# ME338A
# CONTINUUM MECHANICS

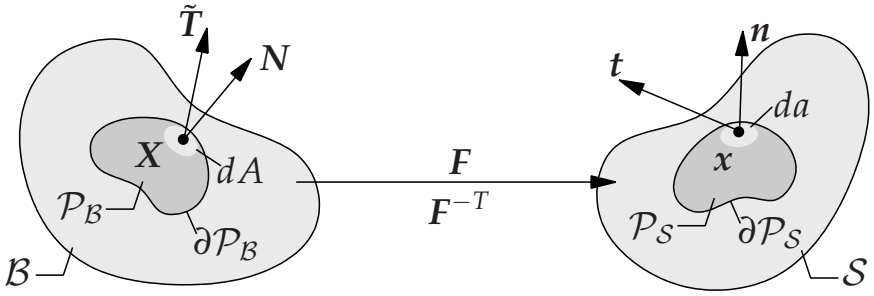
lecture notes 16

thursday, march 4th, 2010

## 5.2 Constitutive Theory

### 5.2.1 Cauchy's Stress Theorem and Fundamental Stress Measures

Consider a part $\mathcal{P}_\mathcal{B} \subset \mathcal{B}$ cut off from the reference body $\mathcal{B}$ and its spatial counterpart $\mathcal{P}_\mathcal{S} \subset \mathcal{S}$ closed by the respective boundaries $\partial\mathcal{P}_\mathcal{B}$ and $\partial\mathcal{P}_\mathcal{S}$.




In the deformed configuration, we introduce the *stress vector* $\boldsymbol{t}$ that acts on the surface element $da$ of $\partial\mathcal{P}_\mathcal{S}$ and represents the force action of the rest of the body at the vicinity $\mathcal{P}_\mathcal{S} \setminus \mathcal{S}$ on $\partial\mathcal{P}_\mathcal{S}$. The *Cauchy stress theorem* states that the spatial traction vector $\boldsymbol{t} \in T_x\mathcal{S}$ linearly depends on the spatial normal $\boldsymbol{n} \in T_x^*\mathcal{S}$ of the surface $\partial\mathcal{P}_\mathcal{S}$, i.e.

$$\boldsymbol{t}(\boldsymbol{x}, t; \boldsymbol{n}) := \boldsymbol{\sigma}(\boldsymbol{x}, t) \cdot \boldsymbol{n} \,, \tag{5.2.1}$$

through the *Cauchy (true) stress tensor* $\boldsymbol{\sigma}$. Cauchy's stress theorem can be proven based on the force equilibrium on a tetrahedron. In the geometrical framework outlined so far, the Cauchy stress tensor can be understood as a contravariant mapping transforming normals $\boldsymbol{n} \in T_x^*\mathcal{S}$ onto tangent vectors $\boldsymbol{t} \in T_x\mathcal{S}$

$$\boldsymbol{\sigma} := \left\{ \begin{array}{rcl} T_x^*\mathcal{S} & \to & T_x\mathcal{S} \,, \\ \boldsymbol{n} & \mapsto & \boldsymbol{t} = \boldsymbol{\sigma} \cdot \boldsymbol{n} \,. \end{array} \right. \tag{5.2.2}$$

Another spatial stress measure, the *Kirchhoff stress tensor*, also known as the *weighted Cauchy stress tensor*, is defined as

$$\boldsymbol{\tau} := J\boldsymbol{\sigma} \tag{5.2.3}$$

and widely used in the spatial description of stress power terms in the reference volume. Owing to the scalar scaling by the Jacobian $J$, the Kirchhoff stresses retain the geometrical transformation characteristics of the Cauchy stress.

Now let us consider another spatial traction vector $\boldsymbol{T} \in T_x\mathcal{S}$ defined through the force equality $\boldsymbol{T}\, dA := \boldsymbol{t}\, da$ by scaling the spatial force term $(\boldsymbol{t}\, da)$ through the reference area element $dA$. Based on this definition, we introduce the *first Piola-Kirchhoff stress tensor* by the reference Cauchy theorem $\boldsymbol{T} := \boldsymbol{P}\cdot\boldsymbol{N}$ leading to $\boldsymbol{P}\cdot\boldsymbol{N}\, dA = \boldsymbol{\sigma}\cdot\boldsymbol{n}\, da$. Using the area map $\boldsymbol{n}da = J\boldsymbol{F}^{-T}\cdot\boldsymbol{N}dA$, we obtain the relation $\boldsymbol{P} = \boldsymbol{\tau}\cdot\boldsymbol{F}^{-T}$ between the first Piola-Kirchhoff stress tensor and the spatial stress measures. Notice that $\boldsymbol{P}$ is a two-point tensor possessing the geometrical mapping properties

$$\boldsymbol{P} := \begin{cases} T^*_X\mathcal{B} \;\rightarrow\; T_x\mathcal{S}\,, \\ \quad \boldsymbol{N} \;\mapsto\; \boldsymbol{T} = \boldsymbol{P}\cdot\boldsymbol{N}\,. \end{cases} \tag{5.2.4}$$

The transformation $(\blacksquare) = J(\bullet)\boldsymbol{F}^{-T}$ devised in obtaining the first Piola-Kirchhoff stress tensor from the Cauchy stress tensor is called the *Piola transformation*. It is widely employed in transforming the objects acting on a *spatial surface* onto their material counterparts. The immediate outcome of the Piola transformation is the *Piola Identity*

$$J\,\mathrm{div}(\bullet) = \mathrm{Div}(\blacksquare) = \mathrm{Div}(J(\bullet)\boldsymbol{F}^{-T}) \tag{5.2.5}$$

that also implies the equality $\mathrm{Div}(J\boldsymbol{F}^{-T}) = \boldsymbol{0}$.

