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# Foundation of Mathematical Elasticity

First lecture for a Short Course on

## Mathematical modelling in Solid Mechanics

Karlsruhe 2005

Version of November 24, 2005

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# Introduction

Following Ciarlet's textbook *Mathematical Elasticity*, we introduce

- Kinematics  
state variables and their basic relationships
- Balance equations  
general equations of equilibrium in continuum mechanics
- Constitutive equations  
specific material laws for elastic materials

establishing a full set of equations determining the deformation of elastic bodies. This part of the lecture serves as an overview and we only sketch parts of the proofs.

Then, we consider some numerical aspects in finite elasticity:

- Newton's method for minimization problems in elasticity  
computation of derivatives
- Homotopy and regularization  
finding a local solution
- Lagrange multipliers  
treatment of additional constraints.

A general problem in solid mechanics is to find a consistent and convenient notation. This is always a compromise, and the choice of a suitable notation depends strongly of the considered application. Thus, we finally summarize two different notations which are both commonly in use.

## References

P. G. Ciarlet: *Mathematical Elasticity*, Vol. I, North Holland 1988

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G. M. Hulbert: *Computational Structural Dynamics*, in: *Encyclopedia of Computational Mechanics*, Vol. 2, ed. E. Stein, R. de Borst, T. R. Hughes, Wiley 2004

J. C. Simo and T. J. R. Hughes: *Computational Inelasticity*, Springer 1998

# 1 Kinematics

## Deformations in $\mathbb{R}^3$

Let  $\Omega \subset \mathbb{R}^3$  be a domain (describing a body in its natural state) and let be the boundary  $\partial\Omega$  sufficiently smooth. Here and in the following, we assume that all functions are sufficiently smooth.

### (1.1) Definition

A deformation is a vector field

$$\varphi: \bar{\Omega} \longrightarrow \mathbb{R}^3$$

which is orientation - preserving and such that  $\varphi|_{\Omega}$  is injective.

We fix the following notations:

$\bar{\Omega}$  reference configuration

$\mathbf{x} \in \bar{\Omega}$  Lagrange variable

$\bar{\Omega}^\varphi := \varphi(\bar{\Omega})$  deformed configuration / current configuration

$\mathbf{x}^\varphi := \varphi(\mathbf{x})$  Euler variable

$$\mathbf{F} := D\varphi = \begin{pmatrix} \partial_1\varphi_1 & \partial_2\varphi_1 & \partial_3\varphi_1 \\ \partial_1\varphi_2 & \partial_2\varphi_2 & \partial_3\varphi_2 \\ \partial_1\varphi_3 & \partial_2\varphi_3 & \partial_3\varphi_3 \end{pmatrix} \quad \text{deformation gradient, where } \partial_i = \frac{\partial}{\partial x_i}$$

$$J := \det \mathbf{F} > 0$$

### (1.2) Lemma

Let  $V \subset \Omega$  be an open subset with sufficiently smooth boundary  $\partial V$ , and let  $A \subset \partial V$ . Then, we have for  $V^\varphi := \varphi(V)$

$$\int_{V^\varphi} d\mathbf{x}^\varphi = \int_V J d\mathbf{x}, \quad \text{volume element } d\mathbf{x}^\varphi$$

and for  $A^\varphi := \varphi(A)$

$$\int_{A^\varphi} da^\varphi = \int_A J |\mathbf{F}^{-T} \mathbf{n}| da \quad \text{area element } da^\varphi,$$

where  $\mathbf{n}: \partial V \longrightarrow S^2 \subset \mathbb{R}^3$  denotes the outer unit normal.

**Remark**  $\mathbf{n}^\varphi: \partial V^\varphi \longrightarrow S^2$  can be computed by

$$\mathbf{n}^\varphi(\mathbf{x}^\varphi) = \frac{1}{|J\mathbf{F}^{-T}(\mathbf{x})\mathbf{n}(\mathbf{x})|} J\mathbf{F}^{-T}(\mathbf{x})\mathbf{n}(\mathbf{x}) = \frac{1}{|\mathbf{F}^{-T}(\mathbf{x})\mathbf{n}(\mathbf{x})|} \mathbf{F}^{-T}(\mathbf{x})\mathbf{n}(\mathbf{x}).$$

## Tensors

For a sufficiently smooth tensor field

$$\mathbf{T}: \bar{\Omega} \longrightarrow \mathbb{R}^{3,3}, \quad \mathbf{T}(x) = \begin{pmatrix} T_{11}(x) & T_{12}(x) & T_{13}(x) \\ T_{21}(x) & T_{22}(x) & T_{23}(x) \\ T_{31}(x) & T_{32}(x) & T_{33}(x) \end{pmatrix}$$

holds the (vector valued) Gauss theorem

$$\int_V \operatorname{div} \mathbf{T} \, d\mathbf{x} = \int_{\partial V} \mathbf{T} \cdot \mathbf{n} \, d\mathbf{a},$$

where

$$\operatorname{div} \mathbf{T} = \begin{pmatrix} \partial_1 T_{11} + \partial_2 T_{12} + \partial_3 T_{13} \\ \partial_1 T_{21} + \partial_2 T_{22} + \partial_3 T_{23} \\ \partial_1 T_{31} + \partial_2 T_{32} + \partial_3 T_{33} \end{pmatrix}.$$

### (1.3) Theorem

Let  $\mathbf{T}^\varphi: \bar{\Omega}^\varphi \longrightarrow \mathbb{R}^{3,3}$  be a tensor field, and let

$$\mathbf{T}(\mathbf{x}) := J(\mathbf{x}) \mathbf{T}^\varphi(\mathbf{x}^\varphi) \mathbf{F}(\mathbf{x})^{-T}$$

be the Piola transform of  $\mathbf{T}^\varphi$ . Then:

$$\operatorname{div} \mathbf{T}(\mathbf{x}) = J(\mathbf{x}) \operatorname{div}^\varphi \mathbf{T}^\varphi(\mathbf{x}^\varphi), \quad \operatorname{div}^\varphi = \sum \frac{\partial}{\partial x_i^\varphi}$$

and therefore

$$\int_{\partial V} \mathbf{T} \cdot \mathbf{n} \, d\mathbf{a} = \int_V \operatorname{div} \mathbf{T} \, d\mathbf{x} = \int_{V^\varphi} \operatorname{div}^\varphi \mathbf{T}^\varphi \, d\mathbf{x}^\varphi = \int_{\partial V^\varphi} \mathbf{T}^\varphi \cdot \mathbf{n}^\varphi \, d\mathbf{a}^\varphi.$$

For the *proof* check first the Piola identity  $\operatorname{div}(J\mathbf{F}^{-T}) = 0$ . Then, inserting the chain rule

$$\begin{aligned} D_{\mathbf{x}} \mathbf{T}^\varphi(\varphi(\mathbf{x})) &= \left( \partial_k (T_{ij}^\varphi(\varphi(\mathbf{x}))) \right)_{ijk} \\ &= \left( \sum_l \partial_l^\varphi T_{ij}^\varphi(\mathbf{x}^\varphi) \partial_k \varphi_l(\mathbf{x}) \right)_{ijk} = D_{\mathbf{x}^\varphi} \mathbf{T}^\varphi(\mathbf{x}^\varphi) D_{\mathbf{x}} \varphi(\mathbf{x}) \end{aligned}$$

gives

$$\begin{aligned} \operatorname{div} \mathbf{T}(\mathbf{x}) &= \operatorname{div} \left( \mathbf{T}^\varphi(\mathbf{x}^\varphi) (J(\mathbf{x}) \mathbf{F}^{-T}(\mathbf{x})) \right) \\ &= \left( \sum_{k,j} (\partial_k T_{ij}^\varphi(\varphi(\mathbf{x}))) J(\mathbf{x}) (\mathbf{F}^{-T}(\mathbf{x}))_{jk} \right)_i + 0 \\ &= J(\mathbf{x}) \left( \sum_{k,j,l} \partial_l^\varphi T_{ij}^\varphi(\mathbf{x}^\varphi) (\mathbf{F}(\mathbf{x}))_{lk} (\mathbf{F}^{-1}(\mathbf{x}))_{kj} \right)_i = J(\mathbf{x}) \operatorname{div}^\varphi \mathbf{T}^\varphi(\mathbf{x}^\varphi). \end{aligned}$$

**(1.4) Definition**

The symmetric tensor field

$$\mathbf{C}(x) := \mathbf{F}(x)^T \mathbf{F}(x)$$

is the (right) Cauchy–Green strain tensor.

**Remark** The strain tensor defines a metric  $g: T\Omega \times T\Omega \longrightarrow \mathbb{R}$  such that

$$(\Omega, g) \xrightarrow{\varphi} (\Omega^\varphi, \text{Euclidian metric})$$

is a diffeomorphism of Riemannian manifolds.

