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1 Laplace equation

For a computational domain $\Omega \subset \mathbb{R}^d$ the Laplace equation is given by

$$\Delta u = 0 \quad \text{on } \Omega. \tag{1}$$

A classical solution $u : \Omega \to \mathbb{R}$ fulfills (1). For a unique solution also boundary conditions have to be specified, e.g.

$$\begin{aligned} \nabla u(\mathbf{x}) \cdot \mathbf{n} &= 0 \qquad \text{on } \Gamma_N, \\ u(\mathbf{x}) &= u_0(\mathbf{x}) \quad \text{on } \Gamma_D, \end{aligned} \tag{2}$$

where the homogeneous Neumann-type boundary conditions for $\mathbf{x} \in \Gamma_N$ set the flux over the boundary in normal direction $\mathbf{n}$ to zero and the Dirichlet-type boundary conditions on Γ_D prescribe a value for u on the boundary.

1.1 Analytical solution

The solution for a 1D case on $\Omega = [0, l]$ with $u_0(0) = a$, $u_0(l) = b$, simply is

$$u(x) = a + (b - a)\, x/l.$$

For the 2D case on $\Omega = [0, 1]^2$ with Dirichlet boundary conditions

$$u_0(x_1, 1) = \sin(k\,\pi\, x_1), \quad k \in \mathbb{N} \qquad \text{“top”},$$

$$u_0(x_1, 0) = u_0(0, x_2) = u_0(1, x_2) = 0 \quad \text{“left, right and bottom”},$$

we have the solution

$$u(x_1, x_2) = c_1\, \sin(k\,\pi\, x_1)\, e^{k\,\pi\, x_2} + c_2\, \sin(k\,\pi\, x_1)\, e^{-k\,\pi\, x_2}, \qquad \text{where}$$

$$c_1 = 1/\big(2\, \sinh(k\,\pi)\big), \quad c_2 = -1/\big(2\, \sinh(k\,\pi)\big).$$

Also see exercise in “Grundlagen des Wissenschaftlichen Rechnens” (2013 3.2d).

1.2 Finite Element formulation

By multiplication of a testfunction $\phi \in H_0^1(\Omega)$ and integration follows the weak formulation of (1):

$$\int_\Omega \Delta u\, \phi \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi \in H_0^1(\Omega) \tag{3}$$

For a definition of H_0^1 see section 1.7.

The Laplace operator can be written as $\Delta u = \nabla \cdot (\nabla u)$. Applying divergence theorem in form of (67) with $f = \phi$ and $\mathbf{F} = \nabla u$ yields

$$-\int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}\mathbf{x} + \int_{\partial\Omega} (\phi\, \nabla u) \cdot \mathbf{n} \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi \in H_0^1(\Omega) \tag{4}$$

Because ϕ is zero on the boundary, the second term vanishes:

$$-\int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi \in H_0^1(\Omega) \tag{5}$$

Now we have to specify a finite-dimensional ansatz space to choose the solution function from. We do this by specifying a basis and take the span of it: $V := \operatorname{span}\{\phi_1, \dots \phi_n\}$.

The numerical solution is given by

$$u_h(\mathbf{x}) = \sum_{i=1}^{N} u_i \, \phi_i(\mathbf{x}). \tag{6}$$

We also take V as the space of testfunctions. Plugging this into (25) yields

$$-\sum_{i=1}^{N} u_i \int_\Omega \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\mathbf{x} = 0 \quad \text{for } j = 1, \dots, N. \tag{7}$$

The minus sign is kept for similarity with later mentioned problem equations that also have a right-hand side.

A reasonable choice of ansatz functions are functions that have limited support. We discretize the domain Ω by Finite Elements Ω_e,

$$\Omega = \bigcup_{e=1}^{M} \Omega_e = \Omega_1 \dot\cup \cdots \dot\cup \Omega_M, \tag{8}$$

and define nodes with global indices $N(e)$ on each element e. Interpolating ansatz functions are now chosen such that they have the value 1 at only one node and the value 0 at all other nodes. The support is contained just within the elements that are adjacent to the node where the function is 1.

1.3 Ansatz functions

A simple choice that fulfills the requirements are first-order Lagrange functions $L_{i,p}, p = 1$ which are defined a follows for $d = 1$ and depicted in fig. 1c.

$$\varphi_i : [0,1] \to \mathbb{R}, \quad \varphi_1(x) = L_{1,1}(x) := 1 - x, \qquad \varphi_2(x) = L_{2,1}(x) := x \tag{9}$$

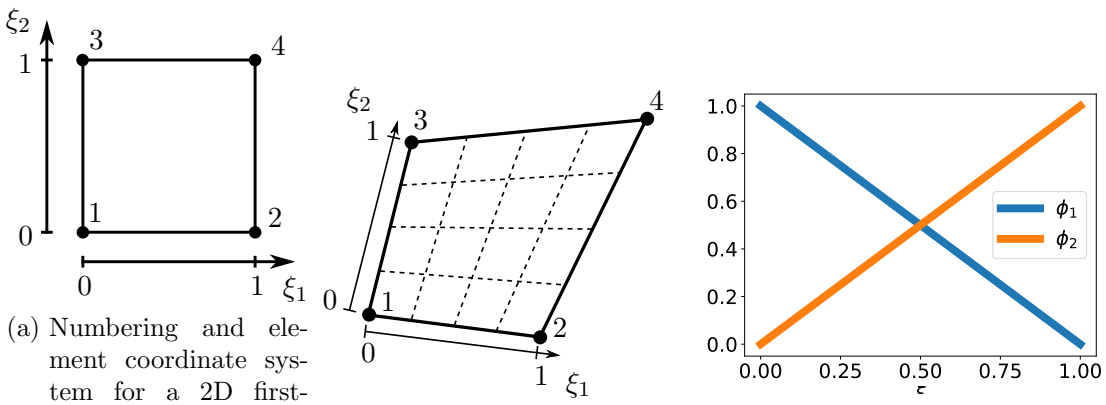
For higher dimensions they are composed by a tensor product ansatz.

$$\varphi_i(\mathbf{x}) = \mathbf{L}_i(\mathbf{x}) := \prod_{k=1}^{d} L_{j,1}(x_k) \tag{10}$$

The local numbering of the ansatz functions of an element proceeds fastest in the first dimension then in the second and so on as shown in fig. 1a

1.4 Transformation of integration domain

The definition of the ansatz functions was in parameter space, i.e. on the unit interval $[0,1]^d$. The corresponding coordinate system is $\boldsymbol{\xi} = \{\xi_1, \dots \xi_d\}$. However, integration over the elements Ω_e of



(a) Numbering and element coordinate system for a 2D first-order Lagrange element

(b) Arbitrarily shaped element

(c) first order Lagrange ansatz functions

Abbildung 1: 2D first-order Lagrange element

the computational domain is required. The node coordinates which define the elements are given in the global coordinate system $\mathbf{x} = \{x_1, \dots x_d\}$. A mapping from $\boldsymbol{\xi}$ to $\mathbf{x}$ can be performed using multi-linear interpolation between the nodal coordinates $\mathbf{x}^i$:

$$\mathbf{x}(\boldsymbol{\xi}) = \Phi(\boldsymbol{\xi}) := \sum_i \mathbf{L}_i(\boldsymbol{\xi})\, \mathbf{x}^i. \tag{11}$$

Note that again Lagrange functions of first order appear, but this is part of the parameter space to global space mapping and independent of the choosen ansatz functions. For 1D and 2D problems Eq. (11) can be written out as:

$$\begin{aligned}
\text{1D:}\quad & \Phi(\xi_1) = && (1-\xi_1)\,\mathbf{x}^1 + \xi_1\,\mathbf{x}^2 \\
\text{2D:}\quad & \Phi(\boldsymbol{\xi}) = && (1-\xi_1)\,(1-\xi_2)\,\mathbf{x}^1 + \xi_1\,(1-\xi_2)\,\mathbf{x}^2 + (1-\xi_1)\,\xi_2\,\mathbf{x}^3 + \xi_1\,\xi_2\,\mathbf{x}^4. \\
\text{3D:}\quad & \Phi(\boldsymbol{\xi}) = && (1-\xi_1)\,(1-\xi_2)\,(1-\xi_3)\,\mathbf{x}^1 + \xi_1\,(1-\xi_2)\,(1-\xi_3)\,\mathbf{x}^2 + (1-\xi_1)\,\xi_2\,(1-\xi_3)\,\mathbf{x}^3 + \xi_1\,\xi_2\,(1-\xi_3)\,\mathbf{x}^4 \\
& && +(1-\xi_1)\,(1-\xi_2)\,\xi_3\,\mathbf{x}^5 + \xi_1\,(1-\xi_2)\,\xi_3\,\mathbf{x}^6 + (1-\xi_1)\,\xi_2\,\xi_3\,\mathbf{x}^7 + \xi_1\,\xi_2\,\xi_3\,\mathbf{x}^8
\end{aligned} \tag{12}$$

The node numbering and coordinate frames are defined by fig. 1b. The Jacobians of Φ, $J_\Phi = \mathrm{d}\mathbf{x}/\mathrm{d}\boldsymbol{\xi}$ for the 1D and 2D case are given by:

$$\begin{aligned}
\text{1D:}\quad & J_\Phi(\xi_1) = \Phi'(\xi_1) = \mathbf{x}^2 - \mathbf{x}^1 \\
\text{2D:}\quad & J_\Phi(\boldsymbol{\xi}) = \begin{pmatrix} (1-\xi_2)\,(\mathbf{x}^2 - \mathbf{x}^1) + \xi_2\,(\mathbf{x}^4 - \mathbf{x}^3) & (1-\xi_1)\,(\mathbf{x}^3 - \mathbf{x}^1) + \xi_1\,(\mathbf{x}^4 - \mathbf{x}^2) \end{pmatrix} \\
\text{3D:}\quad & J_\Phi(\boldsymbol{\xi}) = \begin{pmatrix} J_{\Phi,1}(\boldsymbol{\xi}) & J_{\Phi,2}(\boldsymbol{\xi}) & J_{\Phi,3}(\boldsymbol{\xi}) \end{pmatrix} \\
& J_{\Phi,1}(\boldsymbol{\xi}) = (1-\xi_2)\,(1-\xi_3)\,(\mathbf{x}^2 - \mathbf{x}^1) + \xi_2\,(1-\xi_3)\,(\mathbf{x}^4 - \mathbf{x}^3) + (1-\xi_2)\,\xi_3\,(\mathbf{x}^6 - \mathbf{x}^5) + \xi_2\,\xi_3\,(\mathbf{x}^8 - \mathbf{x}^7) \\
& J_{\Phi,2}(\boldsymbol{\xi}) = (1-\xi_1)\,(1-\xi_3)\,(\mathbf{x}^3 - \mathbf{x}^1) + \xi_1\,(1-\xi_3)\,(\mathbf{x}^4 - \mathbf{x}^2) + (1-\xi_1)\,\xi_3\,(\mathbf{x}^7 - \mathbf{x}^5) + \xi_1\,\xi_3\,(\mathbf{x}^8 - \mathbf{x}^6) \\
& J_{\Phi,3}(\boldsymbol{\xi}) = (1-\xi_1)\,(1-\xi_2)\,(\mathbf{x}^5 - \mathbf{x}^1) + \xi_1\,(1-\xi_2)\,(\mathbf{x}^6 - \mathbf{x}^2) + (1-\xi_1)\,\xi_2\,(\mathbf{x}^7 - \mathbf{x}^3) + \xi_1\,\xi_2\,(\mathbf{x}^8 - \mathbf{x}^4)
\end{aligned}$$

In order to invert the mappings Φ from parameter to world space, we proceed:

$$\text{1D:} \quad \mathbf{x}_i^p = \mathbf{x}_i^1 + \xi_1 \, (\mathbf{x}_i^2 - \mathbf{x}_i^1), \quad \forall i \in \{1,2,3\}$$

$$\Rightarrow \quad \xi_1 = (\mathbf{x}_i^p - \mathbf{x}_1^1)/(\mathbf{x}_i^2 - \mathbf{x}_i^1) \quad \forall i \in \{1,2,3\}$$

2D:

The point in world space, $\mathbf{x}^p$ is computed by the sum over shape functions, ϕ^L and control points of the element, $\mathbf{x}^L$.

$$\mathbf{x}_i^p(\boldsymbol{\xi}) = \Phi_i(\boldsymbol{\xi}) = \sum_L \phi_i^L(\boldsymbol{\xi}) \, \mathbf{x}^L$$
$$\mathbf{x}^p = \mathbf{M}(\boldsymbol{\xi}) \, \mathbf{x},$$

where $\mathbf{M}(\boldsymbol{\xi})$ is a $n \times d$ matrix with n nodes and dimension d and the entries

$$\mathbf{M}_{iL}(\boldsymbol{\xi}) = \phi_i^L(\boldsymbol{\xi})$$

Starting from (7) we now plug in the Lagrange ansatz functions for ϕ. Then the respective functions only have to be integrated over the elements where they are defined. We get

$$-\sum_{e=1}^{M} \sum_{i \in N(e)} u_i \int_{\Omega_e} \nabla \phi_i(\mathbf{x}) \cdot \nabla \phi_j(\mathbf{x}) \, \mathrm{d}\mathbf{x} = 0 \quad \text{for } j = 1, \ldots, N, \tag{13}$$

where the sum over $i \in N(e)$ is over the nodes of element e. The expression $\nabla \phi(\mathbf{x})$ means, that the gradient is with respect to $\mathbf{x}$, despite the function ϕ being defined in parameter space, i.e. $\nabla \phi(\mathbf{x}) = \nabla_{\mathbf{x}} \phi(\Phi^{-1}(\mathbf{x})) = \nabla_{\mathbf{x}} \phi(\boldsymbol{\xi})$.

The integration domain, Ω_e, is described by the mapping from parameter space, $\Omega_e = \Phi([0,1]^d)$. At every point $\mathbf{p} = \Phi(\boldsymbol{\xi})$ the gradients are with respect to orthogonal coordinates in the tangent space of the point. The tangent space coordinates for a particular point given by $\boldsymbol{\xi}$ are introduced as $\boldsymbol{\zeta}(\boldsymbol{\xi}) = (\zeta_1(\boldsymbol{\xi}), \ldots, \zeta_d(\boldsymbol{\xi}))$. The scaling is like in world space, i.e. the following holds:

$$\left| \frac{\partial \zeta_i}{\partial \xi_i} \right| = \left| \frac{\partial \Phi}{\partial \xi_i} \right|.$$

The integral in (13) is then

$$\int_{\Omega_e} \nabla \phi_i(\mathbf{x}) \cdot \nabla \phi_j(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_{\Phi([0,1]^d)} \nabla_{\boldsymbol{\zeta}(\boldsymbol{\xi}(\mathbf{x}))} \phi_i(\mathbf{x}) \cdot \nabla_{\boldsymbol{\zeta}(\boldsymbol{\xi}(\mathbf{x}))} \phi_j(\mathbf{x}) \, \mathrm{d}\mathbf{x}. \tag{14}$$

Depending on dimension this is resolved differently.

1D case. With one dimension, we can choose $\zeta_1 = \xi_1 \cdot s$, where s is the scaling factor between the different length scales in world space (ζ) and parameter space (ξ). Then with $\mathrm{d}\phi/\mathrm{d}\zeta = \mathrm{d}\phi/\mathrm{d}\xi \cdot \mathrm{d}\xi/\mathrm{d}\zeta$ and $\mathrm{d}\xi/\mathrm{d}\zeta = s^{-1}$ we get

$$\int_{\Omega_e} \nabla \phi_i(\mathbf{x}) \cdot \nabla \phi_j(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_{\Phi([0,1])} \frac{\mathrm{d}\phi_i(\mathbf{x})}{\mathrm{d}\xi} \frac{\mathrm{d}\phi_j(\mathbf{x})}{\mathrm{d}\xi} \Big(\underbrace{\frac{\mathrm{d}\xi}{\mathrm{d}\zeta}}_{=:s^{-1}} \Big)^2 \mathrm{d}\mathbf{x}.$$

The scaling factor can be computed by

$$\frac{\partial \Phi}{\partial \xi} = \frac{\partial \zeta}{\partial \xi} = s \quad \Rightarrow \quad s = \Phi'(\xi_1) = \|\mathbf{x}^2 - \mathbf{x}^1\|_2.$$

After transformation of the integration domain to parameter space this yields the following formula for the stiffness matrix:

$$\int_{\Omega_e} \nabla \phi_i(\mathbf{x}) \cdot \nabla \phi_j(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_{[0,1]} \frac{\mathrm{d}\phi_i(\xi)}{\mathrm{d}\xi} \frac{\mathrm{d}\phi_j(\xi)}{\mathrm{d}\xi} \, s^{-2} \mathcal{J}_1(\xi) \, \mathrm{d}\xi$$

3D case. In 3D we use the world coordinate system as $\boldsymbol{\zeta}$-frame, i.e. $\boldsymbol{\zeta}_1 = \mathbf{e}_1, \boldsymbol{\zeta}_2 = \mathbf{e}_2, \boldsymbol{\zeta}_3 = \mathbf{e}_3$. We transform the integration domain from global to local coordinate frame using (73) and get:

$$-\sum_{e=1}^{M} \sum_{i \in N(e)} u_i \int_{[0,1]^d} \nabla_{\boldsymbol{\zeta}(\boldsymbol{\xi})} \phi_i(\boldsymbol{\xi}) \cdot \nabla_{\boldsymbol{\zeta}(\boldsymbol{\xi})} \phi_j(\boldsymbol{\xi}) \, \mathcal{J}_d(\boldsymbol{\xi}) \, \mathrm{d}\boldsymbol{\xi} = 0 \quad \text{for } j = 1, \ldots, N. \tag{15}$$

For a transformation of the gradients to parameter space we need the Jacobian J_Φ of the coordinate mapping, $\mathbf{x} = \Phi(\boldsymbol{\xi})$, which consists of the entries

$$\left(J_\Phi\right)_{i,j} = \frac{\mathrm{d}x_i}{\mathrm{d}\xi_j}.$$

Note that the Jacobian of $\Phi : \mathbb{R}^d \to \mathbb{R}^3$ might not be quadratic in general, but a $3 \times d$ matrix with $d \leq 3$. Only in the special 3D-case it is quadratic and can therefore be inverted.

Assuming that Φ is invertible on Ω the inverse function theorem states

$$J_{\Phi^{-1}} = J_\Phi^{-1}.$$

Executing the chain rule on a derivative in world space, $\mathrm{d}\phi/\mathrm{d}x_k$, yields:

$$\frac{\mathrm{d}\phi(\boldsymbol{\xi})}{\mathrm{d}x_k} = \sum_{\ell=1}^{d} \frac{\mathrm{d}\phi(\boldsymbol{\xi})}{\mathrm{d}\xi_\ell} \frac{\mathrm{d}\xi_\ell(\boldsymbol{\xi})}{\mathrm{d}x_k}$$

and for the whole gradient vector:

$$\nabla_{\mathbf{x}} \phi(\boldsymbol{\xi}) = J_\Phi^{-\top}(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \phi(\boldsymbol{\xi}),$$

where $J_\Phi^{-\top} = (J_\Phi^{-1})^\top$.

Now the expression $\nabla_{\mathbf{x}} \phi_i \cdot \nabla_{\mathbf{x}} \phi_j$ can be computed:

$$\begin{aligned}
\nabla_{\mathbf{x}} \phi_i(\mathbf{x}) \cdot \nabla_{\mathbf{x}} \phi_j(\mathbf{x}) &= \sum_{k=1}^{d} \frac{\mathrm{d}\phi_i(\boldsymbol{\xi})}{\mathrm{d}x_k} \frac{\mathrm{d}\phi_j(\boldsymbol{\xi})}{\mathrm{d}x_k} = \sum_{k=1}^{d} \Big(\sum_{\ell=1}^{d} \frac{\mathrm{d}\phi_i(\boldsymbol{\xi})}{\mathrm{d}\xi_\ell} \frac{\mathrm{d}\xi_\ell(\boldsymbol{\xi})}{\mathrm{d}x_k} \sum_{\ell=1}^{d} \frac{\mathrm{d}\phi_j(\boldsymbol{\xi})}{\mathrm{d}\xi_\ell} \frac{\mathrm{d}\xi_\ell(\boldsymbol{\xi})}{\mathrm{d}x_k} \Big) \\
&= J_\Phi^{-\top}(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \phi_i(\boldsymbol{\xi}) \cdot J_\Phi^{-\top}(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \phi_j(\boldsymbol{\xi}) \\
&= \left(J_\Phi^{-\top}(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \phi_i(\boldsymbol{\xi}) \right)^\top J_\Phi^{-\top}(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \phi_j(\boldsymbol{\xi}) \\
&= \nabla_{\boldsymbol{\xi}} \phi_i(\boldsymbol{\xi})^\top \underbrace{J_\Phi^{-1}(\boldsymbol{\xi}) J_\Phi^{-\top}(\boldsymbol{\xi})}_{=: T_\Phi(\boldsymbol{\xi})} \nabla_{\boldsymbol{\xi}} \phi_j(\boldsymbol{\xi}).
\end{aligned}$$

With the definition of the finite element Laplace operator transformation matrix $T_\Phi(\boldsymbol{\xi}) := J_\Phi^{-1}(\boldsymbol{\xi}) J_\Phi^{-\top}(\boldsymbol{\xi})$ the transformation becomes:

$$\nabla_{\mathbf{x}} \phi_i(\mathbf{x}) \cdot \nabla_{\mathbf{x}} \phi_j(\mathbf{x}) = \nabla_{\boldsymbol{\xi}} \phi_i(\boldsymbol{\xi}) \cdot T_\Phi(\boldsymbol{\xi}) \nabla_{\boldsymbol{\xi}} \phi_j(\boldsymbol{\xi}).$$

The inverse transpose $M_\Phi(\boldsymbol{\xi}) := T_\Phi(\boldsymbol{\xi})^{-\top} = J_\Phi(\boldsymbol{\xi})^\top J_\Phi(\boldsymbol{\xi})$ is called the metric tensor of the mapping Φ.

2D case. In two dimensions we consider the 2D manifold embedded in $\mathbb{R}^3$ with the mapping $\Phi : [0,1]^2 \to \Omega \subset \mathbb{R}^3$. At a fixed point $\mathbf{p} \in \Omega$ with $\Phi(\boldsymbol{\xi}_p) = \mathbf{p}$ we first determine the tangent vectors $\boldsymbol{\zeta}_1(\boldsymbol{\xi}_p), \boldsymbol{\zeta}_2(\boldsymbol{\xi}_z)$. The first tangent vector is defined to lie on the ξ_1 coordinate direction, the second vector is then constructed to be orthogonal to the first. To define the tangent vector $\boldsymbol{\zeta}_1$ we use a curve in parameter space:

$$\gamma(t) = \begin{pmatrix} \gamma_1(t) \\ \gamma_2(t) \end{pmatrix} = \begin{pmatrix} \xi_{p1} + t \\ \xi_{p2} \end{pmatrix}.$$

Then we define

$$\begin{aligned} \boldsymbol{\zeta}_1 &= (\Phi \circ \gamma_1)'(0) = \frac{\partial}{\partial t} \Phi\big(\gamma(t)\big)|_{t=0} \\ &= \frac{\partial \Phi(\gamma(0))}{\partial \xi_1} \underbrace{\gamma_1'(t)}_{=1} + \frac{\partial \Phi(\gamma(0))}{\partial \xi_2} \underbrace{\gamma_2'(t)}_{=0} \\ &= \frac{\partial \Phi(\xi_p)}{\partial \xi_1}. \end{aligned}$$

Similar we define the helper tangent vector $\boldsymbol{\zeta}_h$ along the ξ_2 coordinate, which is then

$$\boldsymbol{\zeta}_h = \frac{\partial \Phi(\xi_p)}{\partial \xi_2}.$$

$\boldsymbol{\zeta}_1$ and $\boldsymbol{\zeta}_h$ are not orthogonal in general. Therefore a third tangent vector $\boldsymbol{\zeta}_2 = \boldsymbol{\zeta}_1 \times \boldsymbol{\zeta}_h \times \boldsymbol{\zeta}_1$ will be defined.