The third fundamental stress measure, the *second Piola-Kirchhoff stress tensor* $\boldsymbol{S}$, is then defined by $\tilde{\boldsymbol{T}} := \boldsymbol{S} \cdot \boldsymbol{N}$ yielding

$$\boldsymbol{S} := \begin{cases} T_X^*\mathcal{B} \;\rightarrow\; T_X\mathcal{B}\,, \\ \quad \boldsymbol{N} \;\mapsto\; \tilde{\boldsymbol{T}} = \boldsymbol{S} \cdot \boldsymbol{N}\,. \end{cases} \tag{5.2.6}$$

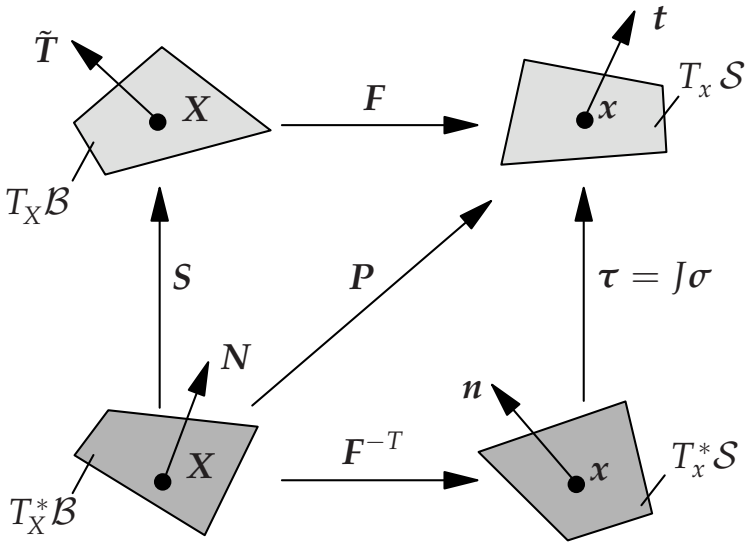
Incorporating the definitions (5.2.2)–(5.2.4) in (5.2.6), we can express the second Piola-Kirchhoff stress tensor in terms of the other stress tensors

$$\boldsymbol{S} := \varphi^*(\boldsymbol{P}) = \boldsymbol{F}^{-1} \cdot \boldsymbol{P} \quad , \quad S_{AB} = (F^{-1})_{Aa} P_{aB}\,,$$

$$\boldsymbol{S} := \varphi^*(\boldsymbol{\tau}) = \boldsymbol{F}^{-1} \cdot \boldsymbol{\tau} \cdot \boldsymbol{F}^{-T} \quad , \quad S_{AB} = (F^{-1})_{Aa} \tau_{ab} (F^{-1})_{Bb}$$

as the pull-back of the contravariant two-point and spatial objects. Apparently the reverse push-forward relations do also hold for the spatial stress tensors

$$\boldsymbol{\tau} = J\boldsymbol{\sigma} = \varphi_*(\boldsymbol{P}) = \boldsymbol{P} \cdot \boldsymbol{F}^T \quad \text{and} \quad \boldsymbol{\tau} = \varphi_*(\boldsymbol{S}) = \boldsymbol{F} \cdot \boldsymbol{S} \cdot \boldsymbol{F}^T\,,$$



### 5.2.2 Closure Problem

The fundamental balance equations are summarized as

| Balance of | Spatial | Material |
|---|---|---|
| Mass | $\dot{\rho_t} + \rho_t \mathrm{div}(\boldsymbol{v}) = 0$ | $\dot{\rho_0} = 0$ |
| Linear M. | $\rho_t \boldsymbol{a} = \mathrm{div}(\sigma) + \rho_t \boldsymbol{b}$ | $\rho_0 \boldsymbol{a} = \mathrm{Div}(\boldsymbol{P}) + \rho_0 \boldsymbol{b}$ |
| Angular M. | $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T, \boldsymbol{\tau} = \boldsymbol{\tau}^T$ | $\boldsymbol{S} = \boldsymbol{S}^T$ |
| | $\boldsymbol{P} \cdot \boldsymbol{F}^T = \boldsymbol{F} \cdot \boldsymbol{P}^T$ | $\boldsymbol{F}^{-1} \cdot \boldsymbol{P} = \boldsymbol{P}^T \cdot \boldsymbol{F}^{-T}$ |
| Energy | $\rho_t \frac{di}{dt} = \sigma : \boldsymbol{d} - \mathrm{div}\, \boldsymbol{q} + R_t$ | $\rho_0 \frac{di}{dt} = \boldsymbol{P} : \dot{\boldsymbol{F}} - \mathrm{Div}\, \boldsymbol{Q} + R_0$ |

where $\rho_0 = J\rho_t, R_0 = JR_t$ and $\boldsymbol{Q} = J\boldsymbol{q} \cdot \boldsymbol{F}^{-T}$.

The number of equations provided by these balance laws and the number of unknowns can be identified as

| Balance of | # | Unknown | # |
|---|---|---|---|
| Mass | 1 | density $\rho_t$ | 1 |
| Linear M. | 3 | Placement $\varphi_t(\boldsymbol{X})$ | 3 |
| Angular M. | 3 | Stresses $\boldsymbol{\sigma}$ | 9 |
| Energy | 1 | Temperature $\theta$ | 1 |
| | | Heat Flux $\boldsymbol{q}$ | 3 |
| $\Sigma$ | 8 | $\Sigma$ | 17 |

where the volume-specific body forces $\boldsymbol{b}$ and the heat source $R_t$ are assumed to be given. Comparison of the number of unknowns with the number of equations indicates that nine additional equations are needed to solve the problem. These additional equations are called the *constitutive equations* which describe the stresses $\hat{\boldsymbol{\sigma}} = \hat{\boldsymbol{\sigma}}^T$ (six equations), and the heat flux $\hat{\boldsymbol{q}}$ (three equations).

In common practice the placement $\varphi_t(\boldsymbol{X})$ and the absolute temperature $\theta$ are considered as the primary unknowns that are solved from the balance of linear momentum and the balance of energy equations.

