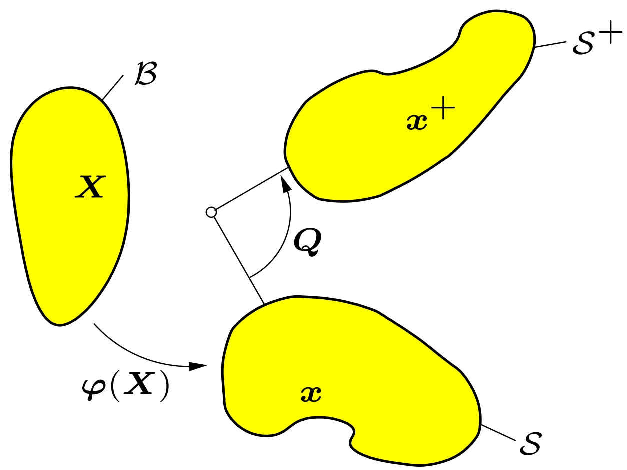
Conflicts with Convexity of $W(\boldsymbol{F})$

$$\Delta \boldsymbol{F} : \hat{\mathbb{C}}(\boldsymbol{F}) : \Delta \boldsymbol{F} > 0 \quad \text{with} \quad \hat{\mathbb{C}} := \partial^2_{(FF)} W(\boldsymbol{F})$$

Incompatible with objectivity



$$W(\boldsymbol{F}) = W(\boldsymbol{QF}) \quad \forall \boldsymbol{Q} \in SO(3), \{\boldsymbol{F} | \det[\boldsymbol{F}] > 0\}$$

Convexity of $W(\boldsymbol{F})$ implies

$$\boldsymbol{\tau} : [\boldsymbol{Q} - \boldsymbol{1}] \leq 0 \quad \forall \boldsymbol{Q} \in SO(3)$$

this leads to impossibilities like

$$\tau_1 + \tau_2 \geq 0, \qquad \tau_2 + \tau_3 \geq 0, \quad \ldots$$

Incompatible with growth condition

$$W(\boldsymbol{F}) \to \infty \qquad \text{if} \qquad \det[\boldsymbol{F}] \to 0^+$$

Excludes instability problems

$$\int_{\mathcal{B}} \Delta \boldsymbol{F} : \hat{\mathbb{C}}(\boldsymbol{F}) : \Delta \boldsymbol{F} \, dV = 0$$

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Convexity Conditions, Definitions

Quasiconvexity, MORREY [1952]

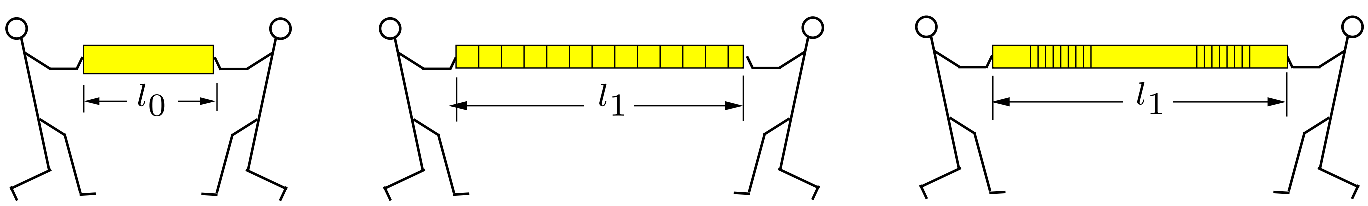
The elastic free energy $W(\boldsymbol{F})$ is quasiconvex whenever forall $\mathcal{B} \subset \mathbb{R}^3$ and all $\boldsymbol{F} \in \mathbb{M}^{3\times 3}$ and all $\boldsymbol{w} \in C_0^\infty(\Omega)$ we have

$$W(\boldsymbol{F}) \cdot |\mathcal{B}| = \int_{\mathcal{B}} W(\boldsymbol{F})\, dV \leq \int_{\mathcal{B}} W(\boldsymbol{F} + \nabla \boldsymbol{w})\, dV$$

Thus the homogeneous solution $\nabla \boldsymbol{\varphi} = \boldsymbol{F}$ of the BVP

$$\mathrm{Div}[D_F W(\nabla \boldsymbol{\varphi})] = \mathbf{0} \quad \text{with} \quad \boldsymbol{u} = \boldsymbol{F}\boldsymbol{X} + \boldsymbol{c} \quad \text{on} \quad \partial\mathcal{B}$$

is a global minimizer.



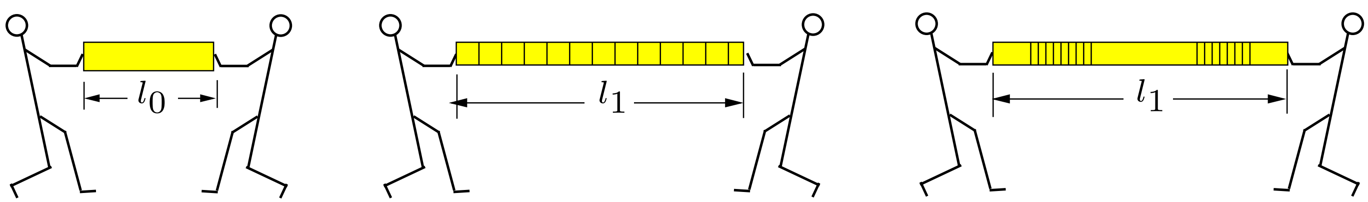
Convexity Conditions, Definitions

Polyconvexity, Ball [1977]

The elastic free energy $W(\boldsymbol{F})$ is polyconvex if and only if there exists a function $P : \mathbb{M}^{3\times3} \times \mathbb{M}^{3\times3} \times \mathbb{R} \mapsto \mathbb{R}$ (in general non unique) such that

$$W(\boldsymbol{F}) = P(\boldsymbol{F}, \mathrm{Cof}\boldsymbol{F}, \det \boldsymbol{F})$$

and the function $\mathbb{R}^{19} \mapsto \mathbb{R}$, $(X, Y, Z) \mapsto P(X, Y, Z)$ is convex.



Polyconvexity ⇒ Quasiconvexity⇒ Ellipticity

Ellipticity

The elastic free energy $W(\boldsymbol{F})$ is uniformly Legendre-Hadamard elliptic whenever $\exists\, c^+ > 0\ \forall\ \boldsymbol{F} \in \mathbb{M}^{3\times3}\ : \forall\ \xi, \eta \in \mathbb{R}^3$

$$D_F^2 W(\boldsymbol{F}).(\xi \otimes \eta, \xi \otimes \eta) \geq c^+ \cdot \|\xi\|^2 \|\eta\|^2$$

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Polyconvexity of some anisotropic functions

Polynomial functions of the form J_4^k are polyconvex

$$\boldsymbol{F} \mapsto (\operatorname{tr}[\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{M}])^k = (\operatorname{tr}[\boldsymbol{C}\boldsymbol{M}])^k = J_4^k \qquad \text{with } k \geq 1$$

Proof: First differential of $(\operatorname{tr}[\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{M}])^k = \langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^k$

$$\begin{aligned} D_F\left(J_4^k\right).\boldsymbol{H} &= k\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-1}\left(\langle \boldsymbol{F}, \boldsymbol{H}\boldsymbol{M}\rangle + \langle \boldsymbol{H}, \boldsymbol{F}\boldsymbol{M}\rangle\right) \\ &= 2k\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-1}\langle \boldsymbol{F}, \boldsymbol{H}\boldsymbol{M}\rangle \end{aligned}$$

Second differential

$$\begin{aligned} D_F^2\left(J_4^k\right).(\boldsymbol{H}, \boldsymbol{H}) &= 4k(k-1)\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-2} \cdot \langle \boldsymbol{F}\boldsymbol{M}, \boldsymbol{H}\rangle^2 + \\ &\quad 2k\langle \boldsymbol{F}, \boldsymbol{F}\boldsymbol{M}\rangle^{k-1}\langle \boldsymbol{H}, \boldsymbol{H}\boldsymbol{M}\rangle \geq 0 \end{aligned}$$

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Polyconvexity of some anisotropic functions

The polynomial function J_5 is not polyconvex

$$\boldsymbol{F} \mapsto \mathrm{tr}\,[\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{M}] = \mathrm{tr}\,[\boldsymbol{C}^2\boldsymbol{M}] = J_5$$

Proof: 2nd differential of $J_5 = \mathrm{tr}\,[\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{M}] = \|\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{a}\|_{\mathbb{R}^3}{}^2$ Special choice of tensors leads after some algebraic manipulations

$$D_F^2\left(\|\boldsymbol{F}_n^T\boldsymbol{F}_n\boldsymbol{a}\|_{\mathbb{R}^3}{}^2\right).(\xi\otimes\eta,\xi\otimes\eta) \quad \leq (-2+\tfrac{2}{3n^2})\tfrac{1}{3}+\tfrac{4}{n} < 0$$

Thus the term is not elliptic and hence not quasi-, polyconvex.

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Polyconvexity of some anisotropic functions

The often used polynomial functions $I_1 J_4$ is not polyconvex

$$\boldsymbol{F} \mapsto \operatorname{tr}(\boldsymbol{F}^T \boldsymbol{F} \boldsymbol{M}) \operatorname{tr}(\boldsymbol{F}^T \boldsymbol{F}) = \operatorname{tr}[\boldsymbol{C}\boldsymbol{M}] \operatorname{tr} \boldsymbol{C} = I_1 \, J_4$$

Proof: $I_1 J_4 = \operatorname{tr}[\boldsymbol{F}^T \boldsymbol{F} \boldsymbol{M}] \operatorname{tr}[\boldsymbol{F}^T \boldsymbol{F}] = \|\boldsymbol{F}\|^2 \|\boldsymbol{F}\boldsymbol{a}\|_{\mathbb{R}^3}{}^2$
Computing the second differential with respect to $\boldsymbol{F}$

$$D_F^2 \, (I_1 J_4) \, .(\boldsymbol{H}, \boldsymbol{H}) = 8 \langle \boldsymbol{F}, \boldsymbol{H} \rangle \langle \boldsymbol{F}\boldsymbol{a}, \boldsymbol{H}\boldsymbol{a} \rangle_{\mathbb{R}^3} + 2 \|\boldsymbol{F}\boldsymbol{a}\|_{\mathbb{R}^3}{}^2 \|\boldsymbol{H}\|^2 + 2 \|\boldsymbol{F}\|^2 \|\boldsymbol{H}\boldsymbol{a}\|_{\mathbb{R}^3}{}^2$$

For $\boldsymbol{F}, \boldsymbol{H} = \xi \otimes \eta$ choose the explicit expressions

$$\boldsymbol{F}_n := \begin{pmatrix} \frac{1}{n} & -1 & 0 \\ 0 & \frac{1}{n} & 0 \\ 0 & 0 & \frac{1}{n} \end{pmatrix}, \quad \xi = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \eta = \begin{pmatrix} 1 \\ n \\ 0 \end{pmatrix}, \quad \boldsymbol{a} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

If we choose $n > 2$, then we get

$$D_F^2 \left(\|\boldsymbol{F}\|^2 \cdot \|\boldsymbol{F}\boldsymbol{a}\|_{\mathbb{R}^3}{}^2 \right) .(\xi \otimes \eta, \xi \otimes \eta) = \frac{16}{n^2} - 4 < 0$$

Thus the term is not elliptic and hence not quasi-, polyconvex.

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Anisotropy - Analysis of Simple Extension

A generalization of small strain to large strain formulations, i.e.
$\boldsymbol{\varepsilon} \to \boldsymbol{E} = \frac{1}{2}[\boldsymbol{C} - \mathbf{1}]$, see e.g. SPENCER [1987], ...

$$\Psi(\boldsymbol{E}) = \alpha_1(\operatorname{tr}\boldsymbol{E})^2 + \alpha_2 \operatorname{tr}[\boldsymbol{E}^2] + \alpha_3 \operatorname{tr}[\boldsymbol{E}\boldsymbol{M}]\operatorname{tr}\boldsymbol{E} + \alpha_4 \operatorname{tr}[\boldsymbol{E}^2\boldsymbol{M}] + \alpha_5(\operatorname{tr}[\boldsymbol{E}\boldsymbol{M}])^2$$

- Advantage: A priori stress free reference configuration.
- Problem: This quadratic form in $\boldsymbol{E}$ is not quasiconvex.