It is the tangent vector of a curve

$$\delta(t) = \begin{pmatrix} \delta_1(t) \\ \delta_2(t) \end{pmatrix} = \begin{pmatrix} \xi_{p1} + \cos(\alpha) t \\ \xi_{p2} + \sin(\alpha) t \end{pmatrix}.$$

The angle β between $\boldsymbol{\zeta}_1$ and $\boldsymbol{\zeta}_h$ is given by

$$\cos(\beta) |\boldsymbol{\zeta}_1| |\boldsymbol{\zeta}_h| = \boldsymbol{\zeta}_1 \cdot \boldsymbol{\zeta}_h \quad \Rightarrow \quad \beta = \arccos\left(\frac{\boldsymbol{\zeta}_1 \cdot \boldsymbol{\zeta}_h}{|\boldsymbol{\zeta}_1| |\boldsymbol{\zeta}_h|} \right)$$

Then by relating angles we get

$$\frac{\pi/2}{\beta} = \frac{\alpha}{\pi/2} \quad \Rightarrow \quad \alpha = \frac{\pi^2}{4\,\beta}.$$

So the tangent vector becomes

$$\boldsymbol{\zeta}_2 = (\Phi \circ \delta)'(0) = \frac{\partial \Phi(\boldsymbol{\xi}_p)}{\partial \xi_1} \cos(\alpha) + \frac{\partial \Phi(\boldsymbol{\xi}_p)}{\partial \xi_2} \sin(\alpha) = \boldsymbol{\zeta}_1 \cos(\alpha) + \boldsymbol{\zeta}_h \sin(\alpha). \tag{16}$$

Another approach is to use the formula

$$\boldsymbol{\zeta}_2 = \boldsymbol{\zeta}_1 \times \boldsymbol{\zeta}_h \times \boldsymbol{\zeta}_1,$$

which leads to the expression

$$\boldsymbol{\zeta}_2 = \begin{pmatrix} -\frac{\partial\Phi_2}{\partial\xi_1}\left(\frac{\partial\Phi_1}{\partial\xi_1}\frac{\partial\Phi_2}{\partial\xi_2} - \frac{\partial\Phi_1}{\partial\xi_2}\frac{\partial\Phi_2}{\partial\xi_1}\right) - \frac{\partial\Phi_3}{\partial\xi_1}\left(\frac{\partial\Phi_1}{\partial\xi_1}\frac{\partial\Phi_3}{\partial\xi_2} - \frac{\partial\Phi_1}{\partial\xi_2}\frac{\partial\Phi_3}{\partial\xi_1}\right) \\ \frac{\partial\Phi_1}{\partial\xi_1}\left(\frac{\partial\Phi_1}{\partial\xi_1}\frac{\partial\Phi_2}{\partial\xi_2} - \frac{\partial\Phi_1}{\partial\xi_2}\frac{\partial\Phi_2}{\partial\xi_1}\right) - \frac{\partial\Phi_3}{\partial\xi_1}\left(\frac{\partial\Phi_2}{\partial\xi_1}\frac{\partial\Phi_3}{\partial\xi_2} - \frac{\partial\Phi_2}{\partial\xi_2}\frac{\partial\Phi_3}{\partial\xi_1}\right) \\ \frac{\partial\Phi_1}{\partial\xi_1}\left(\frac{\partial\Phi_1}{\partial\xi_1}\frac{\partial\Phi_3}{\partial\xi_2} - \frac{\partial\Phi_1}{\partial\xi_2}\frac{\partial\Phi_3}{\partial\xi_1}\right) + \frac{\partial\Phi_2}{\partial\xi_1}\left(\frac{\partial\Phi_2}{\partial\xi_1}\frac{\partial\Phi_3}{\partial\xi_2} - \frac{\partial\Phi_2}{\partial\xi_2}\frac{\partial\Phi_3}{\partial\xi_1}\right) \end{pmatrix}.$$

The mapping between parameter space and tangent space is given by $\Psi_{\mathbf{p}}$:

$$\Psi_{\mathbf{p}} : [0,1]^2 \to T_{\mathbf{p}}\Omega,$$

$$\Psi_{\mathbf{p}}(\boldsymbol{\xi}) = \mathbf{p} + c_1(\boldsymbol{\xi})\,\hat{\boldsymbol{\zeta}}_1 + c_2(\boldsymbol{\xi})\,\hat{\boldsymbol{\zeta}}_2.$$

The basis vectors $\hat{\boldsymbol{\zeta}}_i$ are the normalized tangent vectors, $\hat{\boldsymbol{\zeta}}_i = \boldsymbol{\zeta}_i/|\boldsymbol{\zeta}_i|$. And the coefficients are:

$$c_1(\boldsymbol{\xi}) = \big(\xi_1 - \xi_{p1} - (\xi_2 - \xi_{p2})\cos(\alpha)/\sin(\alpha)\big)\,l_1$$

$$c_2(\boldsymbol{\xi}) = (\xi_2 - \xi_{p2})/\sin(\alpha)\,l_2,$$

with the lengths $l_1 = |\boldsymbol{\zeta}_1|, l_2 = |\boldsymbol{\zeta}_2|$.

The Jacobian of Ψ and its inverse are as follows:

$$J_\Psi = \begin{pmatrix} l_1 & -l_1\cos(\alpha)/\sin(\alpha) \\ 0 & l_2/\sin(\alpha) \end{pmatrix}, \qquad J_\Psi^{-1} = J_{\Psi^{-1}} = \begin{pmatrix} 1/l_1 & \cos(\alpha)/l_2 \\ 0 & \sin(\alpha)/l_2 \end{pmatrix}.$$

The inverse contains the entries

$$(J_\Psi^{-1})_{i,j} = \frac{\mathrm{d}\xi_i}{\mathrm{d}\zeta_j}\,.$$

To compute the gradients of a function with respect to ζ, we use the chain rule:

$$\frac{\mathrm{d}\phi(\boldsymbol{\xi})}{\mathrm{d}\zeta_k} = \sum_{\ell=1}^{d} \frac{\mathrm{d}\phi(\boldsymbol{\xi})}{\mathrm{d}\xi_\ell}\,\frac{\mathrm{d}\xi_\ell(\boldsymbol{\xi})}{\mathrm{d}\zeta_k}\,,$$

so the gradient becomes

$$\nabla_{\boldsymbol{\zeta}}\phi(\boldsymbol{\xi}) = J_\Psi^{-\top}\nabla_{\boldsymbol{\xi}}\phi(\boldsymbol{\xi}),$$

where $J_\Psi^{-\top} = (J_\Psi^{-1})^\top$.

Analogous to the 3D case we define

$$T_\Psi(\boldsymbol{\xi}) := J_\Psi^{-1}(\boldsymbol{\xi})J_\Psi^{-\top}(\boldsymbol{\xi}) = \begin{pmatrix} \cos(\alpha)^2/l_2^2 + 1/l_1^2 & \sin(\alpha)\cos(\alpha)/l_2^2 \\ \sin(\alpha)\cos(\alpha)/l_2^2 & \sin(\alpha)^2/l_2^2 \end{pmatrix}$$

and get:

$$\nabla_{\boldsymbol{\zeta}}\phi_i(\mathbf{x}) \cdot \nabla_{\boldsymbol{\zeta}}\phi_j(\mathbf{x}) = \nabla_{\boldsymbol{\xi}}\phi_i(\boldsymbol{\xi}) \cdot T_\Phi(\boldsymbol{\xi})\nabla_{\boldsymbol{\xi}}\phi_j(\boldsymbol{\xi}).$$

1.5 Evaluation of the integral term

The integral in (15) defines for i and j the entries m_{ij} of the *stiffness matrix* M. The equation can be written in matrix form as

$$M\,\mathbf{u} = \mathbf{0},$$

where M contains the entries

$$m_{ij} = -\int_\Omega \nabla\phi_i \cdot \nabla\phi_j \,\mathrm{d}\mathbf{x} = -\sum_{e=1}^{M} \sum_{i \in N(e)} \int_{[0,1]^d} \nabla\phi_i(\boldsymbol{\xi}) \cdot T_\Phi(\boldsymbol{\xi})\nabla\phi_j(\boldsymbol{\xi})\, \mathcal{J}_d(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}$$

and $\mathbf{u} = (u_1, \ldots, u_N)^\top$ is the solution vector. Given M the solution $\mathbf{u}$ is computed by an appropriate linear system solver.

The integral for $m_{i,j}$ depends via $\mathcal{J}_d$ on the shape of the elements. In general, it has to be evaluated numerically. However, for special simple cases it can be computed analytically. This includes scenarios in $d = 1, 2, 3$ dimensions where the elements are on a rectilinear cartesian grid.

If the grid is arbitrary, analytical computation for 1D is still simple. For $d = 2, 3$ it is still possible, but involves more lengthy derivations that are usually performed using a computer algebra system such as `sympy`. In this section the 1D and 2D cases are derived, the python `sympy` code for 2D and 3D is contained in the `doc` directory for further reference.

For all 1D meshes that are embedded in a 3D domain as well as rectangular cartesian 2D and 3D meshes the terms $T_\Phi(\boldsymbol{\xi})$ and $\mathcal{J}_d(\boldsymbol{\xi})$ are constant within each element, i.e. do not depend on $\boldsymbol{\xi}$. In that case we can take $\mathcal{J}_d$ out of the integral.

1D case. We now compute m_{ij} for $d = 1$. The transformation term $\mathcal{J}_1(\xi)$ is defined as

$$\mathcal{J}_1(\xi) = \|\Phi'(\xi)\|_2.$$

Using the parametric representation of Φ given in (12), we derive

$$\mathcal{J}_1(\xi) = \|\Phi'(\xi)\|_2 = \|\mathbf{x}^2 - \mathbf{x}^1\|_2,$$

which is the length of the element e with nodes $\mathbf{x}^1$ and $\mathbf{x}^2$. We define it to be $l_e := \|\mathbf{x}^2 - \mathbf{x}^1\|_2$, and thus have $\mathcal{J}_1(\xi) = l_e$. The scaling factor is then $s = l_e$ and the total prefactor of the integral becomes

$$\mathcal{J}_1\, s^{-2} = 1/l_e.$$

2D case. For 2D we assume a rectangular element that lies in a z = constant plane with side lengths $l_{1,e}$ and $l_{2,e}$ in ξ_1 and ξ_2 directions. The mapping from $\boldsymbol{\xi} = (\xi_1, \xi_2)$ to $\mathbf{x}$ coordinate frame is given by

$$\Phi(\boldsymbol{\xi}) = \mathbf{x}^1 + \begin{pmatrix} \xi_1\, l_{1,e} \\ \xi_2\, l_{2,e} \end{pmatrix}. \tag{17}$$

Then we derive

$$J_\Phi(\boldsymbol{\xi}) = \begin{pmatrix} l_{1,e} & 0 \\ 0 & l_{2,e} \end{pmatrix}$$

and

$$\mathcal{J}_2 = \sqrt{\det\left(J_\Phi(\boldsymbol{\xi})^\top J_\Phi(\boldsymbol{\xi})\right)} = |l_{1,e}\, l_{2,e}|.$$

The tangent vectors $\boldsymbol{\zeta}_1$ and $\boldsymbol{\zeta}_h$ are computed to be

$$\boldsymbol{\zeta}_1 = \frac{\partial \Phi(\boldsymbol{\xi}_p)}{\partial \xi_1} = (l_{1,e}, 0)^\top, \quad \boldsymbol{\zeta}_h = \frac{\partial \Phi(\boldsymbol{\xi}_p)}{\partial \xi_2} = (0, l_{2,e})^\top, \quad l_1 = |\boldsymbol{\zeta}_1| = l_{1,e}.$$

The angle in between is

$$\beta = \arccos\left(\frac{\boldsymbol{\zeta}_1 \cdot \boldsymbol{\zeta}_h}{|\boldsymbol{\zeta}_1||\boldsymbol{\zeta}_h|}\right) = \frac{\pi}{2}.$$

The angle in parameter space is then also $\alpha = \pi^2/(4\beta) = \pi/2$. Using (16) the orthogonal tangent vector $\boldsymbol{\zeta}_2$ becomes $\boldsymbol{\zeta}_2 = \boldsymbol{\zeta}_h$. Then $l_2 = |\boldsymbol{\zeta}_h| = l_{2,e}$.

This leads to a transformation matrix

$$T_\Psi(\boldsymbol{\xi}) = \begin{pmatrix} \cos(\alpha)^2/l_2^2 + 1/l_1^2 & \sin(\alpha)\,\cos(\alpha)/l_2^2 \\ \sin(\alpha)\,\cos(\alpha)/l_2^2 & \sin(\alpha)^2/l_2^2 \end{pmatrix} = \begin{pmatrix} 1/l_{1,e}^2 & 0 \\ 0 & 1/l_{2,e}^2 \end{pmatrix}.$$

When the mesh resolution is uniform, i.e. $l_{1,e} = l_{2,e} = l_e$, the transformation matrix becomes a scaled identity matrix, $T_\Psi(\boldsymbol{\xi}) = l_e^{-2}\,\mathbf{I}$ and the transformation can be moved out of the integral. The prefactor is then

$$\mathcal{J}_2\, l_e^{-2} = 1.$$

3D case. Similar to the 2D case when a rectangular 3D grid with grid widths $l_{1,e}, l_{2,e}, l_{3,e}$ is assumed, the transformation factor becomes

$$\mathcal{J}_3 = |l_{1,e}\, l_{2,e}\, l_{3,e}|.$$

With the world mapping $\Phi(\boldsymbol{\xi})$ and its Jacobian $J_\Phi(\boldsymbol{\xi})$ given by

$$\Phi(\boldsymbol{\xi}) = \mathbf{x}^1 + \begin{pmatrix} \xi_1\, l_{1,e} \\ \xi_2\, l_{2,e} \\ \xi_3\, l_{3,e} \end{pmatrix}, \quad J_\Phi(\boldsymbol{\xi}) = \begin{pmatrix} l_{1,e} & 0 & 0 \\ 0 & l_{2,e} & 0 \\ 0 & 0 & l_{3,e} \end{pmatrix},$$

the transformation matrix becomes

$$T_\Phi(\boldsymbol{\xi}) := J_\Phi^{-1}(\boldsymbol{\xi}) J_\Phi^{-\top}(\boldsymbol{\xi}) = \begin{pmatrix} l_{1,e}^{-2} & 0 & 0 \\ 0 & l_{2,e}^{-2} & 0 \\ 0 & 0 & l_{3,e}^{-2} \end{pmatrix}.$$

With uniform grid lengths, $l_{1,e} = l_{2,e} = l_{3,e} = l_e$, we get $T_\Phi(\boldsymbol{\xi}) = l_e^{-2}\,\mathbf{I}$. The prefactor of the integral

yields

$$\mathcal{J}_3\, l_e^{-2} = l_e.$$

In the presented special cases with uniform grid resolution $\mathcal{J}_d$ did not depend on the integration domain, which allows to compute the factor separately:

$$\int_\Omega \nabla\phi_i \cdot T\nabla\phi_j \, \mathcal{J}_d \, \mathrm{d}\boldsymbol{\xi} = \mathcal{J}_d \, l_e^{-2} \int_\Omega \nabla\phi_i \cdot \nabla\phi_j \, \mathrm{d}\boldsymbol{\xi}.$$

Now the term $-\int \nabla\phi_i \cdot \nabla\phi_j \, \mathrm{d}\xi$, remains to be computed. We compute values at the nodes and visualize them using *stencil notation*. For a fixed node i we compute the respective values for adjacent nodes j. The result for $i = j$ is underlined in the stencil, the values for adjacent nodes are placed left, right, top and bottom, in the position of the respective nodes.

We first compute element-wise stencils that state the contribution of a single element. If all elements have the same length properties, the element contributions can be summed up to get the total value at the nodes which is shown in the nodal stencils. From these stencils we can easily set up the stiffness matrix for a non-varying, equidistant mesh.

dim	element contribution	node stencil
1D:	$\begin{bmatrix} \underline{-1} & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & \underline{-2} & 1 \end{bmatrix}$
2D:	$\begin{bmatrix} 1/6 & 1/3 \\ \underline{-2/3} & 1/6 \end{bmatrix}$	$\frac{1}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & \underline{-8} & 1 \\ 1 & 1 & 1 \end{bmatrix}$
3D:	center: $\begin{bmatrix} 0 & 1/12 \\ \underline{-1/3} & 0 \end{bmatrix}$ top: $\begin{bmatrix} 1/12 & 1/12 \\ 0 & 1/12 \end{bmatrix}$	bottom: $\frac{1}{12}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 0 & 2 \\ 1 & 2 & 1 \end{bmatrix}$ center: $\frac{1}{12}\begin{bmatrix} 2 & 0 & 2 \\ 0 & \underline{-32} & 0 \\ 2 & 0 & 2 \end{bmatrix}$ top: $\frac{1}{12}\begin{bmatrix} 1 & 2 & 1 \\ 2 & 0 & 2 \\ 1 & 2 & 1 \end{bmatrix}$

Tabelle 1: Stencils of the Finite Element stiffness matrix of $-\Delta u$ for an equidistant mesh with uniform resolution. Note, that for 1D, 2D and 3D elements of mesh width h, the prefactors of the integral over the element domain are $1/h$, 1 and h.

1.6 Boundary Conditions

The Neumann-type boundary condition

$$\nabla u(\mathbf{x}) \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma_N$$

is satisfied automatically by the Galerkin finite element formulation. Starting from the left hand side of (25) and using Divergence theorem we get:

$$-\int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}\mathbf{x} = -\int_{\partial\Omega} \phi \left(\nabla u \cdot \mathbf{n}\right) \mathrm{d}\mathbf{x} + \int_\Omega \Delta u \, \phi \, \mathrm{d}\mathbf{x} = 0 \qquad \forall \phi \in H_0^1(\Omega)$$

Because $\Delta u = 0$ on Ω we get $\nabla u \cdot \mathbf{n} = 0$ on the boundary.

1.6.1 Dirichlet boundary conditions in strong form

Dirichlet boundary conditions can be easily considered at the discretized system. For each condition $u_i = u_{0,i}$ that enforces the degree of freedom $i \in I_{\mathrm{BC}}$ to have the value $u_{0,i}$ we modify the linear system of equations. In the right hand side vector we subtract from the value f_j the product of a_{ji} and the given value $u_{0,i}$ for every $j \neq i$, i.e. the new value is $\hat{f}_j = f_j - a_{ji}\, u_{0,i}$. We set $f_i = u_{0,i}$. In the matrix we zero the row and column that contain the entry a_{ii}, i.e. $a_{ij} = a_{ji} = 0, \forall j \neq i$ and set $a_{ii} = 1$. As an example, consider the system

$$\begin{pmatrix} m_{11} & m_{12} & m_{13} \\ m_{21} & m_{22} & m_{23} \\ m_{31} & m_{32} & m_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

with the Dirichlet boundary condition $u_3 = u_{0,3}$. The modified system is then given by

$$\begin{pmatrix} m_{11} & m_{12} & 0 \\ m_{21} & m_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} -m_{13}\, u_{0,3} \\ -m_{23}\, u_{0,3} \\ u_{0,3} \end{pmatrix}.$$

1.6.2 Dirichlet boundary conditions in weak form

We modify the system (7) and add the weak form of the Dirichlet boundary conditions:

$$-\sum_{i=1}^{N} u_i \int_\Omega \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\mathbf{x} = -\sum_{i \in I_{\mathrm{BC}}} u_{0,i} \int_\Omega \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\mathbf{x} \quad \text{for } j = 1, \ldots, N.$$

1.7 Function spaces

For the weak solutions u of the problems we do not need to request $\mathcal{C}^2(\Omega)$, since only the first derivatives are needed and only in a weak sense. Therefore $u \in H_0^1(\Omega)$ suffices.

The Hilbert space $H^1(\Omega)$ is the Sobolev space $\mathcal{W}^{1,2}(\Omega)$ which is defined using weak derivatives. The concept of weak derivatives generalizes the classical derivatives.

Let $u, v \in \mathcal{L}^1_{\mathrm{loc}}(\Omega)$ and $\alpha \in \mathbb{N}_0^d$ a multi-index. Then v is called *weak derivative* of u of order α if

$$\int_\Omega u(\mathbf{x}) \mathcal{D}^\alpha \phi(\mathbf{x}) \, \mathrm{d}\mathbf{x} = (-1)^{|\alpha|} \int_\Omega v(\mathbf{x})\, \phi(\mathbf{x}) \, \mathrm{d}\mathbf{x} \tag{18}$$

for all $\phi \in \mathcal{C}_0^\infty(\Omega)$. We then write $\mathcal{D}^\alpha u = v$. The derivative with the multi-index, $\mathcal{D}^\alpha$ is given by

$$\mathcal{D}^\alpha = \frac{\partial^{|\alpha|}}{\partial_{x_1}^{\alpha_1} \cdots \partial_{x_d}^{\alpha_d}} \tag{19}$$

If u is differentable in a classical sense, the classical derivatives are also the weak derivatives.

Now we define the *Sobolev* space $\mathcal{W}^{1,2}(\Omega)$ (1=first order weak derivatives, 2=derivatives in $\mathcal{L}^2(\Omega)$)) as follows:

$$\mathcal{W}^{1,2}(\Omega) := \{u \in \mathcal{L}^1_{\text{loc}}(\Omega) \mid |\alpha| \in \mathbb{N}_0^d, |\alpha| \leq 1, \mathcal{D}^\alpha u \text{ exists}, \mathcal{D}^\alpha u \in \mathcal{L}^2(\Omega)\}. \tag{20}$$

With an appropriate Sobolev norm, $\mathcal{W}^{1,2}$ is a Banach space, i.e. complete (Cauchy series converge in it).

Together with the scalar product

$$(u, v)_{H^1} := \sum_{|\alpha| \leq 1} \int_\Omega \mathcal{D}^\alpha u(\mathbf{x})\, \mathcal{D}^\alpha v(\mathbf{x})\, \mathrm{d}\mathbf{x} \tag{21}$$

we get the Hilbert space $H^1(\Omega) := \mathcal{W}^{1,2}(\Omega)$.

With $H_0^1(\Omega) := \{u \in H^1(\Omega) \mid u(\mathbf{x}) = 0 \text{ for } \mathbf{x} \in \partial\Omega\}$ we denote the subspace of functions that are 0 on the boundary.

2 Poisson Equation

The Poisson equation is a generalization of the Laplace equation and is given by

$$\Delta u = f \qquad \text{on } \Omega.$$

It can be subject to the same boundary conditions as Laplace equation, i.e. Neumann-type boundary conditions

$$\nabla u(\mathbf{x}) \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma_N,$$

as well as Dirichlet-type boundary conditions

$$u(\mathbf{x}) = u_0(\mathbf{x}) \qquad \text{on } \Gamma_D.$$

The finite element formulation proceeds similar to Chap. 1, multiplication of a testfunction $\phi \in H_0^1(\Omega)$ and integration yields

$$\int_\Omega \Delta u\, \phi \, \mathrm{d}\mathbf{x} = \int_\Omega f\, \phi \, \mathrm{d}\mathbf{x}, \quad \forall \phi \in H_0^1(\Omega).$$

Applying divergence theorem we get

$$-\int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}\mathbf{x} = \int_\Omega f\, \phi \, \mathrm{d}\mathbf{x} \quad \forall \phi \in H_0^1(\Omega). \tag{22}$$

Like the solution $u(\mathbf{x})$ also the right hand side $f(\mathbf{x})$ has to be spatially discretized by a linear combination of coefficients and basis functions:

$$u_h(\mathbf{x}) = \sum_{i=1}^{N} u_i \, \phi_i(\mathbf{x}),$$
$$f_h(\mathbf{x}) = \sum_{i=1}^{N} f_i \, \phi_i(\mathbf{x}).$$

By again choosing the space of testfunctions to be the same as the span of basis functions, $V = \text{span}\,\{\phi_1, \ldots, \phi_n\}$ we get the Galerkin formulation as

$$-\sum_{i=1}^{N} u_i \int_\Omega \nabla\phi_i \cdot \nabla\phi_j \, \mathrm{d}\mathbf{x} = \sum_{i=1}^{N} f_i \int_\Omega \phi_i \cdot \phi_j \, \mathrm{d}\mathbf{x} \quad \text{for } j = 1, \ldots, N.$$

The domain Ω is again decomposed into disjoint elements $\Omega_e, e = 1, \ldots, M$ and integration has only be performed over the elements where none of the basis function vanish.

The first integral term, $\int_\Omega \nabla\phi_i \cdot \nabla\phi_j \, \mathrm{d}\mathbf{x}$, has to be computed as described in Section 1.5. How to compute the second integral term, $\int_\Omega \phi_i \cdot \phi_j \, \mathrm{d}\mathbf{x}$ is shown in the following.

Similar as before, the integration domain is transferred from element space to parameter space. For this a transformation factor $\mathcal{J}_d$ has to be considered, which is constant for some special cases as discussed in section 1.5.

For the remaining integral, $\int_\Omega \phi_i \cdot \phi_j \, \mathrm{d}\boldsymbol{\xi}$ node stencils are provided in the following table.

dim	element contribution	node stencil
1D:	$\frac{1}{6}\begin{bmatrix} \underline{2} & 1 \end{bmatrix}$	$\frac{1}{6}\begin{bmatrix} 1 & \underline{4} & 1 \end{bmatrix}$
2D:	$\frac{1}{36}\begin{bmatrix} 2 & 1 \\ \underline{4} & 2 \end{bmatrix}$	$\frac{1}{36}\begin{bmatrix} 1 & 4 & 1 \\ 4 & \underline{16} & 4 \\ 1 & 4 & 1 \end{bmatrix}$
3D:	center: $\frac{1}{216}\begin{bmatrix} 4 & 2 \\ \underline{8} & 4 \end{bmatrix}$ top: $\frac{1}{216}\begin{bmatrix} 2 & 1 \\ 4 & 2 \end{bmatrix}$	bottom: $\frac{1}{216}\begin{bmatrix} 1 & 4 & 1 \\ 4 & 16 & 4 \\ 1 & 4 & 1 \end{bmatrix}$ center: $\frac{1}{216}\begin{bmatrix} 4 & 16 & 4 \\ 16 & \underline{64} & 16 \\ 4 & 16 & 4 \end{bmatrix}$ top: $\frac{1}{216}\begin{bmatrix} 1 & 4 & 1 \\ 4 & 16 & 4 \\ 1 & 4 & 1 \end{bmatrix}$

Tabelle 2: Stencils of the Finite Element right hand side for an equidistant mesh with uniform resolution. Note, that for 1D, 2D and 3D elements of mesh width h, the prefactors of the integral over the element domain are h, h^2 and h^3.