It is important to notice that the *stress power* $\mathcal{W} := \boldsymbol{P} : \dot{\boldsymbol{F}}$ per unit reference volume appearing in the balance of energy equation can also be expressed in terms of other stress measures by using the push-forward and pull-back relations among the fundamental stress tensors and the rate of deformation tensors.

$$\mathcal{W} := \boldsymbol{P} : \dot{\boldsymbol{F}} = \boldsymbol{\tau} : \boldsymbol{d} = \boldsymbol{S} : \dot{\boldsymbol{E}} \,.$$

The alternative representations of the reference stress power $\mathcal{W}$ manifest the distinct work conjugate couples

$$(\boldsymbol{P}; \dot{\boldsymbol{F}}) \quad , \quad (\boldsymbol{\tau}; \boldsymbol{d}) \quad , \quad (\boldsymbol{S}; \dot{\boldsymbol{E}}) \,.$$

### 5.2.3 Methodology of Coleman and Gurtin

Let us focus on a problem of thermoelasticity for a homogeneous material, for which the local dissipation $\mathcal{D}_{loc}$ vanishes identically. Being consistent with the *principle of locality*, we assume that the free energy $\psi$ depend upon field variables defined in the neighborhood of the material point $\boldsymbol{X}$

$$\psi = \hat{\psi}(\boldsymbol{F}, \theta, \boldsymbol{\mathcal{G}}) \tag{5.2.7}$$

where $\boldsymbol{\mathcal{G}} := \nabla_X \theta$ denotes the material gradient of the temperature field. Based on this assumption, we can substitute the time derivative of the free energy

$$\dot{\psi} = \partial_{\boldsymbol{F}} \psi : \dot{\boldsymbol{F}} + \partial_\theta \psi : \dot{\theta} + \partial_{\boldsymbol{\mathcal{G}}} \psi : \dot{\boldsymbol{\mathcal{G}}}$$

in the Clausius-Planck inequality

$$J\mathcal{D}_{loc} := (\boldsymbol{P} - \partial_{\boldsymbol{F}}\psi) : \dot{\boldsymbol{F}} - (\eta + \partial_\theta\psi)\,\dot{\theta} - \partial_{\boldsymbol{\mathcal{G}}}\psi \cdot \dot{\boldsymbol{\mathcal{G}}} \;=\; 0\,. \quad (5.2.8)$$

Following the celebrated reasoning of Coleman & Noll (1963) and Coleman & Gurtin (1967) within the framework of thermodynamics with internal variables, we contend that the thermodynamic restriction should be fulfilled for an arbitrary rate of the deformation gradient, temperature and temperature gradient. Therefore, (5.2.8) implies a particular form of constitutive equations such that

$$\boldsymbol{P} := \partial_{\boldsymbol{F}}\psi \quad , \quad \eta := -\partial_\theta\psi \quad \text{and} \quad \partial_{\boldsymbol{\mathcal{G}}}\psi = \boldsymbol{0}\,. \qquad (5.2.9)$$

The first two equations of (5.2.9) state that the free energy acts as a potential for the stresses and the entropy while $(5.2.9)_3$ implies that the free energy does not depend on the temperature gradient $\boldsymbol{\mathcal{G}}$, i.e. $\psi = \hat{\psi}(\boldsymbol{F}, \theta)$.

### 5.2.4 Principle of Material Frame Invariance

We consider a rigid body motion $\xi(\boldsymbol{x}, t) : \mathcal{S} \times \mathcal{R}_+ \longrightarrow \mathcal{R}^3$ superimposed onto a non-linear motion $\varphi_t(\boldsymbol{X})$, i.e.

$$\xi(\boldsymbol{x}, t) := \boldsymbol{c}(t) + \boldsymbol{Q}(t) \cdot \boldsymbol{x}$$

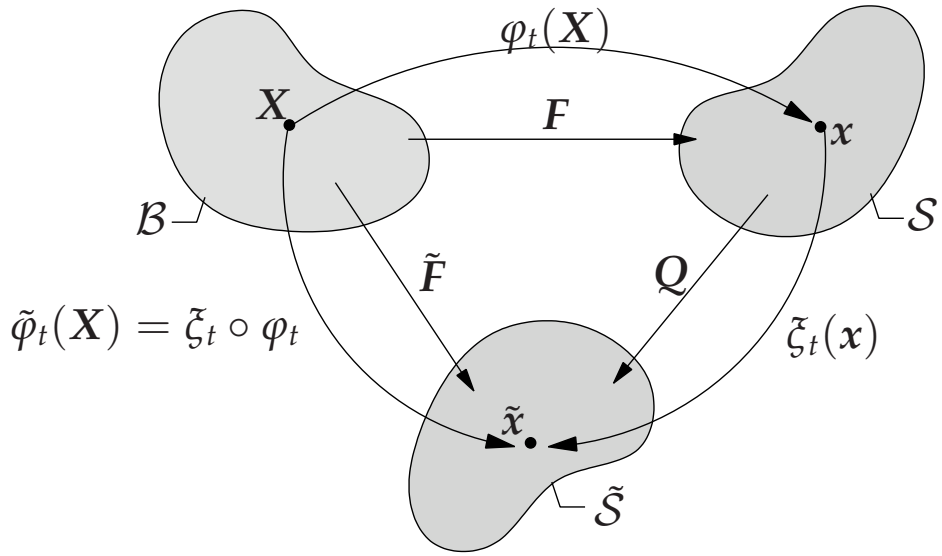
where $\boldsymbol{Q}$ is a proper orthogonal tensor. This definition yields

$$\tilde{\varphi}(\boldsymbol{X}, t) := \xi \circ \varphi = \boldsymbol{c}(t) + \boldsymbol{Q}(t) \cdot \varphi(\boldsymbol{X}, t)\,.$$

Under this superimposed motion, we observe the following transformation relations for:

• **Fundamental Maps:**

$$\tilde{\boldsymbol{F}} := \boldsymbol{Q} \cdot \boldsymbol{F}, \quad \tilde{\boldsymbol{F}}^{-T} = \boldsymbol{Q} \cdot \boldsymbol{F}^{-T}, \quad \tilde{J} = J$$




- **Lagrangian Strain Measures:**

$$\tilde{\boldsymbol{C}} = \tilde{\boldsymbol{F}}^T \cdot \tilde{\boldsymbol{F}} = \boldsymbol{F}^T \cdot \boldsymbol{Q}^T \cdot \boldsymbol{Q} \cdot \boldsymbol{F} = \boldsymbol{C}$$

- **Eulerian Strain Measures:**

$$\tilde{\boldsymbol{b}} = \tilde{\boldsymbol{F}} \cdot \tilde{\boldsymbol{F}}^T = \boldsymbol{Q} \cdot \boldsymbol{F}^T \cdot \boldsymbol{F} \cdot \boldsymbol{Q}^T = \boldsymbol{Q} \cdot \boldsymbol{b} \cdot \boldsymbol{Q}^T$$
$$\tilde{\boldsymbol{c}} = \tilde{\boldsymbol{b}}^{-1} = \boldsymbol{Q} \cdot \boldsymbol{c} \cdot \boldsymbol{Q}^T$$

We call these type of transformation operations *objective transformation of second order tensors*. It is important to note that there also exist spatial tensors that do not fulfill the objective transformation rules, such as the spatial velocity $\boldsymbol{v}$, the spatial velocity gradient $\boldsymbol{l}$, to name a few.