For a curve  $\mathbf{c}: [a, b] \longrightarrow \Omega$  the length of  $\mathbf{c}^\varphi := \varphi \circ \mathbf{c}: [a, b] \longrightarrow \Omega^\varphi$  can be computed by

$$L(\mathbf{c}^\varphi) = \int_a^b \sqrt{\dot{\mathbf{c}}(t)^T \mathbf{C}(\mathbf{c}(t)) \dot{\mathbf{c}}(t)} dt ,$$

i. e., we have  $g(\dot{\mathbf{c}}(t), \dot{\mathbf{c}}(t)) = \dot{\mathbf{c}}(t)^T \mathbf{C}(\mathbf{c}(t)) \dot{\mathbf{c}}(t)$  by identifying  $\dot{\mathbf{c}}(t) \in \mathbb{R}^3$  with  $\dot{\mathbf{c}}(t) \in T_{\mathbf{c}(t)}\Omega$ .

One can identify tensor fields with

$$\mathbf{F}: T\Omega \longrightarrow T\Omega^\varphi \quad \mathbf{T}^\varphi \in T^*\Omega^\varphi \times T^*\Omega^\varphi$$

$$\mathbf{C}: T\Omega \longrightarrow T\Omega \quad \mathbf{T} \in T^*\Omega^\varphi \times T^*\Omega$$

In terms of differential geometry, the Piola transform is the pull back  $\varphi^*$ . The pull back of the Cauchy stress with respect to one component gives the 1. Piola–Kirchhoff stress. The pull back with respect to both components will be introduced later as 2. Piola–Kirchhoff stress  $\Sigma \in T^*\Omega \times T^*\Omega$ .

**(1.5) Theorem**

We have  $\mathbf{C} \equiv \mathbf{I}$  in  $\Omega$  if and only if  $\varphi(\mathbf{x}) = \mathbf{a} + \mathbf{Q}\mathbf{x}$ ,  $\mathbf{Q} \in \text{SO}(3) = \{\mathbf{R} \in \mathbb{R}^{3,3}: \mathbf{R}^T \mathbf{R} = \mathbf{I}, \det(\mathbf{R}) = 1\}$  is a rigid body motion.

## 2 Balance equations

### Cauchy stress

#### (2.1) Cauchy Axiom

For given volume force densities

$$\mathbf{f}^\varphi: \Omega^\varphi \longrightarrow \mathbb{R}^3$$

and traction force densities

$$\mathbf{g}^\varphi: \Gamma_1^\varphi \subset \partial\Omega^\varphi \longrightarrow \mathbb{R}^3$$

a vector field

$$\mathbf{t}^\varphi: \bar{\Omega} \times S^2 \longrightarrow \mathbb{R}^3$$

exists with

- a)  $\mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{n}^\varphi) = \mathbf{g}^\varphi(\mathbf{x}^\varphi)$
- b)  $\int_{V^\varphi} \mathbf{f}^\varphi(\mathbf{x}^\varphi) d\mathbf{x}^\varphi + \int_{\partial V^\varphi} \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{n}^\varphi) d\mathbf{a}^\varphi = 0$
- c)  $\int_{V^\varphi} \mathbf{x}^\varphi \wedge \mathbf{f}^\varphi(\mathbf{x}^\varphi) d\mathbf{x}^\varphi + \int_{\partial V^\varphi} \mathbf{x}^\varphi \wedge \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{n}^\varphi) d\mathbf{a}^\varphi = 0$

for all  $V^\varphi \subset \Omega^\varphi$ .

#### (2.2) Theorem

Then, a tensor field  $\mathbf{T}^\varphi: \Omega^\varphi \longrightarrow \mathbb{R}^{3,3}$  (Cauchy stress tensor) exists such that

$$\mathbf{T}^\varphi(\mathbf{x}^\varphi)\mathbf{n}^\varphi = \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{n}^\varphi)$$

and

- 1)  $\mathbf{T}^\varphi \cdot \mathbf{n}^\varphi = \mathbf{g}^\varphi$  on  $\Gamma_1^\varphi$
- 2)  $-\operatorname{div}^\varphi \mathbf{T}^\varphi = \mathbf{f}^\varphi$  in  $\Omega^\varphi$
- 3)  $(\mathbf{T}^\varphi)^T = \mathbf{T}^\varphi$  in  $\Omega^\varphi$

For the *proof* we consider at some inner point  $\mathbf{x}_0^\varphi \in \Omega^\varphi$  and for  $\mathbf{n}^\varphi \in S^2$  with  $n_i^\varphi > 0$  a small tetrahedron  $\tau$  of diameter  $h > 0$  and faces  $F_i$  with normals  $-\mathbf{e}_i$  (where  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$  is the Euclidian basis in  $\mathbb{R}^3$ ) and face  $F$  with normal  $\mathbf{n}^\varphi$ . Then, we have  $\operatorname{area}(F_i) = n_i^\varphi \operatorname{area}(F)$ . Property b) gives

$$\int_{\partial\tau} \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{n}^\varphi) d\mathbf{a}^\varphi = - \int_\tau \mathbf{f}^\varphi(\mathbf{x}^\varphi) d\mathbf{x}^\varphi$$

i. e.,

$$\frac{1}{|F|} \left( \sum_{i=1}^3 \int_{F_i} \mathbf{t}^\varphi(\mathbf{x}^\varphi, -\mathbf{e}^i) d\mathbf{a}^\varphi + \int_F \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{n}^\varphi) d\mathbf{a}^\varphi \right) = \frac{1}{|F|} \int_\tau \mathbf{f}^\varphi(\mathbf{x}^\varphi) d\mathbf{x}^\varphi$$

Passing to the limit  $h \rightarrow 0$  yields

$$n_i^\varphi t^\varphi(\mathbf{x}_0^\varphi, -\mathbf{e}^i) + t^\varphi(\mathbf{x}_0^\varphi, \mathbf{n}^\varphi) = 0$$

since  $\frac{|\tau|}{|F|} \rightarrow 0$  for  $h \rightarrow 0$ . Thus we obtain

$$\mathbf{t}^\varphi(\mathbf{x}_0^\varphi, \mathbf{n}^\varphi) = - \sum_{i=1}^3 \mathbf{t}^\varphi(\mathbf{x}_0^\varphi, -\mathbf{e}^i) n_i^\varphi$$

and repeating this argument with reflections shows

$$\mathbf{t}^\varphi(\mathbf{x}_0^\varphi, \mathbf{n}^\varphi) = \sum_{i=1}^3 \mathbf{t}^\varphi(\mathbf{x}_0^\varphi, \mathbf{e}^i) n_i^\varphi$$

for all  $\mathbf{n}^\varphi \in S^2$ . Thus,

$$\mathbf{T}^\varphi(\mathbf{x}^\varphi) := \left( \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{e}^1), \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{e}^2), \mathbf{t}^\varphi(\mathbf{x}^\varphi, \mathbf{e}^3) \right)$$

is well defined. This gives 1). The force balance b) gives 2) using the Gauss theorem

$$\int_\tau \mathbf{f}^\varphi d\mathbf{x}^\varphi = - \int_{\partial\tau} \mathbf{T}^\varphi \cdot \mathbf{n}^\varphi d\mathbf{a}^\varphi = - \int_\tau \operatorname{div}^\varphi \mathbf{T}^\varphi d\mathbf{x}^\varphi$$

and by passing to the limit  $h \rightarrow 0$ .

Symmetry follows from the momentum balance c).

## The principle of virtual work

### (2.3) Theorem

Let Piola transform of the Cauchy stress tensor  $\mathbf{T}^\varphi$  defines the first Piola–Kirchhoff stress tensor  $\mathbf{T}(\mathbf{x}) := J(\mathbf{x})\mathbf{T}^\varphi(\mathbf{x}^\varphi)\mathbf{F}^{-T}(\mathbf{x}) : \Omega \rightarrow \mathbb{R}^{3,3}$ .

We set  $\mathbf{f}(\mathbf{x}) = J(\mathbf{x})\mathbf{f}^\varphi(\mathbf{x}^\varphi)$  and  $\mathbf{g}(\mathbf{x}) = J(\mathbf{x})|\mathbf{F}^{-T}\mathbf{n}| \mathbf{g}^\varphi(\mathbf{x}^\varphi)$ . Then,

$$\int_\Omega \mathbf{T} : D\boldsymbol{\theta} d\mathbf{x} = \int_\Omega \mathbf{f} \cdot \boldsymbol{\theta} d\mathbf{x} + \int_{\Gamma_1} \mathbf{g} \cdot \boldsymbol{\theta} d\mathbf{a}$$

holds for all sufficiently smooth vector fields  $\boldsymbol{\theta} : \bar{\Omega} \rightarrow \mathbb{R}^3$  with  $\boldsymbol{\theta}(\mathbf{x}) = \mathbf{0}$  for all  $\mathbf{x} \in \Gamma_0 := \partial\Omega \setminus \Gamma_1$ .