3 Generalized Laplace operator

The Laplace equation $\Delta u = 0$ describes steady-state matter-/heat-/current flow where the computed quantity u designates the potential that induces the flow $\mathbf{F}$, which can be modelled as being directed against the potential gradient, $\mathbf{F} = -\nabla u$. In terms of heat transfer this is *Fick's law*. By considering the conservation law of the flowing quantity we assume $\nabla \cdot \mathbf{F} = 0$ which leads directly to the Laplace equation.

If the medium in which the flow occurs is non-isotropic this can be modelled by adjusting the relationship between the negative potential gradient, $-\nabla u$, and the induced flow direction, F. By applying a linear map A onto the negative gradient vector which can be thought of being the sum of contributions in coordinate directions, each contribution vector of a coordinate direction gets scaled and projected to a new direction. The flow is then $\mathbf{F} = -A\nabla u$ and the resulting equation is called generalized Laplace equation, reading

$$\nabla \cdot (A\nabla u) = 0.$$

The parantheses can also be neglected. $\nabla \cdot A\nabla$ is referred to as generalized Laplace operator.

The derivation of the Finite Element formulation proceeds analoguos to section 1. Multiplication with a testfunction ϕ yields:

$$\int_\Omega \nabla \cdot A\nabla u \, \phi \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi \in H_0^1(\Omega) \tag{23}$$

Applying divergence theorem (67) with $f = \phi$ and $\mathbf{F} = A\nabla u$ yields

$$-\int_\Omega A\nabla u \cdot \nabla \phi \, \mathrm{d}\mathbf{x} + \int_{\partial\Omega} (\phi \, A\nabla u) \cdot \mathbf{n} \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi \in H_0^1(\Omega). \tag{24}$$

Because ϕ is zero on the boundary, the boundary integral vanishes:

$$-\int_\Omega A\nabla u \cdot \nabla \phi \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi \in H_0^1(\Omega). \tag{25}$$

The discretization remains the same and leads to an integral term of

$$m_{ji} = -\int_\Omega A\nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\mathbf{x}.$$

for the stiffness matrix M. For these term the stencil notation cannot be applied in general. The stiffness matrix has to be computed using e.g. numerical quadrature.

4 Diffusion Equation

The diffusion equation is given by

$$u_t = c \, \Delta u, \qquad c \in \mathbb{R} \tag{26}$$

For the finite element formulation it can be seen as a Poisson equation with right hand side u_t, neglecting the constant c for now. We get from (22):

$$-\int_\Omega \nabla u \cdot \nabla \phi \, \mathrm{d}\mathbf{x} = \int_\Omega u_t \, \phi \, \mathrm{d}\mathbf{x} \quad \forall \phi \in H_0^1(\Omega). \tag{27}$$

The derivative in time, u_t can be discretized by a differential quotient as follows:

$$u_t = \frac{u^{(t+1)} - u^{(t)}}{dt},$$

where dt is the time step width. In space we formulate the quantity again with a discrete basis:

$$u_h^{(t)}(\mathbf{x}) = \sum_{i=1}^{N} u_i^{(t)} \, \phi_i(\mathbf{x}).$$

Substituting into (27) yields:

$$\begin{aligned} & -\int_\Omega \nabla u^{(t)} \cdot \nabla \phi \, \mathrm{d}\mathbf{x} = \frac{1}{dt} \int_\Omega \left(u^{(t+1)} - u^{(t)} \right)) \, \phi \, \mathrm{d}\mathbf{x} \quad \forall \phi \in H_0^1(\Omega) \\ \Leftrightarrow \quad & -\sum_{i=1}^{N} u_i^{(t)} \int_\Omega \nabla \phi_i \cdot \nabla \phi_j \, \mathrm{d}\mathbf{x} = \frac{1}{dt} \sum_{i=1}^{N} (u_i^{(t+1)} - u_i^{(t)}) \int_\Omega \phi_i \cdot \phi_j \, \mathrm{d}\mathbf{x} \qquad \text{for } j = 1, \ldots, N. \end{aligned}$$

We use the matrix notation with the stiffness matrix, $\mathbf{K}$, and the mass matrix, $\mathbf{M}$. For the explicit Euler scheme $u^{(t+1)} = u^{(t)} + dt \, f(t, u^{(t)})$, we get

$$\begin{aligned} \mathbf{K}\mathbf{u}^{(t)} &= \frac{1}{dt} \mathbf{M} \left(\mathbf{u}^{(t+1)} - \mathbf{u}^{(t)} \right) \\ \mathbf{u}^{(t+1)} &= \mathbf{u}^{(t)} + dt \, \mathbf{M}^{-1} \mathbf{K} \mathbf{u}^{(t)} \\ &= \left(\mathbf{I} + dt \, \mathbf{M}^{-1} \mathbf{K} \right) \mathbf{u}^{(t)}. \end{aligned}$$

For an implicit Euler scheme $u^{(t+1)} = u^{(t)} + dt \, f(t+1, u^{(t+1)})$, we get

$$\begin{aligned} \mathbf{K}\mathbf{u}^{(t+1)} &= \frac{1}{dt} \mathbf{M} \left(\mathbf{u}^{(t+1)} - \mathbf{u}^{(t)} \right) \\ (I - dt \, \mathbf{M}^{-1} \mathbf{K}) \, \mathbf{u}^{(t+1)} &= \mathbf{u}^{(t)} \end{aligned}$$

or

$$(\mathbf{K} - \frac{\mathbf{M}}{dt}) \mathbf{u}^{(t+1)} = -\frac{\mathbf{M}}{dt} \mathbf{u}^{(t)}$$

The second form may be beneficial in case of variable time step.

For the Crank-Nicolson scheme $u^{(t+1)} = u^{(t)} + dt \, (f(t+1, u^{(t+1)}) + f(t, u^{(t)}))/2$, we get

$$\begin{aligned} \frac{\mathbf{K}(\mathbf{u}^{(t+1)} + \mathbf{u}^{(t)})}{2} &= \frac{1}{dt} \mathbf{M} \left(\mathbf{u}^{(t+1)} - \mathbf{u}^{(t)} \right) \\ (I - \frac{dt}{2} \, \mathbf{M}^{-1} \mathbf{K}) \, \mathbf{u}^{(t+1)} &= \mathbf{u}^{(t)} (I + \frac{dt}{2} \, \mathbf{M}^{-1} \mathbf{K}) \end{aligned}$$

or

$$(\frac{1}{2}\,\mathbf{K} - \frac{1}{dt}\,\mathbf{M})\mathbf{u}^{(t+1)} = (-\frac{1}{2}\,\mathbf{K} - \frac{1}{dt}\,\mathbf{M})\mathbf{u}^{(t)}$$

4.1 Lumped Mass Matrix

For linear or bilinear basis functions

$$\begin{cases} m'_{i,j} = 0 & i \neq j \\ m'_{i,i} = S(i) & i = 1, ..., n \end{cases},$$

where $S(i) = \sum_{j=1}^{n} m_{i,j}$ for $i = 1, ..., n$.
For orders of basis greater than two suggested from Hinton et al. [2]:

$$\begin{cases} m'_{i,j} = 0 & i \neq j \\ m'_{i,i} = \frac{S}{D} m_{i,i} & i = 1, ..., n \end{cases} \tag{28}$$

where $S = \sum_{i=1}^{n} \sum_{j=1}^{n} m_{i,j}$ and $D = \sum_{i=1}^{n} m_{i,i}$.

4.2 Analytical Solution

The analytical solution to the diffusion equation (26) makes use of the fundamental solution

$$H(x,t) = \frac{1}{\sqrt{4\pi\, c\, t}} \exp\left(-\frac{x^2}{4\, c\, t}\right) \quad \text{for 1D}$$
$$H(\mathbf{x},t) = \frac{1}{(4\pi\, c\, t)^{n/2}} \exp\left(-\frac{\|\mathbf{x}\|_2^2}{4\, c\, t}\right) \quad \text{for 2D,3D}$$

For $\Omega = \mathbb{R}^d$ and initial condition

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}) \qquad \mathbf{x} \in \Omega$$

the solution is

$$u(\mathbf{x}, t) = \int_{\mathbb{R}^d} H(\mathbf{x} - \mathbf{y}, t)\, u_0(\mathbf{y})\, \mathrm{d}\mathbf{y}.$$

4.3 Derivation with boundary conditions

4.3.1 Diffusion problem

In general, the weak form of a diffusion problem discretized with Crank-Nicolson,

$$\nabla \cdot (\boldsymbol{\sigma} \nabla u) = u_t, \qquad \frac{\partial u}{\partial \mathbf{n}} = f \quad \text{on } \Gamma_f, \qquad \frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on } \partial\Omega \backslash \Gamma_f$$
$$\Rightarrow \quad \int_\Omega \left(\theta\, \nabla \cdot (\boldsymbol{\sigma} \nabla u^{(i+1)}) + (1-\theta)\, \nabla \cdot (\boldsymbol{\sigma} \nabla u^{(i)})\right) \phi\, \mathrm{d}\mathbf{x} = \frac{1}{dt} \int_\Omega (u^{(i+1)} - u^{(i)})\, \phi\, \mathrm{d}\mathbf{x}, \quad \forall \phi \in V_h \tag{29}$$

Discretize in space with $u = \sum_j u_j\,\varphi_j, V_h = \operatorname{span}\{\varphi_j | j = 1 \dots N\}$ and using Divergence theorem

$$\begin{aligned}\sum_{j=1}^{N} \left(\theta\, u_j^{(i+1)} + (1-\theta)\, u_j^{(i)}\right) \left(-\int_\Omega (\boldsymbol{\sigma} \nabla\varphi_j)\cdot\nabla\phi_k \,\mathrm{d}\mathbf{x} + \int_{\partial\Omega} (\boldsymbol{\sigma}\,\nabla\varphi_j\cdot\mathbf{n})\phi_k \,\mathrm{d}\mathbf{x}\right) \\ = \frac{1}{dt}\sum_{j=1}^{N}\left(u_j^{(i+1)} - u_j^{(i)}\right)\int_\Omega \varphi_j\,\phi_k\,\mathrm{d}\mathbf{x}, \quad \forall k = 1\dots N.\end{aligned} \tag{30}$$

The ansatz functions for discretization and the test functions are chosen to be equal, $\phi_j = \varphi_j$.

The formulation can be written in matrix notation as

$$\mathbf{A}\,\mathbf{u}^{(i+1)} = \mathbf{b}(\mathbf{u}^{(i)}), \tag{31}$$

where

$$\begin{aligned}\mathbf{A} &= \theta\,(\mathbf{K}+\mathbf{B}) - \frac{1}{dt}\,\mathbf{M}, \\ \mathbf{b} &= \left((\theta-1)\,(\mathbf{K}+\mathbf{B}) - \frac{1}{dt}\,\mathbf{M}\right)\mathbf{u}^{(i)},\end{aligned} \tag{32}$$

with

$$\begin{aligned}\mathbf{K}_{kj} &= -\int_\Omega \boldsymbol{\sigma}\,\nabla\varphi_j\cdot\nabla\varphi_k\,\mathrm{d}\mathbf{x} \qquad \text{(note, the minus sign is correct for } +\Delta\text{)}, \\ \mathbf{B}_{kj} &= \int_{\Gamma_f} (\boldsymbol{\sigma}\,\nabla\varphi_j\cdot\mathbf{n})\varphi_k\,\mathrm{d}\mathbf{x}, \\ \mathbf{M}_{kj} &= \int_\Omega \varphi_j\,\varphi_k\,\mathrm{d}\mathbf{x},\end{aligned}$$

or written in component form:

$$\begin{aligned}\mathbf{A}_{kj} &= \theta\,\left(-\int_\Omega \boldsymbol{\sigma}\,\nabla\varphi_j\cdot\nabla\varphi_k\,\mathrm{d}\mathbf{x} + \int_{\partial\Omega}(\boldsymbol{\sigma}\,\nabla\varphi_j\cdot\mathbf{n})\varphi_k\,\mathrm{d}\mathbf{x}\right) - \frac{1}{dt}\int_\Omega \varphi_j\,\varphi_k\,\mathrm{d}\mathbf{x}, \\ \mathbf{b}_k &= \sum_{j=1}^{N} -(1-\theta)\,u_j^{(i)}\,\left(-\int_\Omega \boldsymbol{\sigma}\,\nabla\varphi_j\cdot\nabla\varphi_k\,\mathrm{d}\mathbf{x} + \int_{\partial\Omega}(\boldsymbol{\sigma}\,\nabla\varphi_j\cdot\mathbf{n})\varphi_k\,\mathrm{d}\mathbf{x}\right) + \frac{1}{dt}\sum_{j=1}^{N}(-u_j^{(i)})\int_\Omega \varphi_j\,\varphi_k\,\mathrm{d}\mathbf{x}.\end{aligned}$$

So far we did not plug in the boundary conditions. For $f = 0$ we get $\mathbf{B} = \mathbf{0}$. The case $f \neq 0$ is handled in the next subsection.

4.3.2 Boundary conditions

The boundary condition $\boldsymbol{\sigma}\,\nabla u\cdot\mathbf{n} = f$ can be written as

$$\boldsymbol{\sigma}\,\nabla u\cdot\mathbf{n} = \sum_{j=1}^{N} u_j\,(\boldsymbol{\sigma}\,\nabla\varphi_j\cdot\mathbf{n}) = f,$$

We discretize the flow over the boundary, f, by different ansatz functions, ψ_j, with coefficients f_j:

$$f = \sum_{j=1}^{N} f_j \, \psi_j$$

We get from (30)

$$\begin{aligned}
&\sum_{j=1}^{N} \left(\theta \, u_j^{(i+1)} + (1-\theta) \, u_j^{(i)}\right) \left(-\int_\Omega \boldsymbol{\sigma} \, \nabla\varphi_j \cdot \nabla\varphi_k \, \mathrm{d}\mathbf{x}\right) + \int_{\Gamma_f} \left(\theta \, f^{(i+1)} + (1-\theta) \, f^{(i)}\right) \varphi_k \, \mathrm{d}\mathbf{x} \\
&\quad = \frac{1}{dt} \sum_{j=1}^{N} \left(u_j^{(i+1)} - u_j^{(i)}\right) \int_\Omega \varphi_j \, \varphi_k \, \mathrm{d}\mathbf{x}, \quad \forall k = 1 \ldots N, \\
\Leftrightarrow \quad &\sum_{j=1}^{N} \left(\theta \, u_j^{(i+1)} + (1-\theta) \, u_j^{(i)}\right) \left(-\int_\Omega \boldsymbol{\sigma} \, \nabla\varphi_j \cdot \nabla\varphi_k \, \mathrm{d}\mathbf{x}\right) + \sum_{j=1}^{N} \left(\theta \, f_j^{(i+1)} + (1-\theta) \, f_j^{(i)}\right) \int_{\Gamma_f} \psi_j \, \varphi_k \, \mathrm{d}\mathbf{x} \\
&\quad = \frac{1}{dt} \sum_{j=1}^{N} \left(u_j^{(i+1)} - u_j^{(i)}\right) \int_\Omega \varphi_j \, \varphi_k \, \mathrm{d}\mathbf{x}, \quad \forall k = 1 \ldots N,
\end{aligned}$$

In matrix notation,

$$\mathbf{A} \, \mathbf{u}^{(i+1)} = \mathbf{b}(\mathbf{u}^{(i)}), \tag{33}$$

we have

$$\begin{aligned}
\mathbf{A} &= \theta \, \mathbf{K} - \frac{1}{dt} \, \mathbf{M}, \\
\mathbf{b} &= \left((\theta - 1) \, \mathbf{K} - \frac{1}{dt} \, \mathbf{M}\right) \mathbf{u}^{(i)} - \mathbf{B}_{\Gamma_f} \left(\theta \, \mathbf{f}^{(i+1)} + (1-\theta) \, \mathbf{f}^{(i)}\right),
\end{aligned} \tag{34}$$

with

$$\begin{aligned}
\mathbf{K}_{kj} &= -\int_\Omega \boldsymbol{\sigma} \, \nabla\varphi_j \cdot \nabla\varphi_k \, \mathrm{d}\mathbf{x} \qquad \text{(note, the minus sign is correct for } +\Delta\text{)}, \\
\mathbf{M}_{kj} &= \int_\Omega \varphi_j \, \varphi_k \, \mathrm{d}\mathbf{x}, \\
\mathbf{B}_{\Gamma_f,kj} &= \int_{\Gamma_f} \psi_j \, \varphi_k \, \mathrm{d}\mathbf{x},
\end{aligned}$$

4.3.3 Laplace problem

We consider $\nabla \cdot (\boldsymbol{\sigma} \nabla \mathbf{u}) = 0$ with Neumann boundary condition, $\partial(\boldsymbol{\sigma} \, \mathbf{u})/\partial\mathbf{n} = \mathbf{f}$. This leads to

$$(\mathbf{K} + \mathbf{B}) \, \mathbf{u} = \mathbf{0} \qquad \text{or} \qquad \mathbf{K} \, \mathbf{u} + \mathbf{B}_{\Gamma_f} \, \mathbf{f} = 0.$$

4.3.4 Two coupled Laplace problems

We have the domain as in fig. 2 and the following equations:

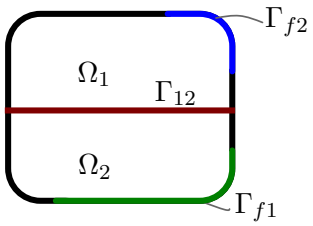


Abbildung 2: Two domains

$$\nabla \cdot (\boldsymbol{\sigma}_1 \nabla u_1) = \mathbf{f}_1, \quad \text{on } \Omega_1 \qquad \partial u_1/\partial \mathbf{n} = g_1 \quad \text{on } \Gamma_{f1}$$

$$\nabla \cdot (\boldsymbol{\sigma}_2 \nabla u_2) = \mathbf{f}_2, \quad \text{on } \Omega_2 \qquad \partial u_2/\partial \mathbf{n} = g_2 \quad \text{on } \Gamma_{f2}$$

$$u_1 = u_2, \quad q := (\boldsymbol{\sigma}_1 \nabla u_1) \cdot \mathbf{n} = (\boldsymbol{\sigma}_1 \nabla u_2) \cdot \mathbf{n} \quad \text{on } \Gamma_{12}$$

The flux over Γ_{12} is

$$q(\mathbf{x}) := (\boldsymbol{\sigma}_1 \nabla u_1(\mathbf{x})) \cdot \mathbf{n} = \sum_{i=1}^{N} u_i \, (\boldsymbol{\sigma}_1 \nabla \varphi_i(\mathbf{x})) \cdot \mathbf{n} \quad \text{for } \mathbf{x} \in \Gamma_{12}.$$

This is only defined for quadratic ansatz functions. The flux condition is therefore forced in a weak form.

The Finite Element formulation leads to

$$\mathbf{K}_{\boldsymbol{\sigma}_1} \, \mathbf{u}_1 = \mathbf{f}_1 - \mathbf{B}_{\Gamma_{f1}} \, \mathbf{g}_1 - \mathbf{B}_{\Gamma_{12}} \, \mathbf{q}_1,$$

$$\mathbf{K}_{\boldsymbol{\sigma}_2} \, \mathbf{u}_2 = \mathbf{f}_2 - \mathbf{B}_{\Gamma_{f2}} \, \mathbf{g}_2 - \mathbf{B}_{\Gamma_{12}} \, \mathbf{q}_2,$$

$$\mathbf{B}_{\Gamma_{12}} \, \mathbf{q}_1 = -\mathbf{B}_{\Gamma_{12}} \, \mathbf{q}_2$$

where

$$\mathbf{K}_{\boldsymbol{\sigma},kj} = -\int_{\Omega} (\boldsymbol{\sigma} \nabla \varphi_j) \cdot \nabla \varphi_k \, \mathrm{d}\mathbf{x} \qquad \text{(note, the minus sign is correct for } +\Delta),$$

$$\mathbf{B}_{\Gamma_f,kj} = \int_{\Gamma_f} \psi_j \, \varphi_k \, \mathrm{d}\mathbf{x}.$$

Combining the two equations we get the system

$$\begin{bmatrix} \mathbf{K}_{\boldsymbol{\sigma}_1} & \\ & \mathbf{K}_{\boldsymbol{\sigma}_2} \end{bmatrix} \begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{f}_1 - \mathbf{B}_{\Gamma_{f1}} \, \mathbf{g}_1 - \mathbf{B}_{\Gamma_{12}} \, \mathbf{q}_1 \\ \mathbf{f}_2 - \mathbf{B}_{\Gamma_{f2}} \, \mathbf{g}_2 - \mathbf{B}_{\Gamma_{12}} \, \mathbf{q}_2 \end{bmatrix}$$

Here, $\mathbf{u}_1$ and $\mathbf{u}_2$ are the degrees of freedom in $\Omega_1 \cup \Gamma_{12}$ and $\Omega_2 \cup \Gamma_{12}$. The degrees of freedom on Γ_{12} appear in $\mathbf{u}_1$ as well as in $\mathbf{u}_2$. $\mathbf{K}_{\boldsymbol{\sigma}_1}$ and $\mathbf{K}_{\boldsymbol{\sigma}_2}$ are computed by integrating only over the domains Ω_1 and Ω_2, respectively. of freedom in $\Omega_1 \backslash \Gamma_{12}$ and $\Omega_2 \backslash \Gamma_{12}$, $\mathbf{K}_{\sigma_{12}} = \mathbf{K}_{\sigma_1} + \mathbf{K}_{\sigma_2}$ on Γ_{12}. Static condensation of $q_1 = -q_2$:

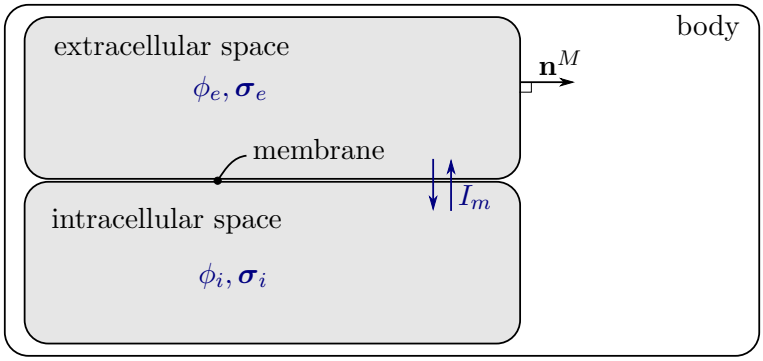


Abbildung 3: Setting of the Bidomain model

$$\mathbf{B}_{\Gamma_{12}}\,\mathbf{q}_2 = \mathbf{f}_2 - \mathbf{B}_{\Gamma_{f2}}\,\mathbf{g}_2 - \mathbf{K}_{\boldsymbol{\sigma}_2}\,\mathbf{u}_2$$

$$\Rightarrow \quad \mathbf{K}_{\boldsymbol{\sigma}_1}\,\mathbf{u}_1 = \mathbf{f}_1 - \mathbf{B}_{\Gamma_{f1}}\,\mathbf{g}_1 + \mathbf{f}_2 - \mathbf{B}_{\Gamma_{f2}}\,\mathbf{g}_2 - \mathbf{K}_{\boldsymbol{\sigma}_2}\,\mathbf{u}_2$$

$$\Rightarrow \quad \mathbf{K}_{\boldsymbol{\sigma}_1}\,\mathbf{u}_1 + \mathbf{K}_{\boldsymbol{\sigma}_2}\,\mathbf{u}_2 = \mathbf{f}_1 - \mathbf{B}_{\Gamma_{f1}}\,\mathbf{g}_1 + \mathbf{f}_2 - \mathbf{B}_{\Gamma_{f2}}\,\mathbf{g}_2$$

$$\begin{bmatrix}\mathbf{K}_{\boldsymbol{\sigma}_1} & \mathbf{K}_{\boldsymbol{\sigma}_2}\end{bmatrix}\begin{bmatrix}\mathbf{u}_1\\ \mathbf{u}_2\end{bmatrix} = \begin{bmatrix}\mathbf{f}_1 + \mathbf{f}_2 - \mathbf{B}_{\Gamma_{f1}}\,\mathbf{g}_1 - \mathbf{B}_{\Gamma_{f2}}\,\mathbf{g}_2\end{bmatrix}$$

This means the systems is solved normally as if there was no separation in Ω_1, Ω_2.

5 Models of Electrophysiology

In the following the Bidomain and Monodomain models are derived.

5.1 The Bidomain Model

The Bidomain model considers two computational domains of intra-cellular and extra-cellular space. In a homogenised view it is assumed that these domains share space such that at each spatial point there coexist both domains at the same time. Both domains have their own conductivity tensors $\boldsymbol{\sigma}_i, \boldsymbol{\sigma}_e$ and electric potential ϕ_i, ϕ_e, as depicted in fig. 3. An electric current I_m between the computational domains is possible and has to pass the cell membrane. For specifying boundary conditions of the Bidomain equations, a third domain, the surrounding body, is assumed, that receives a current from the extracellular domain, but not from the intracellular space. For Monodomain equation this current is later set to 0.