$\Psi(\boldsymbol{E})$ **is not polyconvex.** Proof: CIARLET [1988], set $\alpha_3 = \alpha_4 = \alpha_5 = 0$.

$$W = a_0 + a_1 \operatorname{tr}(\boldsymbol{F}^T\boldsymbol{F}) + a_2 \operatorname{tr}(\boldsymbol{F}^T\boldsymbol{F})^2 + a_3 \operatorname{tr}(\operatorname{cof}[\boldsymbol{F}^T\boldsymbol{F}])$$

Material parameters

$$a_0 = (9\lambda + 6\mu)/8,\ a_1 = -(3\lambda + 2\mu)/4,\ a_2 = (\lambda + 2\mu)/8,\ a_3 = \lambda/4$$

W polyconvex, i.e. P is convex with respect to $\boldsymbol{\xi} := \{\boldsymbol{F}, \det[\boldsymbol{F}]\boldsymbol{F}^{-T}, \det[\boldsymbol{F}]\}$

$$P(\lambda\boldsymbol{\xi}_1 + (1-\lambda)\boldsymbol{\xi}_2) \leq \lambda P(\boldsymbol{\xi}_1) + (1-\lambda)P(\boldsymbol{\xi}_2)$$

Not fullfilled if $a_1 < 0$. Evaluate for $\lambda = 0.5$, $\boldsymbol{F}_1 = \epsilon\,\mathbf{1}$ and $\boldsymbol{F}_2 = \epsilon\,\operatorname{diag}[1,1,3]$.

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Extension of Mooney-Rivlin Material, $\psi(C)$ is PC

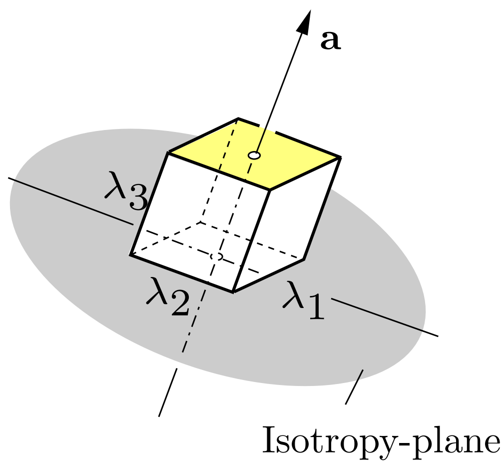
$$\psi(\boldsymbol{C}) = \alpha_1 \mathrm{tr}\,[\boldsymbol{C}] + \eta_1 \mathrm{tr}\,[\mathrm{cof}\boldsymbol{C}] + \delta_1 \det \boldsymbol{C} - \delta_2 \ln\left(\sqrt{\det \boldsymbol{C}}\right) + \ \alpha_3\ (\mathrm{tr}\,[\boldsymbol{C}\boldsymbol{M}])^2$$

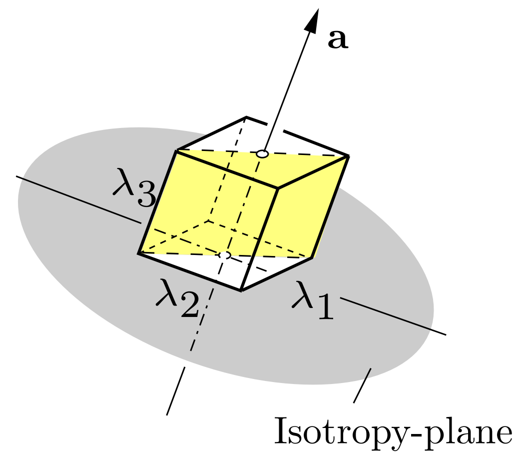
Condition for stress-free reference configuration $\boldsymbol{S}(\mathbf{1}) = \mathbf{0}$

$$\boldsymbol{S} = 2\partial_C \psi|_{C=\mathbf{1}} = (2\alpha_1 + 2\eta_1 + 2\delta_1 - \delta_2)\mathbf{1} + 4\alpha_3 \mathrm{tr}\,[\boldsymbol{M}]\boldsymbol{M} \neq 0\ \forall\ \alpha_3 \in \mathbb{R}^+$$

How to overcome this deficiency?

Construction of qualified polynomial invariants,
Schröder & Neff [2002a,b]





Physical motivation: Deformation of a preferred area element

Construction of new quadratic polynomials

Cayley-Hamilton theorem

$$\boldsymbol{C}^3 - I_1 \boldsymbol{C}^2 + I_2 \boldsymbol{C} - I_3 \boldsymbol{1} = \boldsymbol{0}$$

Multiplication with $\boldsymbol{C}^{-1}\boldsymbol{M}$ yields

$$\boldsymbol{C}^2\boldsymbol{M} - I_1 \boldsymbol{C}\boldsymbol{M} + I_2 \boldsymbol{M} - \mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M} = \boldsymbol{0}$$

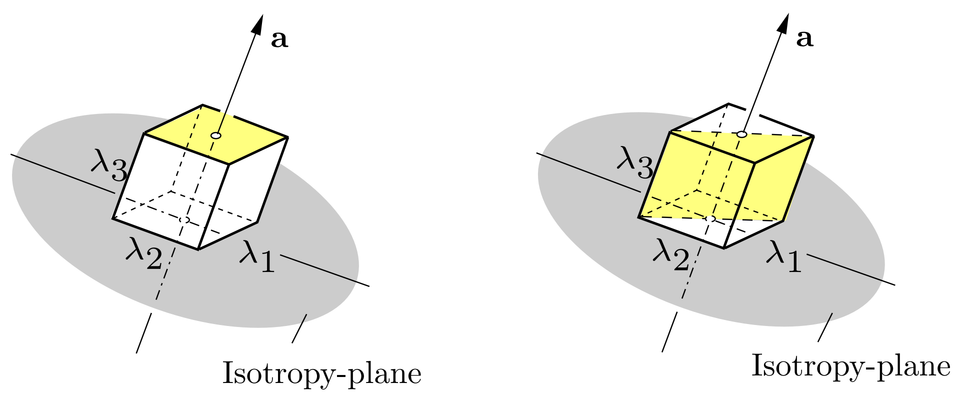
Taking the trace of the equation

$$K_1 := \mathrm{tr}\left[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}\right] = J_5 - I_1\, J_4 + I_2 \bar{I}_M$$

Analogous approach with $\boldsymbol{D} = \boldsymbol{1} - \boldsymbol{M}$ instead of $\boldsymbol{M}$

$$K_3 := \mathrm{tr}\left[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{D}\right] = I_1\, J_4 - J_5 + I_1(1 - \bar{I}_M)$$

K_1 and K_3 are polyconvex polynomial invariants. $\boldsymbol{S}(\boldsymbol{1}) = \boldsymbol{0}$ possible.



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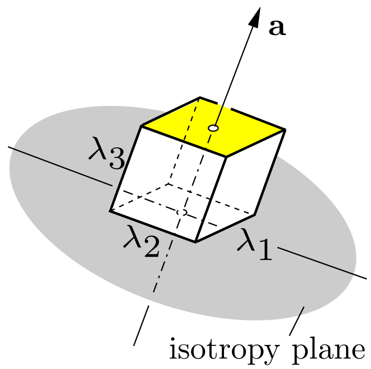
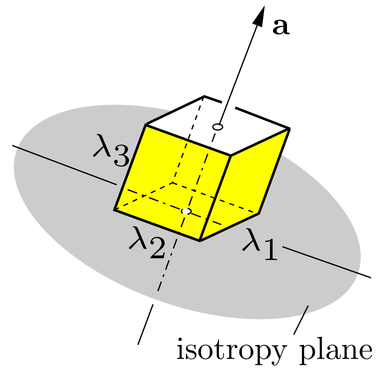
Geometric Interpretation of K_1 and K_3





Polyconvex polynomial invariant

$$K_1 = \mathrm{tr}\,[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}] = \mathrm{Cof}[\boldsymbol{F}^T\boldsymbol{F}] : \boldsymbol{a} \otimes \boldsymbol{a} = (\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a})(\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}) = ||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2$$

$\sqrt{K_1}$ controls the deformation of area element with normal $\boldsymbol{a}$.

Polyconvex polynomial invariant

$$K_3 = \mathrm{tr}\,[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{D}] = ||\mathrm{Cof}[\boldsymbol{F}]||^2 - ||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2$$

We see that $\sqrt{K_3}$ controls the deformation of the sum of area elements with normals in the isotropy plane, perpendicular to $\boldsymbol{a}$.

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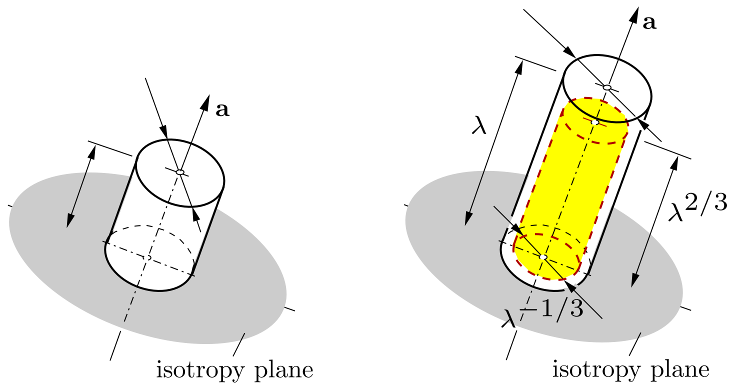
Geometric Interpretation of $I_1/I_3^{1/3}$

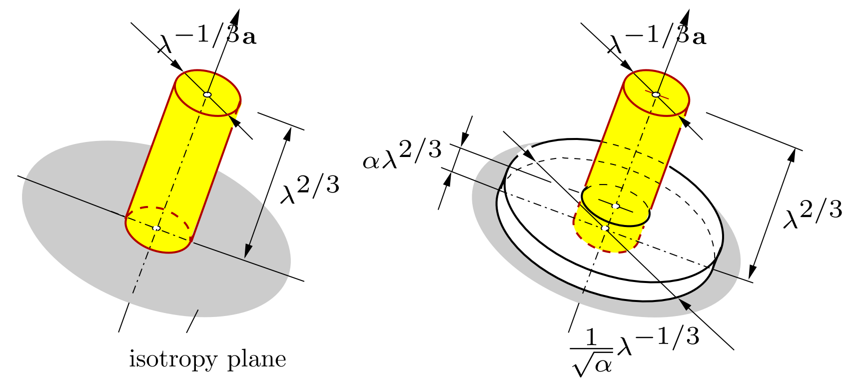


Polynomial invariant

$$I_1/I_3^{1/3} = \operatorname{tr}\boldsymbol{C}/(\det\boldsymbol{C})^{1/3}$$

controlls isochoric part of the deformation.

Geometric Interpretation of $J_4/I_3^{1/3}$, $K_2/I_3^{1/3}$



Polynomial invariants, with $\tilde{\boldsymbol{C}} := \boldsymbol{C}/(\det\boldsymbol{C})^{1/3}$

$$J_4/I_3^{1/3} = \operatorname{tr}[\tilde{\boldsymbol{C}}\boldsymbol{M}]$$

and

$$K_2/I_3^{1/3} = \operatorname{tr}[\tilde{\boldsymbol{C}}\boldsymbol{D}] = (I_1 - J_4)/I_3^{1/3}$$

weight the isochoric part of the deformation.