Here and in the following we use the inner product  $\mathbf{A} : \mathbf{B} = \sum_{i,j=1}^3 A_{ij}B_{ij}$  in  $\mathbb{R}^{3,3}$  and the corresponding Frobenius norm  $|\mathbf{A}| = \sqrt{\mathbf{A} : \mathbf{A}}$ .

For the *proof* apply the Gauss theorem to the (transposed) vector field  $\boldsymbol{\theta}\mathbf{T}$ :

$$\int_{\Omega} \operatorname{div}(\boldsymbol{\theta}\mathbf{T}) \, d\mathbf{x} = \int_{\partial\Omega} (\boldsymbol{\theta}\mathbf{T}) \cdot \mathbf{n} \, da$$

and the chain rule  $\operatorname{div}(\boldsymbol{\theta}\mathbf{T}) = D\boldsymbol{\theta} : \mathbf{T} + \boldsymbol{\theta} \cdot \operatorname{div} \mathbf{T}$ . This gives

$$\int_{\Omega} D\boldsymbol{\theta} : \mathbf{T} \, d\mathbf{x} = - \int_{\Omega} \boldsymbol{\theta} \cdot \operatorname{div} \mathbf{T} \, d\mathbf{x} + \int_{\Gamma_1} (\mathbf{T} \cdot \mathbf{n}) \cdot \boldsymbol{\theta} \, da$$

Now, the assertion follows from

$$- \operatorname{div} \mathbf{T} = -J \operatorname{div}^{\varphi} \mathbf{T}^{\varphi} = J\mathbf{f}^{\varphi} = \mathbf{f}$$

and

$$\mathbf{T} \cdot \mathbf{n} = J\mathbf{T}^{\varphi}\mathbf{F}^{-T} \cdot \mathbf{n} = J\mathbf{T}^{\varphi} \cdot (\mathbf{F}^{-T}\mathbf{n}) = J\mathbf{T}^{\varphi} \cdot \mathbf{n}^{\varphi} |\mathbf{F}^{-T}\mathbf{n}| = J\mathbf{g}^{\varphi} |\mathbf{F}^{-T}\mathbf{n}| = \mathbf{g} .$$

## Conservative Forces

### (2.4) Definition

*Loads  $\mathbf{f}$  and tractions  $\mathbf{g}$  are conservative, if potentials*

$$F(\varphi) = \int_{\Omega} \hat{F}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \, d\mathbf{x}, \quad G(\varphi) = \int_{\Gamma_1} \hat{G}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \, da$$

*exists, such that for the Gâteaux derivative holds:*

$$\begin{aligned} DF(\varphi)[\boldsymbol{\theta}] &= \lim_{h \rightarrow 0} \frac{1}{h} (\mathbf{F}(\varphi + h\boldsymbol{\theta}) - \mathbf{F}(\varphi)) = \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\theta} \, d\mathbf{x} \\ DG(\varphi)[\boldsymbol{\theta}] &= \int_{\Gamma_1} \mathbf{g} \cdot \boldsymbol{\theta} \, da \end{aligned}$$

**Examples**  $\hat{F}(\mathbf{x}, \boldsymbol{\eta}, \mathbf{F}) = -g\eta_3$  defines a gravitational load (with a given pressure constant  $g > 0$  for the acceleration of gravity). Here, the load  $\mathbf{f}$  is not depending on the current configuration; in this case the force is called a *dead load*.

$\hat{G}(\mathbf{x}, \boldsymbol{\eta}, \mathbf{F}) = -\pi(\det \mathbf{F})(\mathbf{F}^{-T}\mathbf{n}(\mathbf{x})) \cdot \boldsymbol{\eta}$  describes a pressure load (with pressure  $\pi > 0$ ). From the Piola identity we can deduce  $\mathbf{T} \cdot \mathbf{n} = -\pi J\mathbf{F}^{-T}\mathbf{n}$ , which corresponds to a constant pressure load  $\mathbf{T}^{\varphi} \cdot \mathbf{n}^{\varphi} = -\pi\mathbf{n}^{\varphi}$  in the deformed configuration. Since the evaluation depends on the current deformation, the pressure load is not a dead load.

### 3 Constitutive relations

#### Elastic materials

We set  $\text{Sym}(3) = \{\mathbf{S} \in \mathbb{R}^{3,3} : \mathbf{S}^T = \mathbf{S}\}$  and  $\mathbb{M}_+^3 = \{\mathbf{F} \in \mathbb{R}^{3,3} : \det \mathbf{F} > 0\}$ .

#### (3.1) Definition

A material is elastic if a response function

$$\hat{\mathbf{T}}^D : \bar{\Omega} \times \mathbb{M}_+^3 \longrightarrow \text{Sym}(3)$$

exists such that

$$\mathbf{T}^\varphi(\mathbf{x}^\varphi) = \hat{\mathbf{T}}^D(\mathbf{x}, D\varphi(\mathbf{x})).$$

We require that the response function is objective/frame-indifferent: for any rigid body transformation of the reference system we obtain the same response, i. e.,

$$\hat{\mathbf{T}}^D(\mathbf{x}, \mathbf{Q}\mathbf{F}) = \mathbf{Q}\hat{\mathbf{T}}^D(\mathbf{x}, \mathbf{F})\mathbf{Q}^T, \quad \mathbf{Q} \in \text{SO}(3)$$

An elastic material is

a) homogeneous, if  $\hat{\mathbf{T}}^D(\mathbf{x}, \mathbf{F}) = \hat{\mathbf{T}}^D(\mathbf{F})$

b) isotropic, if  $\hat{\mathbf{T}}^D(\mathbf{x}, \mathbf{F}\mathbf{Q}) = \hat{\mathbf{T}}^D(\mathbf{x}, \mathbf{F})$ .

In the following we consider only homogeneous materials.

#### (3.2) Definition

We define the 2. Piola–Kirchhoff stress by  $\boldsymbol{\Sigma} = \mathbf{F}^{-1}\mathbf{T}$ .

	Cauchy stress	1. Piola–Kirchhoff stress	2. Piola–Kirchhoff stress
Tensor	$\mathbf{T}^\varphi$	$\mathbf{T} = J\mathbf{T}^\varphi\mathbf{F}^{-T}$	$\boldsymbol{\Sigma} = \mathbf{F}^{-1}\mathbf{T}$
objectivity	$\hat{\mathbf{T}}^D(\mathbf{Q}\mathbf{F}) = \mathbf{Q}\hat{\mathbf{T}}^D(\mathbf{F})\mathbf{Q}^T$	$\hat{\mathbf{T}}(\mathbf{Q}\mathbf{F}) = \mathbf{Q}\hat{\mathbf{T}}(\mathbf{F})$	$\hat{\boldsymbol{\Sigma}}(\mathbf{Q}\mathbf{F}) = \hat{\boldsymbol{\Sigma}}(\mathbf{F})$
isotropy	$\hat{\mathbf{T}}^D(\mathbf{F}\mathbf{Q}) = \hat{\mathbf{T}}^D(\mathbf{F})$	$\hat{\mathbf{T}}(\mathbf{F}\mathbf{Q}) = \hat{\mathbf{T}}(\mathbf{F})\mathbf{Q}$	$\hat{\boldsymbol{\Sigma}}(\mathbf{F}\mathbf{Q}) = \mathbf{Q}^T\hat{\boldsymbol{\Sigma}}(\mathbf{F})\mathbf{Q}$

#### (3.3) Lemma

Since we require that the stress response is objective,  $\hat{\boldsymbol{\Sigma}}(\mathbf{F}) = \tilde{\boldsymbol{\Sigma}}(\mathbf{C})$  is well-defined.

For the *proof* consider the strain tensor  $\mathbf{C} = \mathbf{F}^T\mathbf{F}$  and set  $\mathbf{U} = \sqrt{\mathbf{C}}$ ,  $\mathbf{R} = \mathbf{F}\mathbf{U}^{-1}$ . Then, we have  $\mathbf{R}^T\mathbf{R} = \mathbf{U}^{-1}\mathbf{F}^T\mathbf{F}\mathbf{U}^{-1} = \mathbf{I}$ , i. e.,  $\mathbf{R} \in \text{SO}(3)$ . This defines the *polar decomposition*  $\mathbf{F} = \mathbf{R}\mathbf{U}$ . Thus, we can define

$$\tilde{\boldsymbol{\Sigma}}(\mathbf{C}) := \det(\mathbf{U})\mathbf{U}^{-1}\hat{\mathbf{T}}^D(\mathbf{U})\mathbf{U}^{-1} = \hat{\boldsymbol{\Sigma}}(\mathbf{U}) = \hat{\boldsymbol{\Sigma}}(\mathbf{R}^T\mathbf{F}) = \hat{\boldsymbol{\Sigma}}(\mathbf{F})$$

since the square root is unique for symmetric positive definite matrices.