Starting point of the derivation is a form of Ohm's Law by which the current density J is a result of an electric field E that exists in a medium with electric conductivity $\boldsymbol{\sigma}$:

$$J = \boldsymbol{\sigma}\, E.$$

Assuming quasi static conditions, the field strength E is given by the negative gradient of a potential field:

$$E = -\nabla\phi.$$

For the current densities J_i and J_e in the two domains we then have:

$$J_i = -\boldsymbol{\sigma}_i \nabla\phi_i, \qquad J_e = -\boldsymbol{\sigma}_e \nabla\phi_e.$$

Because of the spatial coexistence of the two domains the divergence of the current density in one domain has to be the negative of the divergence at the same point in the other domain,

$$\nabla \cdot J_i = -\nabla \cdot J_e \quad \Leftrightarrow \quad -\nabla \cdot (\boldsymbol{\sigma}_i \nabla\phi_i) = \nabla \cdot (\boldsymbol{\sigma}_e \nabla\phi_e). \tag{35}$$

The current enabling this relationship is the membrane current I_m such that:

$$\nabla \cdot (\boldsymbol{\sigma}_i \nabla\phi_i) = A_m I_m. \tag{36}$$

The factor A_m characterizes the membrane area to domain volume relationship of the cell membrane. Then I_m is a quantity per area. It is the external current in the Hodgkin-Huxley model, **??**, such that eq. (36) becomes:

$$\nabla \cdot (\boldsymbol{\sigma}_i \nabla\phi_i) = A_m \left(C_m \frac{\partial V_m}{\partial t} + I_{ion}(V_m)\right).$$

Using $V_m = \phi_i - \phi_e$, the intracellular potential ϕ_i can be eliminated yielding

$$\nabla \cdot (\boldsymbol{\sigma}_i \nabla V_m) + \nabla \cdot (\boldsymbol{\sigma}_i \nabla\phi_e) = A_m \left(C_m \frac{\partial V_m}{\partial t} + I_{ion}(V_m)\right). \tag{37}$$

The second equation comes from eq. (35) which is also formulated with V_m instead of ϕ_i:

$$\begin{aligned} &\nabla \cdot \left(\boldsymbol{\sigma}_i \nabla(V_m + \phi_e)\right) = -\nabla \cdot (\boldsymbol{\sigma}_e \nabla\phi_e) \\ \Leftrightarrow \quad &\nabla \cdot \left((\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_e) \nabla\phi_e\right) + \nabla \cdot (\boldsymbol{\sigma}_i \nabla V_m) = 0, \end{aligned} \tag{38}$$

Equations (37) and (38) form the Bidomain Equations.

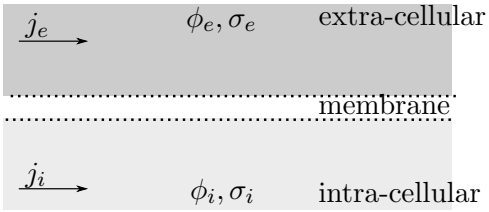
5.2 The Monodomain Model

Under assumption that the anisotropy of the tissue at a point inside and outside the muscle cell is equal, the two Bidomain Equations can be reduced to the single Monodomain Equation. The assumption can be expressed as

$$\boldsymbol{\sigma}_i = k \cdot \boldsymbol{\sigma}_e$$

for a real factor k. Plugging $\boldsymbol{\sigma}_e = \boldsymbol{\sigma}_i / k$ into the second Bidomain Eq. (38) yields

$$\begin{aligned} &\nabla \cdot \left((1 + \frac{1}{k}) \boldsymbol{\sigma}_i \nabla\phi_e\right) + \nabla \cdot (\boldsymbol{\sigma}_i \nabla V_m) = 0 \\ \Leftrightarrow \quad &\nabla \cdot (\boldsymbol{\sigma}_i \nabla\phi_e) = -\frac{k}{k+1} \nabla \cdot (\boldsymbol{\sigma}_i \nabla V_m). \end{aligned} \tag{39}$$



Now eq. (39) can be combined with the first Bidomain Eq. (37) to get:

$$\nabla \cdot (\boldsymbol{\sigma}_i \nabla V_m) - \frac{k}{k+1} \nabla \cdot (\boldsymbol{\sigma}_i \nabla V_m) = A_m \left(C_m \frac{\partial V_m}{\partial t} + I_{ion}(V_m) \right)$$
$$\frac{1}{k+1} \nabla \cdot (\boldsymbol{\sigma}_i \nabla V_m) = A_m \left(C_m \frac{\partial V_m}{\partial t} + I_{ion}(V_m) \right)$$

For the 1D case where the muscle fibre is modeled as a single line this can be simplified to:

$$\nabla \cdot \Big(\underbrace{\frac{\boldsymbol{\sigma}_i}{\boldsymbol{\sigma}_i/\boldsymbol{\sigma}_e + 1}}_{= \frac{\boldsymbol{\sigma}_e \boldsymbol{\sigma}_i}{\boldsymbol{\sigma}_e + \boldsymbol{\sigma}_i}} \nabla V_m \Big) = A_m \left(C_m \frac{\partial V_m}{\partial t} + I_{ion}(V_m) \right)$$

By defining the effective conductivity $\boldsymbol{\sigma}_{\text{eff}} := (\boldsymbol{\sigma}_e \boldsymbol{\sigma}_i)/(\boldsymbol{\sigma}_e + \boldsymbol{\sigma}_i)$ the 1D Monodomain Equation can be written as:

$$\nabla \cdot (\boldsymbol{\sigma}_{\text{eff}} \nabla V_m) = A_m \left(C_m \frac{\partial V_m}{\partial t} + I_{ion}(V_m) \right). \tag{40}$$

This is a 1D PDE in the variable V_m and is usually solved with the boundary condition

$$(\boldsymbol{\sigma}_{\text{eff}} \nabla V_m) \cdot \mathbf{n}^M = 0 \quad \text{on } \Gamma^M.$$

which inhibits current to the outer domain. $\mathbf{n}^M$ is the outward normal vector on the border Γ^M of the muscle fibre surface. The spatial discretization of the diffusion term on the left-hand side of eq. (40) can be achieved by using 1D finite elements.

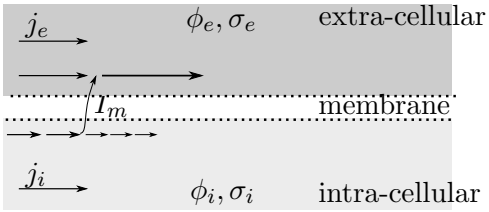
5.3 The 1D Monodomain Equation

We consider 2 domains: intra- and extracellular space. The setting is homogenised such that the domains occupy the same space. The domains have electric potentials ϕ_i, ϕ_e and conductivities σ_i, σ_e, the membrane voltage is defined as $V_m = \phi_i - \phi_e$. The current density can be described by a potential:

$$j_e = -\sigma_e \frac{\partial \phi_e}{\partial x}, \quad j_i = -\sigma_i \frac{\partial \phi_i}{\partial x}$$

Conservation of charges holds, changes in current density affect the other domain.

$$\begin{aligned} & \frac{\partial}{\partial x} j_i = -\frac{\partial}{\partial x} j_e \\ \Leftrightarrow \quad & \frac{\partial}{\partial x} \left(\sigma_i \frac{\partial \phi_i}{\partial x} \right) = -\frac{\partial}{\partial x} \left(\sigma_e \frac{\partial \phi_e}{\partial x} \right) \end{aligned} \tag{41}$$



The current through the domain is given by

$$\begin{aligned} \frac{\partial}{\partial x}\left(\sigma_i \frac{\partial \phi_i}{\partial x}\right) &= I_m \\ &= A_m\Big(C_m \frac{\partial V_m}{\partial t} + I_{\text{ion}}(V_m)\Big) \end{aligned} \tag{42}$$

We assume $\sigma_i = k \cdot \sigma_e$ and substitute $V_m = \phi_i - \phi_e$ to eliminate ϕ_i:

$$\frac{\partial}{\partial x}\left(\sigma_i \frac{\partial \phi_i}{\partial x}\right) = \frac{\partial}{\partial x}\left(k \cdot \sigma_e \frac{\partial (V_m + \phi_e)}{\partial x}\right) \tag{43}$$

Plugging this into (41) yields

$$\begin{aligned} & \frac{\partial}{\partial x}\left(k \cdot \sigma_e \frac{\partial (V_m + \phi_e)}{\partial x}\right) = -\frac{\partial}{\partial x}\left(\sigma_e \frac{\partial \phi_e}{\partial x}\right) \\ \Leftrightarrow \quad & \frac{\partial}{\partial x}\left((k+1) \cdot \sigma_e \frac{\partial \phi_e}{\partial x}\right) = -\frac{\partial}{\partial x}\left(k \cdot \sigma_e \frac{\partial V_m}{\partial x}\right) \\ \Leftrightarrow \quad & \frac{\partial}{\partial x}\left(\sigma_e \frac{\partial \phi_e}{\partial x}\right) = -\frac{\partial}{\partial x}\left(\frac{k}{k+1} \cdot \sigma_e \frac{\partial V_m}{\partial x}\right) \\ \Leftrightarrow \quad & \frac{\partial}{\partial x}\left(k\,\sigma_e \frac{\partial \phi_e}{\partial x}\right) = -\frac{\partial}{\partial x}\left(\frac{k}{k+1} \cdot k\,\sigma_e \frac{\partial V_m}{\partial x}\right) \end{aligned} \tag{44}$$

Using the substitution (43) in (42) yields

$$\frac{\partial}{\partial x}\left(k \cdot \sigma_e \frac{\partial (V_m + \phi_e)}{\partial x}\right) = A_m\Big(C_m \frac{\partial V_m}{\partial t} + I_{\text{ion}}(V_m)\Big)$$

Starting from (41) with (44) we get

$$
\begin{aligned}
& \frac{\partial}{\partial x}\Big(k\cdot\sigma_e\,\frac{\partial(V_m+\phi_e)}{\partial x}\Big) && = A_m\Big(C_m\frac{\partial V_m}{\partial t}+I_{\text{ion}}(V_m)\Big)\\
\Leftrightarrow\quad & \frac{\partial}{\partial x}\Big(k\cdot\sigma_e\,\frac{\partial V_m}{\partial x}\Big)+\frac{\partial}{\partial x}\Big(k\cdot\sigma_e\,\frac{\partial \phi_e}{\partial x}\Big) && = A_m\Big(C_m\frac{\partial V_m}{\partial t}+I_{\text{ion}}(V_m)\Big)\\
\Leftrightarrow\quad & \frac{\partial}{\partial x}\Big(\big(1-\frac{k}{k+1}\big)\cdot k\,\sigma_e\,\frac{\partial V_m}{\partial x}\Big) && = A_m\Big(C_m\frac{\partial V_m}{\partial t}+I_{\text{ion}}(V_m)\Big)\\
\Leftrightarrow\quad & \frac{\partial}{\partial x}\Big(\frac{1}{k+1}\cdot\sigma_i\,\frac{\partial V_m}{\partial x}\Big) && = A_m\Big(C_m\frac{\partial V_m}{\partial t}+I_{\text{ion}}(V_m)\Big)\\
\Leftrightarrow\quad & \frac{\partial}{\partial x}\Big(\frac{1}{\sigma_i/\sigma_e+1}\cdot\sigma_i\,\frac{\partial V_m}{\partial x}\Big) && = A_m\Big(C_m\frac{\partial V_m}{\partial t}+I_{\text{ion}}(V_m)\Big)\\
\Leftrightarrow\quad & \frac{\partial}{\partial x}\Big(\frac{\sigma_i\,\sigma_e}{\sigma_i+\sigma_e}\,\frac{\partial V_m}{\partial x}\Big) && = A_m\Big(C_m\frac{\partial V_m}{\partial t}+I_{\text{ion}}(V_m)\Big)
\end{aligned}
$$

This leads to the Monodomain equation:

$$
\frac{\partial}{\partial x}\Big(\sigma_{\text{eff}}\,\frac{\partial V_m}{\partial x}\Big)=A_m\Big(C_m\frac{\partial V_m}{\partial t}+I_{\text{ion}}(V_m)\Big),\qquad \text{with } \sigma_{\text{eff}}:=\sigma_i||\sigma_e=\frac{\sigma_i\,\sigma_e}{\sigma_i+\sigma_e}
$$

5.4 Numerical treatment

Equation solved for $\dfrac{\partial V_m}{\partial t}$:

$$
\frac{\partial V_m}{\partial t}=-\frac{1}{C_m}\,I_{\text{ion}}(V_m)+\frac{1}{A_m\,C_m}\,\frac{\partial}{\partial x}\Big(\sigma_{\text{eff}}\,\frac{\partial}{\partial x}\,V_m\Big)
$$

Employ finite differences in t and Godunov operator splitting:

$$
\begin{aligned}
\frac{V_m^*-V_m^{(k)}}{\Delta t} &= -\frac{1}{C_m}\;I_{\text{ion}}(V_m^{(k)}),\\
\frac{V_m^{(k+1)}-V_m^*}{\Delta t} &= \frac{1}{A_m\,C_m}\,\frac{\partial}{\partial x}\Big(\sigma_{\text{eff}}\,\frac{\partial}{\partial x}\,V_m^{(k+1)}\Big),
\end{aligned}
$$

$$
V_m^{(k+1)}=V_m^*+\Delta t\cdot\frac{1}{A_m\,C_m}\,\frac{\partial}{\partial x}\Big(\sigma_{\text{eff}}\,\frac{\partial}{\partial x}\,V_m^{(k+1)}\Big),
$$

The CellML model gives the right hand side $f(V_m^{(k)})=-\dfrac{1}{C_m}\;I_{\text{ion}}(V_m^{(k)})$. When solving the diffusion equation the value of C_m should match.

The bidomain equation can be used for computation of EMG (ϕ_e), after the Heidlauf model, when only V_m is known.

$$
\text{div}\,\big((\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_e)\,\text{grad}\,\phi_e\big)=-\text{div}\,(\boldsymbol{\sigma}_i\,\text{grad}\,V_m)
$$

6 Structural mechanics

This section collects theory about structural mechanics formulations and algorithms. Throughout the text the Einstein sum convention is used.

6.1 Introduction of some quantities

No quantities that are completely defined in the actual configuration are considered. $\mathbf{F}$ maps between configurations, $\mathbf{S}, \mathbf{C}, \boldsymbol{\varepsilon}$ are completely in the reference configuration. The definitions are briefly listed here.

- The deformation gradient $\mathbf{F} = \partial\mathbf{x}/\partial\mathbf{X}$ gives the linear approximation to the deformed image $\boldsymbol{\lambda}_{\mathbf{a}_0}$ (stretch vector) of a material vector $\mathbf{a}_0$, i.e. $\boldsymbol{\lambda}_{\mathbf{a}_0} = \mathbf{F}\,\mathbf{a}$ with $\mathbf{y} - \mathbf{x} = \mathbf{F}(\mathbf{X})(\mathbf{Y} - \mathbf{X}) + o(\mathbf{Y} - \mathbf{X})$.
- Polar decomposition of deformation gradient $\mathbf{F}$:

  $$\mathbf{F} = \mathbf{R}\,\mathbf{U}, \quad \mathbf{R}^\top\mathbf{R} = \mathbf{I}, \quad \mathbf{U} = \mathbf{U}^\top \text{ positive definite}$$

  $\mathbf{R}$ rotation tensor, $\mathbf{U}$ right stretch tensor, $\det\mathbf{U} = \det\mathbf{F} = J > 0$.
- Mapping properties between reference $(\mathrm{d}\mathbf{X}, \mathrm{d}\mathbf{S}, \mathrm{d}V)$ and current configuration $(\mathrm{d}\mathbf{x}, \mathrm{d}\mathbf{s}, \mathrm{d}v)$:

  $$\mathrm{d}\mathbf{x} = \mathbf{F}(\mathbf{X})\,\mathrm{d}\mathbf{X} \qquad \text{line map,}$$

  $$\mathrm{d}\mathbf{s} = J\mathbf{F}^{-\top}(\mathbf{X})\,\mathrm{d}\mathbf{S} \quad \text{surface map (Nansons' formula),}$$

  $$\mathrm{d}v = J(\mathbf{X})\,\mathrm{d}V \qquad \text{volume map.}$$

- Right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^\top\mathbf{F}$, symmetric, positive definite, $\det\mathbf{C} = J^2 > 0$.
- Left Cauchy-Green tensor $\mathbf{b} = \mathbf{F}\mathbf{F}^\top$, symmetric, positive definite, $\det\mathbf{b} = J^2 > 0$.
- Green-Lagrange strain tensor $\boldsymbol{\varepsilon} = \mathbf{E} = \dfrac{1}{2}(\mathbf{C} - \mathbf{I})$, symmetric (Both symbols are used here, because of literature). Note that the computation of $\boldsymbol{\varepsilon}$ from a vector of displacement DOFs is nonlinear.
- 2nd Piola-Kirchhoff stress tensor $\mathbf{S} = \dfrac{\partial\Psi(\mathbf{E})}{\partial\mathbf{E}} = 2\dfrac{\partial\psi(\mathbf{C})}{\partial\mathbf{C}}$, symmetric.

6.2 Green-Lagrange strain tensor and derivatives

In this subsection quantities of the reference configuration are denoted by left superscript ${}^{o}\cdot$, quantities in the current configuration at time t are denoted by left superscript ${}^{t}\cdot$. Derivation with respect to the reference configuration are denoted by ${}^{t}_{o}\cdot$.

The position $({}^{t}x_1^M, {}^{t}x_2^M, {}^{t}x_3^M)$ of a material point M at time t is given by

$${}^{t}x_i^M = {}^{o}x_i^M + {}^{t}u_i^M,$$

where ${}^{o}x_i$ is the position in reference configuration and ${}^{t}u_i$ is the displacement. The deformation gradient $\mathbf{F}$ is defined by the entries

$$F_{ij} = {}^{t}_{o}x_{i,j} = \frac{\partial {}^{t}x_i}{\partial {}^{o}x_j}\,.$$

The subscript comma means differentiation. We have ${}^{t}_{o}x_{i,j} = \delta_{ij} + {}^{t}u_{i,j}$. The discretization of ${}^{t}u$ is given by

$${}^{t}u_i(x) = \phi_L(x)\,{}^{t}u_i^L,$$

where ${}^{t}u_i^L$ are the coefficients, i.e. the nodal displacements. Lower case indices $i, j, k, \ldots$ refer to component indices $\{1, 2, 3\}$, capital indices are for dofs $\{1, \ldots, n\}$. The symbol ${}^{t}u_i^L$ stands for the nodal degree of freedom L of the displacement component $i \in \{1, 2, 3\}$.

Differentiation yields

$$\begin{aligned}
&{}^{t}_{o}x_{i,j} = \frac{\partial {}^{t}x_i}{\partial {}^{o}x_j} = \delta_{ij} + \frac{\partial {}^{t}u_i}{\partial {}^{o}x_j} = \delta_{ij} + \phi_{L,j}({}^{o}\mathbf{x})\,{}^{t}u_i^L = \delta_{ij} + u_{i,j}, \quad \text{i.e.}\\
&\mathbf{F} = \mathbf{I} + \nabla_{\mathbf{X}}\mathbf{u}.
\end{aligned}$$

We have

$$\phi_{L,j}({}^{o}\mathbf{x}) = \frac{\mathrm{d}\phi_L\big(\boldsymbol{\xi}({}^{o}\mathbf{x})\big)}{\mathrm{d}\,{}^{o}x_j} = \frac{\partial \phi_L}{\partial \xi_\ell}\,\frac{\partial \xi_\ell}{\partial {}^{o}x_j}\,.$$

The Green-Lagrange strain tensor ${}^{t}_{o}\boldsymbol{\varepsilon}$ is defined as

$${}^{t}_{o}\varepsilon_{kl} = \frac{1}{2}\left({}^{t}_{o}x_{b,k}\,{}^{t}_{o}x_{b,l} - \delta_{kl}\right), \quad \text{or} \quad \mathbf{E} = \frac{1}{2}\left(\mathbf{F}^{\top}\mathbf{F} - \mathbf{I}\right)$$

From that we get

$$\begin{aligned}
{}^{t}_{o}\varepsilon_{kl} &= \frac{1}{2}\left({}^{t}_{o}x_{b,k}\,{}^{t}_{o}x_{b,l} - \delta_{kl}\right) = \frac{1}{2}\left(\left(\delta_{bk} + u_{b,k}\right)\left(\delta_{bl} + u_{b,l}\right) - \delta_{kl}\right)\\
&= \frac{1}{2}\left(\left(\delta_{bk}\,\delta_{bl} + u_{b,k}\,\delta_{bl} + \delta_{bk}u_{b,l} + u_{b,k}\,u_{b,l}\right) - \delta_{kl}\right) = \frac{1}{2}\left(\delta_{kl} + u_{l,k} + u_{k,l} + u_{b,k}\,u_{b,l} - \delta_{kl}\right)\\
&= \frac{1}{2}\left(u_{l,k} + u_{k,l} + u_{b,k}\,u_{b,l}\right), \qquad \text{or}\\
\mathbf{E} &= \frac{1}{2}\left((\nabla\mathbf{u})^{\top} + \nabla\mathbf{u}\right) + \frac{1}{2}\,\nabla\mathbf{u}^{\top}\nabla\mathbf{u}, \qquad \text{where the gradient is w.r.t } \mathbf{X} \text{ (material description).}
\end{aligned}$$

Note that for virtual strain (used later) the virtual displacements are infinitesimally small and the quadratic term can be neglected, yielding

$${}^{t}_{o}\delta\varepsilon_{kl} = \frac{1}{2}\left(\delta u_{l,k} + \delta u_{k,l}\right), \qquad \delta\mathbf{E} = \frac{1}{2}\left((\nabla\delta\mathbf{u})^{\top} + \nabla\delta\mathbf{u}\right).$$

Next the derivative with respect to a nodal displacement u_i^L is considered. Therefore we need

$$\frac{\partial {}^{t}_{o}x_{i,j}}{\partial u_k^L} = \frac{\partial \phi_L\,{}^{t}u_i^L}{\partial u_k^L} = \phi_{L,j}\,\delta_{ik}.$$

We then proceed to compute

$$\frac{\partial^t_o \boldsymbol{\varepsilon}_{kl}}{\partial u^L_i} = \frac{1}{2}\left(\frac{\partial^t_o x_{b,k}}{\partial u^L_i}\,{}^t_o x_{b,l} + {}^t_o x_{b,k}\,\frac{\partial^t_o x_{b,l}}{\partial u^L_i}\right) = \frac{1}{2}\left(\phi_{L,k}\,\delta_{bi}\,{}^t_o x_{b,l} + {}^t_o x_{b,k}\,\phi_{L,l}\,\delta_{bi}\right) = \frac{1}{2}\left({}^t_o x_{i,l}\,\phi_{L,k} + {}^t_o x_{i,k}\,\phi_{L,l}\right).$$

We compute the second derivative (results from [4])

$$\frac{\partial^t_o \boldsymbol{\varepsilon}_{kl}}{\partial u^L_i\,\partial u^M_j} = \cdots = \frac{1}{2}\left(\phi_{L,k}\,\phi_{M,l} + \phi_{L,l}\,\phi_{M,k}\right)\delta_{ij}.$$

6.3 Material modeling

6.3.1 Principal invariants

The principal scalar invariants of the right Cauchy Green Tensor $\mathbf{C} = \mathbf{F}^\top\mathbf{F}$ are defined as

$$I_1(\mathbf{C}) = \mathrm{tr}(\mathbf{C}) = \mathbf{C} : \mathbf{I} = C_{ii} = \lambda_1 + \lambda_2 + \lambda_3$$

$$I_2(\mathbf{C}) = \frac{1}{2}\left(\mathrm{tr}(\mathbf{C})^2 - \mathrm{tr}(\mathbf{C}^2)\right) = \frac{1}{2}\left(C_{ii}\,C_{jj} - C_{ji}\,C_{ij}\right) = \lambda_1\,\lambda_2 + \lambda_1\,\lambda_2 + \lambda_2\,\lambda_3$$

$$I_3(\mathbf{C}) = \det(\mathbf{C}) = \varepsilon_{ijk}\,C_{1i}\,C_{2j}\,C_{3k} = \lambda_1\,\lambda_2\,\lambda_3$$

$$I_4(\mathbf{C}) = \mathbf{a}_0 \cdot \mathbf{C}\,\mathbf{a}_0$$

$$I_5(\mathbf{C}) = \mathbf{a}_0 \cdot \mathbf{C}^2\,\mathbf{a}_0$$

The principal stretches $\lambda_a, a = 1, 2, 3$ are the eigenvalues of the right Cauchy-Green tensor $\mathbf{C}$. ε_{ijk} is the Levi-Civita symbol

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{for } (i,j,k) \in \{(1,2,3),(2,3,1),(3,1,2)\} \\ -1 & \text{for } (i,j,k) \in \{(3,2,1),(1,3,2),(2,1,3)\} \\ 0 & \text{else} \end{cases}$$

Reduced invariants (p.233), with kinematic assumption $\bar{I}_3 = 1$:

$$\bar{I}_1(\bar{\mathbf{C}}) = \mathrm{tr}(\bar{\mathbf{C}}) = \bar{\mathbf{C}} : \mathbf{I} = J^{-2/3} I_1$$

$$\bar{I}_2(\bar{\mathbf{C}}) = \frac{1}{2}\left(\mathrm{tr}(\bar{\mathbf{C}})^2 - \mathrm{tr}(\bar{\mathbf{C}}^2)\right) = J^{-4/3} I_2$$

$$\bar{I}_3(\bar{\mathbf{C}}) = \det(\bar{\mathbf{C}}) = 1$$

6.3.2 Strain energy density function

Strain energy density function $\Psi(\mathbf{C}) = \Psi(I_1, I_2, I_3)$ for isotropic hyperelastic materials. To compute $\mathbf{S} = 2\,\dfrac{\partial \Psi(\mathbf{C})}{\partial \mathbf{C}}$ derivatives w.r.t. to the invariants are required. (p. 216 Holzapfel Nonlinear Solid

