Recent Results on the Construction of Anisotropic Polyconvex Energies

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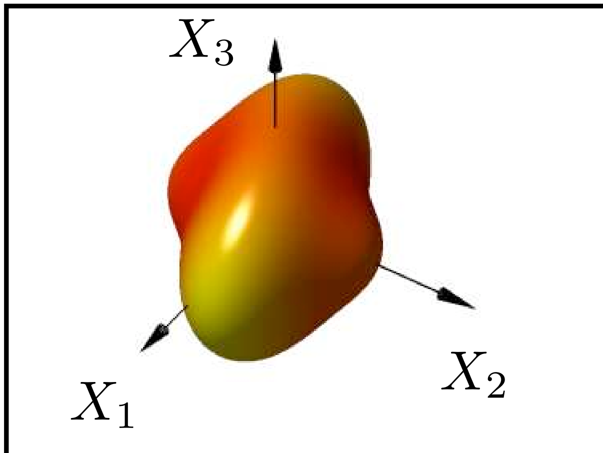
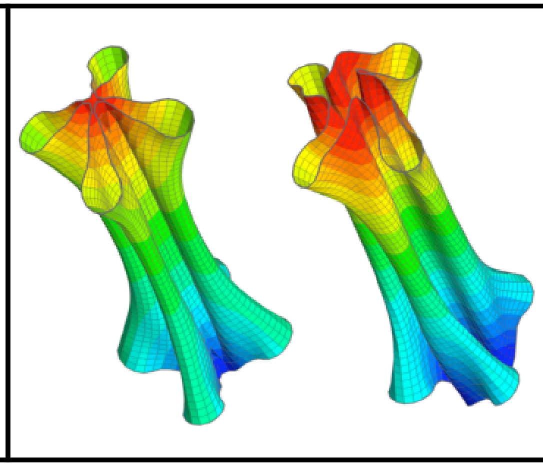
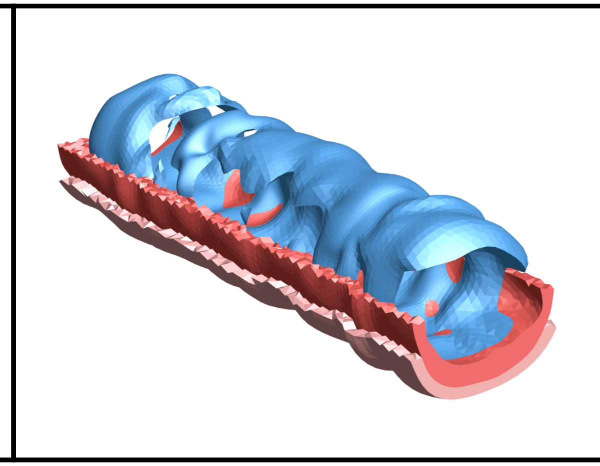






$$\boldsymbol{G},\ J_4 = \mathrm{tr}[\boldsymbol{C}\boldsymbol{G}],\ J_5 = \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{G}]$$

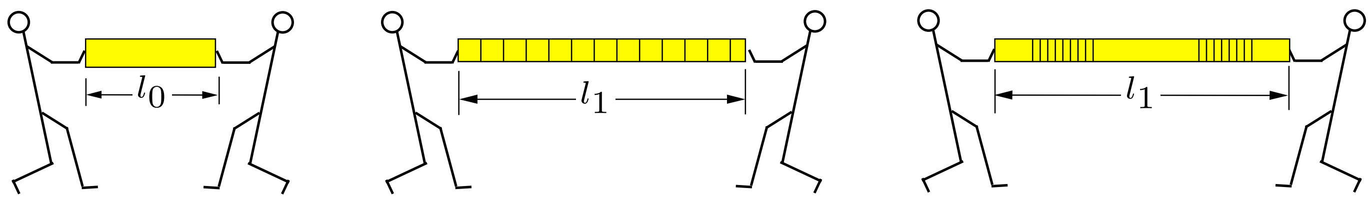
- Polyconvexity Condition
- Crystallographically Motivated Structural Tensors
- Construction of Polyconvex Anisotropic Energies
- Some Applications

DFG-Project: NE 902/2-1 SCHR 570/6-1

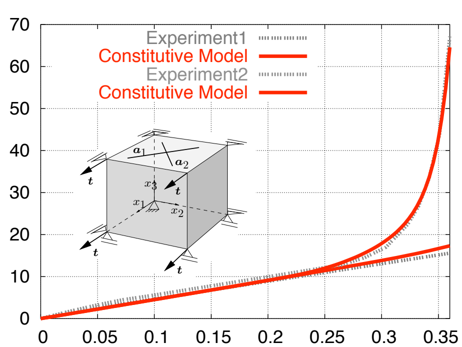
J. Schröder, P. Neff & V. Ebbing [2008], "Anisotropic Polyconvex Energies on the Basis of Crystallographic Motivated Structural Tensors", JMPS, in press

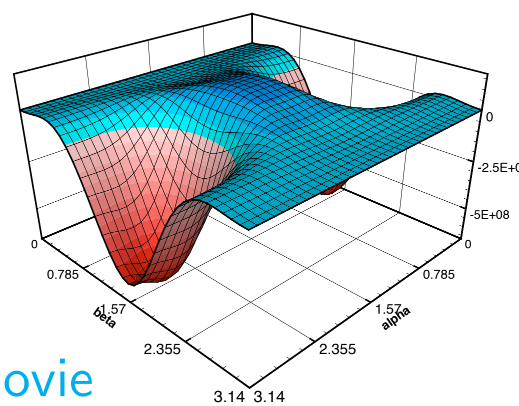
Background and Motivation

- 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], Dacorogna [1989], Silhavý [1997].



- Restricted number of experimental data $\longrightarrow$ fit of data with polyconvex energies guarantees existence of solutions (“of course also in the interpolated region“)





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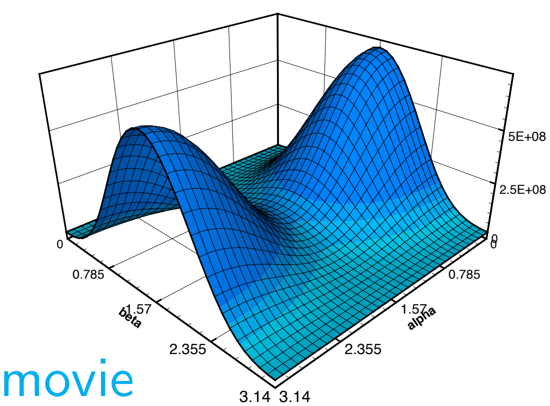

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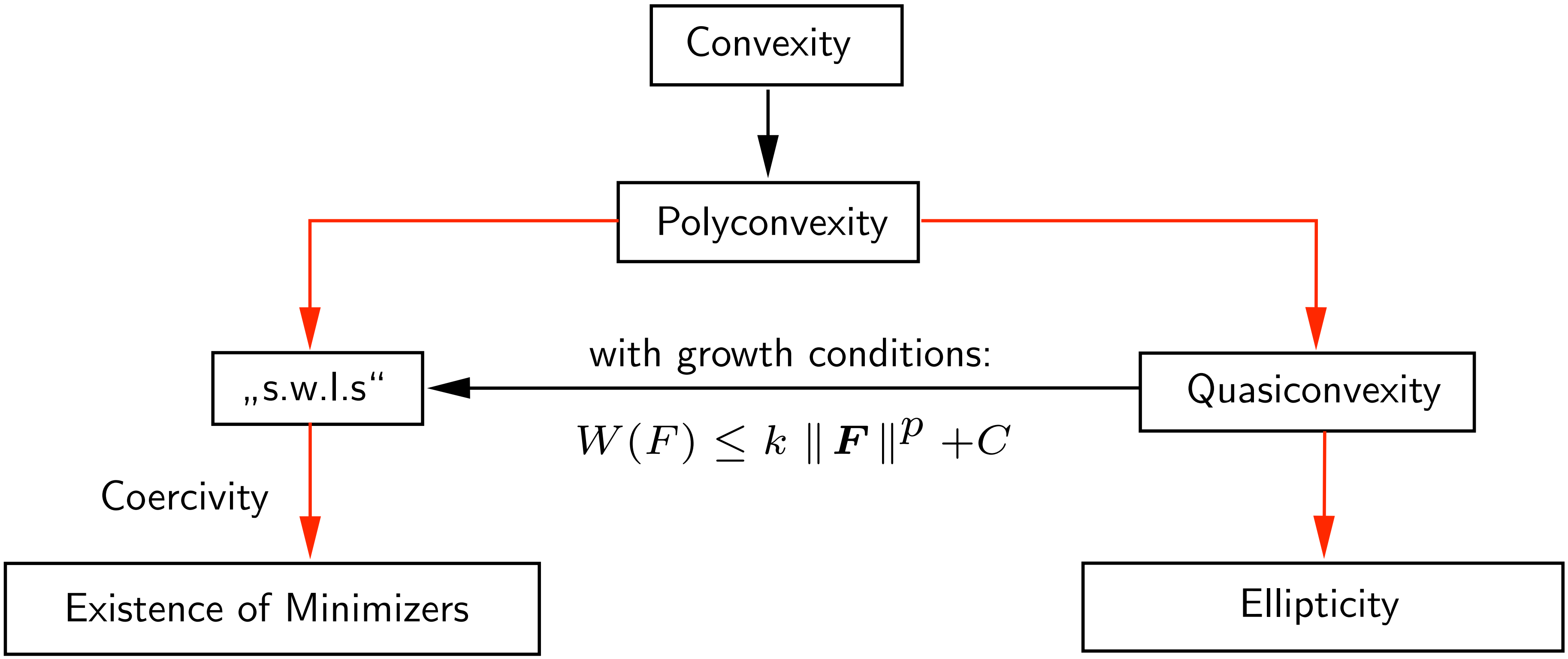
Goal: Construction of polyconvex energies for description of anisotropic materials.

Generalized Convexity Conditions: Implications



Quasiconv.: $W(\bar{\boldsymbol{F}}) \cdot \mathrm{Vol}(\mathcal{B}) \leq \int_{\mathcal{B}} W(\bar{\boldsymbol{F}} + \nabla \boldsymbol{w}) \, dV \;\rightarrow\; \bar{\boldsymbol{F}}$ is global minimizer.

Ellipticity: Positive definite acoustic tensor $\rightarrow$ Real wave speeds.