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Some isotropic polyconvex free energy terms

General functions

$$\boldsymbol{F} \mapsto \alpha^+ \, (\operatorname{tr} \boldsymbol{C})^k \quad k \geq 1$$

$$\boldsymbol{F} \mapsto \alpha^+ \, (\operatorname{tr} [\operatorname{Cof} \boldsymbol{C}])^k \quad k \geq 1$$

$$\boldsymbol{F} \mapsto \alpha^+ \, (\operatorname{tr} \boldsymbol{C})^2 / (\det \boldsymbol{C})^{1/3}$$

$$\boldsymbol{F} \mapsto \alpha^+ \, (\operatorname{tr} [\operatorname{Cof} \boldsymbol{C}])^2 / (\det \boldsymbol{C})^{1/3}$$

Isochoric functions

$$\boldsymbol{F} \mapsto \alpha^+ \, \operatorname{tr} \boldsymbol{C} / (\det \boldsymbol{C})^{1/3}$$

$$\boldsymbol{F} \mapsto \alpha^+ \, \operatorname{tr} [\operatorname{Cof} \boldsymbol{C}] / (\det \boldsymbol{C})^{1/3}$$

Volumetric functions

$$\boldsymbol{F} \mapsto \alpha^+ \, \det \boldsymbol{C}$$

$$\boldsymbol{F} \mapsto \alpha^+ \, 1/\det \boldsymbol{C}$$

$$\boldsymbol{F} \mapsto -\alpha^+ \, \ln(\sqrt{\det \boldsymbol{C}})$$

$$\boldsymbol{F} \mapsto \alpha^+ \, (\det \boldsymbol{C} - 1)^2$$

A priori stress free functions,
Hartmann & Neff [2001]

$$\boldsymbol{F} \mapsto \alpha^+ \, (\operatorname{tr} \boldsymbol{C} / (\det \boldsymbol{C})^{1/3} - 3)^2$$

$$\boldsymbol{F} \mapsto \alpha^+ \, (\operatorname{tr} [\operatorname{Cof} \boldsymbol{C}] / (\det \boldsymbol{C})^{1/3} - 3\sqrt{3})^2$$

$$\boldsymbol{F} \mapsto \alpha^+ \, (\operatorname{tr} [\operatorname{Cof} \boldsymbol{C}])^3 / (\det \boldsymbol{C})^2 - (3\sqrt{3})^2)$$

$$\boldsymbol{F} \mapsto \alpha^+ \, (\exp(\operatorname{tr} \boldsymbol{C} / (\det \boldsymbol{C})^{1/3} - 3) - 1)$$

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Shape functions for anisotropic part

Functions in $\boldsymbol{C}$ and $\boldsymbol{M}$

$\boldsymbol{F} \mapsto \alpha^+ \operatorname{tr}[\boldsymbol{M}\boldsymbol{C}]$

$\boldsymbol{F} \mapsto \alpha^+ (\operatorname{tr}[\boldsymbol{M}\boldsymbol{C}])^2$

$\boldsymbol{F} \mapsto \alpha^+ \operatorname{tr}[(\boldsymbol{M}\boldsymbol{C})^2]$

$\boldsymbol{F} \mapsto \alpha^+ \operatorname{tr}[(\boldsymbol{M}\boldsymbol{C})^2]/(\det \boldsymbol{C})^{1/3}$

Functions in $\mathsf{Cof}\boldsymbol{C}$ and $\boldsymbol{M}$

$\boldsymbol{F} \mapsto \alpha^+ \operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}]$

$\boldsymbol{F} \mapsto \alpha^+ (\operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}])^2$

$\boldsymbol{F} \mapsto \alpha^+ \operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3}$

$\boldsymbol{F} \mapsto \alpha^+ \operatorname{tr}[(\boldsymbol{M}\mathsf{Cof}\boldsymbol{C})^2]$

$\boldsymbol{F} \mapsto \alpha^+ (\operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}])^3$

$\boldsymbol{F} \mapsto \alpha^+ \operatorname{tr}[(\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}])^2]/(\det \boldsymbol{C})^{1/3}$

Functions in $\boldsymbol{M}$ and $\boldsymbol{C}$

$\boldsymbol{F} \mapsto \alpha^+ (2(\operatorname{tr}\boldsymbol{C})^2 + \operatorname{tr}[\boldsymbol{M}\boldsymbol{C}]\operatorname{tr}\boldsymbol{C})$

$\boldsymbol{F} \mapsto \alpha^+ (2(\operatorname{tr}[\mathsf{Cof}\boldsymbol{C}])^2 +$
$\quad + \operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}]\operatorname{tr}[\mathsf{Cof}\boldsymbol{C}])$

$\boldsymbol{F} \mapsto \alpha^+ ((\operatorname{tr}\boldsymbol{C} + 3\operatorname{tr}[\boldsymbol{M}\boldsymbol{C}])/(\det \boldsymbol{C})^{1/3} -$
$\quad -3 \cdot 4^{1/3})$

$\boldsymbol{F} \mapsto \alpha^+ (3\operatorname{tr}\boldsymbol{C} - 2\operatorname{tr}[\boldsymbol{M}\boldsymbol{C}])$

$\boldsymbol{F} \mapsto \alpha^+ (3\operatorname{tr}[\mathsf{Cof}\boldsymbol{C}] - 2\operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}])$

$\boldsymbol{F} \mapsto \alpha^+ ((\operatorname{tr}\boldsymbol{C})^2 - (\operatorname{tr}[\boldsymbol{M}\boldsymbol{C}])^2)$

$\boldsymbol{F} \mapsto \alpha^+ (\operatorname{tr}[\mathsf{Cof}\boldsymbol{C}] - \operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}])$

$\boldsymbol{F} \mapsto \alpha^+ (\operatorname{tr}\boldsymbol{C} - \operatorname{tr}[\boldsymbol{M}\boldsymbol{C}])^2$

$\boldsymbol{F} \mapsto \alpha^+ (\operatorname{tr}[\mathsf{Cof}\boldsymbol{C}] - \operatorname{tr}[\boldsymbol{M}\mathsf{Cof}\boldsymbol{C}])^2$

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Shape functions for anisotropic part

Functions in $\boldsymbol{C}$ or Cof$\boldsymbol{C}$ and $\boldsymbol{D}$

$$\boldsymbol{F} \mapsto \alpha^{+} \operatorname{tr}[\boldsymbol{DC}]$$

$$\boldsymbol{F} \mapsto \alpha^{+} (\operatorname{tr}[\boldsymbol{DC}])^2$$

$$\boldsymbol{F} \mapsto \alpha^{+} \operatorname{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}]$$

$$\boldsymbol{F} \mapsto \alpha^{+} (\operatorname{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}])^2$$

Functions in $\boldsymbol{D}$ and $\boldsymbol{C}$

$$\boldsymbol{F} \mapsto \alpha^{+} \operatorname{tr}[\boldsymbol{DC}]/(\det \boldsymbol{C})^{1/3}$$
$$\boldsymbol{F} \mapsto \alpha^{+} \operatorname{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3}$$

$$\boldsymbol{F} \mapsto \alpha^{+} (\operatorname{tr}[\boldsymbol{DC}])^2/(\det \boldsymbol{C})^{1/3}$$

$$\boldsymbol{F} \mapsto \alpha^{+} (2(\operatorname{tr}\boldsymbol{C})^2 + \operatorname{tr}[\boldsymbol{DC}]\operatorname{tr}\boldsymbol{C})$$

$$\boldsymbol{F} \mapsto \alpha^{+} (2(\operatorname{tr}[\mathrm{Cof}\boldsymbol{C}])^2 + \operatorname{tr}[\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}]\operatorname{tr}[\mathrm{Cof}\boldsymbol{C}])$$

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Stresses and Moduli

Computation of second Piola-Kirchhoff stresses

$$\boldsymbol{S} := 2\frac{\partial \psi}{\partial \boldsymbol{C}} = 2\sum_{j=1}^{n} \sum_{L_i \in P\ \bar{I}_M} \frac{\partial \psi_j}{\partial L_i}\frac{\partial L_i}{\partial \boldsymbol{C}}$$

yields the explicit expression for

$$\boldsymbol{S} = 2\sum_{j=1}^{n}\{(\frac{\partial \psi_j}{\partial I_1} + \frac{\partial \psi_j}{\partial I_2} I_1)\mathbf{1} - \frac{\partial \psi_j}{\partial I_2}\boldsymbol{C} + \frac{\partial \psi_j}{\partial I_3}\mathrm{Cof}\boldsymbol{C} + \frac{\partial \psi_j}{\partial J_4}\boldsymbol{M} + \frac{\partial \psi_j}{\partial J_5}(\boldsymbol{C}\boldsymbol{M} + \boldsymbol{M}\boldsymbol{C})\}$$

The moduli are given by $\mathbb{C} = 4\dfrac{\partial^2 \psi}{\partial \boldsymbol{C} \partial \boldsymbol{C}}$

Remarks

- We choose polyconvex terms ψ_j and then guarantee the ellipticity a priori.
- The advantage of this formulation is that the structure of the stresses and moduli remains unaltered upon introducing additional polynomial invariant terms. Because the tensor generators are the same and only the scalar-valued derivatives of the ψ_j's with respect to the elements of the chosen polynomial basis have to be modified.
- Problem: A priori stress free reference configuration not met. This condition can be fulfilled by choosing appropriate positive parameters α_j^+ in front of the ψ_j's.

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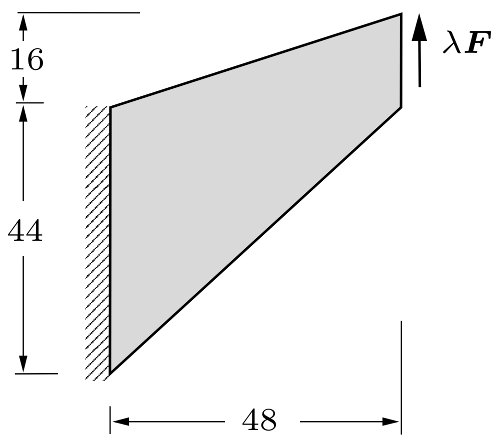
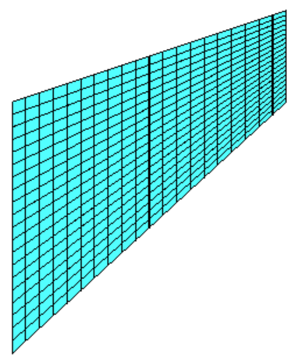
3D-Analysis of a Tapered Cantilever

System and boundary conditions





$$\psi_1(\boldsymbol{C},\boldsymbol{M}) = \alpha_1 \operatorname{tr} \boldsymbol{C}$$
$$\psi_2(\boldsymbol{C},\boldsymbol{M}) = \delta_5 \ 1/\det \boldsymbol{C}$$
$$\psi_3(\boldsymbol{C},\boldsymbol{M}) = \beta_1 \operatorname{tr}[\boldsymbol{M}\boldsymbol{C}]$$
$$\psi_4(\boldsymbol{C},\boldsymbol{M}) = \gamma_3 \operatorname{tr}[\boldsymbol{M}\,\mathsf{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3}$$
$$\psi_5(\boldsymbol{C},\boldsymbol{M}) = \phi_5 \operatorname{tr}[\boldsymbol{D}\mathsf{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3}$$
$$\psi_6(\boldsymbol{C},\boldsymbol{M}) = \phi_7 \ (\operatorname{tr}[\boldsymbol{D}\mathsf{Cof}\boldsymbol{C}])^2/(\det \boldsymbol{C})^{1/3}$$
$$\psi_7(\boldsymbol{C},\boldsymbol{M}) = \kappa_{11} \ (\operatorname{tr}[\mathsf{Cof}\boldsymbol{C}] - \operatorname{tr}[\boldsymbol{M}\,\mathsf{Cof}\boldsymbol{C}])^2$$

Free energy funktion (**MS 1**): $\psi = \sum_{j=1}^{7} \hat{\psi}_j(I_1, I_2, I_3, J_4, J_5, \bar{I}_M)$

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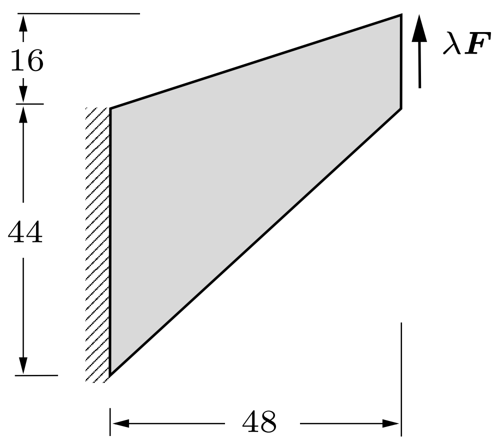
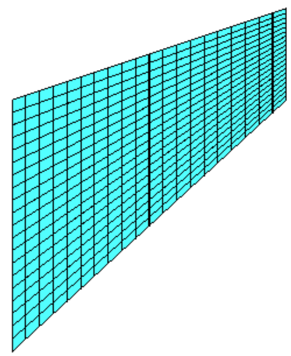
3D-Analysis of a Tapered Cantilever

System and boundary conditions





Parameters of polyconvex functions, MS 1

$$
\begin{aligned}
\alpha_1 &= 2.6875 \\
\delta_5 &= 136.41 \\
\beta_2 &= 112.21 \\
\gamma_3 &= 80.393 \\
\phi_5 &= 162.15 \\
\phi_7 &= 1.1920 \\
\kappa_{11} &= 5.7233
\end{aligned}
$$

Corresponding linearized moduli

$$
\mathbb{C} = \begin{bmatrix}
1215.0 & 445.0 & 581.0 & 0 & 0 & 0 \\
445.0 & 1215.0 & 581.0 & 0 & 0 & 0 \\
581.0 & 581.0 & 2900.0 & 0 & 0 & 0 \\
0 & 0 & 0 & 385.0 & 0 & 0 \\
0 & 0 & 0 & 0 & 500.0 & 0 \\
0 & 0 & 0 & 0 & 0 & 500.0
\end{bmatrix}
$$