One of the fundamental principles of continuum mechanics is the *principle of material frame invariance* that requires the invariance of the energy stored under rigid body rotations superimposed on the current spatial configuration.
Therefore, we locally demand

$$\psi(\boldsymbol{F}, \theta) = \psi(\tilde{\boldsymbol{F}}, \theta) \tag{5.2.10}$$

Since the right Cauchy-Green tensor $\boldsymbol{C} := \boldsymbol{F}^T \cdot \boldsymbol{F} = \tilde{\boldsymbol{F}}^T \cdot \tilde{\boldsymbol{F}}$ satisfies satisfies this condition, a storage function $\hat{\psi}$ constructed in terms of $\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F}$ is *a priori* objective and the form $\hat{\psi}(\boldsymbol{C}, \theta) = \hat{\psi}(\boldsymbol{F}^T \boldsymbol{F}, \theta)$ represents its reduced form.

$$\hat{\psi}(\boldsymbol{C}, \theta) = \hat{\psi}(\boldsymbol{F}^T \cdot \boldsymbol{F}, \theta) \,. \tag{5.2.11}$$

Based on this restriction, we can rewrite the term

$$(\boldsymbol{P} - \partial_{\boldsymbol{F}} \psi) : \dot{\boldsymbol{F}} \quad \text{as} \quad (\boldsymbol{S} - 2\partial_{\boldsymbol{C}} \hat{\psi}) : \tfrac{1}{2} \dot{\boldsymbol{C}}$$

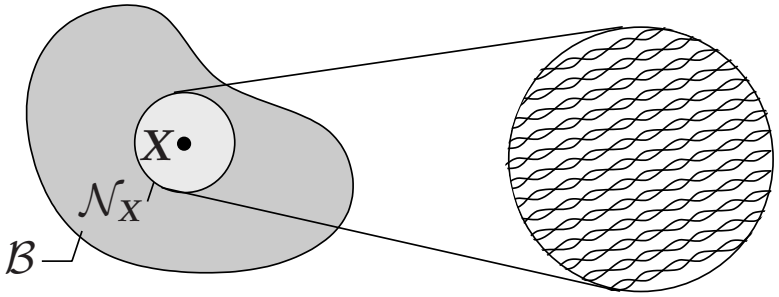
due to the equivalent stress power expressions. This leads us to the functional definition of the second Piola-Kirchhoff stress tensor

$$\boldsymbol{S} = 2\partial_{\boldsymbol{C}} \hat{\psi}(\boldsymbol{C}, \theta) \,. \tag{5.2.12}$$

### 5.2.5 Concept of Material Symmetry

When a material has a particular micro-structure that has to be taken into account in constitutive equations. As we discussed before, in the context continuum modeling of materials, the scale difference between the micro and macro levels is so large that the specific discrete micro-structure can be incorporated in a smeared way. The micro-structure might have an *anisotropic (direction-dependent)* character, which is observed, for example, in crystals, nano-composites, biological tissues to name a few. *Isotropic* material response, however, corresponds to the case where the micro-structure has no direction-dependent pattern.

A particular micro-structure can be classified through *symmetry groups* of rotations, which do not disturb the pattern

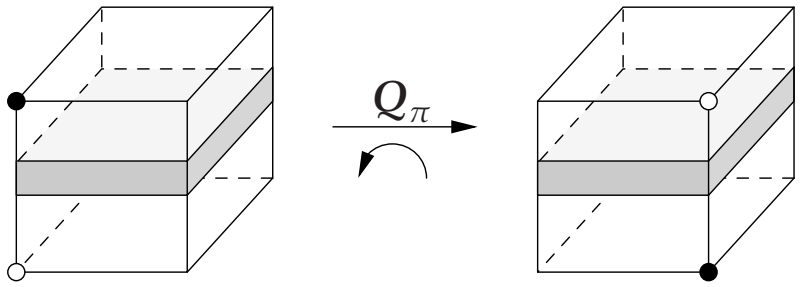



of the micro-structure under consideration. Elementary examples for the symmetry groups are *transverse isotropy* and *orthotropy*. A material symmetry group $G$ is then defined in terms of rotations preserving the material micro-structure

$$G := \{\boldsymbol{Q}_1, \boldsymbol{Q}_2, \ldots\} \subset \mathcal{SO}(3) \tag{5.2.13}$$

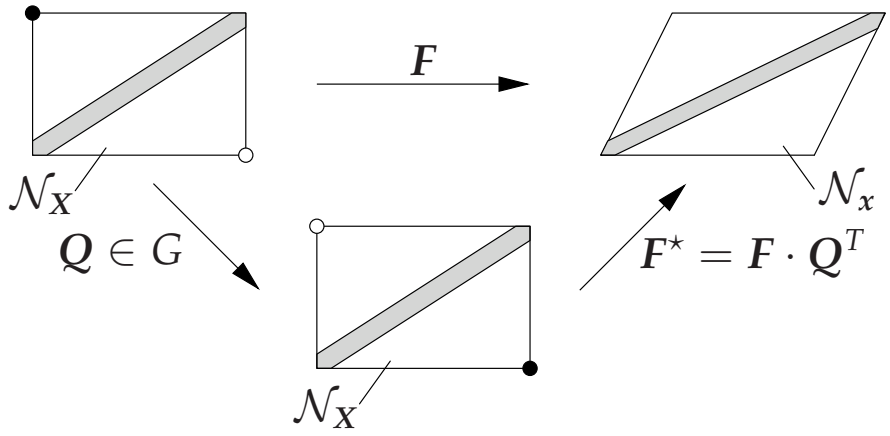
where $\mathcal{SO}(3)$ denotes the *special orthogonal group* defined by

$$\mathcal{SO}(3) := \left\{\boldsymbol{Q} | \boldsymbol{Q} \cdot \boldsymbol{Q}^T = \boldsymbol{1} \wedge \det(\boldsymbol{Q}) = 1\right\} \tag{5.2.14}$$