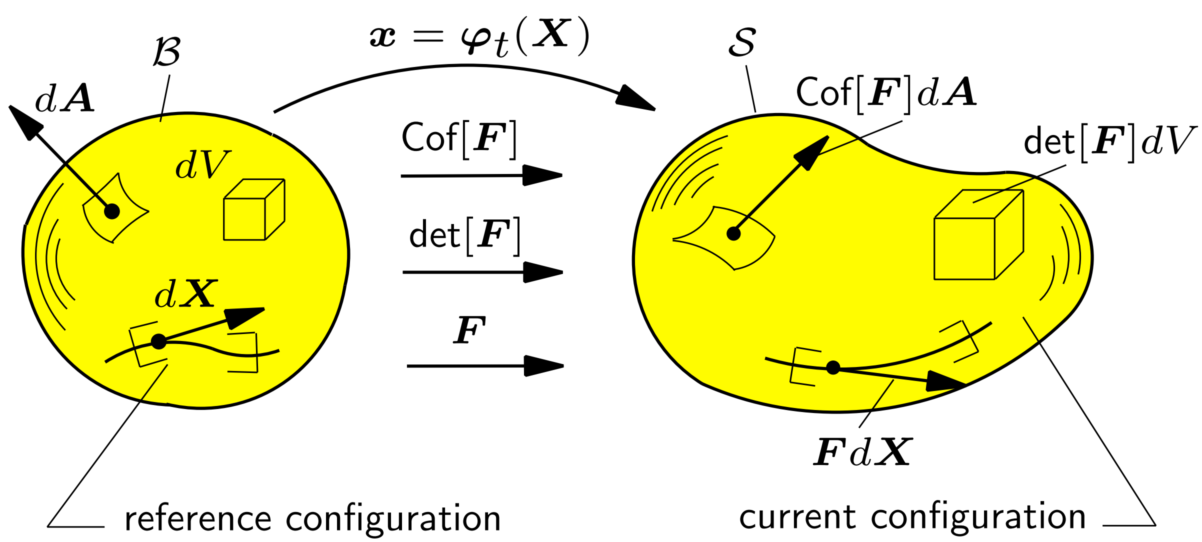
Generalized Convexity Conditions

Polyconvexity, Ball [1977]

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

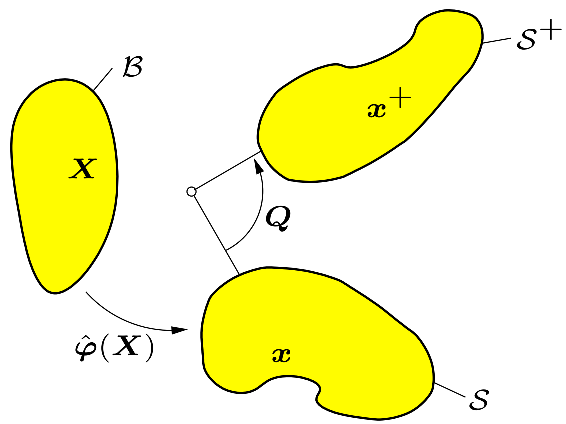
$$\hat{W}(\boldsymbol{F}) = \hat{P}(\boldsymbol{F}, \mathrm{Cof}\,\boldsymbol{F}, \det \boldsymbol{F})$$

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



Material Frame Indifference, Objectivity

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



$$\boldsymbol{x}^+ = \boldsymbol{Q}\boldsymbol{x}$$

Invariance of constitutive equation

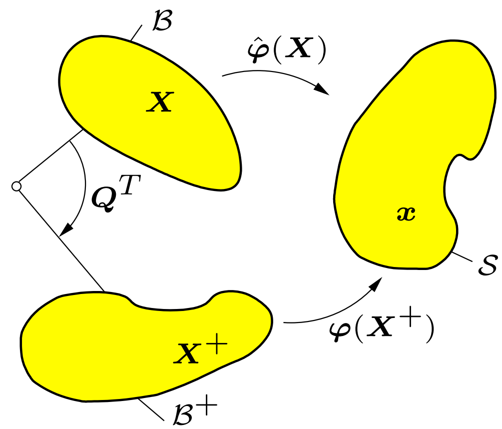
$$\hat{W}(\boldsymbol{F}) = \hat{W}(\boldsymbol{Q}\boldsymbol{F}) \ \forall\, \boldsymbol{Q} \in \mathrm{SO}(3)$$

Reduced form

$\hat{W}(\boldsymbol{F}) = \hat{\psi}(\boldsymbol{C})$ with $\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$

Material Symmetry, Isotropy of Space

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



$$\boldsymbol{X}^+ = \boldsymbol{Q}^T\boldsymbol{X}$$

implies the transformation rules

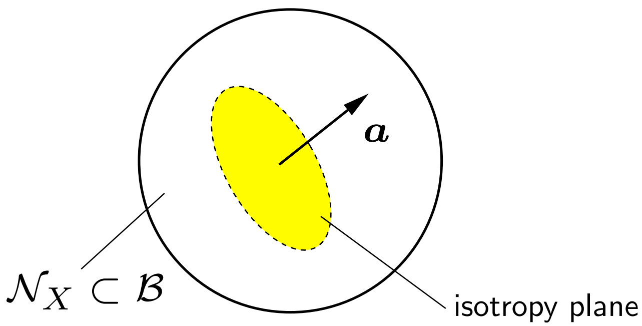
$$\hat{W}(\boldsymbol{F}) = \hat{W}(\boldsymbol{F}\boldsymbol{Q}) \ \forall\, \boldsymbol{Q} \in \mathcal{G}_k, \boldsymbol{F}$$

Goal: Extension of $\mathcal{G}_k$-invariant to $\mathrm{SO}(3)$-invariant functions

$$\hat{\psi}(\boldsymbol{C}) = \hat{\psi}(\boldsymbol{Q}^T\boldsymbol{C}\boldsymbol{Q}, ?) \ \forall\, \boldsymbol{Q} \in \mathrm{SO}(3)$$

Elements of Invariant Theory

Basic idea: Introduce structural tensor $\boldsymbol{M} := \boldsymbol{a} \otimes \boldsymbol{a}$, $\boldsymbol{a}$ is preferred direction in $\mathcal{B}$



Invariance group of $\boldsymbol{M}$:

$$\boldsymbol{M}(\boldsymbol{a}) = \boldsymbol{Q}^T \boldsymbol{M}(\boldsymbol{a}) \boldsymbol{Q} \quad \forall\, \boldsymbol{Q} \in \mathcal{G}_{ti}$$

Isotropic tensor function with respect to $\boldsymbol{C} = \boldsymbol{F}^T \boldsymbol{F}$ and $\boldsymbol{M}$

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

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

Principle and mixed invariants of $\boldsymbol{C}$ and $\boldsymbol{M}$

$$I_1 = \mathrm{tr}\boldsymbol{C}\,,\; I_2 = \mathrm{tr}[\mathrm{Cof}\boldsymbol{C}]\,,\; I_3 = \det\boldsymbol{C}\,,\; J_4 = \mathrm{tr}[\boldsymbol{C}\boldsymbol{M}]\,,\; J_5 = \mathrm{tr}[\boldsymbol{C}^2\boldsymbol{M}]$$

yield the polynomial basis $\mathcal{P}_{ti} := \{I_1, I_2, I_3, J_4, J_5\}$

Common Polyconvex Energy Functions

- **Isotropy**: Polyconvex models, e.g. OGDEN-type models $(\alpha_1, \alpha_2, \delta_1 \geq 0)$

$$\psi^{iso} = \alpha_1 I_1 + \alpha_2 I_2 + \delta_1 I_3^2 - (2\alpha_1 + 4\alpha_2 + 2\delta_1)\ln\sqrt{I_3},$$

formulated in principal invariants $I_1 = \mathrm{tr}\boldsymbol{C},\ I_2 = \mathrm{tr}[\mathrm{Cof}\boldsymbol{C}]$ and $I_3 = \det\boldsymbol{C}$.

BALL [2002], Some open problems in elasticity, **Problem 2:**

“Are there ways of verifying polyconvexity and quasiconvexity for a useful class of anisotropic stored-energy functions? “

- **Anisotropy**: **Transversely isotropic** (a=1) and **orthotropic** (a = 3) polyconvex energy functions first derived in SCHRÖDER & NEFF [2001,2003] formulated in

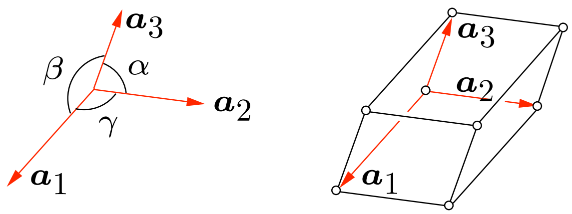
$$\mathrm{tr}[\boldsymbol{C}\boldsymbol{M}^i],\ \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{M}^i],\ \mathrm{tr}[\boldsymbol{C}(\boldsymbol{1} - \boldsymbol{M}^i)],\ \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}](\boldsymbol{1} - \boldsymbol{M}^i)], \quad i = 1, ..., \mathrm{a}.$$

- **Further extensions** and case studies are documented in: STEIGMANN [2003], SNB [2004], ITSKOV & AKSEL [2004], MARKERT, EHLERS & KARAJAN [2005], BALZANI [2006], BNSH [2006], EHRET & ITSKOV [2007].

Are there ways of verifying polyconvexity and quasiconvexity for the further classes of anisotropic stored-energy functions?

General Anisotropy in Polyconvex Framework

Anisotropic elasticity: 12 anisotropy classes / 32 crystal classes / 7 crystal systems

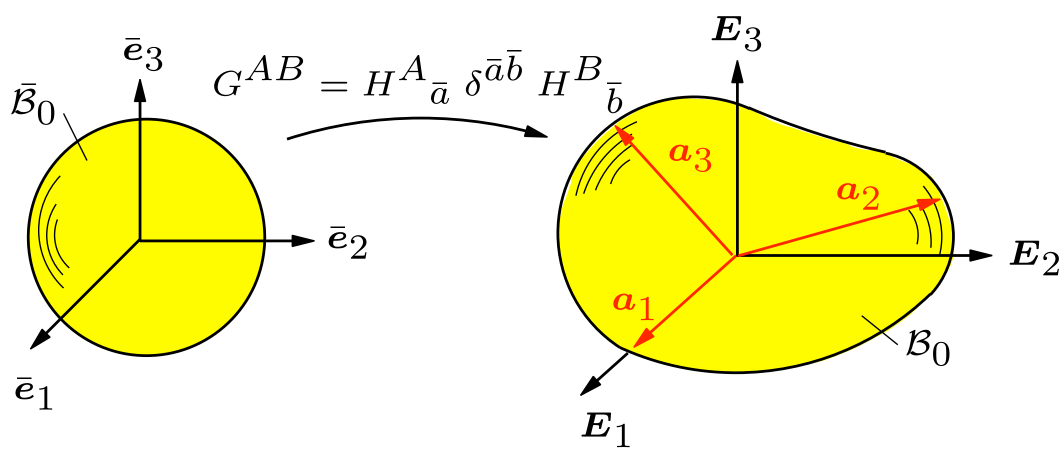


$$
\begin{aligned}
a &= ||\boldsymbol{a}_1|| \\
b &= ||\boldsymbol{a}_2|| \\
c &= ||\boldsymbol{a}_3||
\end{aligned}
$$

Main idea: Crystallographically motivated structural tensor $\boldsymbol{G}$:

- $\boldsymbol{G}$ is a **second-order**, **symmetric** and **positive definite** structural tensor .
- $\boldsymbol{G}$ is the **push-forward** of a cartesian metric of a fictitious reference configuration $\bar{\mathcal{B}}_0$ onto the real reference configuration $\mathcal{B}_0$:

$$
\rightarrow \quad \boldsymbol{G} = \boldsymbol{H}\boldsymbol{H}^T \quad \rightarrow \quad \boldsymbol{G} = \boldsymbol{Q}\boldsymbol{G}\boldsymbol{Q}^T \quad \forall\, \boldsymbol{Q} \in \mathcal{G} \subset \mathrm{O}(3)\,.
$$