**(3.4) Theorem**

The stress response is isotropic if and only if

$$\tilde{\Sigma}(\mathbf{C}) = \gamma_0(\iota_{\mathbf{C}})\mathbf{I} + \gamma_1(\iota_{\mathbf{C}})\mathbf{C} + \gamma_2(\iota_{\mathbf{C}})\mathbf{C}^2$$

$$\text{with } \gamma_j : \mathbb{R}^3 \longrightarrow \mathbb{R} \text{ depending on the invariants } \iota_{\mathbf{C}} = \begin{pmatrix} \iota_1(\mathbf{C}) \\ \iota_2(\mathbf{C}) \\ \iota_3(\mathbf{C}) \end{pmatrix} = \begin{pmatrix} \text{tr } \mathbf{C} \\ \frac{1}{2}((\text{tr } \mathbf{C})^2 - \text{tr } \mathbf{C}^2) \\ \det \mathbf{C} \end{pmatrix}.$$

For the *proof* we observe that

$$\tilde{\Sigma}(\mathbf{Q}^T \mathbf{C} \mathbf{Q}) = \hat{\Sigma}(\mathbf{F} \mathbf{Q}) = \mathbf{Q}^T \hat{\Sigma}(\mathbf{F}) \mathbf{Q} = \mathbf{Q}^T \tilde{\Sigma}(\mathbf{C}) \mathbf{Q}.$$

Now we fix  $\mathbf{Q} = (\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3) \in \text{SO}(3)$  with  $\mathbf{Q}^T \mathbf{C} \mathbf{Q} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$ , i. e.,  $\mathbf{C} \mathbf{q}_i = \lambda_i \mathbf{q}_i$  and  $\mathbf{C} = \sum \lambda_i \mathbf{q}_i \mathbf{q}_i^T$ .

We set  $\mathbf{Q}_1 = \text{diag}(1, -1, -1)$ ,  $\mathbf{Q}_2 = \text{diag}(-1, 1, -1)$ . We have the following characterization:  $\mathbf{S}$  diagonal if and only if  $\mathbf{Q}_j^T \mathbf{S} \mathbf{Q}_j = \mathbf{S}$  for  $j = 1, 2$ . Since

$$\mathbf{Q}_j^T (\mathbf{Q}^T \tilde{\Sigma}(\mathbf{C}) \mathbf{Q}) \mathbf{Q}_j = \tilde{\Sigma}((\mathbf{Q} \mathbf{Q}_j)^T \mathbf{C} (\mathbf{Q} \mathbf{Q}_j)) = \tilde{\Sigma}(\mathbf{Q}^T \mathbf{C} \mathbf{Q}) = \mathbf{Q}^T \tilde{\Sigma}(\mathbf{C}) \mathbf{Q},$$

$\mathbf{Q}^T \tilde{\Sigma}(\mathbf{C}) \mathbf{Q}$  is diagonal, i. e.,

$$\mathbf{Q}^T \tilde{\Sigma}(\mathbf{C}) \mathbf{Q} = \alpha_1(\mathbf{C}) \mathbf{e}_1 \mathbf{e}_1^T + \alpha_2(\mathbf{C}) \mathbf{e}_2 \mathbf{e}_2^T + \alpha_3(\mathbf{C}) \mathbf{e}_3 \mathbf{e}_3^T.$$

Transformation back gives

$$\tilde{\Sigma}(\mathbf{C}) = \alpha_1(\mathbf{C}) \mathbf{q}_1 \mathbf{q}_1^T + \alpha_2(\mathbf{C}) \mathbf{q}_2 \mathbf{q}_2^T + \alpha_3(\mathbf{C}) \mathbf{q}_3 \mathbf{q}_3^T,$$

and recombination of the terms gives

$$\tilde{\Sigma}(\mathbf{C}) = \beta_1(\mathbf{C}) \mathbf{I} + \beta_2(\mathbf{C}) \mathbf{C} + \beta_3(\mathbf{C}) \mathbf{C}^2,$$

(in the case of three different  $\lambda_i$  this follows from  $\text{span}\{\mathbf{q}_1 \mathbf{q}_1^T, \mathbf{q}_2 \mathbf{q}_2^T, \mathbf{q}_3 \mathbf{q}_3^T\} = \text{span}\{\mathbf{I}, \mathbf{C}, \mathbf{C}^2\}$ ).

Now, consider  $\mathbf{D}$  with  $\iota_{\mathbf{D}} = \iota_{\mathbf{C}}$ , i. e.,  $\mathbf{D}$  and  $\mathbf{C}$  have the same eigenvalues. Thus,  $\mathbf{R} \in \text{SO}(3)$  exists with  $\mathbf{R}^T \mathbf{D} \mathbf{R} = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$ , which gives  $\mathbf{Q} \mathbf{R}^T \mathbf{D} \mathbf{R} \mathbf{Q}^T = \mathbf{C}$  and

$$\begin{aligned} \sum \beta_j(\mathbf{C}) \mathbf{C}^j &= \tilde{\Sigma}(\mathbf{C}) = \tilde{\Sigma}(\mathbf{Q} \mathbf{R}^T \mathbf{D} \mathbf{R} \mathbf{Q}^T) = \mathbf{Q} \mathbf{R}^T \tilde{\Sigma}(\mathbf{D}) \mathbf{R} \mathbf{Q}^T \\ &= \mathbf{Q} \mathbf{R}^T \sum \beta_j(\mathbf{D}) \mathbf{R} \mathbf{Q}^T = \sum \beta_j(\mathbf{D}) \mathbf{D}^j. \end{aligned}$$

Thus,  $\gamma_j(\iota_{\mathbf{C}}) = \beta_j(\mathbf{C})$  is well defined.

### (3.5) Definition

We define the Green–St. Venant strain tensor by  $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$ .

The Green–St. Venant strain tensor measures the deviation of the natural state, where  $\varphi \equiv \text{id}$ ,  $\mathbf{F} = \mathbf{C} = \mathbf{I}$  and therefore,  $\mathbf{E} = 0$ .

### (3.6) Theorem

We have near the natural state  $\tilde{\Sigma}(\mathbf{C}) = -\pi\mathbf{I} + \lambda \text{tr}(\mathbf{E})\mathbf{I} + 2\mu\mathbf{E} + o(\mathbf{E})$ .

Here, we use the Landau symbol  $f(\mathbf{E}) = o(\mathbf{E}) \iff \lim_{\mathbf{E} \rightarrow 0} \frac{|f(\mathbf{E})|}{|\mathbf{E}|} = 0$ .

For the *proof* observe the identities

$$\begin{aligned} \mathbf{C} &= \mathbf{I} + 2\mathbf{E} \\ \mathbf{C}^2 &= \mathbf{I} + 4\mathbf{E} + o(\mathbf{E}) \\ \iota_1(\mathbf{C}) &= \text{tr } \mathbf{C} = 3 + 2 \text{tr } \mathbf{E} \\ \iota_2(\mathbf{C}) &= \frac{1}{2}((\text{tr } \mathbf{C})^2 - \text{tr } \mathbf{C}^2) = 3 + 4 \text{tr } \mathbf{E} + o(\mathbf{E}) \\ \iota_3(\mathbf{C}) &= \frac{1}{6}((\text{tr } \mathbf{C})^3 - 3 \text{tr } \mathbf{C} \text{tr } \mathbf{C}^2 + 2 \text{tr } \mathbf{C}^3) = 1 + 2 \text{tr } \mathbf{E} + o(\mathbf{E}) \\ \gamma_j(\iota_{\mathbf{C}}) &= \gamma_j(\iota_{\mathbf{I}}) + \dot{\gamma}_j(\iota_{\mathbf{I}}) \text{tr}(\mathbf{E}) + o(\mathbf{E}) \text{ with } \dot{\gamma}_j(\iota_{\mathbf{I}}) = 2 \frac{\partial \gamma_j}{\partial \iota_1}(\iota_{\mathbf{I}}) + 4 \frac{\partial \gamma_j}{\partial \iota_2}(\iota_{\mathbf{I}}) + 2 \frac{\partial \gamma_j}{\partial \iota_3}(\iota_{\mathbf{I}}). \end{aligned}$$

This gives  $-\pi = \sum \gamma_j(\iota_{\mathbf{I}})$ ,  $\lambda = \sum \dot{\gamma}_j(\iota_{\mathbf{I}})$  and  $\mu = \gamma_1(\iota_{\mathbf{I}}) + 2\gamma_2(\iota_{\mathbf{I}})$ .