Since the rotations belonging to the symmetry group $G$ do not alter the material architecture, we require the free energy must also be invariant with respect to these rotations superimposed on the reference neighborhood of the material $\mathcal{N}_X$.

$$\hat{\psi}(\boldsymbol{F} \cdot \boldsymbol{Q}^T) = \hat{\psi}(\boldsymbol{F}) \qquad \forall \boldsymbol{Q} \in G \subset \mathcal{SO}(3)\ . \tag{5.2.15}$$




### 5.2.6 Isotropic Hyperelasticity

Isotropic materials do not possess a distinct micro-structure. Therefore, the energy storage function, free energy, must be invariant with respect to all rotations. The symmetry group of an isotropic material is the full special orthogonal group

$$G_{iso} \equiv \mathcal{SO}(3) \; . \tag{5.2.16}$$

This property leads us to the simple representation of isotropic free energy functions in terms of principal stretches or invariants. To show this, we consider the spectral representation of the deformation gradient $\boldsymbol{F} = \sum_{\alpha=1}^{3} \lambda_\alpha \boldsymbol{n}_\alpha \otimes \boldsymbol{N}_\alpha$ in the free energy function

$$\begin{aligned} \psi(\boldsymbol{F}) &= \hat{\psi}(\textstyle\sum_{\alpha=1}^{3} \lambda_\alpha \boldsymbol{n}_\alpha \otimes \boldsymbol{N}_\alpha) \\ \psi(\boldsymbol{F} \cdot \boldsymbol{Q}^T) &= \hat{\psi}(\textstyle\sum_{\alpha=1}^{3} \lambda_\alpha \boldsymbol{n}_\alpha \otimes \boldsymbol{Q} \cdot \boldsymbol{N}_\alpha) \end{aligned} \tag{5.2.17}$$

and we require the equality

$$\hat{\psi}(\sum_{\alpha=1}^{3} \lambda_\alpha \boldsymbol{n}_\alpha \otimes \boldsymbol{N}_\alpha) = \hat{\psi}(\sum_{\alpha=1}^{3} \lambda_\alpha \boldsymbol{n}_\alpha \otimes \boldsymbol{Q} \cdot \boldsymbol{N}_\alpha) \quad \forall \boldsymbol{Q} \in \mathcal{SO}(3) \; . \tag{5.2.18}$$

with the Lagrangean eigenvectors $\boldsymbol{N}_\alpha$ mapped to an arbitrary vector $\boldsymbol{Q}\cdot\boldsymbol{N}_\alpha$. This implies that the free energy $\hat{\psi}$ cannot depend upon $\boldsymbol{N}_\alpha$. We also recall that the principle of objectivity requires

$$\begin{aligned}\hat{\psi}(\boldsymbol{Q}\cdot\boldsymbol{F}) &= \hat{\psi}(\boldsymbol{F})\,,\\ \hat{\psi}(\textstyle\sum_{\alpha=1}^{3}\lambda_\alpha\boldsymbol{Q}\cdot\boldsymbol{n}_\alpha\otimes\boldsymbol{N}_\alpha) &= \hat{\psi}(\textstyle\sum_{\alpha=1}^{3}\lambda_\alpha\boldsymbol{n}_\alpha\otimes\cdot\boldsymbol{N}_\alpha)\end{aligned} \tag{5.2.19}$$

for all $\boldsymbol{Q}\in\mathcal{SO}(3)$. In addition to the material symmetry condition, the objectivity principle excludes the functional dependency of the free energy is dependent on the Eulerian eigenvectors $\boldsymbol{n}_\alpha$. Combination of the conclusions we drawn from (5.2.18) and (5.2.19) leads us to simple representation of the free energy of isotropic materials

$$\psi=\bar{\psi}(\lambda_1,\lambda_2,\lambda_3) \tag{5.2.20}$$

Since the principal invariants of the right and left Cauchy Green tensors $\boldsymbol{C}$ and $\boldsymbol{b}$ are symmetric functions of the principal stretches, i.e.

$$\begin{aligned}I_1(\boldsymbol{C})=I_1(\boldsymbol{b}) &= \lambda_1^2+\lambda_2^2+\lambda_3^2\,,\\ I_2(\boldsymbol{C})=I_2(\boldsymbol{b}) &= \lambda_1^2\lambda_2^2+\lambda_2^2\lambda_3^2+\lambda_1^2\lambda_3^2\,,\\ I_3(\boldsymbol{C})=I_3(\boldsymbol{b}) &= \lambda_1^2\lambda_2^2\lambda_3^2\,,\end{aligned} \tag{5.2.21}$$

an alternative representation of isotropic elasticity is obtained in terms of the principal invariants

$$\psi=\tilde{\psi}(I_1,I_2,I_3)\,. \tag{5.2.22}$$

At this point, it is worth noting that the left Cauchy Green tensor remains unaltered under arbitrary rotations of the reference neighborhood $\mathcal{N}_X$

$$\boldsymbol{b}^\star=\boldsymbol{F}\cdot\boldsymbol{Q}^T\cdot\boldsymbol{Q}\cdot\boldsymbol{F}^T=\boldsymbol{F}\cdot\boldsymbol{F}^T=\boldsymbol{b}\,.$$

This suggests that a free energy of hyperelasticity depending solely on $\boldsymbol{b}$, i.e. $\hat{\psi}(\boldsymbol{b})$, is restricted to the isotropic elastic material response.