Mechanics [3])

$$
\begin{aligned}
\frac{\partial I_1}{\partial \mathbf{C}} &= \frac{\partial \mathrm{tr}\mathbf{C}}{\partial \mathbf{C}} = \frac{\partial \mathbf{I} : \mathbf{C}}{\partial \mathbf{C}} = \mathbf{I}, & \frac{\partial I_1}{\partial C_{AB}} &= \delta_{AB} \\
\frac{\partial I_2}{\partial \mathbf{C}} &= \mathrm{tr}\mathbf{C}\,\mathbf{I} - \mathbf{C}, & \frac{\partial I_2}{\partial C_{AB}} &= I_1\,\delta_{AB} - C_{AB} \\
\frac{\partial I_3}{\partial \mathbf{C}} &= I_3\,\mathbf{C}^{-1}, & \frac{\partial I_3}{\partial C_{AB}} &= I_3\,C^{-1}_{AB} \\
\frac{\partial I_4}{\partial \mathbf{C}} &= \mathbf{a}_0 \otimes \mathbf{a}_0 \\
\frac{\partial I_5}{\partial \mathbf{C}} &= \mathbf{a}_0 \otimes \mathbf{C}\,\mathbf{a}_0 + \mathbf{a}_0\,\mathbf{C} \otimes \mathbf{a}_0
\end{aligned}
$$

Note for the reduced invariants (p.234):

$$
\begin{aligned}
\frac{\partial \bar{I}_1}{\partial \bar{\mathbf{C}}} &= \frac{\partial \mathrm{tr}\bar{\mathbf{C}}}{\partial \bar{\mathbf{C}}} = \frac{\partial \mathbf{I} : \bar{\mathbf{C}}}{\partial \bar{\mathbf{C}}} = \mathbf{I} \\
\frac{\partial \bar{I}_2}{\partial \bar{\mathbf{C}}} &= \mathrm{tr}\bar{\mathbf{C}}\,\mathbf{I} - \bar{\mathbf{C}} \\
\frac{\partial \bar{I}_4}{\partial \bar{\mathbf{C}}} &= \mathbf{a}_0 \otimes \mathbf{a}_0 \\
\frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} &= \mathbf{a}_0 \otimes \bar{\mathbf{C}}\,\mathbf{a}_0 + \mathbf{a}_0\,\bar{\mathbf{C}} \otimes \mathbf{a}_0 \quad \text{(p.277)}
\end{aligned}
$$

In total we get

$$
\begin{aligned}
\mathbf{S} &= \frac{\partial \Psi(\mathbf{E})}{\partial \mathbf{E}} = 2\,\frac{\partial \Psi(\mathbf{C})}{\partial \mathbf{C}} = \sum_{a=1}^{3} \frac{\partial \Psi}{\partial I_a}\,\frac{\partial I_a}{\partial \mathbf{C}} \\
&= 2\left(\left(\frac{\partial \Psi}{\partial I_1} + I_1\,\frac{\partial \Psi}{\partial I_2}\right)\mathbf{I} - \frac{\partial \Psi}{\partial I_2}\,\mathbf{C} + I_3\,\frac{\partial \Psi}{\partial I_3}\,\mathbf{C}^{-1}\right)
\end{aligned}
$$

Useful:

$$
\left(\frac{\partial \mathbf{A}^{-1}}{\partial \mathbf{A}}\right)_{ijkl} = -\frac{1}{2}\,(A^{-1}_{ik}\,A^{-1}_{lj} + A^{-1}_{il}\,A^{-1}_{kj}) = -A^{-1} \odot A^{-1}\,.
$$

6.4 Elasticity tensor

For the solution of the nonlinear problem the elasticity tensor $\mathbb{C}$ has to be computed (Holzapfel p.261 [3]):

$$
\begin{aligned}
\mathbb{C} &= \frac{\partial \mathbf{S}}{\partial \mathbf{E}} = 2\frac{\partial \mathbf{S}}{\partial \mathbf{C}} = 4\frac{\partial^2 \Psi(I_1, I_2, I_3)}{\partial \mathbf{C} \partial \mathbf{C}} \\
&= \delta_1\,\mathbf{I} \otimes \mathbf{I} + \delta_2\,(\mathbf{I} \otimes \mathbf{C} + \mathbf{C} \otimes \mathbf{I}) + \delta_3(\mathbf{I} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \mathbf{I}) \\
&\quad + \delta_4 \mathbf{C} \otimes \mathbf{C} + \delta_5(\mathbf{C} \otimes \mathbf{C}^{-1} + \mathbf{C}^{-1} \otimes \mathbf{C}) \\
&\quad + \delta_6 \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} + \delta_7 \mathbf{C}^{-1} \odot \mathbf{C}^{-1} + \delta_8\,\mathbb{I}
\end{aligned}
$$

Recall the definitions:

$$A \otimes B := A_{ab} B_{cd}$$

$$\mathbb{I}_{ABCD} := \frac{\delta_{AC}\delta_{BD} + \delta_{AD}\delta_{BC}}{2}$$

The coefficients $\delta_1, \ldots \delta_8$ are defined by

$$\delta_1 = 4\left(\frac{\partial^2\Psi}{\partial I_1 \partial I_1} + 2\, I_1 \frac{\partial^2\Psi}{\partial I_1 \partial I_2} + \frac{\partial\Psi}{\partial I_2} + I_1^2 \frac{\partial^2\Psi}{\partial I_2 \partial I_2}\right),$$

$$\delta_2 = -4\left(\frac{\partial^2\Psi}{\partial I_1 \partial I_2} + I_1 \frac{\partial^2\Psi}{\partial I_2 \partial I_2}\right),$$

$$\delta_3 = 4\left(I_3 \frac{\partial^2\Psi}{\partial I_1 \partial I_3} + I_1\, I_3 \frac{\partial^2\Psi}{\partial I_2 \partial I_3}\right), \qquad \delta_4 = 4\,\frac{\partial^2\Psi}{\partial I_2 \partial I_2},$$

$$\delta_5 = -4\, I_3 \frac{\partial^2\Psi}{\partial I_2 \partial I_3}, \qquad \delta_6 = 4\left(I_3 \frac{\partial\Psi}{\partial I_3} + I_3^2 \frac{\partial^2\Psi}{\partial I_3 \partial I_3}\right),$$

$$\delta_7 = -4\, I_3 \frac{\partial\Psi}{\partial I_3}, \qquad \delta_8 = -4\,\frac{\partial\Psi}{\partial I_2}.$$

The elasticity tensor $\mathbb{C}$ has the following symmetries:

$$\mathbb{C}_{ijrs} = \mathbb{C}_{jirs} = \mathbb{C}_{ijsr} = \mathbb{C}_{jisr} \quad \text{minor symmetries}$$

$$\mathbb{C}_{ijrs} = \mathbb{C}_{rsij} \quad \text{major symmetries}$$

The minor symmetries are due to the symmetry of the 2nd Piola Kirchhoff tensor, $\mathbf{S}$ and the right Cauchy-Green tensor, $\mathbf{C}$, because

$$\mathbb{C}_{ijrs} = \frac{\partial S_{ij}}{\partial C_{rs}}.$$

The major symmetries are because of the existence of the strain density function because

$$\mathbb{C}_{ijrs} = \frac{\partial^2\Psi(\mathbf{C})}{\partial C_{ij}\, \partial C_{rs}}.$$

The 21 unique entries are:

$\mathbb{C}_{ijrs}$ with $(i, j, r, s) =$

$(1,1,1,1), (1,2,1,1), (1,3,1,1), (2,2,1,1), (2,3,1,1), (3,3,1,1),$

$(1,2,1,2), (1,3,1,2), (2,2,1,2), (2,3,1,2), (3,3,1,2),$

$(1,3,1,3), (2,2,1,3), (2,3,1,3), (3,3,1,3),$

$(2,2,2,2), (2,3,2,2), (3,3,2,2),$

$(2,3,2,3), (3,3,2,3),$

$(3,3,3,3)$

6.5 Constitutive Equations

6.5.1 Incompressible Mooney-Rivlin

The *Mooney-Rivlin* model is used which for incompressible material defines the strain energy function as

$$\Psi_{\text{Mooney-Rivlin}}(I_1, I_2) = c_1(I_1 - 3) + c_2(I_2 - 3),$$

where I_1, I_2 are the strain invariants and c_1, c_2 are material parameters.

For incompressible materials the strain energy function is defined as (p.247)

$$\Psi = \Psi_{\text{Mooney-Rivlin}}(I_1, I_2) - \frac{1}{2}\, p\,(I_3 - 1), \text{ or}$$

$$\Psi = \Psi_{\text{Mooney-Rivlin}}(I_1, I_2) - \frac{1}{2}\, p\,(I_3 - 1)^2$$

and the stress as

$$\begin{aligned}\mathbf{S} &= 2\frac{\partial}{\partial \mathbf{C}}\,\Psi_{\text{Mooney-Rivlin}}(I_1, I_2) - \frac{\partial\big(p(I_3-1)\big)}{\partial \mathbf{C}} = -p\mathbf{C}^{-1} + 2\left(\frac{\partial \Psi}{\partial I_1} + I_1\,\frac{\partial \Psi}{\partial I_2}\right)\mathbf{I} - 2\frac{\partial \Psi}{\partial I_2}\,\mathbf{C} \\ &= -p\mathbf{C}^{-1} + 2\left(c_1 + \operatorname{tr}(\mathbf{C})\, c_2\right)\mathbf{I} - 2\, c_2\, \mathbf{C}\end{aligned}$$

The Cauchy stress:

$$\begin{aligned}\boldsymbol{\sigma} &= -p\mathbf{I} + 2\left(\frac{\partial \Psi}{\partial I_1} + I_1\,\frac{\partial \Psi}{\partial I_2}\right)\mathbf{b} - 2\,\frac{\partial \Psi}{\partial I_2}\,\mathbf{b}^2 \\ &= -p\mathbf{I} + 2(c_1 + I_1\, c_2)\,\mathbf{b} - 2\, c_2\, \mathbf{b}^2\end{aligned}$$

$$\boldsymbol{\sigma} = -p\,\mathbf{I} + 2\, c_1\,\mathbf{b} - 2\, c_2\,\mathbf{b}^{-1} \quad \text{with Left Cauchy-Green tensor } \mathbf{b} = \mathbf{F}\,\mathbf{F}^{\top} \quad \text{(p.238 Holzapfel)}$$

$$\mathbf{b}^2 = \mathbf{b}\,\mathbf{b} = \mathbf{F}\,\mathbf{F}^{\top}\,\mathbf{F}\,\mathbf{F}^{\top}, \quad \mathbf{b}^2_{ij} = \mathbf{b}_{ik}\mathbf{b}_{kj} = \mathbf{F}_{il}\,\mathbf{F}^{\top}_{lk}\,\mathbf{F}_{km}\,\mathbf{F}^{\top}_{mj} = \mathbf{F}_{il}\,\mathbf{F}_{kl}\,\mathbf{F}_{km}\,\mathbf{F}_{jm}$$

(Holzapfel p.224 [3])

The parameter p is here an indeterminate Lagrange multiplier that is identified as the hydrostatic pressure. However it has to be computed from the equilibrium equations and boundary conditions.

6.5.2 Compressible Mooney-Rivlin

The strain-energy function for compressible material can be given in either coupled or decoupled form. The decoupled form uses the modified strain invariants $\bar{I}_1 = J^{-2/3}\, I_1, \bar{I}_2 = J^{-4/3}\, I_2, \bar{I}_3 = 1$. It decouples the strain energy function to a volumetric elastic response, $\Psi_{\text{vol}}(J)$ and the isochoric elastic response $\Psi_{\text{iso}}(\bar{\mathbf{C}})$.

$$\Psi = \Psi_{\text{vol}}(J) + \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)$$

The volumetric part is often given by

$$\Psi_{vol}(J) = \kappa\, G(J) \quad \text{with, e.g.,}$$

$$G(J) = \beta^{-2}(\beta\, \log(J) + J^{-\beta} - 1), \qquad \text{or}$$

$$G(J) = \tfrac{1}{4}(J^2 - 1 - 2\, \log(J))$$

(Holzapfel p.233, p.244/255 [3])

A coupled form uses the normal strain invariants, I_1, I_2, J, e.g. the coupled Mooney-Rivlin model,

$$\Psi(J, I_1, I_2) = c(J-1)^2 - d\, \ln J + c_1(I_1 - 3) + c_2(I_2 - 3), \qquad d = 2(c_1 + 2\, c_2)$$

(Holzapfel p.247 [3])

The stress tensor follows by derivation

$$\begin{aligned}\mathbf{S} &= 2\frac{\partial \Psi}{\partial \mathbf{C}} = 2(c_1 + c_2\, I_1)\mathbf{I} - 2\, c_2\, \mathbf{C} + (2\, c\, J\, (J-1) - d)\mathbf{C}^{-1} \\ &= 2(c_1 + c_2\, \mathrm{tr}\mathbf{C})\mathbf{I} - 2\, c_2\, \mathbf{C} + \Big(2\, c \det(\mathbf{F})\, \big(\det(\mathbf{F}) - 1\big) - d\Big)\mathbf{C}^{-1}\end{aligned}$$

Alternative model:

$$\Psi = \frac{1}{2}\, \kappa (J-1)^2 + c_1(\bar{I}_1 - 3) + c_2(\bar{I}_2 - 3)$$

([4] Sussmann, Bathe p.15)

6.5.3 Transversely isotropic formulation

This formulation assumes a ground matrix and fibres with direction $\mathbf{a}_0$ in reference configuration. Two pseudo-invariants $I_4(\mathbf{C}, \mathbf{a}_0), I_5(\mathbf{C}, \mathbf{a}_0)$ are introduced:

$$I_4(\mathbf{C}, \mathbf{a}_0) = \mathbf{a}_0 \cdot \mathbf{C}\, \mathbf{a}_0,$$

$$I_5(\mathbf{C}, \mathbf{a}_0) = \mathbf{a}_0 \cdot \mathbf{C}^2\, \mathbf{a}_0.$$

The strain energy function is then stated as

$$\Psi = \Psi\big(I_1(\mathbf{C}), I_2(\mathbf{C}), I_3(\mathbf{C}), I_4(\mathbf{C}, \mathbf{a}_0), I_5(\mathbf{C}, \mathbf{a}_0)\big)$$

For the formulation of the stress, derivatives of the pseudo-invariants w.r.t $\mathbf{C}$ are needed:

$$\frac{\partial I_4}{\partial \mathbf{C}} = \mathbf{a}_0 \otimes \mathbf{a}_0, \qquad \frac{\partial I_4}{\partial C_{ij}} = a_{0,i}\, a_{0,j},$$

$$\frac{\partial I_5}{\partial \mathbf{C}} = \mathbf{a}_0 \otimes \mathbf{C}\, \mathbf{a}_0 + \mathbf{a}_0\, \mathbf{C} \otimes \mathbf{a}_0, \quad \frac{\partial I_5}{\partial C_{ij}} = a_{0,i}\, C_{jk}\, a_{0,k} + a_{0,j}\, C_{ik}\, a_{0,k}.$$

6.5.4 Reduced Quantities

For compressible materials reduced quantities are used. The deformation gradient and right Cauchy-Green tensor are multiplicatively decomposed into a volume-changing (volumetric, dilational) and volume-preserving (isochoric, distortional, deviatoric) part as follows:

$$\mathbf{F} = (J^{1/3}\mathbf{I})\,\bar{\mathbf{F}},$$

$$\mathbf{C} = (J^{2/3}\mathbf{I})\,\bar{\mathbf{C}}.$$

The volume preserving measures are given by

$$\bar{\mathbf{F}} = J^{-1/3}\,\mathbf{F} \quad \ldots \quad \text{modified deformation gradient}$$

$$\bar{\mathbf{C}} = J^{-2/3}\,\mathbf{C} \quad \ldots \quad \text{modified right Cauchy-Green tensor}$$

The volume-changing deformations are associated with $J^{1/3}\mathbf{I}$ and $J^{2/3}\mathbf{I}$.

Accordingly, reduced invariants are (p.233)

$$\bar{I_1} = \mathrm{tr}(\bar{\mathbf{C}}) = J^{-2/3}\,I_1,$$

$$\bar{I_2} = \frac{1}{2}\left(\mathrm{tr}(\bar{\mathbf{C}})^2 - \mathrm{tr}(\bar{\mathbf{C}}^2)\right) = J^{-4/3}\,I_2,$$

$$\bar{I_3} = \det(\bar{\mathbf{C}}) = 1.$$

The strain-enery function is now given in a decoupled representation as

$$\Psi(\mathbf{C}) = \Psi_{\mathrm{vol}}(J) + \Psi_{\mathrm{iso}}(\bar{\mathbf{C}}) = \Psi_{\mathrm{vol}}(J) + \Psi_{\mathrm{iso}}(\bar{I_1}, \bar{I_2}),$$

$$\Psi_{\mathrm{vol}}(J) = \kappa\, G(J)$$

with penalty functions $G(J)$ with conditions

$$G(J) = 0 \quad \Leftrightarrow \quad J = 1$$

and $G(J)$ strictly convex

Possible functions in literature are:

$$G_1(J) = \frac{1}{2}\left(J(\mathbf{u}) - 1\right)^2,$$

$$G_2(J) = \frac{1}{2}\left(J(\mathbf{u}) - 1\right).$$

This leads to volumetric and deviatoric/isochoric contribution of stresses

$$
\begin{aligned}
\mathbf{S} &= 2\frac{\partial \Psi(\mathbf{C})}{\partial \mathbf{C}} = \mathbf{S}_{\text{vol}} + \mathbf{S}_{\text{iso}}, \\
\mathbf{S}_{\text{vol}} &= 2\frac{\partial \Psi_{\text{vol}}(J)}{\partial \mathbf{C}} = J\, p\, \mathbf{C}^{-1} \\
\mathbf{S}_{\text{iso}} &= 2\frac{\partial \Psi_{\text{iso}}(\bar{\mathbf{C}})}{\partial \mathbf{C}} = J^{-2/3}\, \mathbb{P} : \bar{\mathbf{S}} \qquad \text{(see Holzapfel p.229 [3] for definition of } \mathbb{P}) \\
p &= \frac{\mathrm{d}\Psi_{\text{vol}}(J)}{\mathrm{d}J}, \quad \bar{\mathbf{S}} = 2\,\frac{\partial \Psi_{\text{iso}}(\bar{\mathbf{C}})}{\partial \bar{\mathbf{C}}}
\end{aligned}
\tag{45}
$$

6.6 Formulation in current configuration

The following spatial quantities are defined in the current configuration.

$\mathbf{x}$	...	position
$\mathbf{v} = \dot{\mathbf{x}}$	...	velocity
ρ	...	density
$\boldsymbol{\sigma}$	...	Cauchy stress

The connection from the symmetric Cauchy stress tensor $\boldsymbol{\sigma}$ to the 2nd Piola-Kirchhoff stress tensor $\mathbf{S}$ is given by

$$
\begin{aligned}
\boldsymbol{\sigma} &= J^{-1}\mathbf{F}\,\mathbf{S}\,\mathbf{F}^{\top} \\
\mathbf{S} &= J\,\mathbf{F}^{-1}\,\boldsymbol{\sigma}\,\mathbf{F}^{-\top} \\
\boldsymbol{\sigma} &= \frac{1}{J}\,\mathbf{P}\,\mathbf{F}^{\top} \quad \Rightarrow \quad \mathbf{P} = J\boldsymbol{\sigma}\,\mathbf{F}^{-\top} \\
\mathbf{S} &= \mathbf{F}^{-1}\mathbf{P} \quad \Rightarrow \quad \mathbf{P} = \mathbf{F}\,\mathbf{S}
\end{aligned}
$$

(Holzapfel [3] p. 135) From the *conservation of mass* we get the spatial equation

$$\dot{\rho}(\mathbf{x},t) + \rho(\mathbf{x},t)\,\nabla\cdot\mathbf{v}(\mathbf{x},t) = 0$$

which for constant density, ρ, reduces to

$$\nabla\cdot\mathbf{v}(\mathbf{x},t) = 0.$$

(Holzapfel [3] p. 145) From the *balance of linear momentum* the equations of motion in spatial description can be derived.

$$\operatorname{div}\boldsymbol{\sigma} + \mathbf{b} = \rho\,\dot{\mathbf{v}} \tag{46}$$

The *balance of angular momentum* enforces the Cauchy stress tensor, $\boldsymbol{\sigma}$ to be symmetric (Holzapfel [3] p. 147).

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\top}$$

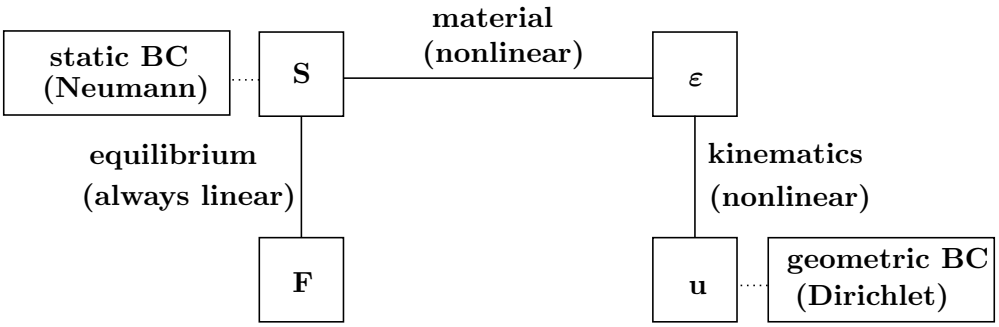


Abbildung 4: Tonti diagram

Equation (46) can be restated in terms of the displacement $\mathbf{u}$ as

$$\rho\,\ddot{\mathbf{u}} - \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} = 0,$$

$$\nabla_{\mathbf{x}} \cdot \dot{\mathbf{u}} = 0.$$

For the quasi-static case, $\dot{\mathbf{u}} = 0$, this reduces to

$$\nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} = 0.$$

Substituting the Cauchy stress $\boldsymbol{\sigma}$ for the material configuration stress, $\mathbf{S}$, yields

$$\nabla_{\mathbf{x}} \cdot (J^{-1}\,\mathbf{F}\,\mathbf{S}\,\mathbf{F}^{\top}) = 0$$

6.7 Incompressible solid mechanics

A material is incompressible if one of the following necessary and sufficient conditions are satisfied (Holzapfel [3] p.103):

$$J = 1, \quad \mathrm{d}v = \text{const}, \quad \dot{J} = 0, \quad \mathbf{F}^{-\top} : \dot{\mathbf{F}} = 0, \quad \operatorname{div}(\mathbf{v}) = 0$$

A nonlinear case occurs if the constitutive relation between $\mathbf{S}$ and $\boldsymbol{\varepsilon}$ is nonlinear or if the relationship between displacement $\mathbf{u}$ and strain $\boldsymbol{\varepsilon}$ is nonlinear, as depicted in the Tonti diagram, fig. 4.

The case of 3D finite elasticity the relation between the displacement vector $\hat{\mathbf{u}}$ and the strain $\mathbf{E} = (\mathbf{C} - \mathbf{I})/2$ is nonlinear because of $\mathbf{C} = \mathbf{F}^{\top}\mathbf{F}$. In addition the material model is often nonlinear, because of the invariants.

For incompressible and nearly incompressible analyses it is necessary to use a mixed formulation to avoid convergence problems (locking). [5], [1].

Sec. 6.7.2 describes the penalty method, Sec. **??** formulates the classical mixed formulation that is used for compressible / nearly incompressible analyses.

6.7.1 Material description

Starting point is the equation of motion in the material description

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} + \mathbf{B} = \rho_0\,\ddot{\mathbf{u}},$$

with body forces in reference configuration, $\mathbf{B} = J\,\mathbf{b}$, and the first Piola-Kirchhoff stress tensor, $\mathbf{P} = J\boldsymbol{\sigma}^{\top}\mathbf{F}^{-\top}$, prescribed surface traction $\bar{T}$, displacement field u in the reference configuration. The principle of virtual work is (Holzapfel [3], p.385)

$$\underbrace{\int_\Omega \mathbf{P} : \nabla_{\mathbf{X}}\delta\mathbf{u}\,\mathrm{d}V}_{=\delta W_{\text{int}}} = \underbrace{\int_\Omega (\mathbf{B} - \rho_0\,\ddot{\mathbf{u}})\cdot\delta\mathbf{u}\,\mathrm{d}V + \int_{\partial\Omega}\bar{\mathbf{T}}\cdot\delta\mathbf{u}\,\mathrm{d}S}_{=\delta W_{\text{ext}}}$$

The internal virtual work δW_{int} can be expressed in terms of Green-Lagrange strain, $\mathbf{E}$, and 2nd Piola-Kirchhoff stress, $\mathbf{S}$,

$$\delta W_{\text{int}} = \int_\Omega \mathbf{P} : \nabla_{\mathbf{X}}\delta\mathbf{u}\,\mathrm{d}V = \int_\Omega \mathbf{S} : \delta\mathbf{E}\,\mathrm{d}V.$$

For the static case, $\ddot{\mathbf{u}} = \mathbf{0}$, the virtual work can be expressed by a potential,

$$\begin{aligned}\Pi_{\text{int}}(\mathbf{u}) &= \int_\Omega \Psi\big(\mathbf{F}(\mathbf{u})\big)\,\mathrm{d}V,\\ \Pi_{\text{ext}}(\mathbf{u}) &= -\int_\Omega \mathbf{B}\mathbf{u}\,\mathrm{d}V - \int_{\partial\Omega}\bar{T}\mathbf{u}\,\mathrm{d}S.\end{aligned} \tag{47}$$

This is useful in order to describe the material behaviour by a scalar strain enery density function, Ψ.