Linearizing the Green–St. Venant strain tensor

$$\mathbf{E} = \text{sym}(D\varphi) + o(D\varphi)$$

gives Hooke's law in linear elasticity:

$$\boldsymbol{\sigma} = -\pi\mathbf{I} + \lambda \text{tr}(D\varphi)\mathbf{I} + 2\mu \text{sym}(D\varphi) = \boldsymbol{\Sigma} + o(D\varphi).$$

## Hyperelastic materials

### (3.7) Definition

An elastic material is hyperelastic if a stored energy function  $\hat{W}: \hat{\Omega} \times \mathbb{M}_+^3 \rightarrow \mathbb{R}$  exists, such that the stress response is of the form  $\hat{\mathbf{T}}(\mathbf{x}, \mathbf{F}) = D_{\mathbf{F}}\hat{W}(\mathbf{x}, \mathbf{F})$ , where the matrix  $D_{\mathbf{F}}\hat{W}(\mathbf{x}, \mathbf{F}) \in \mathbb{R}^{3,3}$  is defined by

$$\begin{aligned} (D_{\mathbf{F}}\hat{W}(\mathbf{x}, \mathbf{F})) : \mathbf{H} &= D_{\mathbf{F}}\hat{W}(\mathbf{x}, \mathbf{F})[\mathbf{H}] \\ &= \lim_{|\mathbf{H}| \rightarrow 0} \frac{1}{|\mathbf{H}|} (\hat{W}(\mathbf{x}, \mathbf{F} + \mathbf{H}) - \hat{W}(\mathbf{x}, \mathbf{F})) \text{ for all } \mathbf{H} \in \mathbb{R}^{3,3}. \end{aligned}$$

We may assume  $\hat{W}(\mathbf{x}, \mathbf{I}) = 0$ .

$\hat{W}$  is homogeneous, if  $\hat{W}(\mathbf{x}, \mathbf{F}) = \hat{W}(\mathbf{F})$  independent of  $\mathbf{x}$ .

**(3.8) Lemma**

*A hyperelastic material is frame-indifferent/objective*

$$\iff \hat{W}(\mathbf{Q}\mathbf{F}) = \hat{W}(\mathbf{F}) \quad \mathbf{Q} \in \text{SO}(3)$$

$$\iff \hat{W}(\mathbf{F}) = \tilde{W}(\mathbf{C}) = \check{W}(\mathbf{E}) \quad \text{is well-defined, where } \mathbf{F}^T\mathbf{F} = \mathbf{C} = \mathbf{I} + 2\mathbf{E}.$$

Then, we have for the 2. Piola–Kirchhoff stress

$$\hat{\Sigma}(\mathbf{F}) = \tilde{\Sigma}(\mathbf{C}) = 2D_{\mathbf{C}}\tilde{W}(\mathbf{C}) = D_{\mathbf{E}}\check{W}(\mathbf{E})$$

where  $D_{\mathbf{C}}\tilde{W}(\mathbf{C}) \in \text{Sym}(3)$  is defined by

$$D_{\mathbf{C}}\tilde{W}(\mathbf{C}) : \mathbf{H} = \lim_{\mathbf{H} \rightarrow 0} \frac{1}{|\mathbf{H}|} (\tilde{W}(\mathbf{C} + \mathbf{H}) - \tilde{W}(\mathbf{C})) \quad \text{for } \mathbf{H} \in \text{Sym}(3).$$

The *proof* of the first part is non-trivial. For the second part, observe that  $\mathbf{A} : (\mathbf{B}\mathbf{C}) = \text{tr}(\mathbf{A}^T\mathbf{B}\mathbf{C}) = \mathbf{B}^T\mathbf{A} : \mathbf{C} = \text{tr}(\mathbf{C}\mathbf{A}^T\mathbf{B}) = \mathbf{C}\mathbf{A}^T : \mathbf{B}^T = \mathbf{A}^T\mathbf{C} : \mathbf{B}$ , which gives

$$\begin{aligned} \hat{W}(\mathbf{F} + \mathbf{H}) - \hat{W}(\mathbf{F}) &= \tilde{W}((\mathbf{F} + \mathbf{H})^T(\mathbf{F} + \mathbf{H})) - \tilde{W}(\mathbf{F}^T\mathbf{F}) \\ &= \tilde{W}(\mathbf{C}) + D_{\mathbf{C}}\tilde{W}(\mathbf{C}) [(\mathbf{F} + \mathbf{H})^T(\mathbf{F} + \mathbf{H}) - \mathbf{C}] + o(\mathbf{H}) - \tilde{W}(\mathbf{C}) \\ &= D_{\mathbf{C}}\tilde{W}(\mathbf{C}) : (\mathbf{F}^T\mathbf{H} + \mathbf{H}^T\mathbf{F}) + o(\mathbf{H}) \end{aligned}$$

and therefore

$$\begin{aligned} D_{\mathbf{F}}\hat{W}(\mathbf{F}) : \mathbf{H} &= D_{\mathbf{C}}\tilde{W}(\mathbf{C}) : (\mathbf{F}^T\mathbf{H} + \mathbf{H}^T\mathbf{F}) \\ &= \mathbf{F}(D_{\mathbf{C}}\tilde{W}(\mathbf{C}) + D_{\mathbf{C}}\tilde{W}(\mathbf{C})^T) : \mathbf{H} = 2\mathbf{F}D_{\mathbf{C}}\tilde{W}(\mathbf{C}) : \mathbf{H}. \end{aligned}$$

**(3.9) Theorem**

*A hyperelastic material is isotropic, if and only if  $\hat{W}(\mathbf{F}) = \hat{W}(\mathbf{F}\mathbf{Q})$  for  $\mathbf{Q} \in \text{SO}(3)$ .*

*Then, we have near to the natural state  $\check{W}(\mathbf{E}) = \frac{\lambda}{2}(\text{tr } \mathbf{E})^2 + \mu \text{tr } \mathbf{E}^2 + o(|\mathbf{E}|^2)$ .*

For the *proof* consider

$$\Delta(\mathbf{E}) = \check{W}(\mathbf{E}) - \frac{\lambda}{2}(\text{tr } \mathbf{E})^2 - \mu \text{tr } \mathbf{E}^2 = \check{W}(\mathbf{E}) - \frac{\lambda}{2}(\mathbf{E} : \mathbf{I})^2 - \mu \mathbf{E} : \mathbf{E},$$

which gives

$$D_{\mathbf{E}}\Delta(\mathbf{E}) : \mathbf{H} = D_{\mathbf{E}}\check{W}(\mathbf{E}) : \mathbf{H} - \lambda \text{tr}(\mathbf{E})\mathbf{I} : \mathbf{H} - 2\mu \mathbf{E} : \mathbf{H},$$

i. e.,  $D_{\mathbf{E}}\Delta(\mathbf{E}) = \check{\Sigma}(\mathbf{E}) - \lambda(\text{tr } \mathbf{E})\mathbf{I} - 2\mu \mathbf{E} = o(\mathbf{E})$  and therefore

$$\Delta(\mathbf{E}) = \Delta(\mathbf{0}) + \int_0^1 \left( \frac{d}{dt} \Delta(t\mathbf{E}) \right) dt = 0 + \int_0^1 D_{\mathbf{E}}\Delta(t\mathbf{E}) : \mathbf{E} dt = o(|\mathbf{E}|^2).$$

**Examples** The quadratic approximation  $\hat{W}(\mathbf{F}) = \frac{\lambda}{2}(\text{tr } \mathbf{E})^2 + \mu \text{tr } \mathbf{E}^2$  is the *St. Venant-Kirchhoff* energy, which is a realistic approximation for small strains. But for large strains, we expect

$$\hat{W}(\mathbf{F}) \rightarrow \infty \text{ for } J \rightarrow 0 \text{ or } J \rightarrow \infty \text{ or } |\mathbf{F}| \rightarrow \infty.$$

This is satisfied, e. g., by energies of Neo-Hooke type  $\hat{W}(\mathbf{F}) = \frac{\mu}{2} \mathbf{F} : \mathbf{F} + \Gamma(J)$ . Then, the theorem gives

$$\Gamma(1) = -\frac{3\mu}{2}, \quad \Gamma'(1) = -\mu, \quad \Gamma''(1) = \lambda + \mu.$$

E.g., this holds for  $\Gamma(J) = \frac{\lambda}{4}J^2 - (\frac{\lambda}{2} + \mu) \log J - \frac{\lambda}{4} - \frac{3}{2}\mu$ .

**(3.10) Theorem**

Let  $W(\varphi) = \int_{\Omega} \hat{W}(\mathbf{x}, D\varphi(\mathbf{x})) \, d\mathbf{x}$  be the strain energy, and assume that a volume load

potential is given by  $F(\varphi) = \int_{\Omega} \hat{F}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \, d\mathbf{x}$  and a surface traction potential is

given by  $G(\varphi) = \int_{\Gamma_1} \hat{G}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \, da$ .