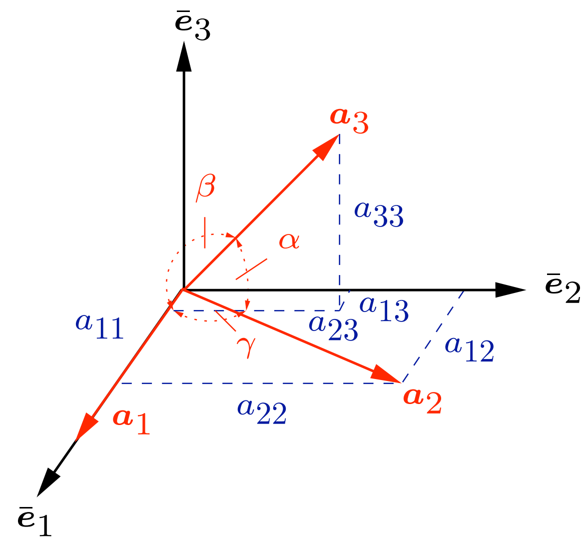
Metric Tensors for the Seven Crystal Systems

Linear Mapping of the cartesian base vectors

$$\boldsymbol{H} : \ \bar{\boldsymbol{e}}_i \ \mapsto \boldsymbol{a}_i \ \rightarrow \ \boldsymbol{H} = [\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3] \quad \text{with} \quad \boldsymbol{a}_i = \boldsymbol{H} \ \bar{\boldsymbol{e}}_i$$

Special choice: $\boldsymbol{a}_1 \parallel \boldsymbol{e}_1, \quad \boldsymbol{a}_2 \perp \boldsymbol{e}_3 :$

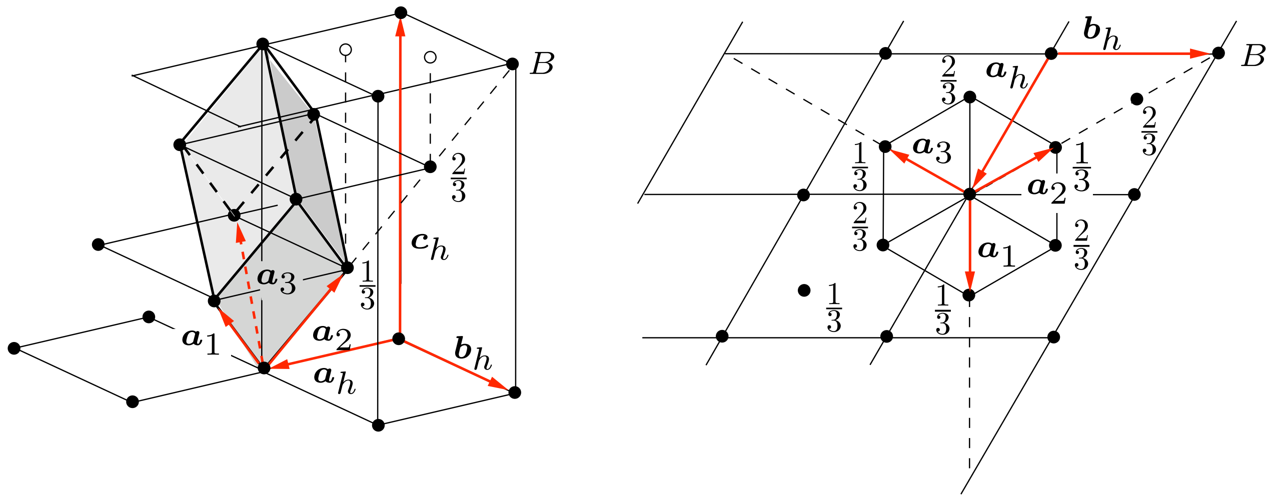
$$\boldsymbol{H} = \begin{bmatrix} a & b \ \cos\gamma & c \ \cos\beta \\ 0 & b \ \sin\gamma & c \ (\cos\alpha - \cos\beta \ \cos\gamma)/\sin\gamma \\ 0 & 0 & c \ [1 + 2 \ \cos\alpha \ \cos\beta \ \cos\gamma - \\ & & (\cos^2\alpha + \cos^2\beta + \cos^2\gamma)]^{1/2}/\sin\gamma \end{bmatrix}$$



E.g. Monoclinic Metric Tensor ($a \neq b \neq c, \alpha = \beta = 90°, \gamma \neq 90°$):

$$\boldsymbol{G}^m = \boldsymbol{H}^m \boldsymbol{H}^{mT} = \begin{bmatrix} a^2 + b^2 \ \cos^2\gamma & b^2 \ \cos\gamma \ \sin\gamma & 0 \\ b^2 \cos\gamma \ \sin\gamma & b^2 \ \sin^2\gamma & 0 \\ 0 & 0 & c^2 \end{bmatrix} \rightarrow \boldsymbol{G}^m = \begin{bmatrix} \tilde{a} & \tilde{d} & 0 \\ \tilde{d} & \tilde{b} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

Crystallographic Motivated Trigonal Metric Tensor



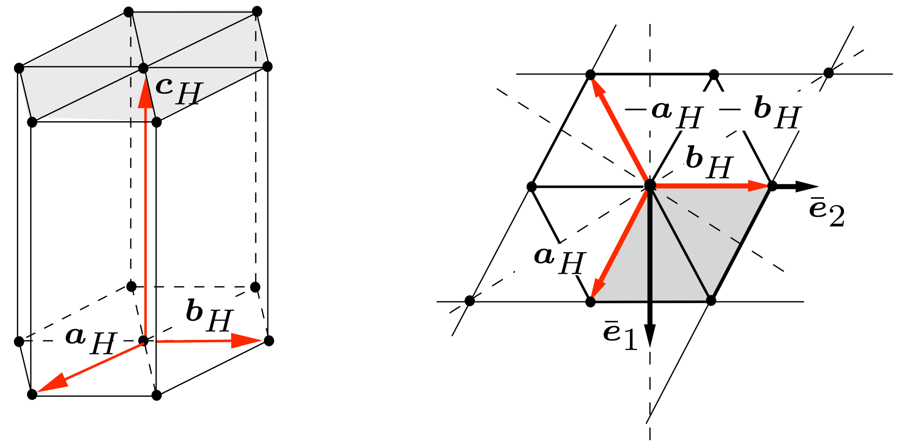
Considering **rhombohedral base vectors** in **hexagonal centered cell**

$$\boldsymbol{a}_1 = \frac{1}{3}(2\boldsymbol{a}_h + \boldsymbol{b}_h + \boldsymbol{c}_h)\,, \quad \boldsymbol{a}_2 = \frac{1}{3}(-\boldsymbol{a}_h + \boldsymbol{b}_h + \boldsymbol{c}_h)\,, \quad \boldsymbol{a}_3 = \frac{1}{3}(-\boldsymbol{a}_h - 2\boldsymbol{b}_h + \boldsymbol{c}_h)\,,$$

with threefold axis $\boldsymbol{c}_h = (\boldsymbol{a}_1 + \boldsymbol{a}_2 + \boldsymbol{a}_3) \;\|\; \boldsymbol{e}_3$, leads to trigonal metric tensor

$$\boldsymbol{G}^{ht} = \boldsymbol{H}^{ht}\boldsymbol{H}^{htT} = \mathrm{diag}(a^2, a^2, c^2) \quad \rightarrow \quad \boldsymbol{G}^{ht} = \boldsymbol{Q}\boldsymbol{G}^{ht}\boldsymbol{Q}^T \;\; \forall\, \boldsymbol{Q} \in \mathcal{G}^{ht}.$$

Crystallographic Motivated Hexagonal Metric Tensor



BRAVAIS [1866]: Inherent sixfold symmetry of **primitive hexagonal cell** is captured by **three hexagonal base vectors** in the $\bar{e}_1 - \bar{e}_2-$plane

$$\boldsymbol{a}_H, \quad \boldsymbol{b}_H, \quad (-\boldsymbol{a}_H - \boldsymbol{b}_H)\,.$$

This symmetry indicates that $\bar{e}_1 - \bar{e}_2-$plane acts as **isotropy plane**, LOVE [1907]. Therefore the fictitious deformation has to be of the type

$$\boldsymbol{H}^h = \operatorname{diag}(a, a, c) \;\rightarrow\; \boldsymbol{G}^h = \operatorname{diag}(a^2, a^2, c^2) \;\rightarrow\; \boldsymbol{G}^h = \boldsymbol{Q}\boldsymbol{G}^h\boldsymbol{Q}^T \;\; \forall\, \boldsymbol{Q} \in \mathcal{G}^h.$$

Proof of Polyconvexity of $\operatorname{tr}[\boldsymbol{C}\boldsymbol{G}]$ and $\operatorname{tr}[\operatorname{Cof}[\boldsymbol{C}]\boldsymbol{G}]$

Generic **polyconvex** anisotropic functions

$$[\operatorname{tr}(\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{G})]^k \quad \text{and} \quad [\operatorname{tr}(\operatorname{Cof}(\boldsymbol{F}^T)\operatorname{Cof}(\boldsymbol{F})\boldsymbol{G})]^k$$

with $k \geq 1$ and $\boldsymbol{G} \in \mathrm{P}_{\mathrm{sym}}$.

Proof of Convexity. With identity $[\operatorname{tr}(\boldsymbol{F}^T\boldsymbol{F}\boldsymbol{G})]^k = \| \boldsymbol{F}\boldsymbol{H} \|^{2k} = \langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^k$ we obtain

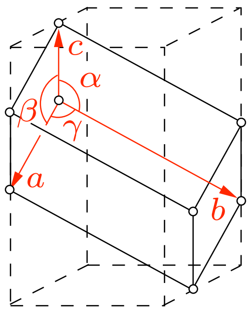
$$\begin{aligned}
D_F(\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^k)\ .\boldsymbol{\xi} = {} & 2k\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^{k-1}\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{\xi}\boldsymbol{H}\rangle \\
D_F^2(\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^k)\ .(\boldsymbol{\xi},\boldsymbol{\xi}) = {} & 2k\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^{k-1}\langle \boldsymbol{\xi}\boldsymbol{H}, \boldsymbol{\xi}\boldsymbol{H}\rangle \\
& +4k(k-1)\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{F}\boldsymbol{H}\rangle^{k-2}\langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{\xi}\boldsymbol{H}\rangle^2 \\
= {} & 2k \| \boldsymbol{F}\boldsymbol{H} \|^{2k-2} \| \boldsymbol{\xi}\boldsymbol{H} \|^2 \\
& +4k(k-1) \| \boldsymbol{F}\boldsymbol{H} \|^{2k-4} \ \langle \boldsymbol{F}\boldsymbol{H}, \boldsymbol{\xi}\boldsymbol{H}\rangle^2 \geq 0.
\end{aligned}$$

Detailed proofs are given in Schröder, Neff & Ebbing [2008].