#### 5.2.6.1 Compressible Neo-Hookean Material

A version of compressible Neo-Hookean material model of hyperelasticity is described by the following free energy

$$\psi = \hat{\psi}(I_1, J) = \frac{\Lambda}{4}(J^2 - 1) - (\mu + \frac{\Lambda}{2}) \ln J + \frac{\mu}{2}(I_1 - 3)$$

where $\Lambda$ and $\mu$ are the material parameters, $I_1 := \boldsymbol{C} : \boldsymbol{1}$ and $J^2 = \det(\boldsymbol{C})$. The second Piola-Kirchhoff stress tensor can be computed by using the result $\boldsymbol{S} = 2\partial_{\boldsymbol{C}}\psi$

$$\boldsymbol{S} = 2\frac{\partial \hat{\psi}}{\partial \boldsymbol{C}} = \frac{\partial \hat{\psi}}{\partial I_1} 2\frac{\partial I_1}{\partial \boldsymbol{C}} + \frac{\partial \hat{\psi}}{\partial J} 2\frac{\partial J}{\partial \boldsymbol{C}}$$

Since $\partial_{\boldsymbol{C}} \det(\boldsymbol{C}) = \det(\boldsymbol{C})\boldsymbol{C}^{-1}$ and $\partial_{\boldsymbol{C}} I_1 = \boldsymbol{1}$, the tensorial derivatives can be shown to be

$$2\partial_{\boldsymbol{C}} I_1 = 2\,\boldsymbol{1} \quad \text{and} \quad 2\partial_{\boldsymbol{C}} J = J\boldsymbol{C}^{-1} \,.$$

Derivatives of the free energy function with respect to the deformation measures $I_1$ and $J$ are

$$\partial_{I_1}\hat{\psi} = \frac{\mu}{2} \quad \text{and} \quad \partial_J \hat{\psi} = \frac{\Lambda}{2} J - (\mu + \frac{\Lambda}{2}) J^{-1} \,.$$

Insertion yields the explicit form of $\boldsymbol{S}$

$$\boldsymbol{S} = 2\frac{\partial \hat{\psi}}{\partial \boldsymbol{C}} = \mu(\boldsymbol{1} - \boldsymbol{C}^{-1}) + \frac{\Lambda}{2}\left(J^2 - 1\right)\boldsymbol{C}^{-1} \,.$$

Having this result at hand, the first Piola-Kirchhoff stress tensor

$$\boldsymbol{P} = \boldsymbol{F} \cdot \boldsymbol{S} = \mu(\boldsymbol{F} - \boldsymbol{F}^{-T}) + \frac{\Lambda}{2}\left(J^2 - 1\right)\boldsymbol{F}^{-T}$$

and the Kirchhoff stresses

$$\tau = \boldsymbol{P} \cdot \boldsymbol{F}^T = \boldsymbol{F} \cdot \boldsymbol{S} \cdot \boldsymbol{F}^T = \mu(\boldsymbol{b} - \mathbf{1}) + \frac{\Lambda}{2}\left(J^2 - 1\right)\mathbf{1}$$

are computed through the push-forward operations.

#### 5.2.6.2 Computation of Homogeneous Stress-Stretch Response

Identification of material parameters of a phenomenological material model is commonly carried out by fitting experimental data. These data often consist of stress-stretch curves acquired from homogeneous experiments, such as uniaxial, biaxial, simple shear deformations. *Purely* homogeneous deformations correspond to the cases where the eigenvectors (both spatial and material) do not evolve during the deformation, but remain parallel to the chosen reference rectangular coordinate system. That is, in purely homogeneous deformations, the deformation gradient $\boldsymbol{F}$ has a diagonal representation

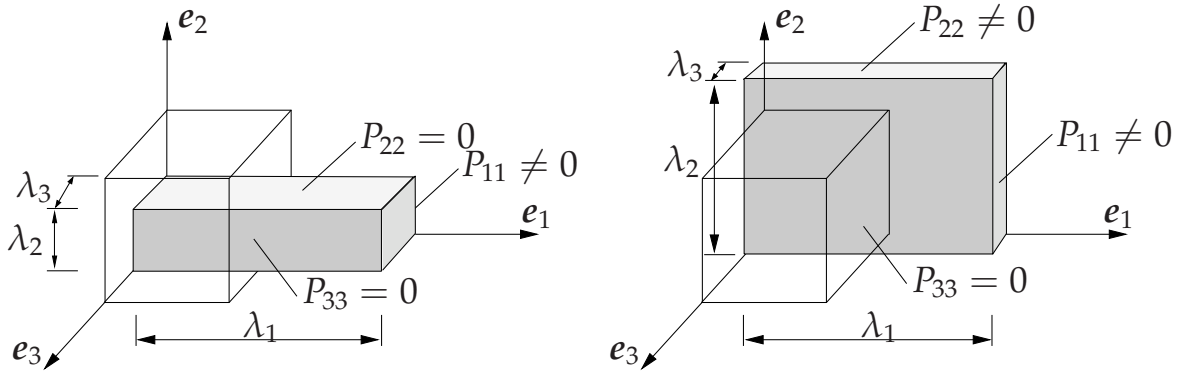
$$\boldsymbol{F} = \mathrm{diag}[F_{11}, F_{22}, F_{33}] = \mathrm{diag}[\lambda_1, \lambda_2, \lambda_3] \tag{5.2.23}$$

in terms of principal stretches with respect to the chosen coordinate system. This form of the deformation gradient results in also diagonal form of the first Piola-Kirchhoff stress for an *isotropic* material

$$\boldsymbol{P} = \hat{\boldsymbol{P}}(\boldsymbol{F}) = \mathrm{diag}[P_{11}(\boldsymbol{F}), P_{22}(\boldsymbol{F}), P_{33}(\boldsymbol{F})]\ . \tag{5.2.24}$$

In different homogeneous deformations, at least one component of the deformation gradient is prescribed and the other components are to be computed from the traction (stress)

boundary conditions associated with the particular experiment considered. The stress component of interest is generally the one in the direction in which we prescribe the deformation. The forthcoming examples illustrate boundary conditions for the uniaxial and biaxial tests.




Component(s) of the stress tensor in the direction(s) where the stretch value is prescribed is/are unknown. On the other hand, stresses in the directions that are free to deform are zero. In a general inhomogeneous boundary value problem, these define the Dirichlet (essential) and Neumann (natural) boundaries whose intersection is an empty set.