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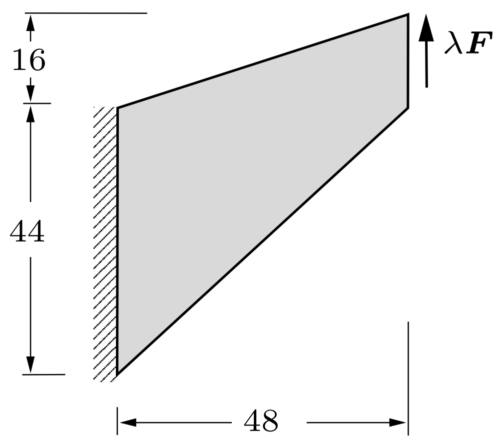
3D-Analysis of a Tapered Cantilever



$$\psi = \sum_{j=1}^{7} \hat{\psi}_j$$

$$\psi_1(\boldsymbol{C}, \boldsymbol{M}) = \alpha_1 \ \mathrm{tr}\, \boldsymbol{C}$$

$$\psi_2(\boldsymbol{C}, \boldsymbol{M}) = \delta_5 \ 1/\det \boldsymbol{C}$$

$$\psi_3(\boldsymbol{C}, \boldsymbol{M}) = \beta_1 \ \mathrm{tr}\, [\boldsymbol{M}\boldsymbol{C}]$$

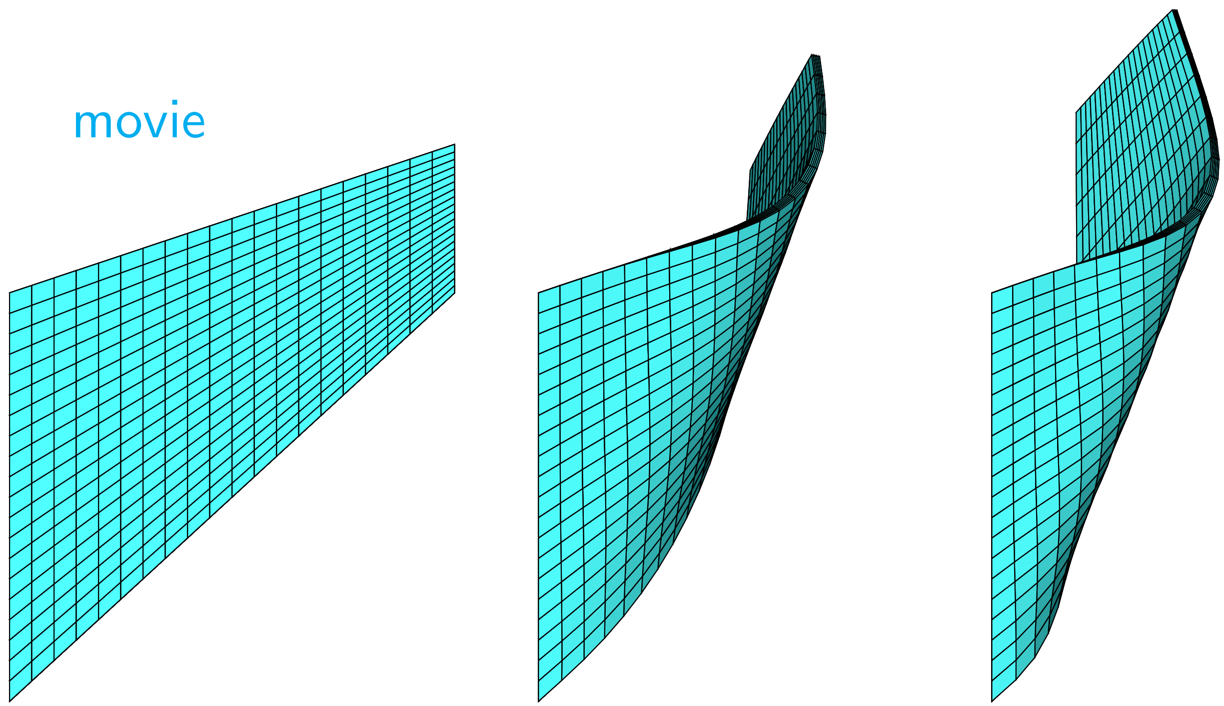
$$\psi_4(\boldsymbol{C}, \boldsymbol{M}) = \gamma_3 \ \mathrm{tr}\, [\boldsymbol{M}\,\mathrm{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3}$$

$$\psi_5(\boldsymbol{C}, \boldsymbol{M}) = \phi_5 \ \mathrm{tr}\, [\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3}$$

$$\psi_6(\boldsymbol{C}, \boldsymbol{M}) = \phi_7 \ (\mathrm{tr}\, [\boldsymbol{D}\mathrm{Cof}\boldsymbol{C}])^2/(\det \boldsymbol{C})^{1/3}$$

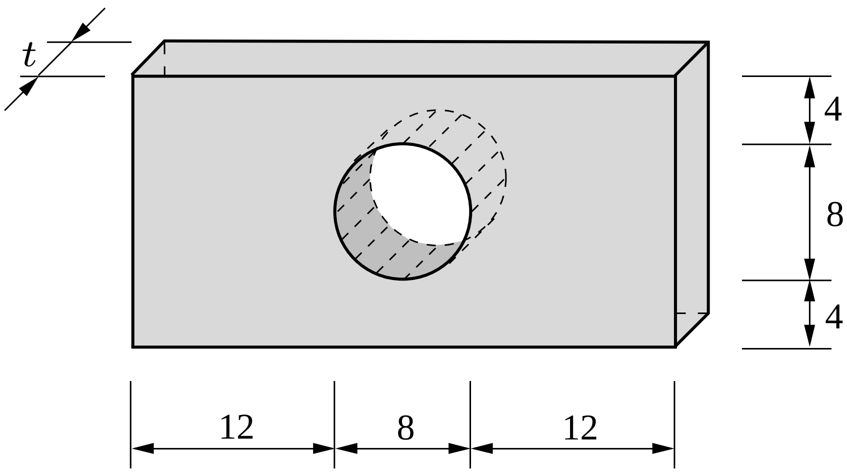
$$\psi_7(\boldsymbol{C}, \boldsymbol{M}) = \kappa_{11} \ (\mathrm{tr}\, [\mathrm{Cof}\boldsymbol{C}] - \mathrm{tr}\, [\boldsymbol{M}\,\mathrm{Cof}\boldsymbol{C}])^2$$

movie



Perforated Plate with Centered Hole

Dimension of specimen



$$\psi_1(\boldsymbol{C},\boldsymbol{M}) = \alpha_1 \; \mathrm{tr}\,\boldsymbol{C}$$
$$\psi_2(\boldsymbol{C},\boldsymbol{M}) = \delta_2 \; \mathsf{ln}[\sqrt{\det \boldsymbol{C}}]$$
$$\psi_3(\boldsymbol{C},\boldsymbol{M}) = \gamma_5 \; (\mathrm{tr}\,[\boldsymbol{M}\,\mathsf{Cof}\boldsymbol{C}])^3$$
$$\psi_4(\boldsymbol{C},\boldsymbol{M}) = \phi_2 \; (\mathrm{tr}\,[\boldsymbol{D}\boldsymbol{C}])^2$$
$$\psi_5(\boldsymbol{C},\boldsymbol{M}) = \phi_4 \; (\mathrm{tr}\,[\boldsymbol{D}\mathsf{Cof}\boldsymbol{C}])^2$$
$$\psi_6(\boldsymbol{C},\boldsymbol{M}) = \phi_6 \; \mathrm{tr}\,[\boldsymbol{D}\mathsf{Cof}\boldsymbol{C}]/(\det \boldsymbol{C})^{1/3}$$
$$\psi_7(\boldsymbol{C},\boldsymbol{M}) = \phi_7 \; (\mathrm{tr}\,[\boldsymbol{D}\mathsf{Cof}\boldsymbol{C}])^2/(\det \boldsymbol{C})^{1/3}$$

Free energy funktion (**MS 2**): $\psi = \sum_{j=1}^{7} \hat{\psi}_j(I_1, I_2, I_3, J_4, J_5, \bar{I}_M)$

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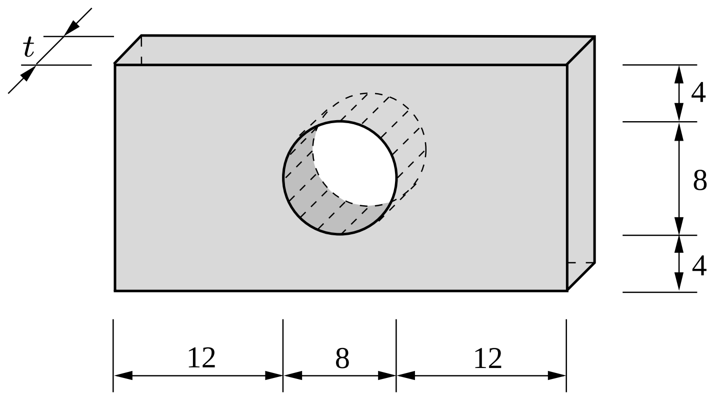
Perforated Plate with Centered Hole

Dimension of specimen



Parameters of polyconvex functions, MS 2

$$\begin{aligned} \alpha_1 &= 14.0625 \\ \delta_2 &= 325.0 \\ \gamma_5 &= 3.64583 \\ \phi_2 &= 3.515625 \\ \phi_4 &= 20.3125 \\ \phi_6 &= 4.6875 \\ \phi_7 &= 15.234375 \end{aligned}$$

Corresponding linearized moduli

$$\mathbb{C} = \begin{bmatrix} 1000.0 & 300.0 & 600.0 & 0 & 0 & 0 \\ 300.0 & 1000.0 & 600.0 & 0 & 0 & 0 \\ 600.0 & 600.0 & 1400.0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 350.0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 200.0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 200.0 \end{bmatrix}$$

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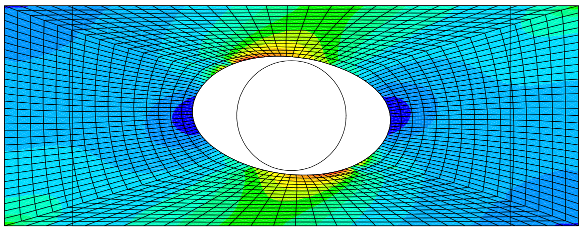
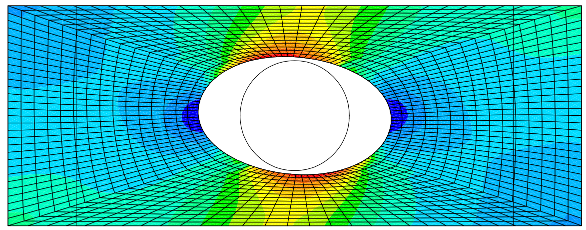
Perforated Plate with Centered Hole

Material set MS 1

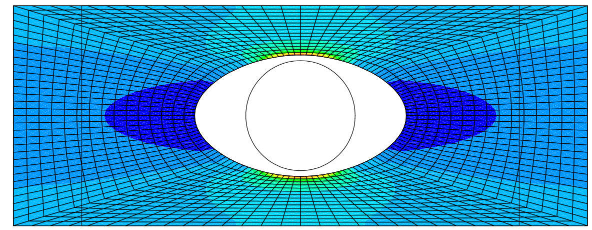
$\boldsymbol{a} = [1, 1, 0]^T/\sqrt{2}$



$\boldsymbol{a} = [0.5, 1, 0]^T/\sqrt{1.25}$

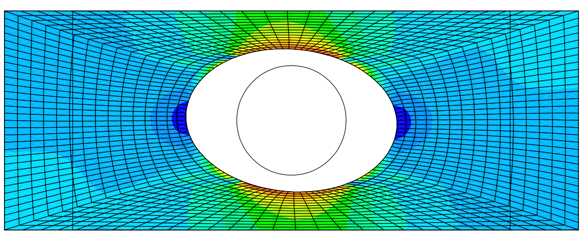


$\boldsymbol{a} = [1, 0, 0]^T$

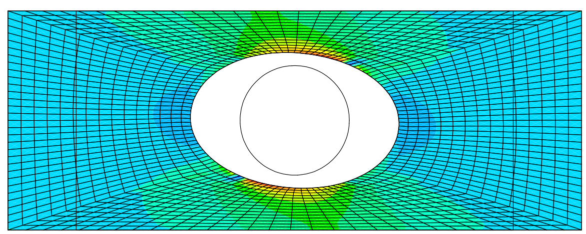


Material set MS 2

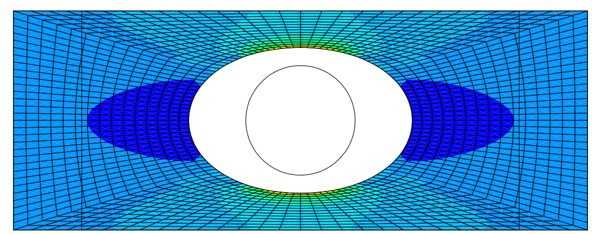
$\boldsymbol{a} = [1, 1, 0]^T/\sqrt{2}$



$\boldsymbol{a} = [0.5, 1, 0]^T/\sqrt{1.25}$



$\boldsymbol{a} = [1, 0, 0]^T$



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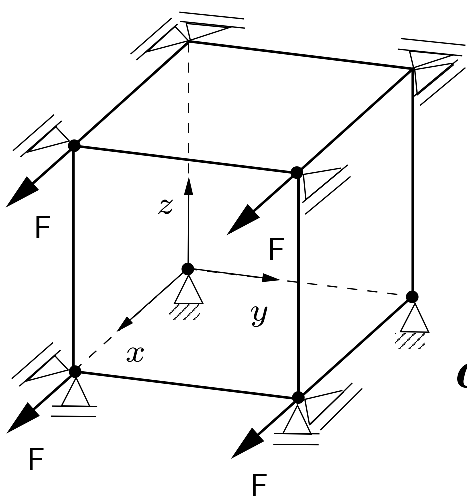
Free Energy for Soft Tissues