Polyconvex Functional Bases $\mathcal{P}$

– Evaluation of Polyconvex Invariants $\boldsymbol{C} \cdot \boldsymbol{G}$ and $\mathrm{Cof}\boldsymbol{C} \cdot \boldsymbol{G}$ –

Triclinic system: 2nd-order SST



$$\boldsymbol{G}^a = \begin{bmatrix} \tilde{a} & \tilde{d} & \tilde{e} \\ \tilde{d} & \tilde{b} & \tilde{f} \\ \tilde{e} & \tilde{f} & \tilde{c} \end{bmatrix}$$

Ordering with respect to individual entries of $\boldsymbol{G}$ yields

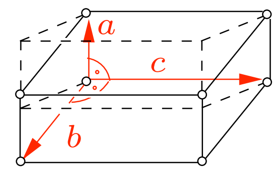
$$\mathcal{P}^a := \{\, C_{11}\,,\ C_{22}\,,\ C_{33}\,,\ C_{12}\,,\ C_{13}\,,\ C_{23}\,\}.$$

Classical Basis:

$$\mathcal{I}^a := \{\, C_{11}\,,\ C_{22}\,,\ C_{33}\,,\ C_{12}\,,\ C_{13}\,,\ C_{23}\,\}.$$

$\longrightarrow$ complete description

Monoclinic system: 2nd-order SST



$$\boldsymbol{G}^m = \begin{bmatrix} \tilde{a} & \tilde{d} & 0 \\ \tilde{d} & \tilde{b} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

$$\begin{aligned} \mathcal{P}^m := \{\, & C_{11}\,,\ C_{22}\,,\ C_{33}\,,\ C_{12}, \\ & \mathrm{Cof}C_{11} = C_{22}C_{33} - C_{23}^2\,, \\ & \mathrm{Cof}C_{22} = C_{11}C_{33} - C_{13}^2\,, \\ & \mathrm{Cof}C_{33} = C_{11}C_{22} - C_{12}^2\,, \\ & \mathrm{Cof}C_{12} = C_{13}C_{23} - C_{12}C_{33}\,\}. \end{aligned}$$

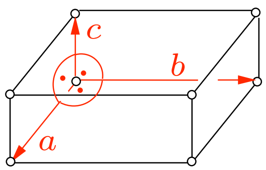
Classical Basis:

$$\mathcal{I}^m := \{\, C_{11}\,,\ C_{22}\,,\ C_{33}\,,\ C_{12}\,,\ C_{13}^2\,,\ C_{23}^2\,,\ C_{13}C_{23}\,\}.$$

$\longrightarrow$ complete description

Polyconvex Functional Bases $\mathcal{P}$

Rhombic system: 2nd-order SST

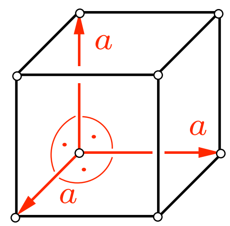


$$\boldsymbol{G}^o = \begin{bmatrix} \tilde{a} & 0 & 0 \\ 0 & \tilde{b} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

$$\mathcal{P}^o := \{\ C_{11}\ ,\ \ C_{22}\ ,\ \ C_{33}\ , C_{22}C_{33} \\ -C_{23}^2\ ,\ \ C_{11}C_{33} - C_{13}^2\ , \\ C_{11}C_{22} - {C_{12}}^2\ \}.$$

$\longrightarrow$ complete description

Cubic system: 4th-order SST

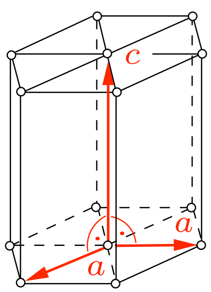


$$\boldsymbol{G}^c = \begin{bmatrix} \tilde{a} & 0 & 0 \\ 0 & \tilde{a} & 0 \\ 0 & 0 & \tilde{a} \end{bmatrix}$$

$$\mathcal{P}^c := \{I_1,\ \ I_2\}.$$

$\longrightarrow$ incomplete description

Hexagonal system: 6th-order SST

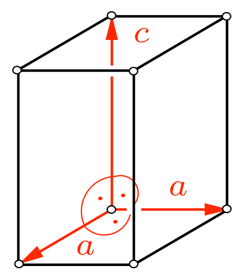


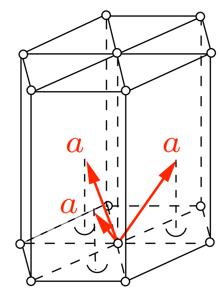
$$\boldsymbol{G}^h = \begin{bmatrix} \tilde{a} & 0 & 0 \\ 0 & \tilde{a} & 0 \\ 0 & 0 & \tilde{c} \end{bmatrix}$$

$$\mathcal{P}^h := \{\ C_{11}\ +\ C_{22}\ ,\ \ C_{33}\ ,\ \ C_{22}C_{33} \\ +C_{11}C_{33} - (C_{23}^2 + C_{13}^2)\ , \\ C_{11}C_{22} - C_{12}^2\}\ .$$

$\longrightarrow$ complete description

Tetragonal, Trigonal system: 4th-order SSTs





$$\boldsymbol{G}^t = \boldsymbol{G}^{ht} = \boldsymbol{G}^h$$
$$\mathcal{P}^t = \mathcal{P}^{ht} = \mathcal{P}^h$$

$\longrightarrow$ incomplete description

Generic Polyconvex Anisotropic Energy Functions

Additive decomposition of the free energy in isotropic and anisotropic terms, i.e.,

$$\psi = \psi^{iso}(I_1, I_2, I_3) + \psi^{aniso}(I_3, J_{4j}, J_{5j}),$$

with $J_{4j} = \mathrm{tr}[\boldsymbol{C}\boldsymbol{G}_j]$, $J_{5j} = \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{G}_j]$, j-th metric tensor $\boldsymbol{G}_j$, $g_j := \mathrm{tr}\boldsymbol{G}_j$.

For the isotropic part ψ^{iso} we choose a compressible MOONEY-RIVLIN model,i.e.,

$$\psi^{iso} = \alpha_1\; I_1 + \alpha_2\; I_2 + \delta_1\; I_3 - \delta_2 \ln(\sqrt{I_3}), \quad \forall\; \alpha_1,\; \alpha_2,\; \delta_1,\; \delta_2 \geq 0.$$

Polyconvex isotropic f_{3rj} & anisotropic functions $f_{4rj}, f_{5rj}, f_{6rj}, f_{7rj}$ are used for

$$\boxed{\begin{aligned}
\psi_1^{aniso} &= \sum_{r=1}^{n}\sum_{j=1}^{m}\left[f_{3rj}(I_3) + f_{4rj}(J_{4j}) + f_{5rj}(J_{5j})\right],\\
\psi_2^{aniso} &= \sum_{r=1}^{n}\sum_{j=1}^{m}\left[f_{3rj}(I_3) + f_{6rj}(I_3, J_{4j}) + f_{7rj}(I_3, J_{5j})\right],\\
\psi_3^{aniso} &= \sum_{r=1}^{n}\sum_{j=1}^{m}\left[f_{3rj}(I_3) + f_{4rj}(J_{4j}) + f_{5rj}(J_{5j})\right.\\
&\qquad \left. + f_{6rj}(I_3, J_{4j}) + f_{7rj}(I_3, J_{5j})\right].
\end{aligned}}$$

Further details: SCHRÖDER, NEFF & EBBING [2008].

Generic Polyconvex Anisotropic Functions

Some specific functions which **automatically** satisfy the condition $\boldsymbol{S}|_{C=1} = \boldsymbol{0}$

$$\psi_I^{aniso} = \sum_{r=1}^{n}\sum_{j=1}^{m} \xi_{rj} \left\{ \begin{aligned} &\left[\frac{1}{\alpha_{rj}+1}\frac{1}{(g_j)^{\alpha_{rj}}}(J_{4j})^{\alpha_{rj}+1}\right. \\ &\left. + \frac{1}{\beta_{rj}+1}\frac{1}{(g_j)^{\beta_{rj}}}(J_{5j})^{\beta_{rj}+1} + \frac{g_j}{\gamma_{rj}}(I_3)^{-\gamma_{rj}}\right] \end{aligned} \right\},$$

with $\xi_{rj}, \alpha_{rj}, \beta_{rj} \geq 0\,,$ $\gamma_{rj} \geq -1/2\,.$ $\longrightarrow$ coercive

$$\psi_{II}^{aniso} = \sum_{r=1}^{n}\sum_{j=1}^{m} \xi_{rj} \left\{ \begin{aligned} &\left[\frac{1}{\alpha_{rj}+1}\frac{1}{(g_j)^{\alpha_{rj}}}(J_{4j})^{\alpha_{rj}+1}\right. \\ &\left. + \frac{1}{\beta_{rj}+1}\frac{1}{(g_j)^{\beta_{rj}}}(J_{5j})^{\beta_{rj}+1} - \ln(I_3^{g_j})\right] \end{aligned} \right\},$$

with $\xi_{rj},\ \alpha_{rj},\ \beta_{rj} \geq 0\,.$

$$\psi_{III}^{aniso} = \sum_{r=1}^{n}\sum_{j=1}^{m} \left[\frac{J_{4j}^{\alpha_{rj}}}{I_3^{1/3}} + \frac{J_{5j}^{\alpha_{rj}}}{I_3^{1/3}} + \frac{g_j^{\alpha_{rj}}}{\beta_{rj}}\, I_3^{-\beta_{rj}}\right],$$

with $\alpha_{rj} = 5/3\,,$ $\beta_{rj} \geq -1/2\,.$

$$\psi_{IV}^{aniso} = \sum_{r=1}^{n}\sum_{j=1}^{m} \left[\frac{J_{4j}^{\alpha_{rj}}}{I_3^{1/3}} + \frac{J_{5j}^{\alpha_{rj}}}{I_3^{1/3}} - g_j^{\alpha_{rj}}\, \beta_{rj}\, \ln(I_3)\right],$$

with $\alpha_{rj} \geq 1\,,$ $\beta_{rj} = \alpha_{rj} - 2/3\,.$

A priori stress free reference configuration: Itskov & Aksel [2004].
Proof of coercivity: Schröder, Neff & Ebbing [2008].