Since the first Piola-Kirchhoff stress tensor and the deformation gradient have diagonal representations, we can store them in $3 \times 1$ vector format

$$[\boldsymbol{F}] = \begin{bmatrix} F_{11} \\ F_{22} \\ F_{33} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_u \\ \boldsymbol{F}_k \end{bmatrix} \quad \text{and} \quad [\boldsymbol{P}] = \begin{bmatrix} P_{11} \\ P_{22} \\ P_{33} \end{bmatrix} = \begin{bmatrix} \boldsymbol{P}_k \\ \boldsymbol{P}_u \end{bmatrix} \tag{5.2.25}$$

where the subscripts $k$ and $u$ denote the *known* and *unknown* components, respectively. The known components of the

stress tensor $\boldsymbol{P}_k$ are generally zero, $\boldsymbol{P}_k = \boldsymbol{0}$. Therefore, these equations serve as a residual vector. That is, for a given $\boldsymbol{F}_k$, the following equality

$$\boldsymbol{P}_k = \hat{\boldsymbol{P}}_k(\boldsymbol{F}_u) = \boldsymbol{0} \tag{5.2.26}$$

has to be solved for $\boldsymbol{F}_u$. In general, the residual is a nonlinear function of $\boldsymbol{F}_u$ and therefore should be solved iteratively. To this end, for a given $\boldsymbol{F}_k$ we linearize $\boldsymbol{P}_k$ at some intermediate value of $\boldsymbol{F}_u$ during iteration, say $\bar{\boldsymbol{F}}_u$,

$$\mathrm{Lin}\, \boldsymbol{P}_k|_{\bar{\boldsymbol{F}}_u} = \boldsymbol{P}_k|_{\bar{\boldsymbol{F}}_u} + \boldsymbol{A}_{ku} \cdot (\boldsymbol{F}_u - \bar{\boldsymbol{F}}_u) = \boldsymbol{0} \tag{5.2.27}$$

where $\boldsymbol{A}_{ku} := \partial_{\boldsymbol{F}_u} \boldsymbol{P}_k\big|_{\bar{\boldsymbol{F}}_u}$ stands for the tangent matrix containing appropriate components of the fourth-order elasticity tensor (moduli) $\mathbb{A} := \partial_{\boldsymbol{F}} \boldsymbol{P} = \partial^2_{\boldsymbol{F}\boldsymbol{F}} \psi$. Solution of the linearized residual expression (5.2.27) for $\boldsymbol{F}_u$ leads us to the update equation of $\boldsymbol{F}_u$

$$\boldsymbol{F}_u \longleftarrow \bar{\boldsymbol{F}}_u - \boldsymbol{A}_{ku}^{-1} \cdot \boldsymbol{P}_k|_{\bar{\boldsymbol{F}}_u} \ , \tag{5.2.28}$$

which is performed until the desired accuracy $||\boldsymbol{P}_k|| < \texttt{tol}$ is obtained. The following box summarizes the algorithm

1. For a given $\boldsymbol{F}_k$, set $\boldsymbol{F}_u = \bar{\boldsymbol{F}}_u (= \boldsymbol{1})$
2. Compute the residual $\boldsymbol{P}_k|_{\bar{\boldsymbol{F}}_u}$ and the tangent $\boldsymbol{A}_{ku} := \partial_{\boldsymbol{F}_u} \boldsymbol{P}_k\big|_{\bar{\boldsymbol{F}}_u}$
3. Update $\boldsymbol{F}_u \longleftarrow \bar{\boldsymbol{F}}_u - \boldsymbol{A}_{ku}^{-1} \cdot \boldsymbol{P}_k|_{\bar{\boldsymbol{F}}_u}$
4. Check `IF` $||\boldsymbol{P}_k|| < \texttt{tol}$
5. `NO` set $\bar{\boldsymbol{F}}_u = \boldsymbol{F}_u$ `GOTO 2.`
6. `ELSE` compute $\boldsymbol{P}_u(\boldsymbol{F})$ and
7. Assign new value to $\boldsymbol{F}_k$ and `GOTO 1.`

**Example: Uniaxial Tension at Finite Strains**

We now consider a uniaxial extension of a hyperelastic material in $x_1$ direction. For this purpose, we prescribe $\boldsymbol{F}_k \equiv F_{11}(t)$ as some function of time and want to compute the engineering stress $\boldsymbol{P}_u \equiv P_{11}$ in that direction for a given value of $F_{11}$. The lateral faces of the specimen are stress-free, i.e. $\boldsymbol{P}_k \equiv [P_{22} \;\; P_{33}]^T = \boldsymbol{0}$. Therefore, the stretches in $x_2$ and $x_3$ directions are unkown, $\boldsymbol{F}_u \equiv [F_{22} \;\; F_{33}]^T$.

Recall the compressible neo-Hookean material model we discussed in Section 5.2.6.1

$$P_{aA} = \mu(F_{aA} - F^{-1}_{Aa}) + \frac{\Lambda}{2}\left(J^2 - 1\right) F^{-1}_{Aa} \, .$$

Having the first Piola-Kirchhoff stresses at hand, the associated moduli can be computed as

$$\begin{aligned} \mathbb{A}_{aAbB} := \partial_{F_{bB}} P_{aA} \;\; = \;\; & \mu\delta_{ab}\delta_{AB} + (\mu - \tfrac{\Lambda}{2}(J^2 - 1))F^{-1}_{Ab}F^{-1}_{Ba} \\ & + \Lambda J^2 F^{-1}_{Aa}F^{-1}_{Bb} \, . \end{aligned}$$

The residual vector and the tangent matrix that we need during the Newton iterations can then be shown to be