FUNG [1973], TONG & FUNG [1973], FUNG [1993]

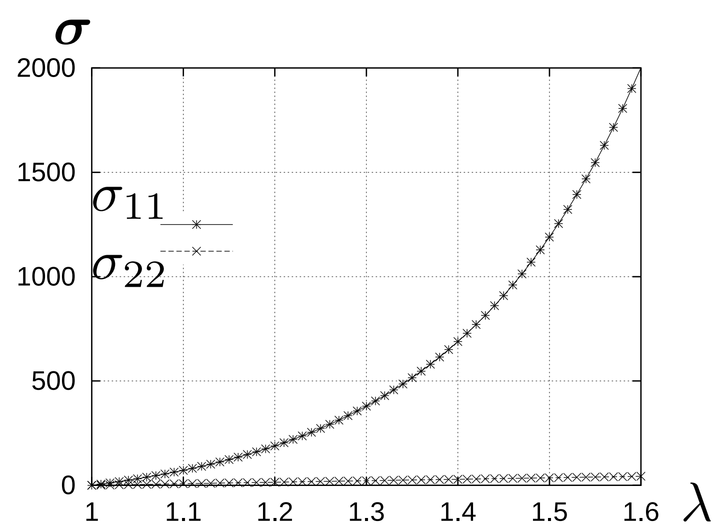
$$\psi = \hat{\psi}_1(\alpha_i, \boldsymbol{E}) + c\,\mathsf{exp}[\hat{F}(\beta_k, \boldsymbol{E})] \quad i, k = 1, ...4$$

WEISS, MAKER & GOVINDJEE [1996]

$$\tilde{\psi}(I_1, I_2, I_3, J_4) = \beta_1(\frac{I_1}{I_3^{1/3}} - 3) + \beta_2(\frac{I_2}{I_3^{2/3}} - 3) + \beta_3(\mathsf{exp}[\frac{J_4}{I_3^{1/3}} - 1] - \frac{J_4}{I_3^{1/3}}) + \beta_4(I_3 - \ln(I_3))$$



$$\boldsymbol{a} = (1, 0, 0)^T$$



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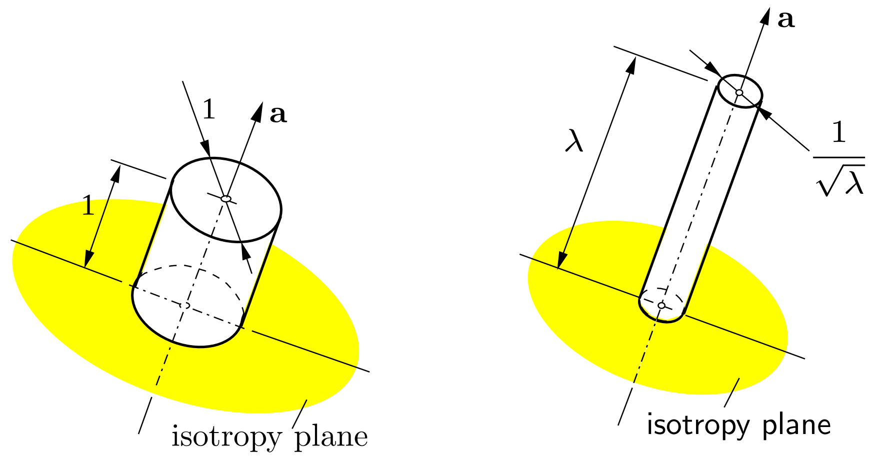
Polyconvex Free Energy for Soft Tissues



Split of ψ in an isotropic and an anisotropic part

$$\hat{\psi}(I_1, I_2, I_3, J_4, J_5) = \hat{\psi}^{iso}(I_1, I_2, I_3) + \hat{\psi}^{ti}(I_1, I_2, I_3, J_4, J_5)$$

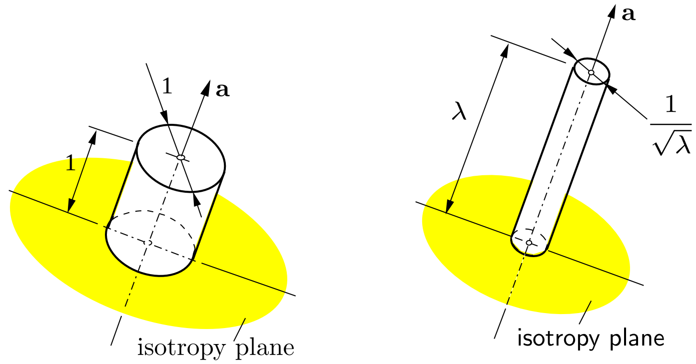
Isotropic part

$$\psi^{iso} = \alpha_1 \frac{I_1}{I_3^{1/3}} + \alpha_2 \frac{I_2}{I_3^{1/3}} - \alpha_3 \ln(I_3) + \alpha_4 (I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2)$$

Third and fouth term are associated to volumetric deformation.

Polyconvex Transversely Isotropic Free Energy

Motivation: unimodular deformation of a cylinder



Deformation of cross section, of generated surface, stretch in fiber-direction

$$||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||^k, \qquad ||\mathrm{Cof}[\boldsymbol{F}]||^2 - ||\mathrm{Cof}[\boldsymbol{F}]\boldsymbol{a}||^2, \qquad ||\boldsymbol{F}\boldsymbol{a}||^k$$

For the anisotropic part we choose

$$\psi^{ti} = \alpha_6(J_5 - I_1 J_4 + I_2) + \alpha_7 \frac{J_4^{\alpha_8}}{I_3^{1/3}} + \alpha_9(I_1 J_4 - J_5) + \alpha_{10} J_4^{\alpha_{11}}$$

Stress free reference configuration

$$2 \sum_{j=1}^{n} \left\{ \left(\frac{\partial \psi_j}{\partial I_1} + 2\,\frac{\partial \psi_j}{\partial I_2} + \frac{\partial \psi_j}{\partial I_3}\right)\mathbf{1} + \left(\frac{\partial \psi_j}{\partial J_4} + 2\frac{\partial \psi_j}{\partial J_5}\right)\boldsymbol{M} \right\} = \mathbf{0}$$

leads to dependent parameters

$$\alpha_7 = (\alpha_3 - \alpha_2 - 2\alpha_9 - \alpha_{10}\alpha_{11})/(\alpha_8 - 1/3); \qquad \alpha_6 = \alpha_7\alpha_8 + \alpha_9 + \alpha_{10}\alpha_{11}$$

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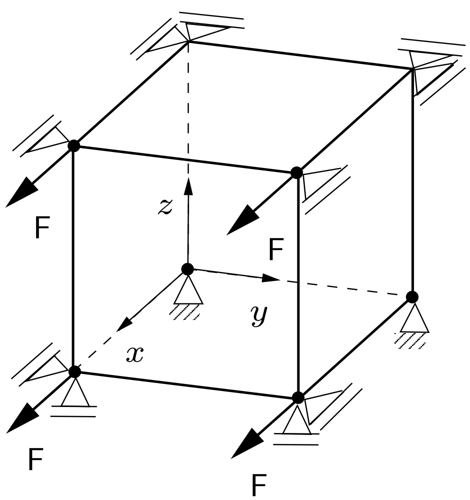
Constrained Tension Test $(\mathrm{WMG} \rightleftharpoons \mathrm{SN})$

Parameters of WMG [1996]

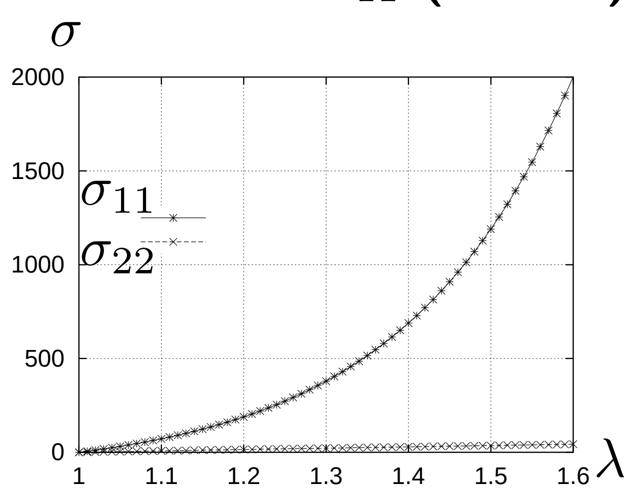
$$\beta_1 = 10. \quad \beta_2 = 10. \quad \beta_3 = 100. \quad \beta_4 = 10^5 \quad [\beta_i] = N/mm^2$$

Parameters of polyconvex functions

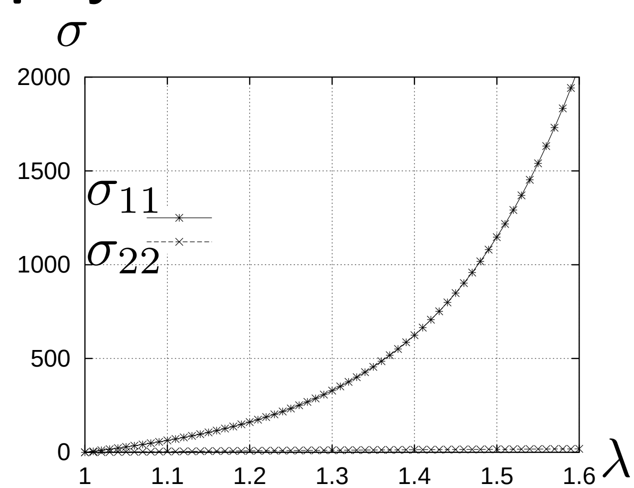
$$\left.\begin{array}{c} \alpha_1 = 10. \quad \alpha_2 = 1. \quad \alpha_3 = 30.5 \quad \alpha_4 = 10000 \\ \alpha_8 = 5. \quad \alpha_9 = 1. \quad \alpha_{10} = 10. \quad \alpha_{11} = 2 \end{array}\right\} \begin{array}{c}\text{dependent} \\ \longrightarrow \\ \text{parameters}\end{array} \left\{\begin{array}{c} \alpha_6 = 1.6071 \\ \alpha_7 = 29.0357 \end{array}\right.$$



Cauchy stress σ_{11} versus stretch $\lambda := F_{11}$ (WMG)