Proof of Coercivity

The polyconvex anisotropic free-energy function

$$\psi_I^{aniso}(\boldsymbol{F}) = \frac{1}{1+\alpha}\frac{1}{g^\alpha}J_4^{1+\alpha} + \frac{1}{1+\beta}\frac{1}{g^\beta}J_5^{1+\beta} + \frac{g}{\gamma}I_3^{-\gamma}, \quad \alpha,\beta \geq 0, \gamma \geq -\frac{1}{2}$$

is **coercive**, because $\forall\, \boldsymbol{F} \in \mathbb{M}^{3\times 3}$:

$$\psi_I^{aniso}(\boldsymbol{F}) \geq C_1\ (\|\ \boldsymbol{F}\|^p + \|\ \mathrm{Cof}\boldsymbol{F}\|^q) - C_2\,, \quad p \geq 2\,,\ q \geq \frac{3}{2},\ C_1, C_2 \geq 0,\ C_1 > 0.$$

Proof. Case 1: $\gamma \geq 0$:

$$\begin{aligned}
\psi_I^{aniso}(\boldsymbol{F}) &\geq \tfrac{1}{1+\alpha}\tfrac{1}{g^\alpha}J_4 + \tfrac{1}{1+\beta}\tfrac{1}{g^\beta}J_5 + \tfrac{g}{\gamma}I_3^{-\gamma} \\
&\geq \tfrac{1}{1+\alpha}\tfrac{1}{g^\alpha}\lambda_{\min}(\boldsymbol{G}_j)\ \|\ \boldsymbol{F}\ \|^2 + \tfrac{1}{1+\beta}\tfrac{1}{g^\beta}\lambda_{\min}(\boldsymbol{G}_j)\ \|\ \mathrm{Cof}\boldsymbol{F}\ \|^2 + \tfrac{g}{\gamma}I_3^{-\gamma} \\
&= c_1^+\ \|\ \boldsymbol{F}\ \|^2 + c_2^+\ \|\ \mathrm{Cof}\boldsymbol{F}\ \|^2 + \tfrac{g}{\gamma}(\det\boldsymbol{F})^{-2\gamma}\,, \quad \forall c_1^+,\ c_2^+ > 0
\end{aligned}$$

$C_1 = \min(c_1^+, c_2^+),\ C_2 = 0$ and $p = q = 2 \quad \rightarrow \quad \psi_I^{aniso}$ is **coercive**.

Proof of Coercivity

Proof. Case 2: $0 \geq \gamma \geq -\frac{1}{2}$:

$$
\begin{aligned}
\psi_I^{aniso}(\boldsymbol{F}) &\geq c_1^+ \parallel \boldsymbol{F} \parallel^2 + c_2^+ \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^2 + \frac{g}{\gamma} (\det \boldsymbol{F})^{-2\gamma} \\
&\geq c_1^+ \parallel \boldsymbol{F} \parallel^2 + c_2^+ \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^2 - c_3^+ (\det \boldsymbol{F})^{-2\gamma} , \\
&= c_1^+ \parallel \boldsymbol{F} \parallel^2 + c_2^+ \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^2 - c_3^+ ((\det \boldsymbol{F})^2)^{|\gamma|} , \\
&\geq c_1^+ \parallel \boldsymbol{F} \parallel^2 + c_2^+ \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^2 - c_3^+ [\det \boldsymbol{F} + 1] , \quad 0 \leq |\gamma| \leq \frac{1}{2} \\
&\geq c_1^+ \parallel \boldsymbol{F} \parallel^2 + c_2^+ \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^2 - c_3^+ [\frac{1}{\sqrt{3\sqrt{3}}} \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^{\frac{3}{2}} + 1] .
\end{aligned}
$$

Applying $\forall\, x \in \mathbb{R}^+ : \quad k_1 x^2 - k_2 x^{3/2} \geq \tilde{k}_1 x^{3/2} - \tilde{k}_2 , \quad \forall\, k_1, k_2 > 0,\ \tilde{k}_1, \tilde{k}_2 > 0$

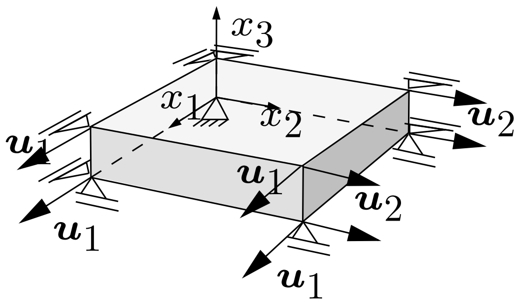
with $x = \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel$ yields

$$
\begin{aligned}
\psi_I^{aniso}(\boldsymbol{F}) &\geq c_1^+ \parallel \boldsymbol{F} \parallel^2 + c_2^+ \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^2 - c_3^+ [\frac{1}{\sqrt{3\sqrt{3}}} \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^{\frac{3}{2}} + 1] \\
&\geq c_1^+ \parallel \boldsymbol{F} \parallel^2 + C_2^+ \parallel \mathrm{Cof}\,\boldsymbol{F} \parallel^{3/2} - C_3^+
\end{aligned}
$$

$C_1 = \min(c_1^+, C_2^+)$ and $p = 2,\ q = \frac{3}{2} \quad \rightarrow \quad \psi_I^{aniso}$ is **coercive**.

A First Applications to Transverse Isotropy

Biaxial Homogeneous Tension Test

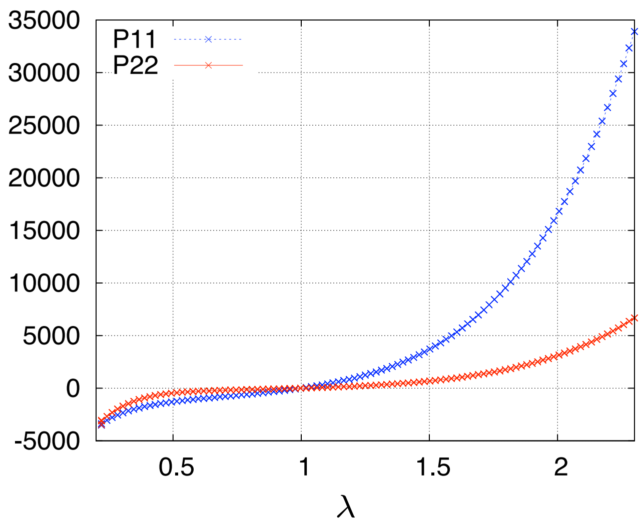


Unimodular metric tensor:

$$\boldsymbol{G}^{ti} = \mathrm{diag}(\gamma, \frac{1}{\sqrt{\gamma}}, \frac{1}{\sqrt{\gamma}})$$

Additive construction of energy function $\psi = \psi^{iso} + \psi^{ti}$, with

$$\begin{aligned} \psi^{iso} &= \alpha_1 I_1 + \alpha_2 I_2 + \delta_1 I_3 - \delta_2 \ln\sqrt{I_3} \\ \psi^{ti} &= \eta_1 (J_4^{\alpha_4} + \beta_1 J_5^{\alpha_5}) \end{aligned}$$



$J_4 = \mathrm{tr}[\boldsymbol{C}\boldsymbol{G}^{ti}], \quad J_5 = \mathrm{tr}[\mathrm{Cof}[\boldsymbol{C}]\boldsymbol{G}^{ti}]$

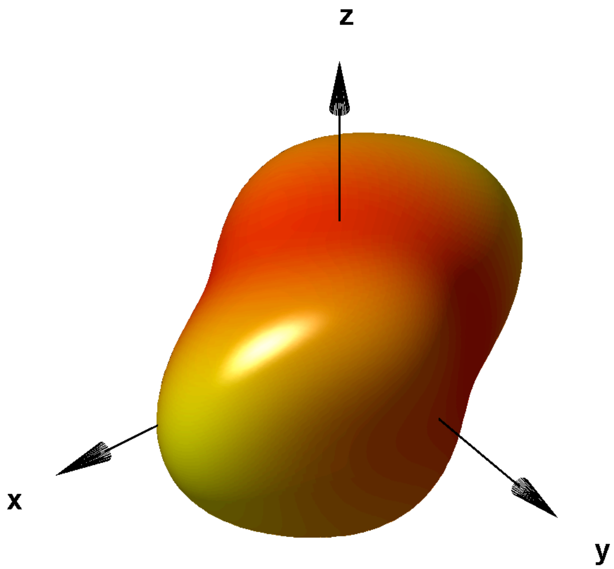
$\gamma = 4.0,\ \alpha_1 = 2.0,\ \alpha_2 = 0.0,$

$\delta_1 = 10.0,\ \delta_2 = 786,\ \eta_1 = 1.0,\ \beta_1 = 7.5,$

$\alpha_4 = 2.0,\ \alpha_5 = 3.0$ [MPa]

Fitting of Monoclinic Moduli $\mathbb{C} = 4\partial^2_{CC}\psi$: Augite

Characteristic surface of Young's moduli:



movie

Elasticities in [GPa], Simmons [1971]:

$$\mathbb{C}^{(V)exp} = \begin{bmatrix} 217.8 & 72.4 & 33.9 & 24.6 & 0 & 0 \\ & 181.6 & 73.4 & 19.9 & 0 & 0 \\ & & 150.7 & 16.6 & 0 & 0 \\ & & & 51.1 & 0 & 0 \\ & sym. & & & 55.8 & 4.3 \\ & & & & & 69.7 \end{bmatrix}$$

Error for $\psi = \psi_I^{aniso}$ and $n = m = 3$:

$$e = \frac{\| \mathbb{C}^{(V)comp} - \mathbb{C}^{(V)exp} \|}{\| \mathbb{C}^{(V)exp} \|} \approx 3.48[\%]$$

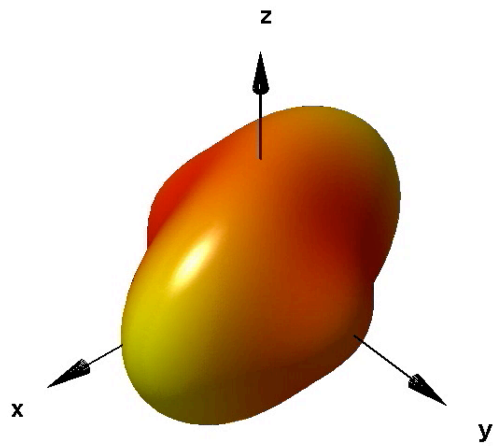
Transversely isotropic and monoclinic metric tensors:

$$\boldsymbol{G}^{ti} = \begin{bmatrix} 0.419 & 0 & 0 \\ 0 & 0.419 & 0 \\ 0 & 0 & 1.953 \end{bmatrix}, \quad \boldsymbol{G}_2^m = \begin{bmatrix} 1.503 & -0.513 & 0 \\ -0.513 & 0.934 & 0 \\ 0 & 0 & 1.572 \end{bmatrix}, \quad \boldsymbol{G}_3^m = \begin{bmatrix} 2.719 & 0.496 & 0 \\ 0.496 & 0.547 & 0 \\ 0 & 0 & 1.008 \end{bmatrix}$$