Set  $\mathbf{V}(\varphi_0) = \{\varphi : \bar{\Omega} \rightarrow \mathbb{R}^3 : \varphi(\mathbf{x}) = \varphi_0(\mathbf{x}) \text{ on } \Gamma_0\}$ .

Then, any minimizer  $\varphi \in \mathbf{V}(\varphi_0)$  of the total energy

$$I(\varphi) = W(\varphi) - F(\varphi) - G(\varphi)$$

is a critical point of the energy functional  $I$  satisfying  $D_{\varphi}I(\varphi)[\boldsymbol{\theta}] = 0$ , i. e., it satisfies the variational equation

$$\int_{\Omega} \mathbf{T}(D\varphi(\mathbf{x})) : D\boldsymbol{\theta}(\mathbf{x}) \, d\mathbf{x} = \int_{\Omega} \hat{\mathbf{f}}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \cdot \boldsymbol{\theta}(\mathbf{x}) \, d\mathbf{x} + \int_{\Gamma_1} \hat{\mathbf{g}}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \cdot \boldsymbol{\theta}(\mathbf{x}) \, da$$

for all  $\boldsymbol{\theta} \in \mathbf{V}(\mathbf{0})$ , where

$$\begin{aligned} D_{\varphi}W(\varphi)[\boldsymbol{\theta}] &= \int_{\Omega} D_{\mathbf{F}}\hat{W}(D\varphi(\mathbf{x})) : D\boldsymbol{\theta}(\mathbf{x}) \, d\mathbf{x} \\ D_{\varphi}F(\varphi)[\boldsymbol{\theta}] &= \int_{\Omega} \hat{\mathbf{f}}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \cdot \boldsymbol{\theta}(\mathbf{x}) \, d\mathbf{x} \\ D_{\varphi}G(\varphi)[\boldsymbol{\theta}] &= \int_{\Gamma_1} \hat{\mathbf{g}}(\mathbf{x}, \varphi(\mathbf{x}), D\varphi(\mathbf{x})) \cdot \boldsymbol{\theta}(\mathbf{x}) \, d\mathbf{x}. \end{aligned}$$

## 4 Newton's method for energy minimization problems in finite elasticity

*Objective:* Find a (local) minimum  $\varphi \in \mathbf{V}(\varphi_0)$  of the total energy  $I$ .

*Algorithm:*

- 1) Choose start iterate  $\varphi^0$  with  $\varphi^0(\mathbf{x}) = \varphi_0(\mathbf{x})$  for  $\mathbf{x} \in \Gamma_0$ . For  $k = 0, 1, 2, \dots$
- 2) Compute the residual  $D_\varphi I(\varphi^k)$ ; if  $\|D_\varphi I(\varphi^k)\|$  is small enough, STOP.
- 3) Compute the second variation  $D^2 I_\varphi(\varphi^k)$  and solve

$$\mathbf{v} \in \mathbf{V}(\mathbf{0}): D_\varphi^2 I(\varphi^k)[\mathbf{v}, \boldsymbol{\theta}] = -D_\varphi I(\varphi^k)[\boldsymbol{\theta}] \text{ for all } \boldsymbol{\theta} \in \mathbf{V}(\mathbf{0}) .$$

- 4) Choose  $s \in (0, 1]$  such that

$$I(\varphi^k + s\mathbf{v}) < I(\varphi^k) \quad \text{and / or} \quad \|D_\varphi I(\varphi^k + s\mathbf{v})\| < \|D_\varphi I(\varphi^k)\| .$$

STOP, if this fails.

- 5) Set  $\varphi^{k+1} = \varphi^k + s\mathbf{v}$ ,  $k := k + 1$ , and go to 2).

### (4.1) Theorem

*If for the start iterate  $\varphi^0 \in \mathbf{V}(\varphi_0)$  the second variation is positive definite and the residual is small enough, Newton's method is well-defined and  $\varphi^k$  converges to a local minimum.*

*Remark:* In computations, one uses in general the displacement field

$$\mathbf{u}: \bar{\Omega} \rightarrow \mathbb{R}^3 \quad \text{with} \quad \varphi(\mathbf{x}) = \mathbf{x} + \mathbf{u}(\mathbf{x})$$

instead of the deformation.

**(4.2) Lemma**

a)  $D_{\boldsymbol{\varphi}}^2 W(\boldsymbol{\varphi})[\mathbf{v}, \mathbf{w}] = \int_{\Omega} D_{\mathbf{F}}^2 \hat{W}(D\boldsymbol{\varphi})[D\mathbf{v}, D\mathbf{w}] dx$  is a symmetric bilinear form.

b) For  $\hat{W}(\mathbf{F}) = \tilde{W}(\mathbf{C}) = \check{W}(\mathbf{E})$  we have

$$\begin{aligned} D_{\mathbf{F}}^2 \hat{W}(\mathbf{F})[\mathbf{G}, \mathbf{H}] &= D_{\mathbf{C}} \tilde{W}(\mathbf{C})[\mathbf{G}^T \mathbf{H} + \mathbf{H}^T \mathbf{G}] + D_{\mathbf{C}}^2 \tilde{W}(\mathbf{C})[\mathbf{G}^T \mathbf{F} + \mathbf{F}^T \mathbf{G}, \mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}] \\ &= 2D_{\mathbf{C}} \tilde{W}(\mathbf{C})[\text{sym}(\mathbf{G}^T \mathbf{H})] + 4D_{\mathbf{C}}^2 \tilde{W}(\mathbf{C})[\text{sym}(\mathbf{F}^T \mathbf{G}), \text{sym}(\mathbf{F}^T \mathbf{H})] \\ &= D_{\mathbf{E}} \check{W}(\mathbf{E})[\text{sym}(\mathbf{G}^T \mathbf{H})] + D_{\mathbf{E}}^2 \check{W}(\mathbf{E})[\text{sym}(\mathbf{F}^T \mathbf{G}), \text{sym}(\mathbf{F}^T \mathbf{H})] . \end{aligned}$$

*Examples*

A) For the St. Venant-Kirchhoff energy  $\hat{W}(\mathbf{F}) = \frac{\lambda}{2}(\text{tr } \mathbf{E})^2 + \mu \text{tr } \mathbf{E}^2$  we have

$$D_{\mathbf{F}} \hat{W}(\mathbf{F})[\mathbf{H}] = \mathbf{F} \hat{\boldsymbol{\Sigma}}(\mathbf{F}) : \mathbf{H} = (\lambda(\text{tr } \mathbf{E})\mathbf{F} + 2\mu\mathbf{F}\mathbf{E}) : \mathbf{H}$$

and

$$\begin{aligned} D_{\mathbf{F}}^2 \hat{W}(\mathbf{F})[\mathbf{G}, \mathbf{H}] &= \frac{1}{2}(\lambda(\text{tr } \mathbf{E})\mathbf{I} + 2\mu\mathbf{E}) : (\mathbf{G}^T \mathbf{H} + \mathbf{H}^T \mathbf{G}) \\ &\quad + \frac{1}{4}\lambda \text{tr}(\mathbf{G}^T \mathbf{F} + \mathbf{F}^T \mathbf{G}) \text{tr}(\mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}) \\ &\quad + \frac{1}{2}\mu(\mathbf{G}^T \mathbf{F} + \mathbf{F}^T \mathbf{G}) : (\mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}) \\ &= \lambda((\text{tr } \mathbf{E})\mathbf{G} : \mathbf{H} + \text{tr}(\mathbf{F}^T \mathbf{G}) \text{tr}(\mathbf{F}^T \mathbf{H})) \\ &\quad + 2\mu(\mathbf{E} : \text{sym}(\mathbf{G}^T \mathbf{H}) + \text{sym}(\mathbf{F}^T \mathbf{G}) : \text{sym}(\mathbf{F}^T \mathbf{H})) , \end{aligned}$$

since

$$\begin{aligned} D_{\mathbf{E}} \check{W}(\mathbf{E}) &= \lambda(\text{tr } \mathbf{E})\mathbf{I} + 2\mu\mathbf{E} , \\ D_{\mathbf{E}}^2 \check{W}(\mathbf{E})[\mathbf{G}, \mathbf{H}] &= \lambda \text{tr } \mathbf{G} \text{tr } \mathbf{H} + 2\mu\mathbf{G} : \mathbf{H} . \end{aligned}$$