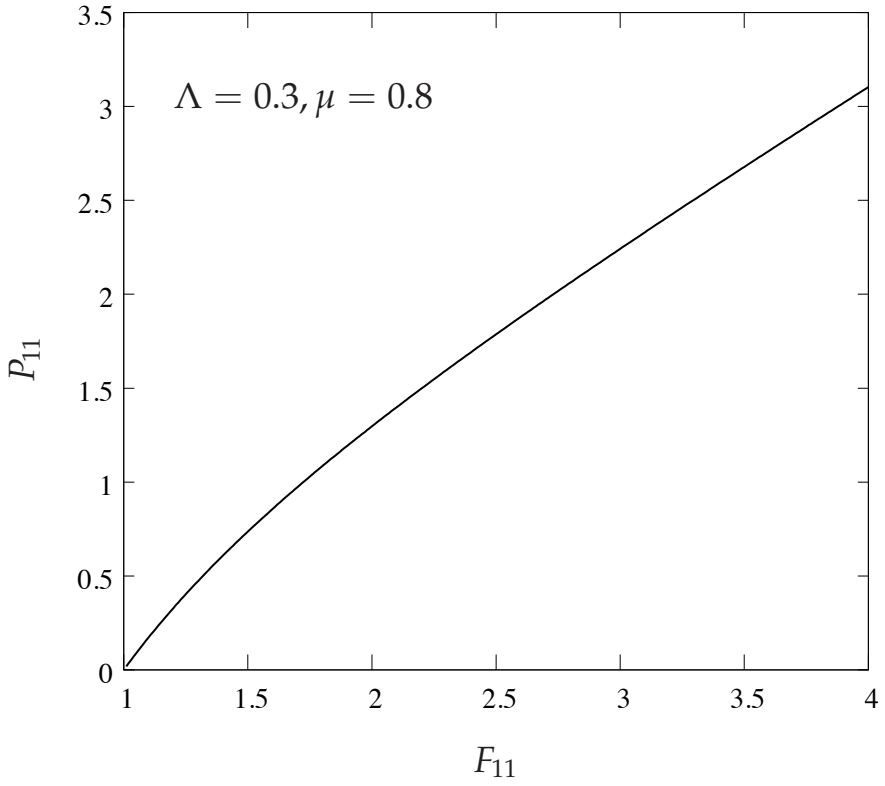
$$\boldsymbol{P}_k(\boldsymbol{F}) = \begin{bmatrix} P_{22} \\ P_{33} \end{bmatrix} = \begin{bmatrix} \mu(F_{22} - F^{-1}_{22}) + \frac{\Lambda}{2}\left(J^2 - 1\right) F^{-1}_{22} \\ \mu(F_{33} - F^{-1}_{33}) + \frac{\Lambda}{2}\left(J^2 - 1\right) F^{-1}_{33} \end{bmatrix}$$

$$\boldsymbol{A}_{ku}(\boldsymbol{F}) = \partial_{\boldsymbol{F}_u}\boldsymbol{P}_k = \frac{\partial [P_{22}\, P_{33}]^T}{\partial [F_{22}\, F_{33}]^T} = \begin{bmatrix} \mathbb{A}_{2222} & \mathbb{A}_{2233} \\ \mathbb{A}_{3322} & \mathbb{A}_{3333} \end{bmatrix}$$

for the uniaxial tension.

```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
/*_______________________________________

  ME 338A Continuum Mechanics
  Stanford University
  E. Kuhl, S. Goktepe
  Driver routine for uniaxial tension
  _______________________________________*/

int main()
{

  // open file for output
  FILE *fp;
  fp = fopen("data.out","w");
  if (fp==NULL){
    printf("Cannot create the output file!!\n");
    exit(1);
  }

  int  i,j;
  // solution parameters
  double dlam=1.e-2, lam_max=4., nres=0.,tol=1.e-12;
  int   niter, nitermax=50;
  //material parameters
  double Lam=0.3, mu=0.8;
  //deformation measures, stresses and moduli
  double J,F[3],P[3],AA[3][3];
  //residual, tangent for iterations
  double res[2],tang[2][2],det,temp;

  //initialize F
  for(i=0;i<3;i++)  F[i]=1.;

  // loop for loading
  do {
      niter = 0;
      F[0] +=dlam;
      printf("STRETCH=%4e\n", F[0]);
      // loop of iterations
      do {
  niter +=1 ;
// compute Jacobi, det(F)
```

```
J = F[0]*F[1]*F[2];

// MATERIAL MODEL specific computation of stresses and moduli
//-------------------------------------------------------------
// Compressible Neo-Hookean Material
for (i=0;i<3;i++) {
  P[i] = mu*(F[i]-1./F[i]) + Lam*(J*J-1.)/F[i]/2;
  for (j=0;j<3;j++) {
    AA[i][j] = Lam*J*J/F[i]/F[j];
    if(i==j) AA[i][j] += (mu - (-mu+Lam*(J*J-1.)/2.)/F[i]/F[j]);
  }
//-------------------------------------------------------------
}
//compute residual vector and its norm
res[0] = P[1]; res[1] = P[2];
nres = sqrtl(res[0]*res[0] + res[1]*res[1]);

//construct tangent matrix
tang[0][0] = AA[1][1]; tang[0][1] = AA[1][2];
tang[1][0] = AA[2][1]; tang[1][1] = AA[2][2];

// invert tanget matrix
det =  tang[0][0] *tang[1][1] - tang[0][1] *tang[1][0];
temp = tang[0][0];
tang[0][0] =  tang[1][1]/det;
tang[1][1] =        temp/det;
tang[0][1] = -tang[0][1]/det;
tang[1][0] = -tang[1][0]/det;

// update lateral stretches
F[1]  = F[1] - (tang[0][0]*res[0]+tang[0][1]*res[1]);
F[2]  = F[2] - (tang[1][0]*res[0]+tang[1][1]*res[1]);

// print iteration counter and norm of residual
printf("Iteration %4d, residual=%4e\n", niter,nres);
      } while (tol<nres && niter<nitermax);  // Check convergence
      if (niter==nitermax) {printf("No convergence!\n"); break;};

      // print stretch and PK1 stresses
      fprintf(fp,"%4e, %4e\n",F[0],P[0]);

  } while ((lam_max-F[0])>1.e-8); // check loading
  fclose(fp);//close file
  return 0;
}
```


$\Lambda = 0.3, \mu = 0.8$
$P_{11}$
$F_{11}$
0
0.5
1
1.5
2
2.5
3
3.5
4