Fitting of Anisotropic Moduli

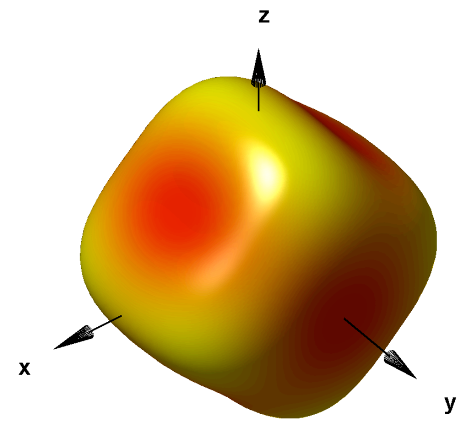
Monoclinic Materials

Rhombic Materials



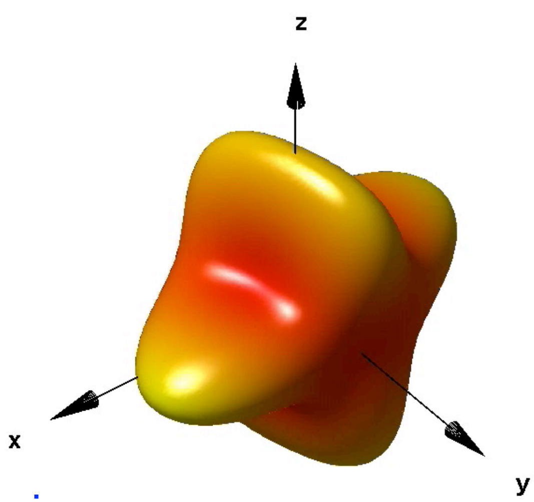
movie

Aegirite: $e = 1.65\%$



movie

Ammonium Sulfate: $e = 3.46\%$



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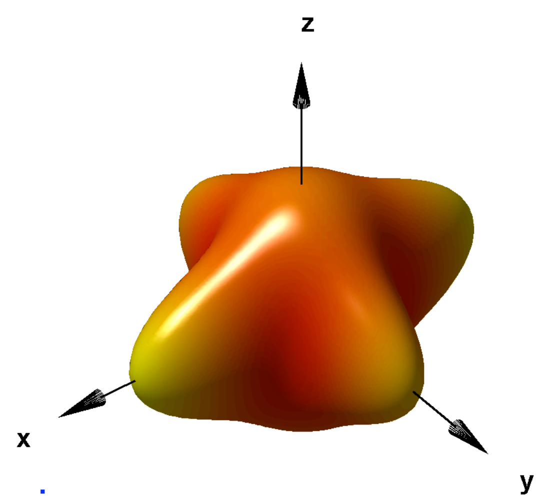
Feldspar(Labradorite): $e = 5.28\%$

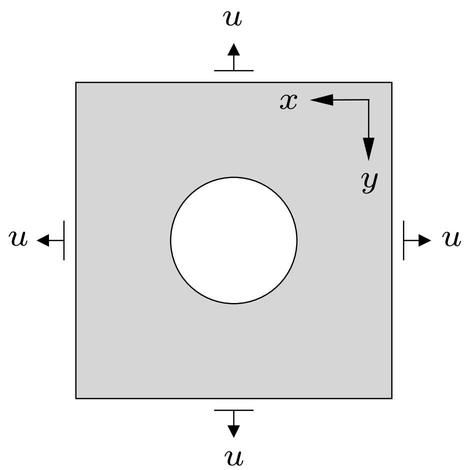


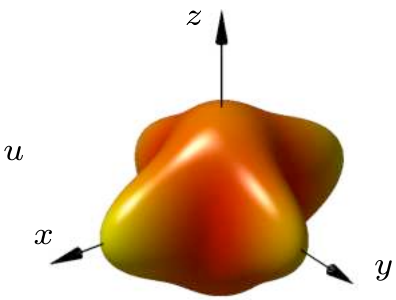
movie

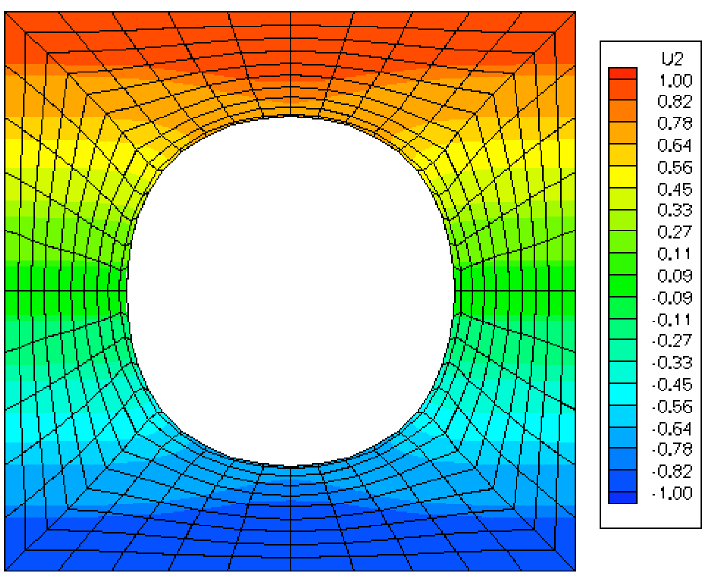
Acenaphthene: $e = 2.28\%$

Biaxial Tension Test of Perforated Plate with Centered Hole

Rhombic Acenaphthene







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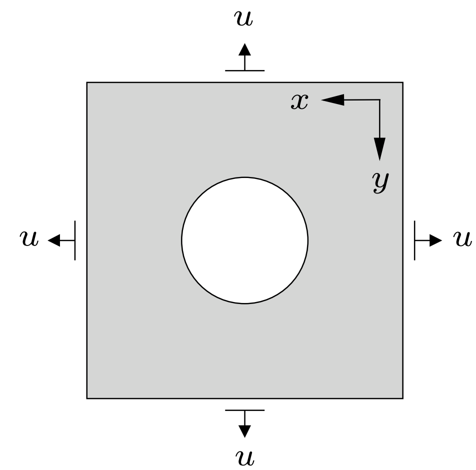
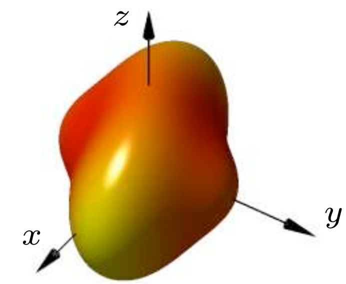
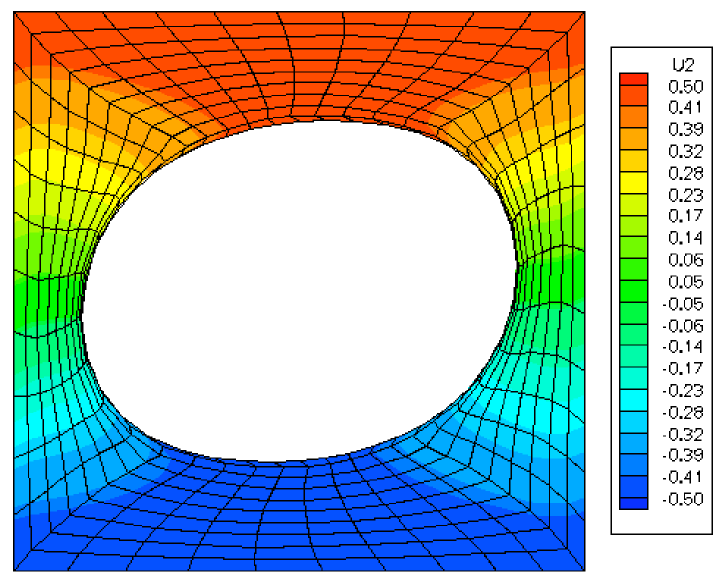
Monoclinic Aegirite



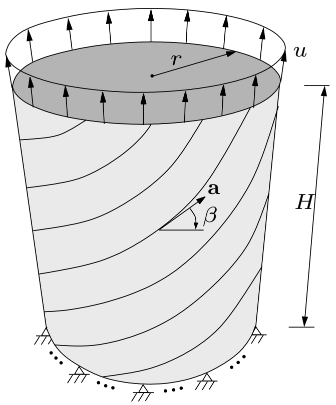




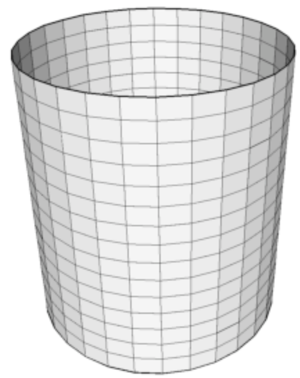
movie

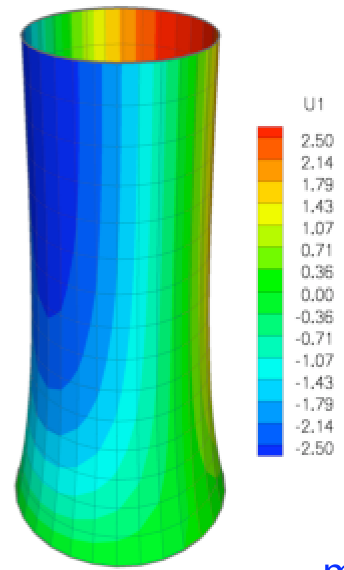
Axial Stretch of a Thin-Walled Cylinder

System

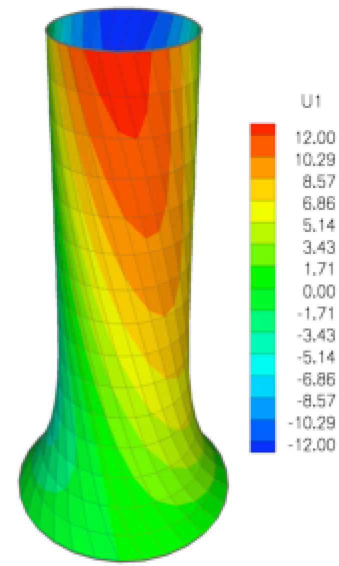


Mesh





movie



$H = 20.0$ cm, $r = 10.0$ cm

$\beta = 45.0^\circ$, $h = 0.05$ cm

Isotropic

Anisotropic

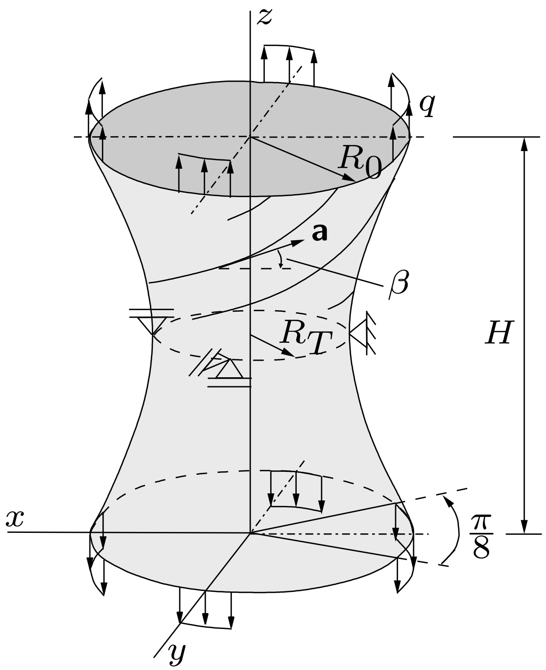
Anisotropic calculation: consider energy for one fiber direction

$$\psi = c_1 \left(\frac{I_1}{I_3^{1/3}} - 3 \right) + \epsilon_1 \left(I_3^{\epsilon_2} + \frac{1}{I_3^{\epsilon_2}} - 2 \right) + \alpha_1 \langle \mathrm{tr}[(\mathbf{1} - \boldsymbol{M})\mathrm{Cof}\boldsymbol{C}] - 2 \rangle^{\alpha_2}$$