Compare with polyconvex function



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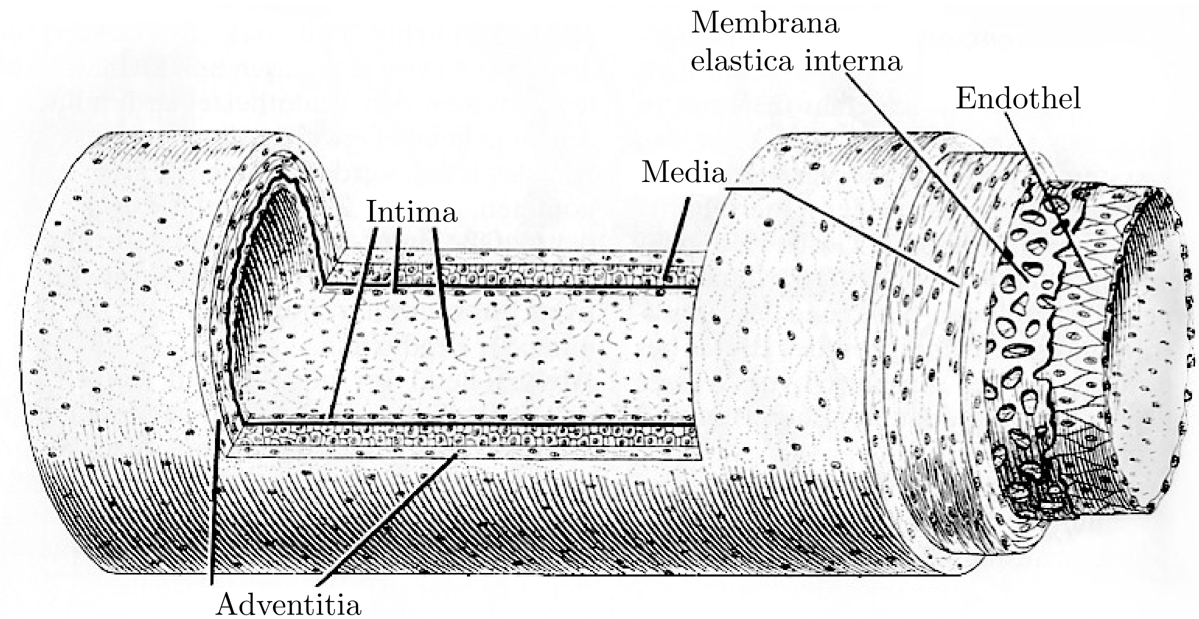
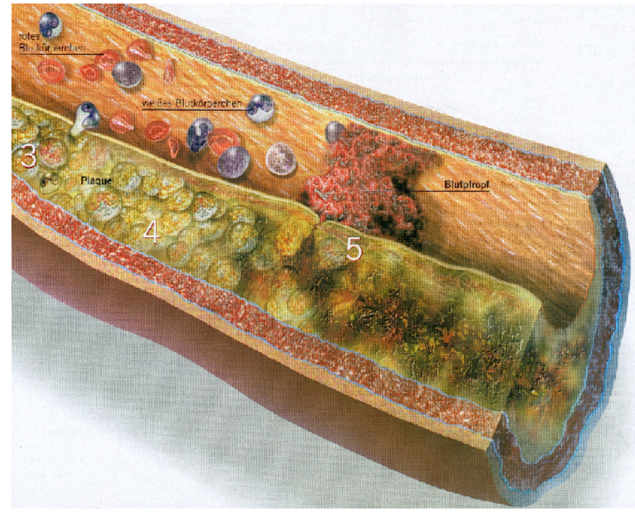
Histology of Arterial Walls

Healthy elastic artery



(Junqueira [1991])

Unhealthy artery



(Spektrum der Wissenschaft)

Differentiate two types:

- Elastic arteries (large diameter, located close to heart, e.g. aorta)
- Muscular arteries (located at periphery, e.g. cerebral arteries)

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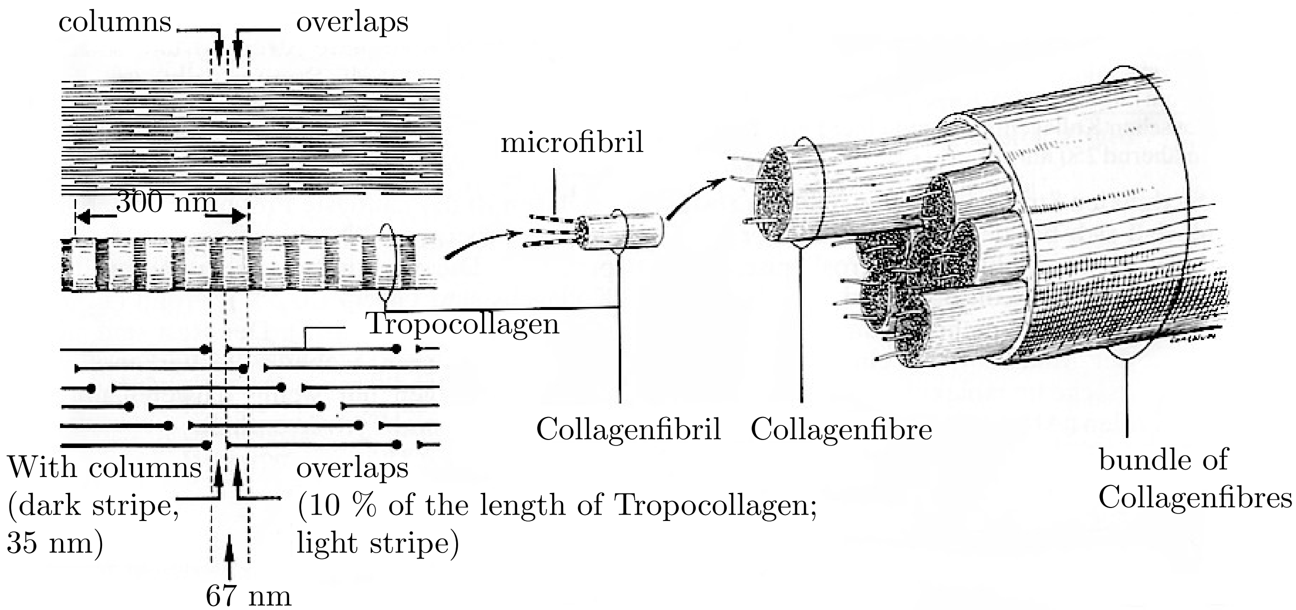
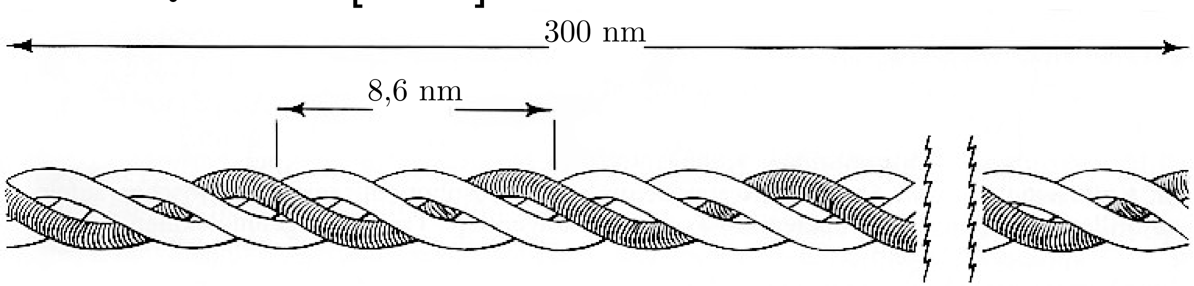
Histology of Arterial Walls

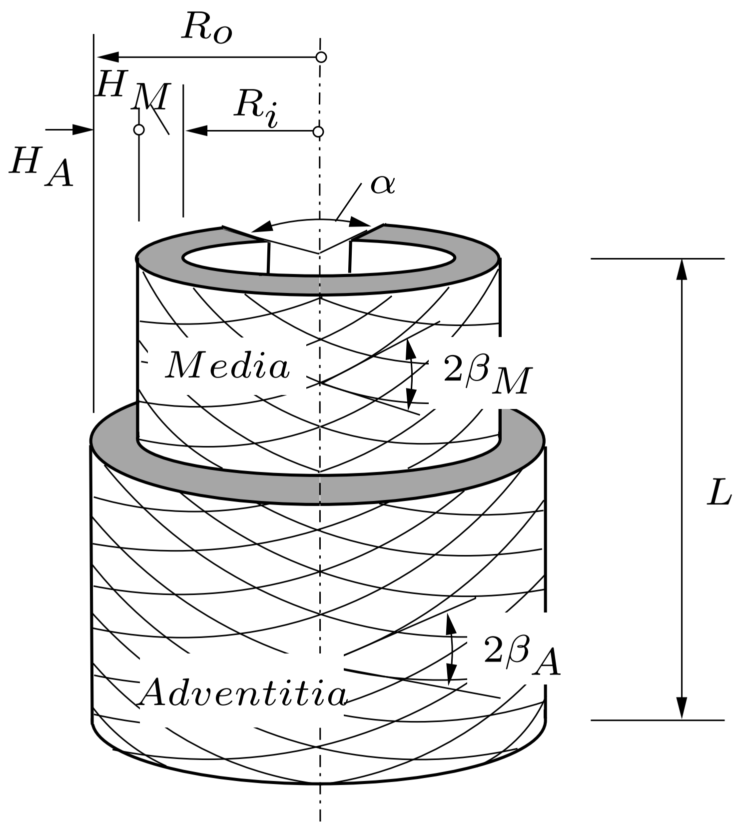
Composition of a collagen fiber, Junqueira [1991]



Tropocollagen, Junqueira [1991]



Geometric Data of Arterial Wall



$R_i = 3.1[mm]$

Media:

$H_M = 0.6[mm]$

$\beta_M = 29.0°$

Adventitia:

$H_A = 0.3[mm]$

$\beta_A = 62.0°$

Two-layer thick-walled tube with two superimposed preferred directions representing two fiber directions in each layer.

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Reference Model

Modified free energy function of Holzapfel, Gasser & Ogden [2000]:

$$\tilde{\psi}^{iso}(I_1, I_3) = \frac{\mu}{2}(\frac{I_1}{I_3^{1/3}} - 3) + \alpha_1(I_3^{\alpha_2} + \frac{1}{I_3^{\alpha_2}} - 2)$$

$$\tilde{\psi}^{ti}(I_3, {}^1J_4, {}^2J_4) = \sum_{i=1}^{2} \frac{k_1}{2k_2}\{\mathsf{exp}[k_2(\frac{{}^iJ_4}{I_3^{1/3}} - 1)^2] - 1\}$$

with the parameters for the Media and Adventitia

$$\begin{array}{lllll} \mu_M = 3.0, & \alpha_{1,M} = 23.0, & \alpha_{2,M} = 29.0, & k_{1,M} = 2.3632, & k_{2,M} = 0.8393 \\ \mu_A = 0.3, & \alpha_{1,A} = 23.0, & \alpha_{2,A} = 29.0, & k_{1,A} = 0.5620, & k_{2,A} = 0.7112 \end{array}$$

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Proposed Model

Proposed polyconvex free energy function:

$$\psi^{iso} = \alpha_1 \frac{I_1}{I_3^{1/3}} + \alpha_2 \frac{I_2}{I_3^{1/3}} - \alpha_3 \ln(I_3) + \alpha_4 (I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2)$$

$$\psi^{ti} = \sum_{i=1}^{2} [\alpha_6 ({}^iJ_5 - I_1 {}^iJ_4 + I_2) + \alpha_7 \frac{{}^iJ_4{}^{\alpha_8}}{I_3^{1/3}} + \alpha_9 (I_1 {}^iJ_4 - {}^iJ_5) + \alpha_{10} {}^iJ_4{}^{\alpha_{11}}]$$

with the parameters for the Media and Adventitia

$$\begin{array}{llll} \alpha_{1,M} = 0.097, & \alpha_{2,M} = 0.001, & \alpha_{3,M} = 0.710, & \alpha_{4,M} = 4.077, \\ \alpha_{5,M} = 6.614, & \alpha_{6,M} = 0.394, & \alpha_{7,M} = 10^{-5}, & \alpha_{8,M} = 2.975, \\ \alpha_{9,M} = 0.315, & \alpha_{10,M} = 0.011, & \alpha_{11,M} = 7.180 & \end{array}$$

$$\begin{array}{llll} \alpha_{1,A} = 0.014, & \alpha_{2,A} = 0.001, & \alpha_{3,A} = 0.208, & \alpha_{4,A} = 5.112, \\ \alpha_{5,A} = 8.481, & \alpha_{6,A} = 0.153, & \alpha_{7,A} = 0.031, & \alpha_{8,A} = 2.236, \\ \alpha_{9,A} = 0.064, & \alpha_{10,A} = 0.003, & \alpha_{11,A} = 6.811 & \end{array}$$

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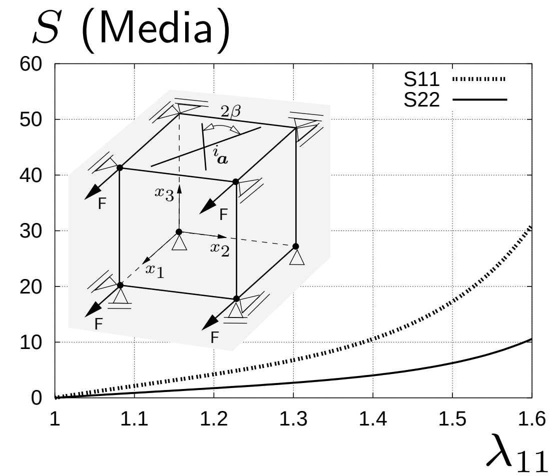
Considered Hyperelastic Models