By taking the directional derivative,

$$D_{\delta\mathbf{u}}\Pi(\mathbf{u}) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\Pi(\mathbf{u} + \varepsilon\delta\mathbf{u})\big|_{\varepsilon=0},$$

we get back to the virtual work terms.

$$D_{\delta\mathbf{u}}\Pi_{\text{int}} = \delta W_{\text{int}}, \qquad D_{\delta\mathbf{u}}\Pi_{\text{ext}} = -\delta W_{\text{ext}}.$$

6.7.2 Penalty method

For incompressible materials we use the decoupled representation of the strain energy function,

$$\Psi(\mathbf{C}) = \Psi_{\text{vol}}\big(J(\mathbf{u})\big) + \Psi_{\text{iso}}(\bar{\mathbf{C}}(\mathbf{u})), \quad \text{with } \Psi_{\text{vol}}(J) = \kappa\,G(J), \quad G(J) := \frac{1}{2}\,(J-1)^2$$

The derivative yields

$$\begin{aligned}\delta W_{\text{int}} &= D_{\delta\mathbf{u}}\Pi_{\text{int}} = \int_\Omega \left(\frac{\partial\Psi_{\text{vol}}\big(J(\mathbf{u})\big)}{\partial\mathbf{C}} + \frac{\partial\Psi_{\text{iso}}(\bar{\mathbf{C}}(\mathbf{u})}{\partial\mathbf{C}}\right) : D_{\delta\mathbf{u}}\mathbf{C}(\mathbf{u})\,\mathrm{d}V\\ &= \int_\Omega \Big(\underbrace{\underbrace{J\frac{\mathrm{d}\Psi_{\text{vol}}}{\mathrm{d}J}}_{=p}\,\mathbf{C}^{-1}}_{=\mathbf{S}_{\text{vol}}} + \underbrace{2\frac{\partial\Psi_{\text{iso}}}{\partial\mathbf{C}}}_{=\mathbf{S}_{\text{iso}}}\Big) : \delta\mathbf{E}\,\mathrm{d}V = \int_\Omega \big(\mathbf{S}_{\text{vol}} + \mathbf{S}_{\text{iso}}\big) : \delta\mathbf{E}\,\mathrm{d}V\end{aligned}$$

In comparison with (45) we identify the split of the 2nd Piola-Kirchhoff stress tensor, $\mathbf{S} = \mathbf{S}_{\text{vol}} + \mathbf{S}_{\text{iso}}$. The pressure p is artifical and does not represent the physical volumetric pressure.

$$p = \frac{\mathrm{d}\Psi_{\text{vol}}}{\mathrm{d}J} = \kappa \frac{\mathrm{d}G(J)}{\mathrm{d}J} = \kappa\big(J(\mathbf{u}) - 1\big).$$

The penalty parameter κ is a numerical parameter, for $\kappa \to \infty$ the problem gets incompressible, but ill-conditioned.

The variation of the Green-Lagrange strain tensor, $\delta\mathbf{E}$ is given by (p.375)

$$\begin{aligned} \delta\mathbf{E} &= \operatorname{sym}\left(\mathbf{F}^\top \nabla\delta u\right) = \frac{1}{2}\left((\mathbf{F}^\top\nabla\delta\mathbf{u})^\top + \mathbf{F}^\top\nabla\delta\mathbf{u}\right), \\ \delta E_{AB} &= \frac{1}{2}\left(F_{aB}\frac{\partial\delta u_a}{\partial X_A} + F_{aA}\frac{\partial\delta u_a}{\partial X_B}\right) \end{aligned} \tag{48}$$

The governing equations are given by the principle of virtual work,

$$\delta W_{\text{int}}(\mathbf{u}) - \delta W_{\text{ext}} = 0. \tag{49}$$

The extern virtual energy is assumed to not depend on the displacements.

(49) has to hold for arbitrary virtual displacements, $\delta\mathbf{u}$. The system of equations is thus

$$\underbrace{\int_\Omega \mathbf{S} : \delta\mathbf{E}(\delta\mathbf{u})\,\mathrm{d}V}_{=\delta W_{\text{int}}} - \underbrace{\int_\Omega (\mathbf{B} - \rho_0\,\ddot{\mathbf{u}})\cdot\delta\mathbf{u}\,\mathrm{d}V + \int_{\partial\Omega}\bar{\mathbf{T}}\cdot\delta\mathbf{u}\,\mathrm{d}s}_{=\delta W_{\text{ext}}} = 0, \qquad \forall\,\delta\mathbf{u} \tag{50}$$

With the usual discretization,

$$u_a = u_a^L\,\phi_L, \quad \delta u_a = \delta u_a^L\,\phi_L, \qquad \hat{\mathbf{u}} = (u_a^L)_{a=1,2,3}, \quad \delta\hat{\mathbf{u}} = (\delta u_a^L)_{a=1,2,3},$$

we get from (48) and (50) in index form

$$\begin{aligned} &\int_\Omega \frac{1}{2}\,S_{AB}\left(F_{aB}\frac{\partial\delta u_a}{\partial X_A} + F_{aA}\frac{\partial\delta u_a}{\partial X_B}\right)\mathrm{d}V - \int_\Omega (B_a - \rho_0\,\ddot{u}_a)\delta u_a\,\mathrm{d}V + \int_{\partial\Omega}\bar{T}_a\delta u_a\,\mathrm{d}s = 0 \\ \Leftrightarrow\quad &\int_\Omega \frac{1}{2}\,S_{AB}(\hat{\mathbf{u}})\,\delta u_a^L\left(F_{aB}(\hat{\mathbf{u}})\frac{\partial\phi_L}{\partial X_A} + F_{aA}(\hat{\mathbf{u}})\frac{\partial\phi_L}{\partial X_B}\right)\mathrm{d}V - \text{rhs} = 0 \end{aligned} \tag{51}$$

where the constant rhs, which is the discretized δW_{ext}, is given by

$$\text{rhs} = \int_\Omega (B_a - \rho_0\,\ddot{u}_a)\delta u_a^L\,\phi_L\,\mathrm{d}V - \int_{\partial\Omega}\bar{T}_a\delta u_a^L\,\phi_L\,\mathrm{d}s.$$

This defines a nonlinear function, $\mathbf{R}(\hat{\mathbf{u}}) \in \mathbb{R}^{3N}$, with one value for each $\delta u_a^L, a = 1,2,3, L = 1,\ldots,N$ (I.e. entry (a,L) of the vector $\mathbf{R}$ contains formula (51) with $\delta u_{\bar{a}}^{\bar{L}} = 1$ for $\bar{a} = a, \bar{L} = L$ and $\delta u_{\bar{a}}^{\bar{L}} = 0$ otherwise). The aim is to find $\hat{\mathbf{u}}$ such that $\mathbf{R}(\hat{\mathbf{u}}) = 0$.

Within the Newton-Raphson scheme the equation is linearized around iterative values $\hat{\mathbf{u}}^{(k)}$.

$$\mathbf{R}(\hat{\mathbf{u}}^{(k+1)}) = \mathbf{R}\Big|_{\hat{\mathbf{u}}=\hat{\mathbf{u}}^{(k)}} + D_{\Delta\hat{\mathbf{u}}^{(k)}}\delta W_{\text{int}}(\hat{\mathbf{u}}, \delta\hat{\mathbf{u}}) + \mathcal{O}\big((\Delta\hat{\mathbf{u}}^{(k)})^2\big).$$

The iterative procedure starts with an initial value $\hat{\mathbf{u}}^{(0)} = \hat{\mathbf{u}}_0$ and repeatedly computes

$$\hat{\mathbf{u}}^{(k+1)} = \hat{\mathbf{u}}^{(k)} + \Delta\hat{\mathbf{u}}^{(k)}.$$

The increment $\Delta\hat{\mathbf{u}}^{(k)}$is computed by assuming $\mathbf{R}(\hat{\mathbf{u}}^{(k+1)}) = 0$ and solving

$$D_{\Delta\hat{\mathbf{u}}^{(k)}}\delta W_{\text{int}}(\hat{\mathbf{u}}, \delta\hat{\mathbf{u}}) = -\mathbf{R}(\hat{\mathbf{u}}^{(k)}). \tag{52}$$

This is a linear system that has to be solved. It is repeated until the residual norm $\|\mathbf{R}(\hat{\mathbf{u}}^{(k)})\|$ gets below a threshold.

The left-hand side term of (52) is derived from (49) (Holzapfel p.396),

$$D_{\Delta\hat{\mathbf{u}}^{(k)}}\delta W_{\text{int}}(\hat{\mathbf{u}}, \delta\hat{\mathbf{u}}) = \int_\Omega \frac{\partial\delta u_a}{\partial X_B} \underbrace{(\delta_{ab}\, S_{BD} + F_{aA}\, F_{bC}\, C_{ABCD})}_{=\tilde{k}_{abBD}} \frac{\partial\Delta u_b}{\partial X_D}\, \mathrm{d}V \tag{53}$$

with

$B, D = 1, \ldots, 3$	...	indices over spatial dimensions
$a, b = 1,$	...	indices over degrees of freedom
$\mathbf{S},$	...	current 2nd Piola-Kirchhoff stress tensor
$\mathbb{C} = \dfrac{\partial\mathbf{S}(\mathbf{E})}{\partial\mathbf{E}},$	...	elasticity tensor
$\tilde{k}_{abBD},$	...	integrand to be used for tangent stiffness matrix.

Note that the expression is a scalar value in total with the inner parantheses term being a forth-order tensor. The expression is bilinear in δu and Δu. The virtual displacements, $\delta\mathbf{u}$ and increments, $\Delta\mathbf{u}$ are discretized as usual, leading to the stiffness matrix $\mathbf{k}$.

Herein, $\partial\delta u_a/\partial X_B$ is a virtual displacement in component $a = 1, 2, 3$, derivative B. In discretized form it is $\delta\hat{u}^L_{a,B}$ with dof index (L, B) and component number a. Eq. (53) has to hold for all $\delta\hat{u}^L_{a,B}$, these are the equations or rows in the stiffness matrix. The columns of the stiffness matrix correspond to the unknown increments, Δu_d, discretized as

$$\frac{\partial\Delta u_b}{\partial X_D} = \Delta\hat{u}^M_b \phi^M_{b,D}.$$

The coefficients, $\Delta\hat{u}^M_b$, are also the same for the real increments, not the derivatives, i.e.

$$\Delta u_b = \Delta\hat{u}^M_b \phi^M_b.$$

The entries of the tangent stiffness matrix, k_{ij} are thus

$$k_{ij} = \int_\Omega \frac{\partial\phi^L_a}{\partial X_B}\, \tilde{k}_{abBD} \frac{\partial\phi^M_b}{\partial X_D}\, \mathrm{d}V \qquad \text{(sum over } B \text{ and } D\text{)}$$

with appropriate mappings $i \mapsto (a, L)$ and $j \mapsto (b, M)$.

The stress, $\mathbf{S}$ is computed by

$$\mathbf{S} = \mathbf{S}_{\text{vol}} + \mathbf{S}_{\text{iso}} = J\, p\, \mathbf{C}^{-1} + 2\frac{\partial \Psi_{\text{iso}}}{\partial \mathbf{C}}$$

The elasticity tensor

$$\mathbb{C} = \mathbb{C}_{\text{vol}} + \mathbb{C}_{\text{iso}} = 2\frac{\partial \mathbf{S}_{\text{vol}}}{\partial \mathbf{C}} + 2\frac{\partial \mathbf{S}_{\text{iso}}}{\partial \mathbf{C}}$$

According to Holzapfel [3] the required quantities are as follows:

$$J = \det(\mathbf{F}), \quad \mathbf{C} = \mathbf{F}^{\top}\mathbf{F}$$

$$\bar{\mathbf{C}} = J^{-2/3}\mathbf{C} \tag{p.228}$$

$$\bar{\gamma}_1 = 2\left(\frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_1} + \bar{I}_1 \frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_2}\right) \tag{p.234}$$

$$\bar{\gamma}_2 = -2\frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_2} \tag{p.234}$$

$$\bar{\mathbf{S}} = 2\frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{\mathbf{C}}} = \bar{\gamma}_1 \mathbf{I} + \bar{\gamma}_2 \bar{\mathbf{C}} \tag{p.234}$$

$$(\mathbb{I})_{abcd} = \delta_{ac}\,\delta_{bd} \tag{p.23}$$

$$\mathbb{P} = \mathbb{I} - \frac{1}{3}\mathbf{C}^{-1} \otimes \mathbf{C} \tag{p.229}$$

$$\mathbf{S}_{\text{iso}} = J^{-2/3}\mathbb{P} : \bar{\mathbf{S}} \tag{p.234}$$

$$p = \frac{\mathrm{d}\Psi_{\text{vol}}(J)}{\mathrm{d}J} \tag{p.230}$$

$$\mathbf{S}_{\text{vol}} = J\,p\,\mathbf{C}^{-1} \tag{p.230, p.245}$$

$$\mathbf{S} = \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{vol}} \tag{p.233}$$

$$\tilde{p} = p + J\frac{\mathrm{d}p}{\mathrm{d}J} \tag{p.255}$$

$$\left(\mathbf{C}^{-1} \odot \mathbf{C}^{-1}\right)_{abcd} = \frac{1}{2}\left(C^{-1}_{ac}\,C^{-1}_{bd} + C^{-1}_{ad}\,C^{-1}_{bc}\right) \tag{p.254}$$

$$\mathbb{C}_{\text{vol}} = J\,\tilde{p}\,\mathbf{C}^{-1} \otimes \mathbf{C}^{-1} - 2\,J\,p\,\mathbf{C}^{-1} \odot \mathbf{C}^{-1} \tag{p.254}$$

$$\bar{\delta}_1 = 4\left(\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_1\,\partial \bar{I}_1} + 2\,\bar{I}_1\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_1\,\partial \bar{I}_2} + \frac{\partial \Psi_{\text{iso}}}{\partial \bar{I}_2} + \bar{I}_1^2\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\,\partial \bar{I}_2}\right) \tag{p.262}$$

$$\bar{\delta}_2 = -4\left(\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_1\,\partial \bar{I}_2} + \bar{I}_1\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\,\partial \bar{I}_2}\right) \tag{p.262}$$

$$\bar{\delta}_3 = 4\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\,\partial \bar{I}_2} \tag{p.262}$$

$$\bar{\delta}_4 = -4\frac{\partial \Psi_{\text{iso}}}{\partial \bar{I}_2} \tag{p.262}$$

$$\bar{\mathbb{C}} = J^{-4/3}\left(\bar{\delta}_1\,\mathbf{I} \otimes \mathbf{I} + \bar{\delta}_2\left(\mathbf{I} \otimes \bar{\mathbf{C}} + \bar{\mathbf{C}} \otimes \mathbf{I}\right) + \bar{\delta}_3\bar{\mathbf{C}} \otimes \bar{\mathbf{C}} + \bar{\delta}_4\,\mathbb{I}\right) \tag{p.262}$$

$$\tilde{\mathbb{P}} = \mathbf{C}^{-1} \odot \mathbf{C}^{-1} - \frac{1}{3}\mathbf{C}^{-1} \otimes \mathbf{C}^{-1} \tag{p.255}$$

$$\mathbb{C}_{\text{iso}} = \mathbb{P} : \bar{\mathbb{C}} : \mathbb{P}^{\top} + \frac{2}{3}\,J^{-2/3}\bar{\mathbf{S}} : \mathbf{C}\,\tilde{\mathbb{P}} - \frac{2}{3}\left(\mathbf{C}^{-1} \otimes \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{iso}} \otimes \mathbf{C}^{-1}\right) \tag{p.255}$$

$$\mathbb{C} = \mathbb{C}_{\text{vol}} + \mathbb{C}_{\text{iso}} \tag{p.254}$$

6.7.3 Linear elasticity

For linear elasticity we have $\mathbf{x} \approx \mathbf{X}$ and

$$\mathbf{K}\,\mathbf{u} = \mathbf{f}$$

with right hand side

$$\mathbf{f} = \int_{\partial\Omega} \bar{T}_a\,\delta u_a^L\,\phi_L\,\mathrm{d}s$$

and stiffness matrix

$$\mathbf{K}(\delta\mathbf{u})\,\mathbf{u} = \int_\Omega \boldsymbol{\sigma} : \delta\boldsymbol{\varepsilon}\,\mathrm{d}\mathbf{x}$$

where $\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}$ with

$$\mathbb{C}_{abcd} = K\,\delta_{ab}\,\delta_{cd} + \mu\,(\delta_{ac}\,\delta_{bd} + \delta_{ad}\,\delta_{bc} - \frac{2}{3}\,\delta_{ab}\,\delta_{cd}),$$

with bulk modulus K and shear modulus μ.

The following symmetry properties hold:

$$\mathbb{C}_{abcd} = \mathbb{C}_{bacd} = \mathbb{C}_{abdc} = \mathbb{C}_{badc} \quad \text{minor symmetries}$$

$$\mathbb{C}_{abcd} = \mathbb{C}_{cdab} \quad \text{major symmetries}$$

Discretization yields:

$$\mathbf{u}_a(\mathbf{x}) = u_a^M\,\phi^M(\mathbf{x}),$$

$$\frac{\partial \mathbf{u}_a(\mathbf{x})}{\partial x_b} = u_a^M\,\frac{\partial \phi^M(\mathbf{x})}{\partial x_b}\,.$$

As before, $a, b = 1, \ldots, D$ indicate components, L, M indicate nodes / dofs. Strain $\boldsymbol{\varepsilon}$ is computed linearly from displacements:

$$\boldsymbol{\varepsilon}_{ab}(\mathbf{x}) = \frac{1}{2}\left(\frac{\partial \mathbf{u}_{(b)}(\mathbf{x})}{\partial x_{(a)}} + \frac{\partial \mathbf{u}_{(a)}(\mathbf{x})}{\partial x_{(b)}}\right) = \frac{1}{2}\left(u_{(b)}^L\,\frac{\partial \phi^L(\mathbf{x})}{\partial x_{(a)}} + u_{(a)}^M\,\frac{\partial \phi^M(\mathbf{x})}{\partial x_{(b)}}\right)$$

This results in

$$\begin{aligned}
\mathbf{K}\,\mathbf{u} &= \delta\boldsymbol{\varepsilon}_{ab}(\mathbf{x})\,\mathbb{C}_{abcd}\,\boldsymbol{\varepsilon}_{cd}(\mathbf{x}) \\
&= \mathbb{C}_{abcd}\,\frac{1}{2}\left(\delta u_{(d)}^L\,\frac{\partial \phi^L(\mathbf{x})}{\partial x_{(c)}} + \delta u_{(c)}^M\,\frac{\partial \phi^M(\mathbf{x})}{\partial x_{(d)}}\right)\frac{1}{2}\left(u_{(b)}^N\,\frac{\partial \phi^N(\mathbf{x})}{\partial x_{(a)}} + u_{(a)}^O\,\frac{\partial \phi^O(\mathbf{x})}{\partial x_{(b)}}\right) \\
&= \frac{1}{4}\,\mathbb{C}_{abcd}\Big(\delta u_{(d)}^L\,u_{(b)}^N\,\frac{\partial \phi^L(\mathbf{x})}{\partial x_{(c)}}\,\frac{\partial \phi^N(\mathbf{x})}{\partial x_{(a)}} + \delta u_{(d)}^L\,u_{(a)}^O\,\frac{\partial \phi^L(\mathbf{x})}{\partial x_{(c)}}\,\frac{\partial \phi^O(\mathbf{x})}{\partial x_{(b)}} \\
&+ \delta u_{(c)}^M\,u_{(b)}^N\,\frac{\partial \phi^M(\mathbf{x})}{\partial x_{(d)}}\,\frac{\partial \phi^N(\mathbf{x})}{\partial x_{(a)}} + \delta u_{(c)}^M\,u_{(a)}^O\,\frac{\partial \phi^M(\mathbf{x})}{\partial x_{(d)}}\,\frac{\partial \phi^O(\mathbf{x})}{\partial x_{(b)}}\Big).
\end{aligned}$$

For matrix entry $\mathbf{M}_{LaMb}$, we have

$$\begin{aligned}
\mathbf{M}_{LaMb} &= \frac{1}{4}\,\mathbb{C}_{cbda}\frac{\partial\phi^L(\mathbf{x})}{\partial x_d}\,\frac{\partial\phi^M(\mathbf{x})}{\partial x_c} + \frac{1}{4}\,\mathbb{C}_{bcda}\frac{\partial\phi^L(\mathbf{x})}{\partial x_d}\,\frac{\partial\phi^M(\mathbf{x})}{\partial x_c} \\
&+\frac{1}{4}\,\mathbb{C}_{cbad}\frac{\partial\phi^L(\mathbf{x})}{\partial x_d}\,\frac{\partial\phi^M(\mathbf{x})}{\partial x_c} + \frac{1}{4}\,\mathbb{C}_{bcad}\frac{\partial\phi^L(\mathbf{x})}{\partial x_d}\,\frac{\partial\phi^M(\mathbf{x})}{\partial x_c} \\
&= \frac{1}{4}\left(\mathbb{C}_{cbda} + \mathbb{C}_{bcda} + \mathbb{C}_{cbad} + \mathbb{C}_{bcad}\right)\frac{\partial\phi^L(\mathbf{x})}{\partial x_d}\,\frac{\partial\phi^M(\mathbf{x})}{\partial x_c} \\
&= \mathbb{C}_{adbc}\frac{\partial\phi^L(\mathbf{x})}{\partial x_d}\,\frac{\partial\phi^M(\mathbf{x})}{\partial x_c}
\end{aligned}$$

6.7.4 Using active stress

For the stress inside the muscle we have $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\text{passive}} + \boldsymbol{\sigma}_{\text{active}}$.

$$\mathbf{I}(\mathbf{u}, \delta\mathbf{u}) = \int_\Omega (\boldsymbol{\sigma}_{\text{passive}} + \boldsymbol{\sigma}_{\text{active}}) : \delta\boldsymbol{\varepsilon}\,\mathrm{d}\mathbf{x} = \int_\Omega (\mathbb{C} : \boldsymbol{\varepsilon} + \boldsymbol{\sigma}_{\text{active}}) : \delta\boldsymbol{\varepsilon}\,\mathrm{d}\mathbf{x} = \mathbf{K}(\delta\mathbf{u})\,\mathbf{u} + \mathbf{f}_{\text{active}}$$

The additional term can be computed by

$$\mathbf{f}_{\text{active}} = \int_\Omega \boldsymbol{\sigma}^{\text{active}}_{ab}\,\delta\boldsymbol{\varepsilon}_{ab}\,\mathrm{d}\mathbf{x} = \int_\Omega \boldsymbol{\sigma}^{\text{active}}_{ab}\frac{1}{2}\left(\delta u^L_b\,\frac{\partial\phi^L(\mathbf{x})}{\partial x_a} + \delta u^M_a\,\frac{\partial\phi^M(\mathbf{x})}{\partial x_b}\right)\mathrm{d}\mathbf{x}.$$

The entry of $\mathbf{f}$ is

$$\mathbf{f}^{\text{active}}_{La} = \int_\Omega \left(\frac{1}{2}\,\boldsymbol{\sigma}^{\text{active}}_{ba}\,\frac{\partial\phi^L(\mathbf{x})}{\partial x_b} + \frac{1}{2}\,\boldsymbol{\sigma}^{\text{active}}_{ab}\,\frac{\partial\phi^L(\mathbf{x})}{\partial x_b}\right)\mathrm{d}\mathbf{x}.$$

Because of symmetry of $\boldsymbol{\sigma}$, we have

$$\mathbf{f}^{\text{active}}_{La} = \int_\Omega \boldsymbol{\sigma}^{\text{active}}_{ab}\,\frac{\partial\phi^L(\mathbf{x})}{\partial x_b}\,\mathrm{d}\mathbf{x}.$$

Care must be taken when setting up the principle of virtual work, $\delta W_{\text{int}} = \delta W_{\text{ext}}$. Normally, we would have

$$\delta W_{\text{int}} = \mathbf{I}(\mathbf{u}, \delta\mathbf{u})$$

and

$$\delta W_{\text{int}}(\mathbf{u}, \delta\mathbf{u}) = \delta W_{\text{ext}}(\mathbf{u}, \delta\mathbf{u}), \quad \forall\delta\mathbf{u} \in H^1_0(\Omega).$$

This gives one scalar equation for each basis vector of the discretized space. Each equation can be thought of as equating the work that is needed externally and transferred to elastic energy internally, if one particular node is displaced along one coordinate axis by an infinitesimal amount. This would lead to strains around the particular node. The strain itself produce a stress response. This stress together with the strain, again, produces the work.

In this formulation, the active stress term, $(\boldsymbol{\sigma}^{\text{active}} : \delta\boldsymbol{\varepsilon})$, is part of the internal virtual work. However, this makes no sense as it is not the strain that causes the stress in this case, but the

stress acts independent of the strain. This active stress actively adds virtual work to the system and should therefore be considered as external virtual work.