B) For energy of Neo-Hooke type  $\hat{W}(\mathbf{F}) = \frac{\mu}{2}\mathbf{F} : \mathbf{F} + \Gamma(J)$  we have

$$D_{\mathbf{F}} \hat{W}(\mathbf{F})[\mathbf{H}] = \mu\mathbf{F} : \mathbf{H} + \Gamma'(J)J\mathbf{F}^{-T} : \mathbf{H}$$

using  $D_{\mathbf{F}} J[\mathbf{H}] = J\mathbf{F}^{-T} : \mathbf{H}$ , and

$$\begin{aligned} D_{\mathbf{F}}^2 \hat{W}(\mathbf{F})[\mathbf{G}, \mathbf{H}] &= \mu\mathbf{G} : \mathbf{H} \\ &\quad + (\Gamma'(J)J)' J(\mathbf{F}^{-T} : \mathbf{G})(\mathbf{F}^{-T} : \mathbf{H}) \\ &\quad - \Gamma'(J)J \text{tr}(\mathbf{F}^{-1} \mathbf{G} \mathbf{F}^{-1} \mathbf{H}) . \end{aligned}$$



C) For Hencky type energies  $\hat{W}(\mathbf{F}) = \bar{W}(\mathbf{C}) = \frac{\mu}{4} |\text{dev}(\ln \mathbf{C})|^2 + \frac{\kappa}{8} (\text{tr}(\ln \mathbf{C}))^2$  we have

$$\begin{aligned} \mathbf{T} = D_{\mathbf{F}}\hat{W}(\mathbf{F}) &= 2\mathbf{F}D_{\mathbf{C}}\bar{W}(\mathbf{C}) = 2\mathbf{F}D_{\mathbf{C}}\left(\frac{\mu}{4} |\text{dev}(\ln \mathbf{C})|^2 + \frac{\kappa}{8} (\text{tr}(\ln \mathbf{C}))^2\right) \\ &\text{using the Sansours formula and replacing } \mathbf{X} = \ln \mathbf{C} : \\ &= \frac{\mu\mathbf{F}}{2} D_{\mathbf{X}}(\text{tr}(\text{dev}(\mathbf{X}))^2)\mathbf{C}^{-1} + \frac{\kappa\mathbf{F}}{4} 2 \text{tr}(\ln \mathbf{C}) D_{\mathbf{X}}(\text{tr}(\mathbf{X}))\mathbf{C}^{-1} \\ &= \mu\mathbf{F} \text{dev}(\ln \mathbf{C})\mathbf{F}^{-1}\mathbf{F}^{-T} + \frac{\kappa}{2} \text{tr}(\ln \mathbf{C})\mathbf{F}^{-T} \\ \text{Sansours formula for } \bar{W}(\mathbf{C}) \in \mathbb{R} \text{ and } \mathbf{C} = \mathbf{C}^T \in \mathbb{R}^{3,3} \\ D_{\mathbf{C}}(\bar{W}(\mathbf{C})) &= D_{(\ln \mathbf{C})}(\tilde{W}(\ln \mathbf{C}))\mathbf{C}^{-1} \end{aligned}$$

D) For Ogden materials with

$$\begin{aligned} \hat{W}(\mathbf{F}) &= \sum_{i=1}^3 \frac{\mu_i}{\alpha_i} \sum_j \lambda_j^{\alpha_i} + \mu_4 \alpha_4^{-2} J^{-\alpha_4} + \left( \mu_4 \alpha_4^{-1} - \sum_{i=1}^3 \mu_i \right) \log J + \mu_5 J^{2/3} (J-1) \sum_j \lambda_j^{-2} \\ &= \sum_{i=1}^3 \frac{\mu_i}{\alpha_i} \text{tr}(\mathbf{C}^{\alpha_i}) + \mu_4 \alpha_4^{-2} J^{-\alpha_4} + \left( \mu_4 \alpha_4^{-1} - \sum_{i=1}^3 \mu_i \right) \log J + \mu_5 J^{2/3} (J-1) \text{tr}(\mathbf{C}^{-2}) \end{aligned}$$

we have

$$\begin{aligned} \mathbf{T} = D_{\mathbf{F}}\hat{W}(\mathbf{F}) &= 2\mathbf{F} \sum_{i=1}^3 \mu_i \mathbf{C}^{\alpha_i-1} \\ &+ \left( \frac{\mu_4}{\alpha_4} (1 - J^{-\alpha_4}) - \sum_{i=1}^3 \mu_i + \mu_5 \left( \frac{5}{3} J^{5/3} - \frac{2}{3} J^{2/3} \right) \text{tr}(\mathbf{C}^{-2}) \right) \mathbf{F}^{-T} \\ &- 4\mu_5 J^{2/3} (J-1) \mathbf{F}\mathbf{C}^{-3} \end{aligned}$$

E) For materials with an energy as introduced by Ciarlet and Geymonat, where

$$\begin{aligned} \hat{W}(\mathbf{F}) &= c_1(\iota_1 - 3) + c_2(\iota_2 - 3) + a(\iota_3 - 1) - (c_1 + 2c_2 + a) \log \iota_3 \\ &= c_1(\text{tr} \mathbf{C} - 3) + c_2 \left( \frac{1}{2} [(\text{tr} \mathbf{C})^2 - \text{tr} \mathbf{C}^2] - 3 \right) + a(\det \mathbf{C} - 1) - (c_1 + 2c_2 + a) \log(\det \mathbf{C}) \end{aligned}$$

subject to the restrictions:

$$\begin{aligned} \lambda &= 4c_2 + 4a \\ \mu &= 2c_1 + 2c_2 \end{aligned}$$

we have

$$\mathbf{T} = D_{\mathbf{F}}\hat{W}(\mathbf{F}) = 2(c_1 \mathbf{F} + c_2 (\text{tr}(\mathbf{C})\mathbf{F} - \mathbf{F}\mathbf{C})) + a \det(\mathbf{C})\mathbf{F}^{-T} - (c_1 + 2c_2 + a) \mathbf{F}^{-T}$$

and

$$D_{\mathbf{F}}\hat{W}(\mathbf{F})[\mathbf{H}] = c_1 \operatorname{tr}(\mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}) + c_2 (\operatorname{tr}(\mathbf{C}) \operatorname{tr}(\mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}) - \operatorname{tr}(\mathbf{C}(\mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}))) \\ + 2a \operatorname{tr}(\mathbf{H}\mathbf{F}^{-1}) \det \mathbf{C} - 2(c_1 + 2c_2 + a) \operatorname{tr}(\mathbf{H}\mathbf{F}^{-1})$$

as well as

$$D_{\mathbf{F}}^2 \hat{W}(\mathbf{F})[\mathbf{G}, \mathbf{H}] = c_1 \operatorname{tr}(\mathbf{H}^T \mathbf{G} + \mathbf{G}^T \mathbf{H}) + c_2 (2 \operatorname{tr}(\mathbf{F}^T \mathbf{G}) \operatorname{tr}(\mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}) + \operatorname{tr} \mathbf{C} \operatorname{tr}(\mathbf{H}^T \mathbf{G} + \mathbf{G}^T \mathbf{H}) \\ - \operatorname{tr}((\mathbf{G}^T \mathbf{F} + \mathbf{F}^T \mathbf{G})(\mathbf{H}^T \mathbf{F} + \mathbf{F}^T \mathbf{H}) + \mathbf{C}(\mathbf{H}^T \mathbf{G} + \mathbf{G}^T \mathbf{H})) \\ + 2a \det \mathbf{C} (2 \operatorname{tr}(\mathbf{H}\mathbf{F}^{-1}) \operatorname{tr}(\mathbf{G}\mathbf{F}^{-1}) - \operatorname{tr}(\mathbf{H}\mathbf{F}^{-1} \mathbf{G}\mathbf{F}^{-1})) \\ + 2(c_1 + 2c_2 + a) \operatorname{tr}(\mathbf{H}\mathbf{F}^{-1} \mathbf{G}\mathbf{F}^{-1})$$

## 5 Homotopy and regularization

For given data, in general there is no unique solution of the energy minimization problem. Therefore, consider a (artificial time or homotopy) parameter  $t \in [a, b]$  and data

$$\begin{aligned}\varphi_0 & : [a, b] \times \Gamma_0 \rightarrow \mathbb{R}^3 \\ \mathbf{f} & : [a, b] \times \Omega \rightarrow \mathbb{R}^3 \\ \mathbf{g} & : [a, b] \times \Gamma_1 \rightarrow \mathbb{R}^3\end{aligned}$$

such that  $\varphi_0(a) \equiv 0$ ,  $\mathbf{f}(a) \equiv 0$ ,  $\mathbf{g}(a) \equiv 0$  corresponds to the natural state  $\varphi = \text{id}$ .