Modified free energy function of Holzapfel, Gasser & Ogden [2000]:

$$\tilde{\psi}^{iso} = \frac{\mu}{2}(\frac{I_1}{I_3^{1/3}} - 3) + \alpha_1(I_3^{\alpha_2} + \frac{1}{I_3^{\alpha_2}} - 2)$$

$$\tilde{\psi}^{ti}(I_3, {}^iJ_4) = \sum_{i=1}^{2} \frac{k_1}{2k_2}\{\exp[k_2(\frac{{}^iJ_4}{I_3^{1/3}} - 1)^2] - 1\}$$

with ${}^iJ_4 = {}^i\boldsymbol{a} \cdot \boldsymbol{C} \cdot {}^i\boldsymbol{a}$

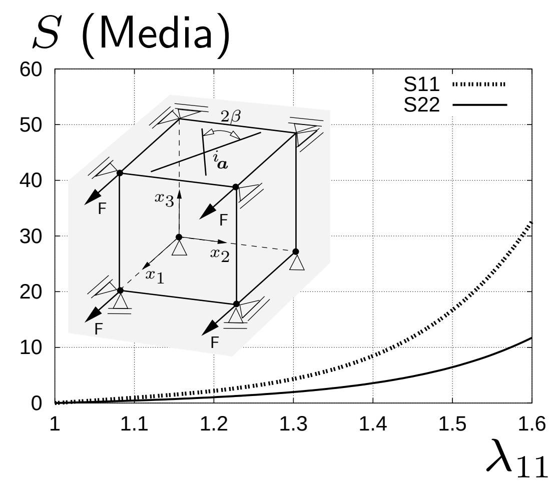


Proposed polyconvex free energy function:

$$\psi^{iso} = \alpha_1\frac{I_1}{I_3^{1/3}} + \alpha_2\frac{I_2}{I_3^{1/3}} - \alpha_3\ln(I_3) + \alpha_4(I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2)$$

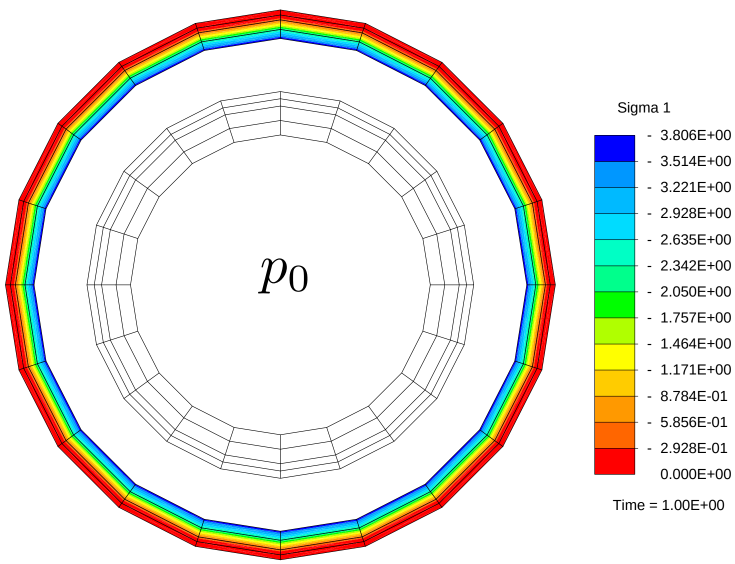
$$\psi^{ti} = \sum_{i=1}^{2}[\alpha_6({}^iJ_5 - I_1{}^iJ_4 + I_2) + \alpha_7\frac{{}^iJ_4^{\alpha_8}}{I_3^{1/3}} + \alpha_9(I_1{}^iJ_4 - {}^iJ_5) + \alpha_{10}{}^iJ_4^{\alpha_{11}}]$$

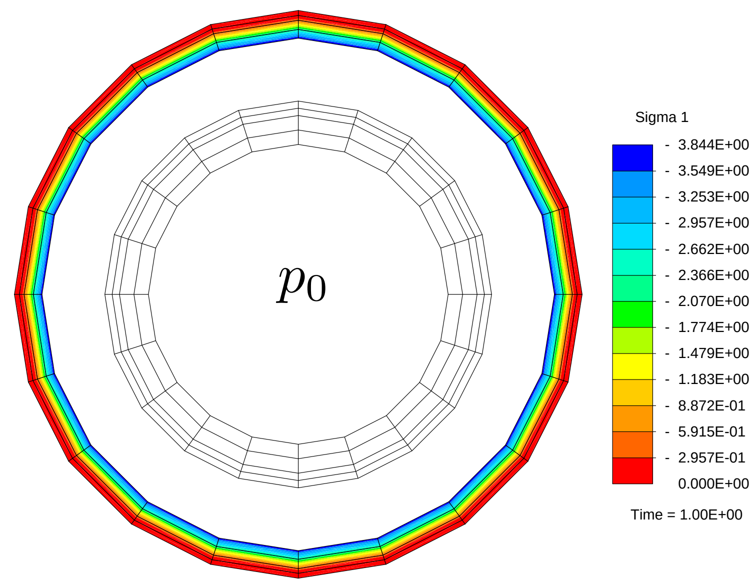
with ${}^iJ_5 = {}^i\boldsymbol{a} \cdot \boldsymbol{C}^2 \cdot {}^i\boldsymbol{a}$



Modelling of Arterial Wall

Radial Kirchhoff stresses, Internal pressure: $p_0 = 11.3\ kPa$





Reference model, HOLZAPFEL ET AL. [2000]

$$\tilde{\psi}^{iso} = \frac{\mu}{2}\left(\frac{I_1}{I_3^{1/3}} - 3\right) + \alpha_1\left(I_3^{\alpha_2} + \frac{1}{I_3^{\alpha_2}} - 2\right)$$

$$\tilde{\psi}^{ti}(I_3, {}^iJ_4) = \sum_{i=1}^{2} \frac{k_1}{2k_2}\{\exp[k_2(\frac{{}^iJ_4}{I_3^{1/3}} - 1)^2] - 1\}$$

Proposed model

$$\psi^{iso} = \alpha_1 \frac{I_1}{I_3^{1/3}} + \alpha_2 \frac{I_2}{I_3^{1/3}} - \alpha_3 \ln(I_3) +$$
$$+\alpha_4\left(I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2\right)$$

$$\psi^{ti} = \sum_{i=1}^{2} [\alpha_6({}^iJ_5 - I_1\,{}^iJ_4 + I_2) + \alpha_7 \frac{{}^iJ_4^{\alpha_8}}{I_3^{1/3}} +$$
$$+\alpha_9(I_1\,{}^iJ_4 - {}^iJ_5) + \alpha_{10}\,{}^iJ_4^{\alpha_{11}}]$$

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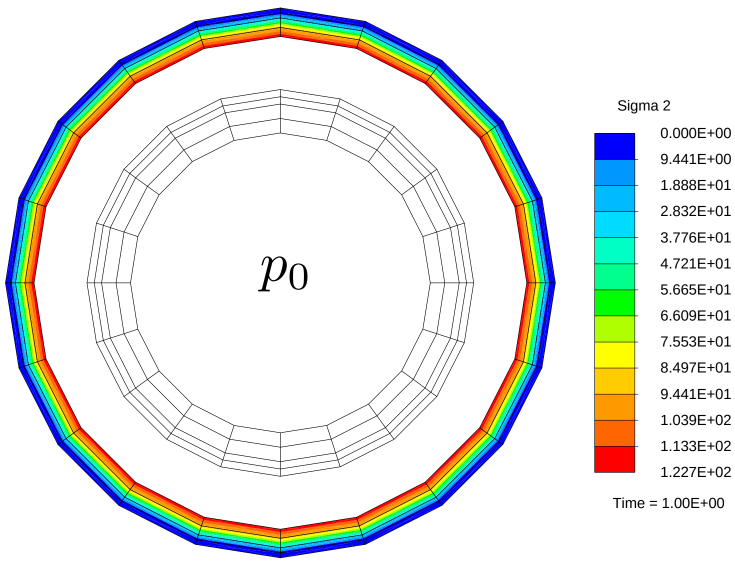
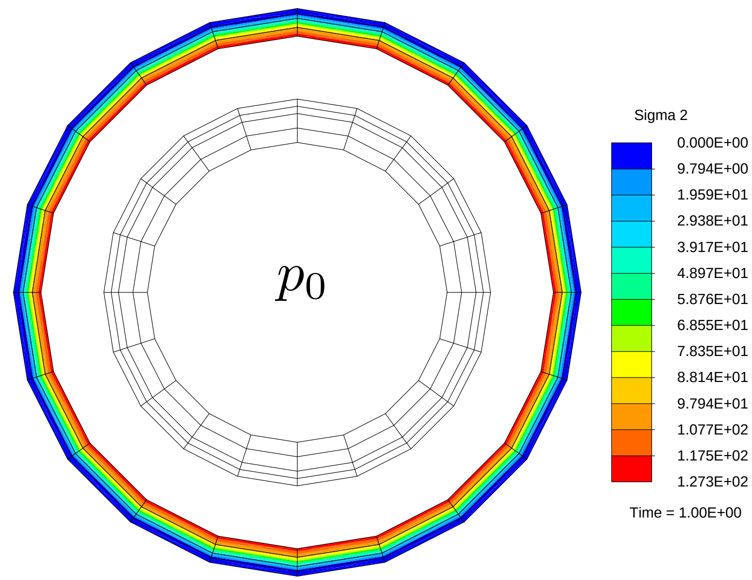
Modelling of Arterial Wall

Peripheral Kirchhoff stresses, Internal pressure: $p_0 = 11.3\ kPa$





Reference model, Holzapfel et al. [2000]

$$\tilde{\psi}^{iso} = \frac{\mu}{2}\left(\frac{I_1}{I_3^{1/3}} - 3\right) + \alpha_1\left(I_3^{\alpha_2} + \frac{1}{I_3^{\alpha_2}} - 2\right)$$

$$\tilde{\psi}^{ti}(I_3, {}^iJ_4) = \sum_{i=1}^{2} \frac{k_1}{2k_2}\{\exp[k_2(\frac{{}^iJ_4}{I_3^{1/3}} - 1)^2] - 1\}$$

Proposed model

$$\psi^{iso} = \alpha_1 \frac{I_1}{I_3^{1/3}} + \alpha_2 \frac{I_2}{I_3^{1/3}} - \alpha_3 \ln(I_3) +$$
$$+\alpha_4\left(I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2\right)$$

$$\psi^{ti} = \sum_{i=1}^{2} [\alpha_6({}^iJ_5 - I_1{}^iJ_4 + I_2) + \alpha_7 \frac{{}^iJ_4^{\alpha_8}}{I_3^{1/3}} +$$
$$+\alpha_9(I_1{}^iJ_4 - {}^iJ_5) + \alpha_{10}{}^iJ_4^{\alpha_{11}}]$$