The quantity $\boldsymbol{\sigma}^{\text{active}}$ in the equation can be seen as an additive part of the stress that results not from the material response to the strain, but from an external active stress, $\boldsymbol{\sigma}^{\text{active,applied}}$, which is independently magically applied everywhere in the muscle continuum. Therefore we have to set

$$\boldsymbol{\sigma}^{\text{active}} = -\boldsymbol{\sigma}^{\text{active,applied}}$$

This leads to the following equation which has no minus signs.

$$\int_\Omega \mathbb{C} : \boldsymbol{\varepsilon} : \delta\boldsymbol{\varepsilon}\, \mathrm{d}\mathbf{x} = \int_\Omega \boldsymbol{\sigma}^{\text{active,applied}} : \delta\boldsymbol{\varepsilon}\, \mathrm{d}\mathbf{x}.$$

Furthermore, there will only be external virtual work by the active stress when the strain is negative (which means compression/contraction). Therefore, we have to use

$$\int_\Omega \mathbb{C} : \boldsymbol{\varepsilon} : \delta\boldsymbol{\varepsilon}\, \mathrm{d}\mathbf{x} = \int_\Omega \boldsymbol{\sigma}^{\text{active,applied}} : (\delta\boldsymbol{\varepsilon})_-\, \mathrm{d}\mathbf{x},$$

with

$$(x)_- = \begin{cases} x & \text{if } x < 0, \\ 0 & \text{else.} \end{cases}$$

(Not completely sure about the argumentation, at least this gives reasonable numerical results, while other signs and omitting the $(\cdot)_-$ fails.)

6.7.5 Handling of Dirichlet boundary conditions

The Newton algorithm to solve the nonlinear equation $f(\mathbf{x}) = \mathbf{b}$ for $\mathbf{x}$ with respect to Dirichlet boundary conditions $\mathbf{x}_i = \mathbf{x}_{0i}$ for $i \in \mathcal{I}$ can be summarized as follows:

set initial $\mathbf{x}_0$
$\mathbf{x}_i := \mathbf{x}_{0i}$ (initial values satisfy boundary conditions)
$\mathbf{f} := f(\mathbf{x}_i)$
while $\|\mathbf{b} - \mathbf{f}\| \geq \text{tol}$
  `apply_BC_to_f`
  $\mathbb{C}_i := J_f(\mathbf{x}_i)$
  `apply_BC_to_`$\mathbb{C}_i$
  solve $\mathbb{C}_i\, \Delta\mathbf{x}_i = \mathbf{b} - \mathbf{f}$ for $\Delta\mathbf{x}_i$
  $\mathbf{x}_{i+1} := \mathbf{x}_i + \Delta\mathbf{x}_i$
  $\mathbf{f} := f(\mathbf{x}_{i+1})$

The operation `apply_BC_to_f` sets values $\mathbf{f}_i = \mathbf{b}_i$ for all $i \in \mathcal{I}$. The operation `apply_BC_to_`$\mathbb{C}_i$ sets rows and columns for which BC are specified to the identity matrix, i.e. set

$$\mathbb{C}_{ii} = 1 \quad \forall\, i \in \mathcal{I}$$

$$\mathbb{C}_{ij} = \mathbb{C}_{ji} = 0, \quad \forall j \neq i\, \forall i \in \mathcal{I}.$$

By doing so the system of linear equation $\mathbb{C}_i \, \Delta \mathbf{x}_i = \mathbf{b} - \mathbf{f}$ contains the equations $\Delta x_i = b_i - f_i = 0$ for $i \in \mathcal{I}$. Therefore the variables $\mathbf{x}_i$ don't change their value in the loop and keep the initially assigned Dirichlet BC value.

6.8 Nonlinear hyperelasticity

This section is a rewrite of the theory.

We assume a stationary problem. We use a mixed formulation, meaning that the displacement, $\mathbf{u}(\mathbf{X})$, and the pressure, $p(\mathbf{X})$, are discretized separately. The formulation is described in material configuration.

We define the Hellinger-Reissner energy functional, $\Pi_L(\mathbf{u}, p)$ which describes the potential energy of the system. It is additively composed of internal and external potential energy,

$$\Pi_L(\mathbf{u}, p) = \Pi_{\text{int}}(\mathbf{u}, p) + \Pi_{\text{ext}}(\mathbf{u}).$$

The external energy functional is given by

$$\Pi_{\text{ext}}(\mathbf{u}) = -\int_{\Omega_0} \mathbf{B}\mathbf{u} \, \mathrm{d}V - \int_{\partial\Omega_0} \bar{T}\mathbf{u} \, \mathrm{d}S,$$

with body forces, $\mathbf{B} = J\,\mathbf{b}$, in reference configuration, Ω_0, and prescribed surface traction $\bar{T}$.

The internal energy functional can be expressed by

$$\Pi_{\text{int}}(\mathbf{u}) = \int_{\Omega_0} \Big(p\,\big(J(\mathbf{u}) - 1\big) + \Psi_{\text{iso}}\big(\bar{\mathbf{C}}(\mathbf{u})\big) \Big) \, \mathrm{d}V.$$

Here, Ψ_{iso} is a strain-energy density function, and is defined on the reference configuration, Ω_0. It describes the isochoric elastic response of the material and depends on the modified right Cauchy-Green tensor,

$$\bar{\mathbf{C}}(\mathbf{u}) = J^{-2/3}\,\mathbf{C}.$$

p is the Lagrange multiplier to the the incompressibility constraint, $J(\mathbf{u}) = 1$. It is also the hydrostatic pressure in this case.

According to the principle of stationary potential energy, the system is in equilibrium if the potential energy functional is stationary. This is the case if the first variation of the potential, $\delta\Pi_L$, is zero.

The variation is defined as

$$D_{\delta\mathbf{u}}\Pi(\mathbf{u}) = \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\Pi(\mathbf{u} + \varepsilon\delta\mathbf{u})\big|_{\varepsilon=0}. \tag{54}$$

Using the additive structure of Π_L, we can express the principle of stationary as

$$\begin{aligned} 0 &= D_{\delta\mathbf{u}}\Pi_L(\mathbf{u}, p) = D_{\delta\mathbf{u}}\Pi_{\text{int}}(\mathbf{u}, p) + D_{\delta\mathbf{u}}\Pi_{\text{ext}}(\mathbf{u}), \\ 0 &= D_{\delta p}\Pi_L(\mathbf{u}, p) = D_{\delta p}\Pi_{\text{int}}(\mathbf{u}, p) \end{aligned} \tag{55}$$

The variations of the internal energy functionals are identified as the internal and external virtual work,

$$D_{\delta\mathbf{u}}\Pi_{\text{int}}(\mathbf{u},p) = \delta W_{\text{int}}, \quad D_{\delta\mathbf{u}}\Pi_{\text{ext}}(\mathbf{u}) = -\delta W_{\text{ext}}.$$

The first equation of eq. (54) can be rewritten as

$$\delta W_{\text{int}} - \delta W_{\text{ext}} \quad = 0.$$

Next, we derive the expressions for eq. (55). We start with the directional derivative in the direction of the virtual pressure, δp.

$$\begin{aligned} D_{\delta p}\Pi_{\text{int}}(\mathbf{u},p) &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\Pi_{\text{int}}(\mathbf{u},p+\varepsilon\delta p)\big|_{\varepsilon=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\Omega_0}\Big((p+\varepsilon\delta p)\,\big(J(\mathbf{u})-1\big)+\Psi_{\text{iso}}\big(\bar{\mathbf{C}}(\mathbf{u})\big)\Big)\,\mathrm{d}V\big|_{\varepsilon=0} \\ &= \int_{\Omega_0}\big(J(\mathbf{u})-1\big)\delta p\,\mathrm{d}V. \end{aligned}$$

The corresponding Euler-Lagrange equation is the incompressibility constraint, $J = 1$.

For the directional derivative of the internal energy functional with respect to $\delta\mathbf{u}$ we get

$$\begin{aligned} D_{\delta\mathbf{u}}\Pi_{\text{int}}(\mathbf{u},p) &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\,\Pi_{\text{int}}(\mathbf{u}+\varepsilon\delta\mathbf{u},p)\big|_{\varepsilon=0} \\ &= \frac{\mathrm{d}}{\mathrm{d}\varepsilon}\int_{\Omega_0}\Big(p\,\big(J(\mathbf{u}+\varepsilon\delta\mathbf{u})-1\big)+\Psi_{\text{iso}}\big(\bar{\mathbf{C}}(\mathbf{u}+\varepsilon\delta\mathbf{u})\big)\Big)\,\mathrm{d}V\big|_{\varepsilon=0} \\ &= \int_{\Omega_0}\Big(\underbrace{J(\mathbf{u})\,p\,\mathbf{C}^{-1}(\mathbf{u})}_{=\mathbf{S}_{\text{vol}}(\mathbf{u},p)}+2\underbrace{\frac{\partial\Psi_{\text{iso}}(\bar{\mathbf{C}}(\mathbf{u}))}{\partial\mathbf{C}}}_{=\mathbf{S}_{\text{iso}}(\mathbf{u})}\Big):\delta\mathbf{E}(\mathbf{u})\,\mathrm{d}V \\ &= \int_{\Omega_0}\mathbf{S}(\mathbf{u},p):\delta\mathbf{E}(\mathbf{u})\,\mathrm{d}V \\ &= \delta W_{\text{int,vol}}(\mathbf{u},p)+\delta W_{\text{int,iso}}(\mathbf{u}) = \delta W_{\text{int}}. \end{aligned} \tag{56}$$

(See [3] eq. (8.105) for the missing steps.) As can be seen, the internal virtual work is decomposed into volumentric and isochoric portions.

The external virtual work is given by

$$D_{\delta\mathbf{u}}\Pi_{\text{ext}}(\mathbf{u}) = -\delta W_{\text{ext}} = -\int_{\Omega_0}\mathbf{B}\cdot\delta\mathbf{u}\,\mathrm{d}V - \int_{\partial\Omega_0^{\text{traction}}}\bar{\mathbf{T}}\cdot\delta\mathbf{u}\,\mathrm{d}S$$

Discretization

The displacements, $\mathbf{u}$, have components, u_a, i.e., $\mathbf{u} = u_a\,\mathbf{e}_a$. Indices $a, b, c, A, B, C, \ldots$ denote dimensions and always run from 1 to dimension D, e.g. $i = 1, \ldots, 3$. Lower-case letters are for current configuration, upper-case letters denote reference configuration. Indices $L, M, N, \ldots$ denote degrees of freedom and run from 1 to the number of nodes. Einstein sum convention is used, indices in parantheses mean no summation over this index.

We discretize the displacements, u_a, pressure, p, increments $\Delta u_a, \Delta p$ and the virtual displacements and virtual pressure, $\delta u_a, \delta p$, using two different ansatz functions for displacements and pressure, $\phi(\mathbf{X})$ and $\psi(\mathbf{X})$, respectively,

$$\begin{aligned}
u_a &= \hat{u}_a^L \phi_{(a)}^L, & \frac{\partial u_a}{\partial X_A} &= \hat{u}_a^M \phi_{(a),A}^M, & p &= \hat{p}^L \psi^L \\
\Delta u_a &= \Delta\hat{u}_a^L \phi_{(a)}^L, & \frac{\partial \Delta u_a}{\partial X_A} &= \Delta\hat{u}_a^M \phi_{(a),A}^M, & \Delta p &= \Delta\hat{p}^L \psi^L \\
\delta u_a &= \delta\hat{u}_a^L \phi_{(a)}^L, & \frac{\partial \delta u_a}{\partial X_A} &= \delta\hat{u}_a^M \phi_{(a),A}^M, & \delta p &= \delta\hat{p}^L \psi^L
\end{aligned}$$

We choose

$$\phi_{(a)}^M(\mathbf{X}) = \phi^M(\mathbf{X}) = \phi^{M_1}(X_1) \cdot \phi^{M_2}(X_2) \cdot \phi^{M_3}(X_3) \quad \Rightarrow \quad \phi_{(a),2}^M(\mathbf{X}) = \phi^{M_1}(X_1) \cdot \phi'^{M_2}(X_2) \cdot \phi^{M_3}(X_3)$$

The variation of the Green-Lagrange strain tensor, $\delta\mathbf{E}$ is given by ([3] p.375)

$$\begin{aligned}
\delta\mathbf{E} &= \operatorname{sym}\left(\mathbf{F}^\top \nabla\delta u\right) = \frac{1}{2}\left((\mathbf{F}^\top\nabla\delta\mathbf{u})^\top + \mathbf{F}^\top\nabla\delta\mathbf{u}\right), \\
\delta E_{AB} &= \frac{1}{2}\left(F_{aB}\frac{\partial\delta u_a}{\partial X_A} + F_{aA}\frac{\partial\delta u_a}{\partial X_B}\right) \\
&= \frac{1}{2}\left(F_{aB}\,\delta\hat{u}_a^M\phi_{(a),A}^M + F_{aA}\,\delta\hat{u}_a^M\phi_{(a),B}^M\right) \\
&= \frac{1}{2}\left(F_{aB}\,\phi_{(a),A}^M + F_{aA}\,\phi_{(a),B}^M\right)\delta\hat{u}_a^M
\end{aligned} \tag{57}$$

Starting from eq. (56) we get with eq. (57)

$$\delta W_{\text{int}}(\mathbf{u}, p) = \int_\Omega \frac{1}{2}\, S_{AB}(\mathbf{u}, p)\,\left(F_{aB}\,\phi_{(a),A}^M + F_{aA}\,\phi_{(a),B}^M\right)\delta\hat{u}_a^M\,\mathrm{d}V$$

We derive an expression for S_{AB}. From eq. (56) we know

$$\begin{aligned}
S_{AB} &= J(\mathbf{u})\,p\,C_{AB}^{-1}(\mathbf{u}) + 2\frac{\partial\Psi_{\text{iso}}(\bar{\mathbf{C}}(\mathbf{u}))}{\partial C_{AB}} \\
&= J(\mathbf{u})\,p\,C_{AB}^{-1}(\mathbf{u}) + 2\frac{\partial\Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2}{\partial C_{AB}})
\end{aligned}$$

with ([3] p.234)

$$S_{AB} = J^{-2/3}\cdot\left(\frac{1}{2}\left(\delta_{AC}\delta_{BD} + \delta_{AD}\delta_{BC}\right) - \frac{1}{3}C_{AB}^{-1}\,C_{CD}\right)\bar{S}_{CD} + J\,p\,C_{AB}^{-1}$$

with (p.228,229)

$$\begin{aligned}
\bar{S}_{CD} &= \bar{\gamma}_1\,\delta_{CD} + \bar{\gamma}_2\,\bar{C}_{CD} \\
&= \bar{\gamma}_1\,\delta_{CD} + \bar{\gamma}_2\,J^{-2/3}\,C_{CD}, \qquad \bar{\gamma}_1 = 2\left(\frac{\partial\Psi_{\text{iso}}(\bar{I}_1,\bar{I}_2)}{\partial\bar{I}_1} + \bar{I}_1\,\frac{\partial\Psi_{\text{iso}}(\bar{I}_1,\bar{I}_2)}{\partial\bar{I}_2}\right), \quad \bar{\gamma}_2 = -2\,\frac{\partial\Psi_{\text{iso}}(\bar{I}_1,\bar{I}_2)}{\partial\bar{I}_2}
\end{aligned}$$

So in summary we get

$$S_{AB} \;= J^{-2/3}\Big(\frac{1}{2}\left(\delta_{AC}\delta_{BD}+\delta_{AD}\delta_{BC}\right)-\frac{1}{3}C^{-1}_{AB}\,C_{CD}\Big)\left(\bar{\gamma}_1\,\delta_{CD}+\bar{\gamma}_2\,J^{-2/3}\,C_{CD}\right)+J\,p\,C^{-1}_{AB}.$$

S_{AB}, which is the 2nd Piola-Kirchhoff stress tensor, is symmetric, since $\mathbf{C}$ and $\mathbf{C}^{-1}$ are symmetric.

The jacobian determinant, J, can be computed from discretized quantities as follows.

$$F_{aA} = \delta_{aA} + \frac{\partial u_a}{\partial X_A} \;= \delta_{aA} + \hat{u}^M_a \phi^M_{(a),A}$$
$$J = \det \mathbf{F}$$

The external virtual work for the dynamic case is given by

$$\begin{aligned} D_{\delta\mathbf{u}}\Pi_{\text{ext}} = -\delta W_{\text{ext}} \;&= -\int_\Omega (B_a - \rho_0\,\ddot{u}_a)\delta u_a \,\mathrm{d}V - \int_{\partial\Omega} \bar{T}_a \delta u_a \,\mathrm{d}S \\ &= -\int_\Omega \left(B^L_a\,\phi^L_{(a)} - \rho_0\,\hat{\ddot{u}}^L_a\,\phi^L_{(a)}\right)\delta\hat{u}^M_a\,\phi^M_{(a)}\,\mathrm{d}V - \int_{\partial\Omega}\bar{T}^L_a\phi^L_{(a)}\delta\hat{u}^M_a\,\phi^M_{(a)}\,\mathrm{d}S \end{aligned}$$

In summary, the nonlinear equations are

$$\begin{aligned} &\begin{cases} D_{\delta\mathbf{u}}\Pi_{\text{int}}(\mathbf{u},p) + D_{\delta\mathbf{u}}\Pi_{\text{ext}}(\mathbf{u}) = 0 & \forall\,\delta\mathbf{u}, \\ D_{\delta p}\Pi_{\text{int}}(\mathbf{u},p) = 0 & \forall\,\delta p, \end{cases} \\ \Leftrightarrow\quad &\begin{cases} \delta W_{\text{int}} - \delta W_{\text{ext}} = 0 & \forall\,\delta\mathbf{u}, \\ D_{\delta p}\Pi_L = 0 & \forall\,\delta p, \end{cases} \end{aligned}$$

where

$$\begin{aligned} \delta W_{\text{int}}(\mathbf{u},p) &= \int_\Omega \frac{1}{2}\,S_{AB}(\mathbf{u},p)\,\left(F_{aB}\,\phi^M_{(a),A} + F_{aA}\,\phi^M_{(a),B}\right)\delta\hat{u}^M_a\,\mathrm{d}V \\ \delta W_{\text{ext}} &= \int_\Omega (B_a - \rho_0\,\ddot{u}_a)\phi^M_{(a)}\,\delta\hat{u}^M_a\,\mathrm{d}V + \int_{\partial\Omega}\bar{T}^L_a\,\phi^L_{(a)}\,\phi^M_{(a)}\,\delta\hat{u}^M_a\,\mathrm{d}S \\ D_{\delta p}\Pi_L(\mathbf{u}) &= \int_\Omega \left(J(\mathbf{u})-1\right)\delta p\,\mathrm{d}V \end{aligned} \tag{58}$$

Solution

To illustrate the algorithm, we define $(\hat{\mathbf{u}},\hat{p}) =: \mathbf{z}$ and the governing equations to be $W(\mathbf{u},p) =: \mathcal{W}(z) = 0$. We proceed by linearization:

$$\mathcal{W}(z+\Delta z) = \mathcal{W}(z) + \mathcal{J}\,\Delta z + o(z+\Delta z)$$

$$\mathcal{W}(z) + \mathcal{J}\,\Delta z \stackrel{!}{=} 0$$

This leads to the iterative Newton scheme, which in its simplest form uses the iteration

$$\mathcal{J}\,\Delta z^{(i)} = -\mathcal{W}(z^{(i)}),$$
$$z^{(i+1)} = z^{(i)} + \Delta z^{(i)}$$

In terms of $\mathbf{u}$ and p, this can be expressed as

$$\begin{aligned} D^2_{\delta\mathbf{u},\Delta\mathbf{u}}\Pi_L(\mathbf{u},p)\,\Delta\mathbf{u} + D^2_{\delta\mathbf{u},\Delta p}\Pi_L(\mathbf{u},p)\,\Delta p &= -D_{\delta\mathbf{u}}\Pi_L(\mathbf{u},p) \quad \forall\,\delta\mathbf{u} \\ D^2_{\delta p,\Delta\mathbf{u}}\Pi_L(\mathbf{u},p)\,\Delta\mathbf{u} + D^2_{\delta p,\Delta p}\Pi_L(\mathbf{u},p)\,\Delta p &= -D_{\delta p}\Pi_L(\mathbf{u},p) \quad \forall\,\delta p \end{aligned}$$

To compute the second directional derivatives we recall the first derivatives eq. (64):

$$\begin{aligned} D_{\delta\mathbf{u}}\Pi_L(\mathbf{u},p) = &\int_\Omega \frac{1}{2}\,S_{AB}(\mathbf{u},p)\,\Big(F_{aB}\,\phi^L_{(a),A} + F_{aA}\,\phi^L_{(a),B}\Big)\,\delta\hat{u}^L_a\,\mathrm{d}V \\ &- \int_\Omega (B_a - \rho_0\,\hat{\ddot{u}}_a)\phi^L_{(a)}\,\delta\hat{u}^L_a\,\mathrm{d}V - \int_{\partial\Omega}\bar{T}_a\,\phi^L_{(a)}\,\delta\hat{u}^L_a\,\mathrm{d}S \\ D_{\delta p}\Pi_L(\mathbf{u},p) = &\int_\Omega \big(J(\mathbf{u})-1\big)\,\delta p\,\mathrm{d}V = \int_\Omega \big(J(\mathbf{u})-1\big)\,\psi^L\,\delta\hat{p}^L\,\mathrm{d}V \end{aligned} \tag{59}$$

Linearization yields (p.396)

$$\begin{aligned} D^2_{\delta\mathbf{u},\Delta\mathbf{u}}\Pi_L(\mathbf{u},p) &= \int_{\Omega_0}\big(\nabla\delta\mathbf{u} : \nabla\Delta\mathbf{u}\,\mathbf{S} + \mathbf{F}^\top\nabla\delta\mathbf{u} : (\mathbb{C}_{\text{vol}} + \mathbb{C}_{\text{iso}}) : \mathbf{F}^\top\nabla\Delta\mathbf{u}\big)\,\mathrm{d}V \\ &= \int_{\Omega_0}\Big(\underbrace{\frac{\partial\delta u_a}{\partial X_B}\,\frac{\partial\Delta u_a}{\partial X_D}\,S_{BD}}_{\substack{\text{geometrical}\\ \text{stress contribution}}} + \underbrace{F_{aA}\frac{\partial\delta u_a}{\partial X_B}\,\mathbb{C}_{ABCD}\,F_{bC}\frac{\partial\Delta u_b}{\partial X_D}}_{\substack{\text{material}\\ \text{contribution}}}\Big)\,\mathrm{d}V \\ &= \int_{\Omega_0}\frac{\partial\delta u_a}{\partial X_B}\,(\delta_{ab}S_{BD} + F_{aA}\,F_{bC}\,\mathbb{C}_{ABCD})\frac{\partial\Delta u_b}{\partial X_D}\,\mathrm{d}V \\ &= \int_{\Omega_0}\delta\hat{u}^L_a\,\phi^L_{(a),B}\big(\delta_{ab}S_{BD} + F_{aA}\,F_{bC}\,\mathbb{C}_{ABCD}\big)\phi^M_{(b),D}\,\Delta\hat{u}^M_b\,\mathrm{d}V \\ D^2_{\delta p,\Delta\mathbf{u}}\Pi_L(\mathbf{u},p) &= \int_{\Omega_0} J(\mathbf{u})\,\delta p\,\nabla_{\mathbf{x}}\cdot\Delta\mathbf{u}\,\mathrm{d}V \\ D^2_{\delta\mathbf{u},\Delta p}\Pi_L(\mathbf{u},p) &= \int_{\Omega_0} J(\mathbf{u})\,\nabla_{\mathbf{x}}\cdot\delta\mathbf{u}\,\Delta p\,\mathrm{d}V \\ D^2_{\delta p,\Delta p}\Pi_L(\mathbf{u},p) &= 0 \end{aligned} \tag{60}$$

with $\mathbb{C} = \partial\mathbf{S}(\mathbf{E})/\partial\mathbf{E} = 2\partial\mathbf{S}(\mathbf{C})/\partial\mathbf{C} = \mathbb{C}_{\text{vol}} + \mathbb{C}_{\text{iso}}$ from Holzapfel [3] ($\mathbb{C}_{\text{vol}}$ p.254, $\mathbb{C}_{\text{iso}}$ p.255)

$$\mathbb{C}_{\text{vol}} = \frac{\partial J(\mathbf{u})p\mathbf{C}^{-1}(\mathbf{u})}{\partial\mathbf{C}}\ ,$$
$$\mathbb{C}_{\text{iso}} = 4\frac{\partial^2\Psi_{\text{iso}}(\bar{\mathbf{C}})}{\partial\mathbf{C}\partial\mathbf{C}}\ .$$

Note that the term for $D^2_{\delta\mathbf{u},\Delta\mathbf{u}}\Pi_L(\mathbf{u},p)$ is the same as in (53), while we can expand the term $\nabla_{\mathbf{x}}\cdot\delta\mathbf{u}$

as (Holzapfel [3] p.405)

$$\begin{aligned}
\nabla_{\mathbf{x}} \cdot \delta\mathbf{u} &= \mathbf{C}^{-1} : \delta\mathbf{E} \\
&= \mathbf{C}^{-1} : \mathrm{sym}(\mathbf{F}^T \nabla_{\mathbf{X}} \delta\mathbf{u}) \\
&= \mathbf{C}^{-1} : \mathbf{F}^T \nabla_{\mathbf{X}} \delta\mathbf{u} \\
(A : BC &= B^T A : C) \\
&= \mathbf{F}\mathbf{C}^{-1} : \nabla_{\mathbf{X}} \delta\mathbf{u} \\
&= \mathbf{F}^{-T} : \nabla_{\mathbf{X}} \delta\mathbf{u}\,.
\end{aligned}$$