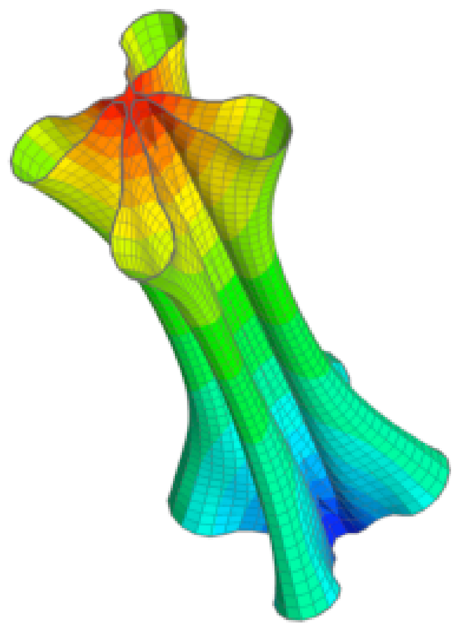
$c_1 = 100.0$ kN/cm^2, $\epsilon_1 = 2000.0$ kN/cm^2, $\epsilon_2 = 10.0$, $\alpha_1 = 14000.0$ kN/cm^2 , $\alpha_2 = 2.3$

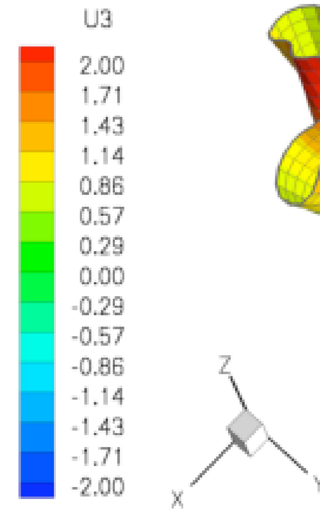
Balzani, D.; Gruttmann, F. & Schröder, J. [2008], "Analysis of Thin Shells using Anisotropic Polyconvex Energy Densities", *Computer Methods in Applied Mechanics and Engineering*, Vol. 197, 1015-1032

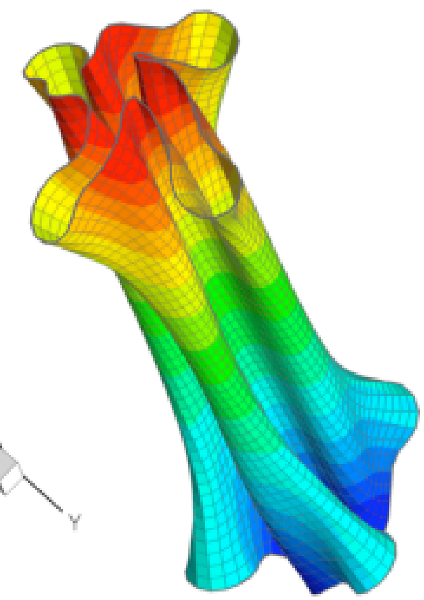
Hyperbolic Shell with Locally Distributed Loads



$R_0 = 5.0$ m, $R_T = 3.0$ m
$\beta = 45.0^{\circ}$, $H = 12.0$ m







movie

Isotropic

Anisotropic

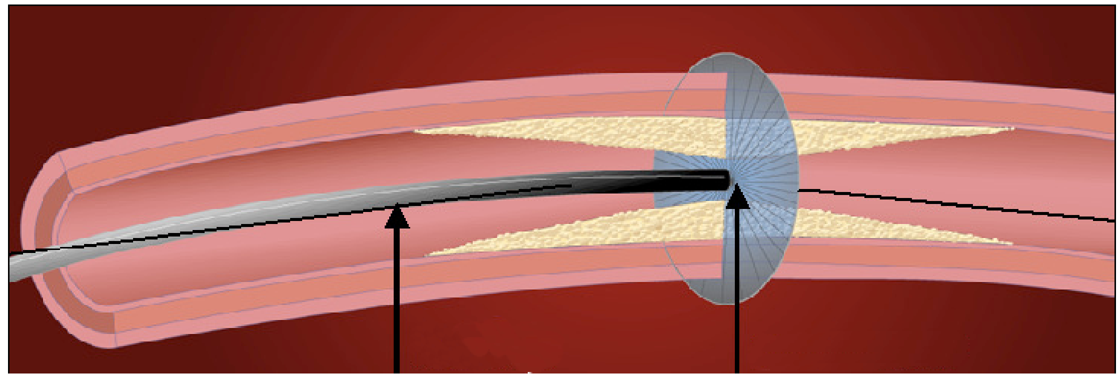
The radius of the hyperbolic shell is defined as (cf. BAŞAR ET AL. [1997,2004])

$$R = \hat{R}(z) = R_T \sqrt{1 + \left(\frac{z - \frac{H}{2}}{4.5} \right)^2}$$

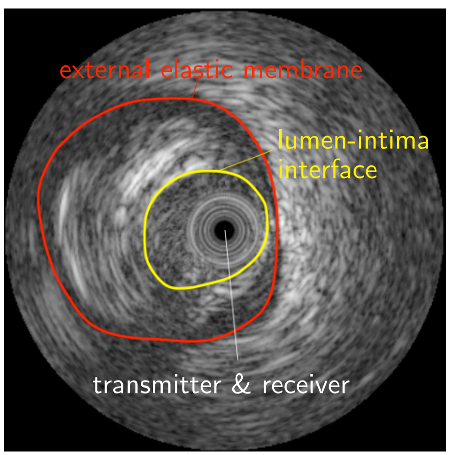
$c_1 = 100.0$ kN/cm^2, $\epsilon_1 = 2000.0$ kN/cm^2, $\epsilon_2 = 10.0$, $\alpha_1 = 1000.0$ kN/cm^2, $\alpha_2 = 2.3$

Motivation: Atherosclerotic Degenerated Artery

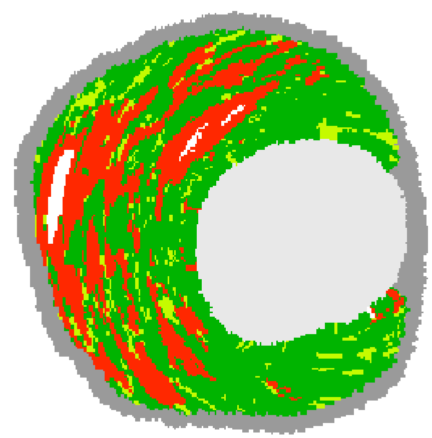
Arterial segment[1]



Intravascular Ultrasound (IVUS) examination[2]



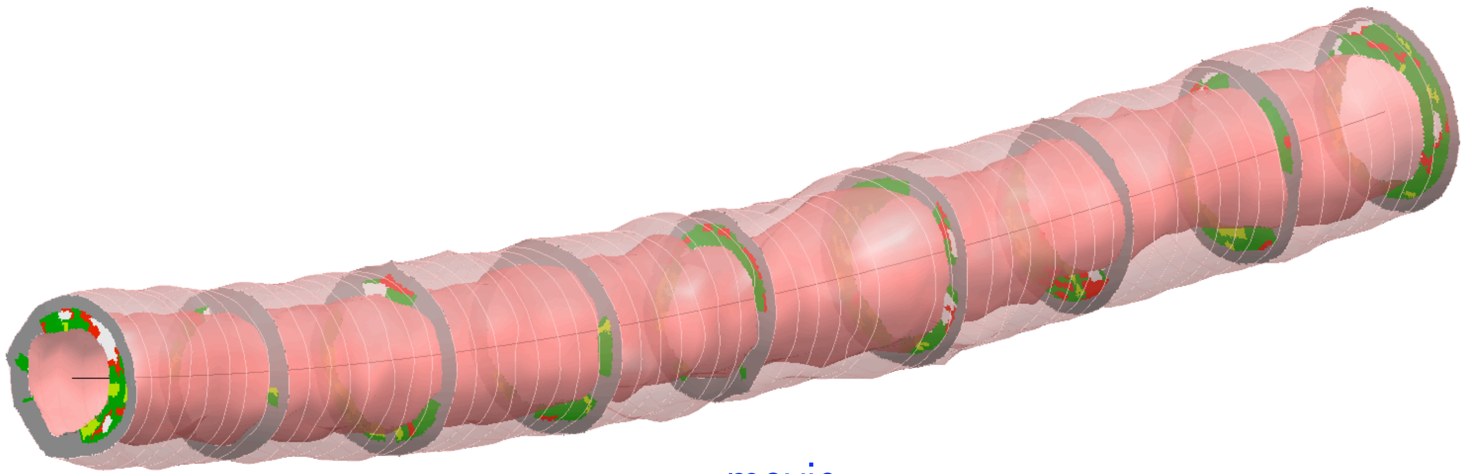
IVUS image[3]



Virtual Histology (VH) - IVUS[3]

[1]HOLZAPFEL, SOMMER, REGITNIG [2004], [2]BERSCH [2005]
[3]Westdeutsches Herzzentrum Essen, Prof. Erbel

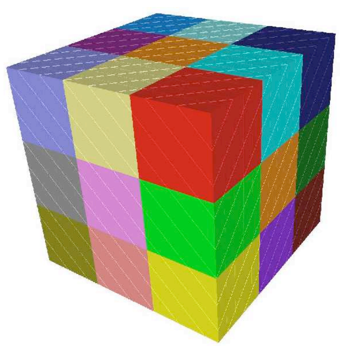
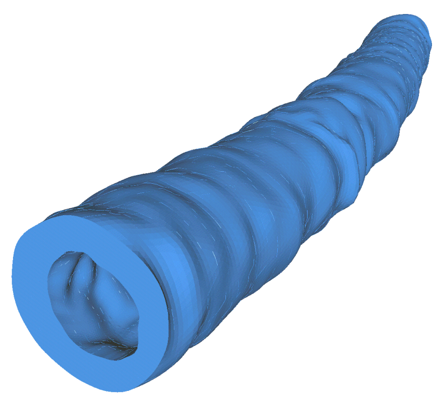
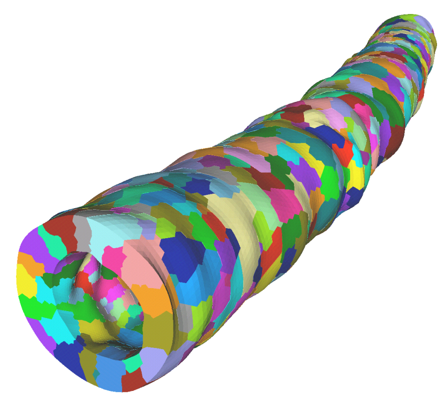
Visualization of 3-D Reconstruction



movie

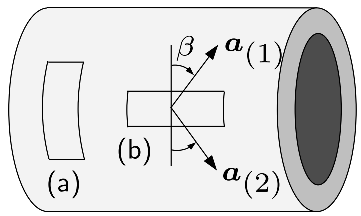
Finite **E**lement **T**earing and **I**nterconnecting - **D**ual-**P**rimal

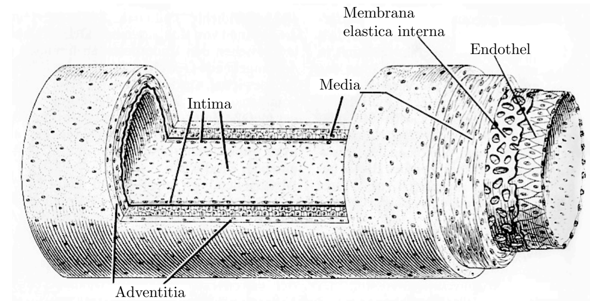
- Decompose domain Ω into N nonoverlapping subdomains.
- Parallel computing: Allocate one or several subdomains to each processor.