Choose a step size parameter  $\tau_0 > 0$ , and for  $k = 0, 1, 2, 3, \dots$

- 1) set  $t = \min\{t_k + \tau_k, b\}$
- 2) apply Newton's method with the data at  $t$  (starting, e. g., with  $\varphi^k$  at  $t_k$ )
- 3) in case of no convergence within a few Newton steps, diminish  $\tau_k$  and go to 1)
- 4) otherwise, set  $\varphi^{k+1}$  to the Newton solution and set  $t_{k+1} = t$ ,  $\tau_{k+1} = \tau_k$
- 5) in case of very fast convergence, increase  $\tau_{k+1}$
- 6)  $k := k + 1$  and go to 1)

In general, along this homotopy the equations can degenerate:  $D_{\varphi}^2 I(\varphi(t))$  gets singular at bifurcation points!

A standard remedy is to add (artificial) inertia effects. For given (artificial) density  $\rho: \bar{\Omega} \rightarrow \mathbb{R}^3$  the momentum equations reads

$$\rho \ddot{\varphi} - \text{div } \mathbf{T} = f$$

(where  $\ddot{\varphi} = \frac{d^2}{dt^2} \varphi$ ). An implicit time-stepping reads as follows:

- 0) Start with deformation  $\varphi^0 \in \mathbf{V}(\varphi_0(a))$ , velocity  $\mathbf{v}^0 = \mathbf{0}$  and  $t_0 = a$ . Set  $n = 1$ .
- 1) Choose  $\tau_n > 0$  and set  $t = \min\{t_{n-1} + \tau_n, b\}$  and  $k = 0$ .  
Choose start iterate  $\varphi^{n,0} \in \mathbf{V}(\varphi_0(t + \tau_n))$  for the acceleration.
- 2) For  $\mathbf{v}^{n,k} = \frac{1}{\tau_n}(\varphi^{n,k} - \varphi^{n-1})$  and  $\mathbf{a}^{n,k} = \frac{1}{\tau_n}(\mathbf{v}^{n,k} - \mathbf{v}^{n-1})$  compute the residual

$$R^{n,k}[\boldsymbol{\theta}] = \int_{\Omega} \rho \mathbf{a}^{n,k} \cdot \boldsymbol{\theta} \, dx + D_{\varphi} I(\varphi^{n,k})[\boldsymbol{\theta}] ;$$

if  $\|R^{n,k}\|$  is small enough, go to 4).

- 3) Compute the second variation  $D_{\varphi}^2 I(\varphi^{n,k})$  and solve

$$\mathbf{w} \in \mathbf{V}(\mathbf{0}) : \quad \frac{1}{\tau_n^2} \int_{\Omega} \rho \mathbf{w} \cdot \boldsymbol{\theta} \, dx + D_{\varphi}^2 I(\varphi^{n,k})[\mathbf{w}, \boldsymbol{\theta}] = -R^{n,k}(\varphi^{n,k})[\boldsymbol{\theta}] \text{ for all } \boldsymbol{\theta} \in \mathbf{V}(\mathbf{0}) .$$

and set  $\varphi^{n,k+1} = \varphi^{n,k} + \mathbf{w}$ ,  $k := k + 1$  and go to 2).

- 4) Set  $\mathbf{v}^n = \mathbf{v}^{n,k}$ ,  $\varphi^n = \varphi^{n,k}$ ,  $t_n = t$ ,  $n := n + 1$  and go to 1).

This (first order method in time) can be modified to a second order method, e. g., by replacing the full implicit acceleration  $\mathbf{a}^{n,k}$  with the midpoint rule  $\frac{1}{2\tau_n}(\mathbf{v}^{n,k} - \mathbf{v}^{n-1})$ .

Caution: dynamic instabilities may occur. Then, e. g., use stabilized Newmark schemes.

## 6 Lagrange multipliers for constraint problems

As an example we consider the incompressibility constraint  $J \equiv 1$ . This corresponds to an energy minimizing problem in the constraint space  $\mathbf{W}(\varphi_0) = \{\boldsymbol{\psi} \in V(\varphi_0) : \det D\boldsymbol{\psi} = 1\}$ :

find  $\boldsymbol{\varphi} \in \mathbf{W}(\varphi_0)$  with  $I(\boldsymbol{\varphi}) \leq I(\boldsymbol{\psi})$  for all  $\boldsymbol{\psi} \in \mathbf{W}(\varphi_0)$ .

Introducing a Lagrange parameter  $p: \bar{\Omega} \rightarrow \mathbb{R}$  (hydrostatic pressure), the (local) minima correspond to critical points of the Lagrange functional

$$L(\boldsymbol{\varphi}, p) = I(\boldsymbol{\varphi}) + \int_{\Omega} p (\det D\boldsymbol{\varphi} - 1) d\mathbf{x}$$

characterized by the saddle point problem: find  $\boldsymbol{\varphi} \in V(\varphi_0)$  and  $p$  with

$$\begin{aligned} 0 &= D_{\boldsymbol{\varphi}}L(\boldsymbol{\varphi}, p)[\boldsymbol{\theta}] = \int_{\Omega} \mathbf{T}(\mathbf{F}) : D\boldsymbol{\theta} + p\mathbf{F}^{-T} : D\boldsymbol{\theta} d\mathbf{x} - \int_{\Omega} \mathbf{f} \cdot \boldsymbol{\theta} d\mathbf{x} - \int_{\Gamma_1} \mathbf{g} \cdot \boldsymbol{\theta} da \\ 0 &= D_pL(\boldsymbol{\varphi}, p)[q] = \int_{\Omega} (\det D\boldsymbol{\varphi} - 1) q d\mathbf{x} \end{aligned}$$

for all  $\boldsymbol{\theta} \in \mathbf{V}(\mathbf{0})$  and all  $q$ . Note that a finite element discretization requires an inf-sup condition for the displacement and pressure spaces.

The corresponding equations in the reference configuration  $\Omega$  are

$$-\operatorname{div}(\mathbf{T} + p\mathbf{F}^{-T}) = \mathbf{f} \quad (\mathbf{T} + p\mathbf{F}^{-T})\mathbf{n} = \mathbf{g}$$

and in the current configuration  $\Omega^{\varphi}$

$$-\operatorname{div}^{\varphi}(\mathbf{T}^{\varphi} + p) = \mathbf{f}^{\varphi} \quad (\mathbf{T}^{\varphi} + p)\mathbf{n}^{\varphi} = \mathbf{g}^{\varphi}.$$

We indicate shortly how this extends to inequality constraints. Therefore, we consider a model for an elastic foam where the pores are filled with air. Obviously, the composed material is compressible. If all air is pressed out of the pores, we assume that the remaining material cannot be compressed further. This is formalized by the following problem: find  $\boldsymbol{\varphi} \in \mathbf{V}(\varphi_0)$  with minimal energy subject to the constraint  $\det D\boldsymbol{\varphi} \geq J_0$  for a given constant  $J_0 \in (0, 1)$  describing the porosity of the material. Again, local minima are characterized by critical points of the Lagrange functional

$$L(\boldsymbol{\varphi}, p) = I(\boldsymbol{\varphi}) + \int_{\Omega} p (\det D\boldsymbol{\varphi} - J_0) d\mathbf{x} ,$$

complemented by complementary conditions (Kuhn-Tucker)

$$(\det D\boldsymbol{\varphi} - J_0)p = 0, \quad p \leq 0, \quad \det D\boldsymbol{\varphi} \geq J_0 .$$

# Synopsis of Notations

	Ciarlet	Simo/Hughes
reference configuration	$\bar{\Omega}$	$\mathcal{B}$
current configuration	$\bar{\Omega}^\varphi$	$\mathcal{S}$
Lagrangian/material variable	$x$	$\mathbf{X}$
Eulerian/spatial variable	$x^\varphi$	$\mathbf{x}$
deformation	$\varphi$	$\varphi$
deformation gradient	$\mathbf{F} = \nabla \varphi$	$\mathbf{F} = D\varphi$
deformation gradient determinant	$J = \det(\mathbf{F})$	$J = \det(\mathbf{F})$
right Cauchy-Green strain tensor	$\mathbf{C} = \mathbf{F}^T \mathbf{F}$	$\mathbf{C} = \mathbf{F}^T \mathbf{F}$
left Cauchy-Green strain tensor	$\mathbf{B} = \mathbf{F} \mathbf{F}^T$	$\mathbf{b} = \mathbf{F} \mathbf{F}^T$
Lagrangian strain	$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$	$\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$
invariants	$\iota_1, \iota_2, \iota_3$	$I_1, I_2, I_3$
divergence operator (ref. conf)	div	DIV
divergence operator (cur. conf.)	$\operatorname{div}^\varphi$	div
stored energy	$\hat{W}$	$\hat{W}$
Cauchy stress tensor	$\mathbf{T}^\varphi$	$\boldsymbol{\sigma}$
1. Piola–Kirchhoff stress tensor	$\mathbf{T}$	$\mathbf{P}$
2. Piola–Kirchhoff stress tensor	$\boldsymbol{\Sigma}$	$\mathbf{S}$