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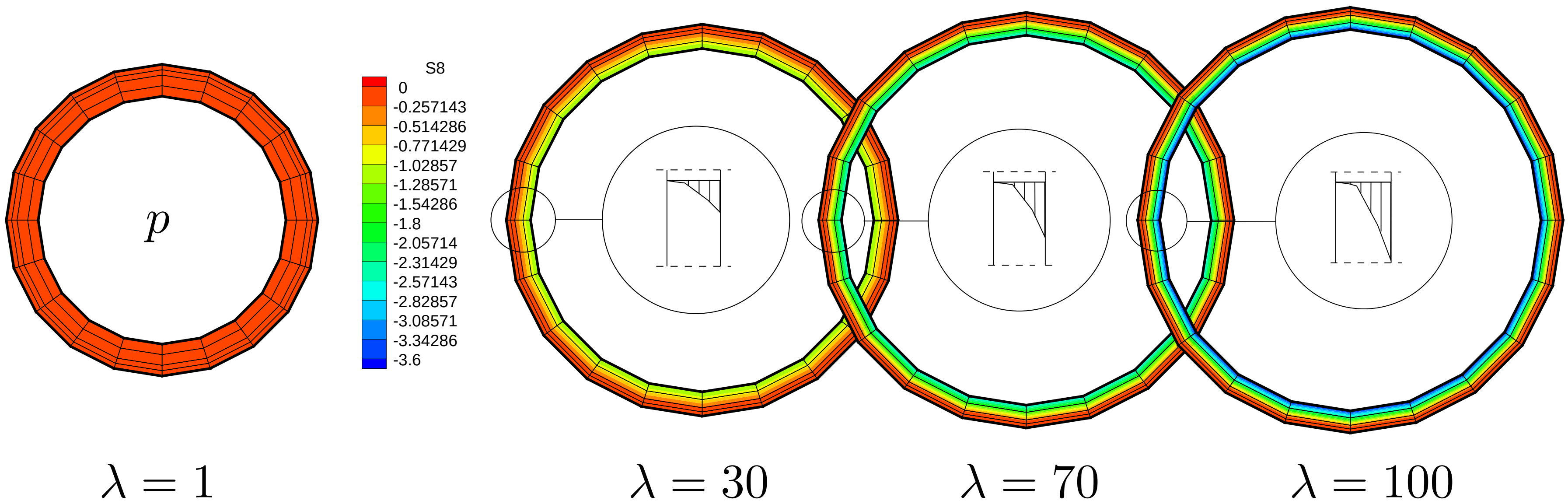
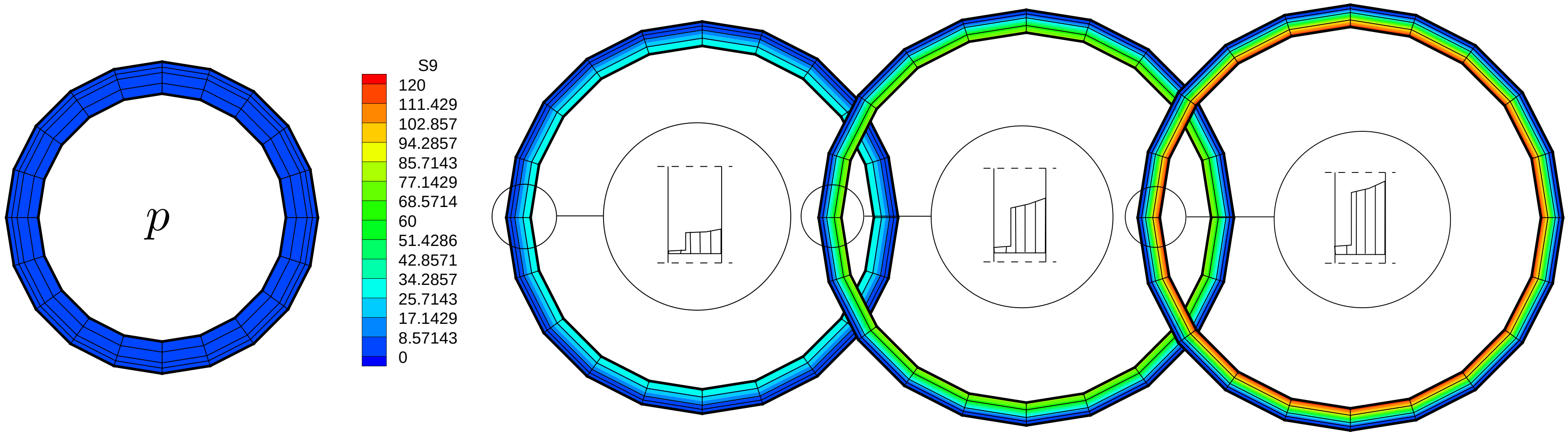
Modelling of Arterial Wall

Radial Kirchhoff stresses, Internal pressure: $p = \lambda\, p_0,$ with $p_0 = 0.113\ kPa$



Modelling of Arterial Wall

Peripheral Kirchhoff stresses, Internal pressure: $p = \lambda\, p_0$, with $p_0 = 0.113\; kPa$



$\lambda = 1$ $\lambda = 30$ $\lambda = 70$ $\lambda = 100$

Localization Analysis

Accoustic tensor $\boldsymbol{Q}$ in direction $\boldsymbol{N}$

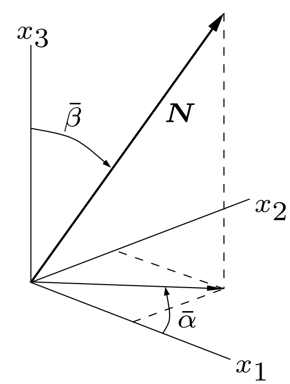
$$Q^a{}_b = \mathbb{A}^{aB}{}_b{}^D \, N_B \, N_D$$

with the nominal moduli

$$\mathbb{A}^{aB}{}_b{}^D = (\mathbb{C}^{ABCD} \, F^a{}_A \, F^c{}_C + S^{BD} \, g^{ac}) \, g_{bc}$$

and the norm vector defined by

$$\boldsymbol{N}(\bar{\alpha}, \bar{\beta}) = \begin{bmatrix} \sin(\bar{\beta}) \cos(\bar{\alpha}) \\ \sin(\bar{\beta}) \sin(\bar{\alpha}) \\ \cos(\bar{\beta}) \end{bmatrix}$$



Material is instable if the following condition holds

$$\det[\boldsymbol{Q}(\boldsymbol{N})] \leq 0$$

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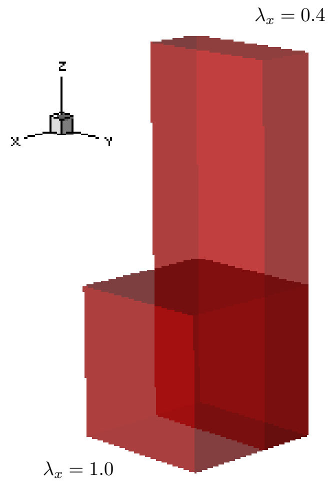
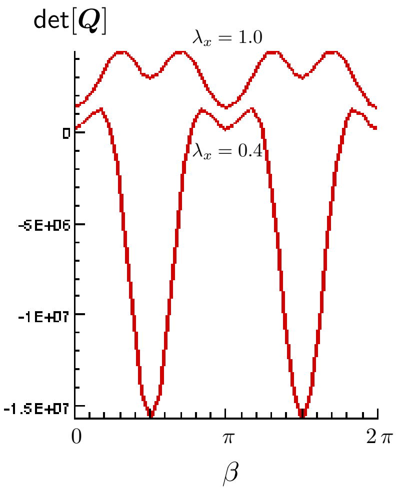
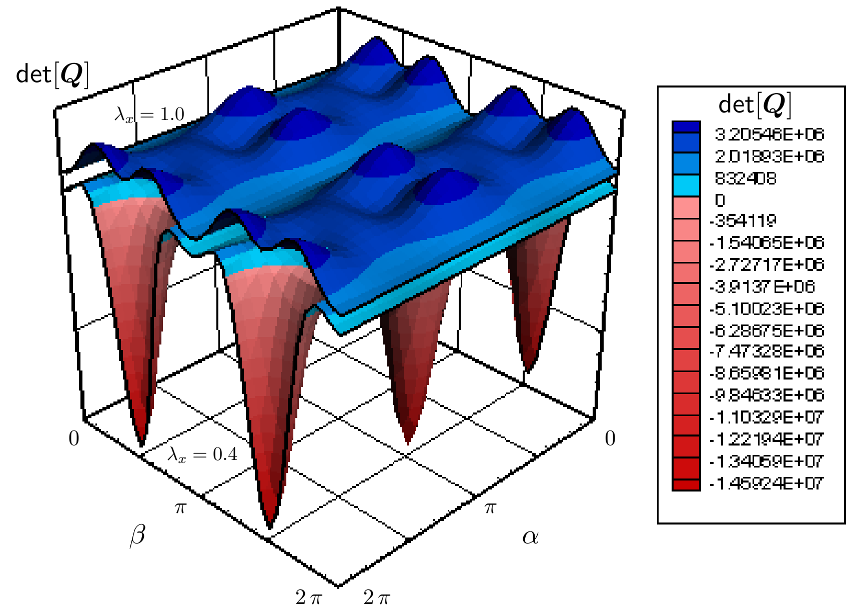
Acoustic Tensor in Constrained Compression







Test material: Media of a healthy elastic artery in its natural alignment

Modified free energy function of Holzapfel et al. [2000]:

$$\tilde{\psi}^{iso} = \frac{\mu}{2}(\frac{I_1}{I_3^{1/3}} - 3) + \alpha_1(I_3^{\alpha_2} + \frac{1}{I_3^{\alpha_2}} - 2)$$

$$\tilde{\psi}^{ti}(I_3, {}^iJ_4) = \sum_{i=1}^{2} \frac{k_1}{2k_2}\{\exp[k_2(\frac{{}^iJ_4}{I_3^{1/3}} - 1)^2] - 1$$

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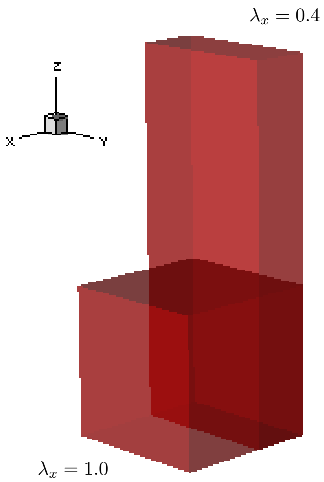
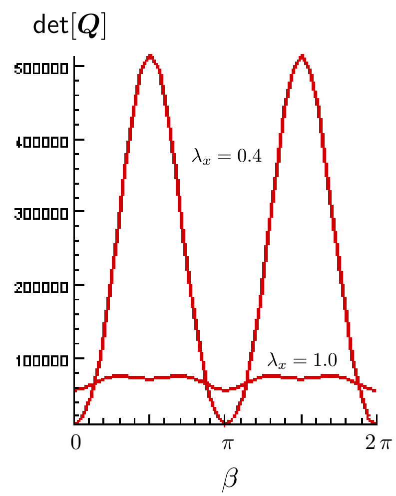
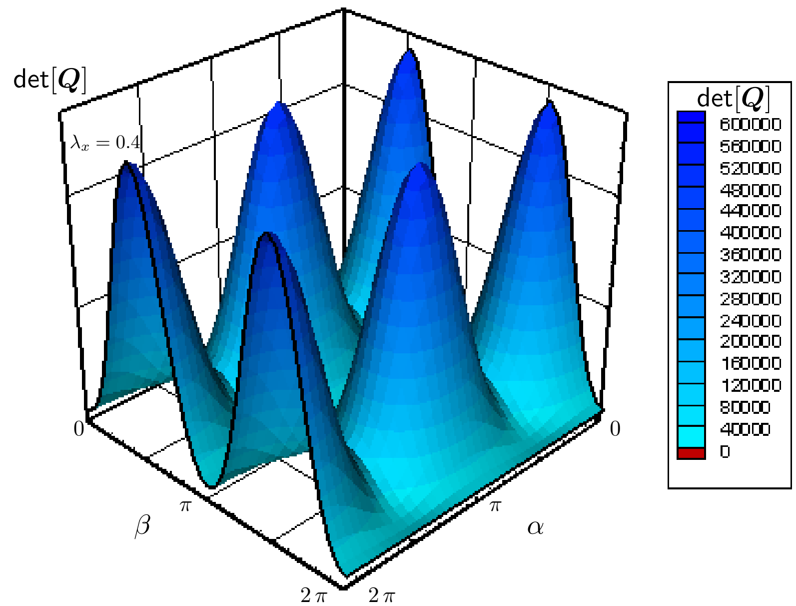
Acoustic Tensor in Constrained Compression







Test material: Media of a healthy elastic artery in its natural alignment

Polyconvex free energy function of S & N [2002]:

$$\psi^{iso} = \alpha_1 \frac{I_1}{I_3^{1/3}} + \alpha_2 \frac{I_2}{I_3^{1/3}} - \alpha_3 \ln(I_3) + \alpha_4 (I_3^{\alpha_5} + \frac{1}{I_3^{\alpha_5}} - 2)$$

$$\psi^{ti} = \sum_{i=1}^{2} [\alpha_6 ({}^iJ_5 - I_1 {}^iJ_4 + I_2) + \alpha_7 \frac{{}^iJ_4^{\alpha_8}}{I_3^{1/3}} + \alpha_9 (I_1 {}^iJ_4 - {}^iJ_5)$$

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On the Construction of Polyconvex Free Energy Functions

Conclusions

- Polyconvexity has been applied to finite anisotropic elasticity.
- Existence of minimizers is guaranteed.
- Often used standard terms like $I_1 J_4, J_5$ have to be excluded.
- A variety of isotropic and anisotropic free energy terms has been developed.
- Stress free reference configuration necessitates the introduction of alternative polynomial invariant terms like $\mathrm{tr}\,[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}]$. This motivates the introduction of a more physically based integrity basis, e.g. $\mathcal{P} = \{I_1, I_2, I_3, J_4, K_1\}$.
- The characteristic (exponential) behavior of soft tissues can be modeled with polyconvex anisotropic functions.
- The localization has been analyzed.