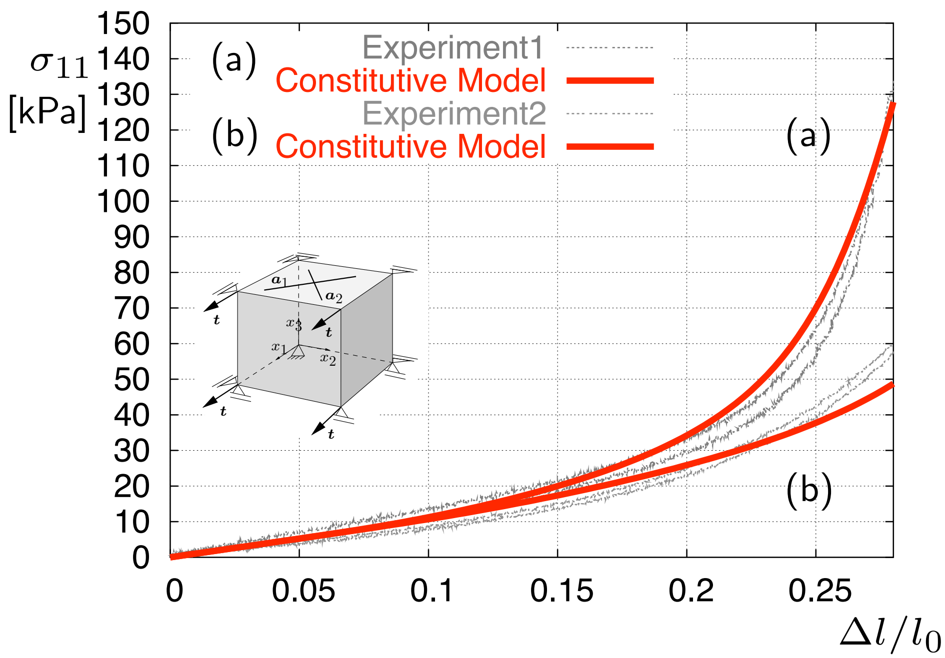
Adjustment to Experimental Stress-Strain Curves

Test stripes:

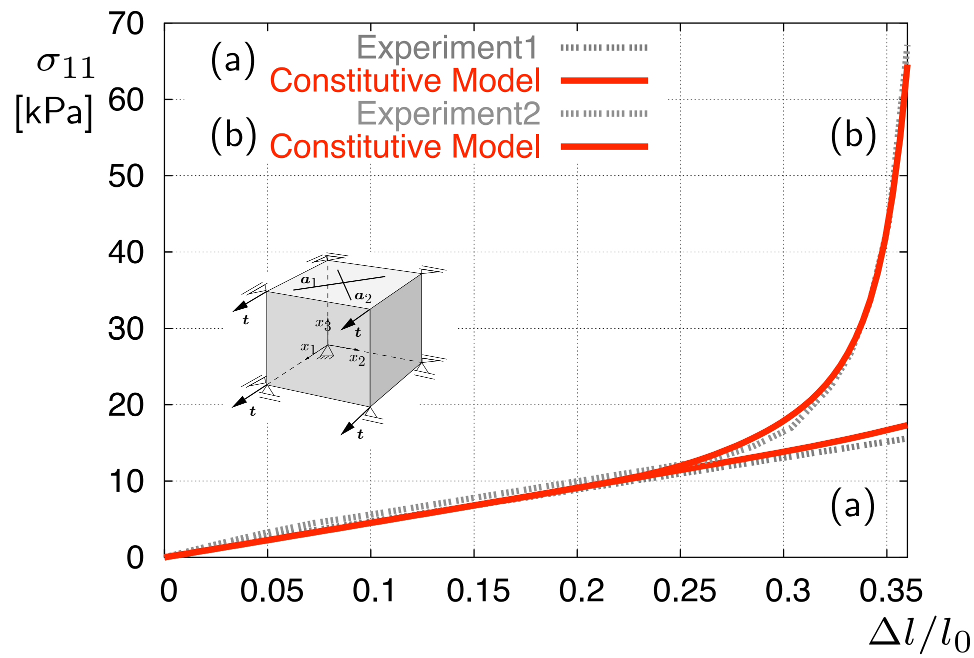




Media:



Adventitia:



$$\psi_{(BNSH)} = C_1 \left(\frac{I_1}{I_3^{1/3}} - 3 \right) + \epsilon_1 \left(I_3^{\epsilon_2} + \frac{1}{I_3^{\epsilon_2}} - 2 \right) + \sum_{a=1}^{2} \alpha_1 \left\langle K_3^{(a)} - 2 \right\rangle^{\alpha_2}$$

BNSH [2005]

in cooperation with G.A. Holzapfel

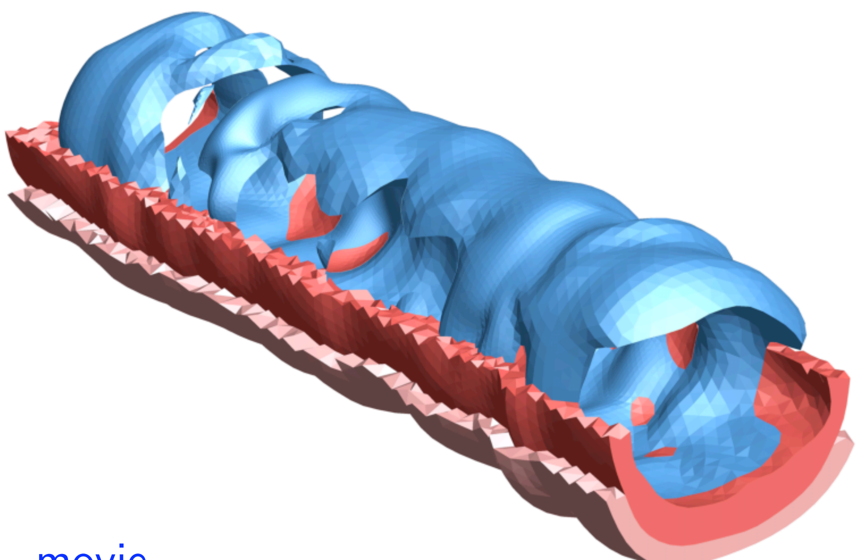
3-D Simulation Using Patient Specific Arterial Geometries

Model:

- 25 cross-sectional images,
- Average distance: 0.5mm,
- 10-noded tetrahedral finite elements.

Computation:

- FEAP – FETI-DP environment,
- $1\,303\,551$ dofs; $305\,033$ elements,
- $p_{\max} = 19.2\,\mathrm{kPa} \approx 144\,\mathrm{mmHg}$.



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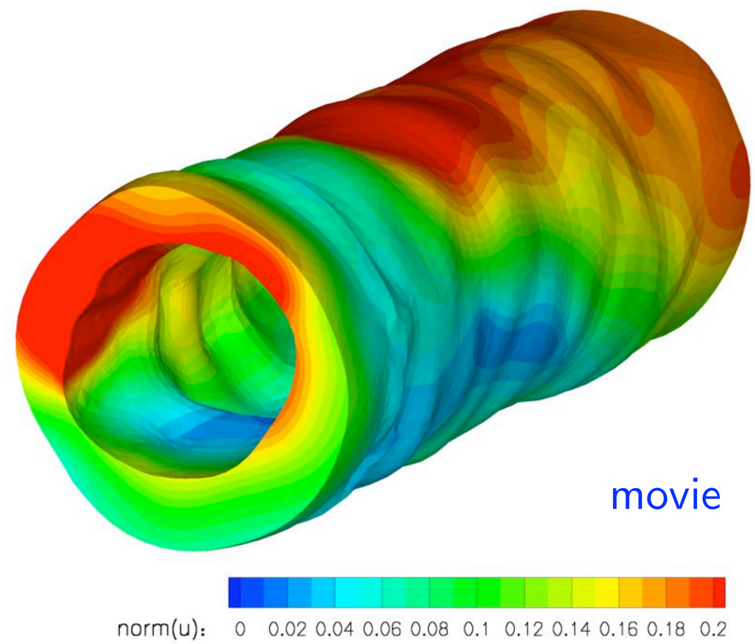


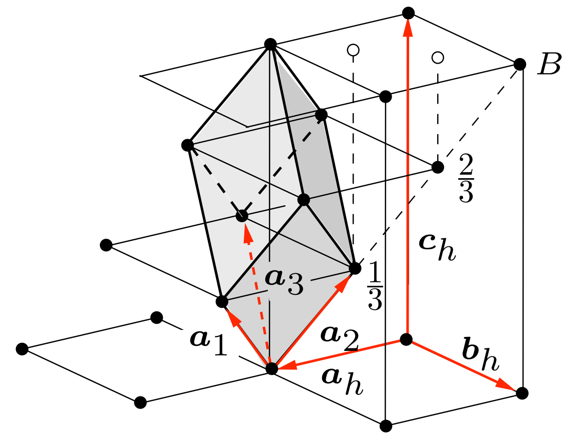
movie

Brands, D.; Klawonn, A.; Rheinbach, O. & Schröder, J. [2008], "Modelling and convergence in arterial wall simulations using a parallel FETI solution strategy.", *Computer Methods in Biomechanics and Biomedical Engineering*, Vol. 11, pp. 569-583

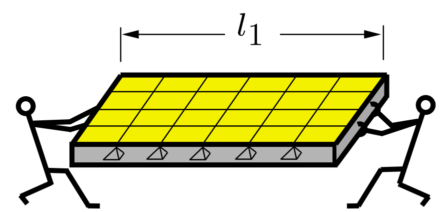
Brands, D.; Klawonn, A.; Rheinbach, O. & Schröder, J. [2008], "On the Visualization of Patient Specific Arterial Geometries Using the Virtual Histology.", *PAMM*, submitted for publication

Recent Results on the Construction of Anisotropic Polyconvex Energies

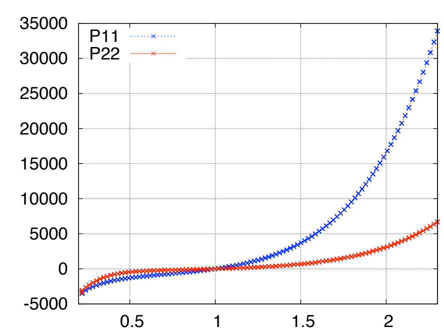
- Arbitrary anisotropy can be *“completely described “* by generic invariant functions in terms of **single, second-order and fourth-order positive definite crystallographically motivated structural tensors**.



- These invariant functions **automatically fulfill** the **polyconvexity condition**.



- The polyconvex anisotropic free energy functions in terms of the proposed invariant functions also **automatically satisfy** the requirement of a **stress-free reference configuration**.



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