Equation (60) is given in index notation by:

$$\begin{aligned}
D^2_{\delta\mathbf{u},\Delta\mathbf{u}}\Pi_L(\mathbf{u},p) &= \int_\Omega \frac{\partial \delta u_a}{\partial X_B}\left(\delta_{ab}\, S_{DB} + F_{aA}\, F_{bC}\, C_{ABCD}\right)\frac{\partial \Delta u_b}{\partial X_D}\,\mathrm{d}V \\
D^2_{\delta p,\Delta\mathbf{u}}\Pi_L(\mathbf{u},p) &= \int_\Omega J\,\delta p\,(F^{-1})_{Ba}\frac{\partial \Delta u_a}{\partial X_B}\,\mathrm{d}V = \int_\Omega J\,\delta p\,(F^{-1})_{Ba}\phi^L_{(a),B}\,\Delta\hat{u}^L_a\,\mathrm{d}V \\
D^2_{\delta\mathbf{u},\Delta p}\Pi_L(\mathbf{u},p) &= \int_\Omega J\,\Delta p\,(F^{-1})_{Ba}\frac{\partial \delta u_a}{\partial X_B}\,\mathrm{d}V = \int_\Omega J\,\Delta p\,(F^{-1})_{Ba}\phi^L_{(a),B}\,\delta\hat{u}^L_a\,\mathrm{d}V \\
D^2_{\delta p,\Delta p}\Pi_L(\mathbf{u},p) &= 0
\end{aligned}$$

In summary we get

$$\begin{aligned}
D^2_{\delta\mathbf{u},\Delta\mathbf{u}}\Pi_L(\mathbf{u},p) &= \int_\Omega \frac{\partial \delta u_a}{\partial X_B}\left(\delta_{ab}\, S_{DB} + F_{aA}\, F_{bC}\, C_{ABCD}\right)\frac{\partial \Delta u_b}{\partial X_D}\,\mathrm{d}V \\
&= \delta\hat{u}^L_a\,\Delta\hat{u}^M_b \int_\Omega \phi^L_{(a),B}\left(\delta_{ab}\, S_{DB} + F_{aA}\, F_{bC}\, C_{ABCD}\right)\phi^M_{(b),D}\,\mathrm{d}V, \\
D^2_{\delta p,\Delta\mathbf{u}}\Pi_L(\mathbf{u},p) &= \int_\Omega J\,\delta p\,(F^{-1})_{Ba}\,\frac{\partial \Delta u_a}{\partial X_B}\,\mathrm{d}V, \\
&= \delta\hat{p}^L\,\Delta\hat{u}^M_a \int_\Omega J\,\psi^L\,(F^{-1})_{Ba}\,\phi^M_{(a),B}\,\mathrm{d}V \\
D^2_{\delta\mathbf{u},\Delta p}\Pi_L(\mathbf{u},p) &= \int_\Omega J\,\Delta p\,(F^{-1})_{Ba}\,\frac{\partial \delta u_a}{\partial X_B} \\
&= \Delta\hat{p}^L\,\delta\hat{u}^M_a \int_\Omega J\,\psi^L\,(F^{-1})_{Ba}\phi^M_{(a),B}\,\mathrm{d}V \\
D^2_{\delta p,\Delta p}\Pi_L(\mathbf{u},p) &= 0,
\end{aligned}$$

leading to the matrix formulation of the Newton iteration:

$$\begin{bmatrix} \mathbf{k}_{\delta\mathbf{u},\Delta\mathbf{u}} & \mathbf{k}^\top_{\delta p,\Delta\mathbf{u}} \\ \mathbf{k}_{\delta p,\Delta\mathbf{u}} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Delta\hat{\mathbf{u}} \\ \Delta\hat{p} \end{bmatrix} = \begin{bmatrix} \mathbf{R}_{\delta\mathbf{u}} \\ \mathbf{R}_{\delta p} \end{bmatrix}. \tag{61}$$

The stiffness matrix is symmetric.

Given the number of spatial dimensions $a, b = 1, \ldots, D = 3$, the blocks of the Jacobian or tangent

stiffness matrix are given by:

$$\mathbf{k}_{\delta\mathbf{u},\Delta\mathbf{u},(L,a),(M,b)} = \int_\Omega \phi^L_{(a),B} \tilde{k}_{abBD} \phi^M_{(b),D}\, \mathrm{d}V \qquad \text{with} \qquad \tilde{k}_{abBD} = \delta_{ab}\, S_{BD} + F_{aA}\, F_{bC}\, \mathbb{C}_{ABCD}$$

$d \times d$ blocks of submatrices, each with size $(u_{\text{dofs}} \times u_{\text{dofs}})$

$$\mathbf{k}_{\delta p,\Delta\mathbf{u},L,(M,a)} = \int_\Omega J\, \psi^L\, (F^{-1})_{Ba}\, \phi^M_{(a),B}\, \mathrm{d}V$$

$1 \times d$ blocks of submatrices, each with size $(p_{\text{dofs}} \times u_{\text{dofs}})$

The blocks of the residual on the righ-hand side (quasi-static case and neglecting gravity) follow from eq. (59) and are given by

$$-\mathbf{R}_{\delta\mathbf{u},(L,a)} = D_{\delta\mathbf{u},(L,a)} \Pi_L(\mathbf{u}, p) = \delta W_{\text{int},(L,a)} - \delta W_{\text{ext},(L,a)} = -\big(\mathbf{R}^{\text{int}}_{\delta\mathbf{u},(L,a)} + \mathbf{R}^{\text{ext}}_{\delta\mathbf{u},(L,a)}\big) \text{ with}$$

$$-\mathbf{R}^{\text{int}}_{\delta\mathbf{u},(L,a)} = \int_\Omega \frac{1}{2}\, S_{AB} \left(F_{aB} \phi^L_{(a),A} + F_{aA} \phi^L_{(a),B} \right) \mathrm{d}V$$

$$-\mathbf{R}^{\text{ext}}_{\delta\mathbf{u},(L,a)} = -\int_\Omega \big(B^M_a\, \phi^M_{(a)} - \rho_0\, \hat{\ddot{u}}^M_a\, \phi^M_{(a)}\big) \phi^L_{(a)}\, \mathrm{d}V - \int_{\partial\Omega} \bar{T}^M_a\, \phi^M_{(a)}\, \phi^L_{(a)}\, \mathrm{d}S$$

d blocks of subvectors with length u_{dofs}

$$-\mathbf{R}_{\delta p,L} = D_{\delta p,L} \Pi_L(\mathbf{u}, p) = \int_\Omega (J - 1)\, \psi^L\, \mathrm{d}V$$

1 subvector of length p_{dofs}

The tensors inside $\mathbf{k}$ and $\mathbf{R}$ are computed using the current iterates $\hat{\mathbf{u}}^{(i)}$, $\hat{p}^{(i)}$. The new values $\hat{\mathbf{u}}^{(i+1)}, \hat{p}^{(i+1)}$ are computed by adding the increments $\Delta\hat{\mathbf{u}}^{(i)}, \Delta\hat{p}^{(i)}$:

$$\hat{\mathbf{u}}^{(i+1)} = \hat{\mathbf{u}}^{(i)} + \Delta\hat{\mathbf{u}}^{(i)}$$

$$\hat{p}^{(i+1)} = \hat{p}^{(i)} + \Delta\hat{p}^{(i)}$$

The following is a summary of the steps to compute the 2nd Piola-Kirchhoff stress, $\mathbf{S}$ and the

tangent stiffness tensor, $\mathbb{C}$. The pages of the derivation in the book [3] are given as reference.

$$J = \det(\mathbf{F}), \quad \mathbf{C} = \mathbf{F}^{\top}\mathbf{F}$$

$$\bar{\mathbf{C}} = J^{-2/3}\mathbf{C} \tag{p.228}$$

$$\bar{\gamma}_1 = 2\left(\frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_1} + \bar{I}_1 \frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_2}\right) \tag{p.234}$$

$$\bar{\gamma}_2 = -2\frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_2}, \quad \text{note, there is no } \bar{\gamma}_3 \tag{p.234}$$

$$\bar{\gamma}_4 = 2\frac{\partial \Psi_{\text{iso}}}{\partial \bar{I}_4} \tag{p.273}$$

$$\bar{\gamma}_5 = 2\frac{\partial \Psi_{\text{iso}}}{\partial \bar{I}_5} \tag{p.273}$$

$$\bar{\mathbf{S}} = 2\frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{\mathbf{C}}} = \bar{\gamma}_1 \mathbf{I} + \bar{\gamma}_2 \bar{\mathbf{C}} \quad \text{(isotropic)} \tag{p.234}$$

$$\bar{\mathbf{S}} = 2\frac{\partial \Psi_{\text{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{\mathbf{C}}} = \bar{\gamma}_1 \mathbf{I} + \bar{\gamma}_2 \bar{\mathbf{C}} + \bar{\gamma}_4 \mathbf{a}_0 \otimes \mathbf{a}_0 + \bar{\gamma}_5 (\mathbf{a}_0 \otimes \bar{\mathbf{C}}\mathbf{a}_0 + \mathbf{a}_0 \bar{\mathbf{C}} \otimes \mathbf{a}_0) \quad \text{(trans-isotropic)} \tag{p.271}$$

$$(\mathbb{I})_{abcd} = \delta_{ac}\delta_{bd} \tag{p.23}$$

$$\mathbb{P} = \mathbb{I} - \frac{1}{3}\mathbf{C}^{-1} \otimes \mathbf{C} \tag{p.229}$$

$$\mathbf{S}_{\text{iso}} = J^{-2/3}\mathbb{P} : \bar{\mathbf{S}} \tag{p.234}$$

$$\mathbf{S}_{\text{vol}} = J\, p\, \mathbf{C}^{-1} \tag{p.230, p.245}$$

$$\mathbf{S} = \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{vol}} \quad \text{symmetric} \tag{p.233}$$

$$\left(\mathbf{C}^{-1} \odot \mathbf{C}^{-1}\right)_{abcd} = \frac{1}{2}\left(C^{-1}_{ac}\, C^{-1}_{bd} + C^{-1}_{ad}\, C^{-1}_{bc}\right) \tag{p.254}$$

$$\mathbb{C}_{\text{vol}} = J\, p\, \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} - 2\, J\, p\, \mathbf{C}^{-1} \odot \mathbf{C}^{-1} \tag{p.254, p.406}$$

$$\bar{\delta}_1 = 4\left(\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_1\, \partial \bar{I}_1} + 2\,\bar{I}_1 \frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_1\, \partial \bar{I}_2} + \frac{\partial \Psi_{\text{iso}}}{\partial \bar{I}_2} + \bar{I}_1^2\, \frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\, \partial \bar{I}_2}\right) \tag{p.262}$$

$$\bar{\delta}_2 = -4\left(\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_1\, \partial \bar{I}_2} + \bar{I}_1\, \frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\, \partial \bar{I}_2}\right) \tag{p.262}$$

$$\bar{\delta}_3 = 4 \frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\, \partial \bar{I}_2} \tag{p.262}$$

$$\bar{\delta}_4 = -4 \frac{\partial \Psi_{\text{iso}}}{\partial \bar{I}_2} \tag{p.262}$$

$$\bar{\delta}_5 = 4\left(\frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_1\, \partial \bar{I}_4} + \bar{I}_1 \frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\, \partial \bar{I}_4}\right) \tag{p.272}$$

$$\bar{\delta}_6 = -4 \frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_2\, \partial \bar{I}_4} \tag{p.272}$$

$$\bar{\delta}_7 = 4 \frac{\partial^2 \Psi_{\text{iso}}}{\partial \bar{I}_4\, \partial \bar{I}_4} \tag{p.272}$$

$$\mathbb{S} = (\mathbb{I} + \bar{\mathbb{I}})/2, \quad \mathbb{I}_{abcd} = \delta_{ac}\, \delta_{bd}, \quad \bar{\mathbb{I}}_{abcd} = \delta_{ad}\, \delta_{bc} \tag{p.262, p.23}$$

$$\bar{\mathbb{C}} = J^{-4/3}\, 2\, \frac{\partial \bar{\mathbf{S}}}{\partial \bar{\mathbf{C}}} = J^{-4/3}\left(\bar{\delta}_1\, \mathbf{I} \otimes \mathbf{I} + \bar{\delta}_2\left(\mathbf{I} \otimes \bar{\mathbf{C}} + \bar{\mathbf{C}} \otimes \mathbf{I}\right) + \bar{\delta}_3 \bar{\mathbf{C}} \otimes \bar{\mathbf{C}} + \bar{\delta}_4\, \mathbb{S}\right) \quad \text{isotropic} \tag{p.262}$$

$$\frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} = \mathbf{a}_0 \otimes \bar{\mathbf{C}}\, \mathbf{a}_0 + \mathbf{a}_0\, \bar{\mathbf{C}} \otimes \mathbf{a}_0, \quad \left(\frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}}\right)_{ij} = a_{0,i}\, a_{0,k}\, \underbrace{\bar{C}_{kj}}_{=\bar{C}_{jk}} + a_{0,j}\, a_{0,k}\, \underbrace{\bar{C}_{ki}}_{=\bar{C}_{ik}} \tag{p.277}$$

$$\frac{\partial^2 \bar{I}_5}{\partial \bar{\mathbf{C}} \partial \bar{\mathbf{C}}} = \frac{\partial}{\partial \bar{\mathbf{C}}}\left(\mathbf{a}_0 \otimes \bar{\mathbf{C}}\, \mathbf{a}_0 + \mathbf{a}_0\, \bar{\mathbf{C}} \otimes \mathbf{a}_0\right),$$

$$\frac{\partial^2 \bar{I}_5}{\partial \bar{\mathbf{C}}_{ij} \partial \bar{\mathbf{C}}_{lm}} = \frac{1}{2}\left(\delta_{jm}\, a_{0,i}\, a_{0,l} + \delta_{im}\, a_{0,j}\, a_{0,l} + \delta_{jl}\, a_{0,i}\, a_{0,m} + \delta_{il}\, a_{0,j}\, a_{0,m}\right)$$

$$\begin{aligned}
\bar{\mathbb{C}} = J^{-4/3}\Big(&\bar{\delta}_1\, \mathbf{I} \otimes \mathbf{I} + \bar{\delta}_2\left(\mathbf{I} \otimes \bar{\mathbf{C}} + \bar{\mathbf{C}} \otimes \mathbf{I}\right) + \bar{\delta}_3 \bar{\mathbf{C}} \otimes \bar{\mathbf{C}} + \bar{\delta}_4\, \mathbb{S} \\
&+\bar{\delta}_5\left(\mathbf{I} \otimes \mathbf{a}_0 \otimes \mathbf{a}_0 + \mathbf{a}_0 \otimes \mathbf{a}_0 \otimes \mathbf{I}\right) \\
&+\bar{\delta}_6\left(\bar{\mathbf{C}} \otimes \mathbf{a}_0 \otimes \mathbf{a}_0 + \mathbf{a}_0 \otimes \mathbf{a}_0 \otimes \bar{\mathbf{C}}\right) \\
&+\bar{\delta}_7\left(\mathbf{a}_0 \otimes \mathbf{a}_0 \otimes \mathbf{a}_0 \otimes \mathbf{a}_0\right) + \bar{\delta}_8\left(\mathbf{I} \otimes \frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} + \frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} \otimes \mathbf{I}\right) \\
&+\bar{\delta}_9\left(\bar{\mathbf{C}} \otimes \frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} + \frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} \otimes \bar{\mathbf{C}}\right) + \bar{\delta}_{10}\left(\frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} \otimes \frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}}\right) \\
&+\bar{\delta}_{11}\left(\mathbf{a}_0 \otimes \mathbf{a}_0 \otimes \frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} + \frac{\partial \bar{I}_5}{\partial \bar{\mathbf{C}}} \otimes \mathbf{a}_0 \otimes \mathbf{a}_0\right) + \bar{\delta}_{12} \frac{\partial^2 \bar{I}_5}{\partial \bar{\mathbf{C}} \partial \bar{\mathbf{C}}}\Big) \quad \text{trans-isotropic}
\end{aligned} \tag{p.272}$$

$$\tilde{\mathbb{P}} = \mathbf{C}^{-1} \odot \mathbf{C}^{-1} - \frac{1}{3}\, \mathbf{C}^{-1} \otimes \mathbf{C}^{-1} \tag{p.255}$$

$$\mathbb{C}_{\text{iso}} = \mathbb{P} : \bar{\mathbb{C}} : \mathbb{P}^{\top} + \frac{2}{3}\, J^{-2/3} \bar{\mathbf{S}} : \mathbf{C}\, \tilde{\mathbb{P}} - \frac{2}{3}\left(\mathbf{C}^{-1} \otimes \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{iso}} \otimes \mathbf{C}^{-1}\right) \tag{p.255}$$

$$\mathbb{C} = \mathbb{C}_{\text{vol}} + \mathbb{C}_{\text{iso}} \quad \text{minor symmetries} \tag{p.254}$$

6.8.1 Compressible Hyperelasticity

Compressible materials in decoupled form have the same equations for stress, $\mathbf{S}$, and material tangent tensor, $\mathcal{C}$, except the hydrostatic pressure, p, is computed from the volumetric strain energy function,

$$p = \frac{\partial \Psi_{\text{vol}}(J)}{\partial J}$$

(Holzapfel p.245)

The computation is analogous to the Penalty method 6.7.2 and is the same as for the incompressible case, except for computation of p and $\tilde{p}$ that is used for $\mathbb{C}$.

For the coupled form, the algorithm is different:

$$J = \det(\mathbf{F}), \quad \mathbf{C} = \mathbf{F}^{\top}\mathbf{F}$$

$$\gamma_1 = 2\left(\frac{\partial \Psi(I_1, I_2, I_3)}{\partial I_1} + I_1 \frac{\partial \Psi(I_1, I_2, I_3)}{\partial I_2}\right) \quad \text{(p.248)}$$

$$\gamma_2 = -2\frac{\partial \Psi(I_1, I_2, I_3)}{\partial I_2} \quad \text{(p.248)}$$

$$\gamma_3 = 2\, I_3 \frac{\partial \Psi(I_1, I_2, I_3)}{\partial I_3} \quad \text{(p.248)}$$

$$\mathbf{S} = 2\frac{\partial \Psi(I_1, I_2, I_3)}{\partial \mathbf{C}} = \gamma_1 \mathbf{I} + \gamma_2 \mathbf{C} + \gamma_3 \mathbf{C}^{-1}$$

$$\left(\mathbf{C}^{-1} \odot \mathbf{C}^{-1}\right)_{abcd} = \frac{1}{2}\left(C^{-1}_{ac}\, C^{-1}_{bd} + C^{-1}_{ad}\, C^{-1}_{bc}\right) \quad \text{(p.254)}$$

$$\delta_1 = 4\left(\frac{\partial^2\Psi}{\partial I_1\,\partial I_1} + 2\,I_1\frac{\partial^2\Psi}{\partial I_1\,\partial I_2} + \frac{\partial\Psi}{\partial I_2} + I_1^2\,\frac{\partial^2\Psi}{\partial I_2\,\partial I_2}\right) \quad \text{(p.261)}$$

$$\delta_2 = -4\left(\frac{\partial^2\Psi}{\partial I_1\,\partial I_2} + I_1\,\frac{\partial^2\Psi}{\partial I_2\,\partial I_2}\right)$$

$$\delta_3 = 4\left(I_3\,\frac{\partial^2\Psi}{\partial I_1\,\partial I_3} + I_1\,I_3\,\frac{\partial^2\Psi}{\partial I_2\,\partial I_3}\right)$$

$$\delta_4 = 4\frac{\partial^2\Psi}{\partial I_2\,\partial I_2}$$

$$\delta_5 = -4\,I_3\,\frac{\partial^2\Psi}{\partial I_2\,\partial I_3}$$

$$\delta_6 = 4\left(I_3\,\frac{\partial\Psi}{\partial I_3} + I_3^2\,\frac{\partial^2\Psi}{\partial I_3\,\partial I_3}\right)$$

$$\delta_7 = -4\,I_3\,\frac{\partial\Psi}{\partial I_3}$$

$$\delta_8 = -4\,\frac{\partial\Psi}{\partial I_2}$$

$$\mathbb{S} = (\mathbb{I} + \bar{\mathbb{I}})/2, \quad \mathbb{I}_{abcd} = \delta_{ac}\,\delta_{bd}, \quad \bar{\mathbb{I}}_{abcd} = \delta_{ad}\,\delta_{bc} \quad \text{(p.262, p.23)}$$

$$\mathbb{C} = 2\,\frac{\partial\mathbf{S}}{\partial\mathbf{C}} = \delta_1\,\mathbf{I}\otimes\mathbf{I} + \delta_2\left(\mathbf{I}\otimes\mathbf{C} + \mathbf{C}\otimes\mathbf{I}\right) + \delta_3\left(\mathbf{I}\otimes\mathbf{C}^{-1} + \mathbf{C}^{-1}\otimes\mathbf{I}\right) + \delta_4\,\mathbf{C}\otimes\mathbf{C}$$
$$+\delta_5\left(\mathbf{C}\otimes\mathbf{C}^{-1} + \mathbf{C}^{-1}\otimes\mathbf{C}\right) + \delta_6\left(\mathbf{C}^{-1}\otimes\mathbf{C}^{-1}\right) + \delta_7\left(\mathbf{C}^{-1}\odot\mathbf{C}^{-1}\right) + \delta_8\,\mathbb{S} \quad \text{(p.261)}$$

6.9 Dynamic elasticity

6.9.1 Dynamic linear elasticity

For the linear case we have the governing equation,

$$\mathbf{M}\,\ddot{\mathbf{u}} + \mathbf{C}\,\dot{\mathbf{u}} + \mathbf{K}\,\mathbf{u} - \mathbf{f} = \mathbf{0}$$

with

$$\mathbf{M}_{ij} = \int_\Omega \mathbf{N}_i^\top \rho \mathbf{N}_j \,\mathrm{d}V: \quad \text{mass matrix, density } \rho$$

$$\mathbf{C}_{ij} = \int_\Omega \mathbf{N}_i^\top \boldsymbol{\mu} \mathbf{N}_j \,\mathrm{d}V: \quad \text{damping matrix, viscosity parameters } \boldsymbol{\mu}$$

(Zienkiewicz I p.470)

In the case $\mathbf{C} = \mathbf{0}$ we can use the second order, symplectic *Leapfrog* integration. There is also an extension to using damping. But since we don't have conservation of energy anyways, use a RK4 scheme instead:

In the general case with damping we use a transformation to a system of first order ODEs.

$$\mathbf{w} = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} \mathbf{u} \\ \dot{\mathbf{u}} \end{pmatrix}$$
$$\mathbf{w}' = \begin{pmatrix} \mathbf{v} \\ \mathbf{M}^{-1}(\mathbf{f} - \mathbf{K}\,\mathbf{u} - \mathbf{C}\,\mathbf{v}) \end{pmatrix} =: \begin{pmatrix} \mathbf{v} \\ \mathbf{a}(\mathbf{u}, \mathbf{v}) \end{pmatrix}$$

Applying the 4th order Runge-Kutta scheme gives the following algorithm:

$$\begin{aligned}
&\mathbf{k}_1 = \Delta t\, \mathbf{a}(\mathbf{u}^{(n)}, \mathbf{v}^{(n)}, t^{(n)}), && \mathbf{l}_1 = \Delta t\, \mathbf{v}^{(n)} \\
&\mathbf{k}_2 = \Delta t\, \mathbf{a}(\mathbf{u}^{(n)} + \tfrac{1}{2}\mathbf{l}_1, \mathbf{v}^{(n)} + \tfrac{1}{2}\mathbf{k}_1, t^{(n+\frac{1}{2})}), && \mathbf{l}_2 = \Delta t\, (\mathbf{v}^{(n)} + \tfrac{1}{2}\mathbf{k}_1) \\
&\mathbf{k}_3 = \Delta t\, \mathbf{a}(\mathbf{u}^{(n)} + \tfrac{1}{2}\mathbf{l}_2, \mathbf{v}^{(n)} + \tfrac{1}{2}\mathbf{k}_2, t^{(n+\frac{1}{2})}), && \mathbf{l}_3 = \Delta t\, (\mathbf{v}^{(n)} + \tfrac{1}{2}\mathbf{k}_2) \\
&\mathbf{k}_4 = \Delta t\, \mathbf{a}(\mathbf{u}^{(n)} + \mathbf{l}_3, \mathbf{v}^{(n)} + \mathbf{k}_3, t^{(n+1)}), && \mathbf{l}_4 = \Delta t\, (\mathbf{v}^{(n)} + \mathbf{k}_3) \\
&\mathbf{v}^{(n+1)} = \mathbf{v}^{(n)} + \tfrac{1}{6}(\mathbf{k}_1 + 2\,\mathbf{k}_2 + 2\,\mathbf{k}_3 + \mathbf{k}_4), && \mathbf{u}^{(n+1)} = \mathbf{u}^{(n)} + \tfrac{1}{6}(\mathbf{l}_1 + 2\,\mathbf{l}_2 + 2\,\mathbf{l}_3 + \mathbf{l}_4)
\end{aligned}$$

Computing $\mathbf{a}(\mathbf{u}, \mathbf{v})$ is done by

$$\mathbf{a}(\mathbf{u}, \mathbf{v}) = \mathbf{M}^{-1}(\mathbf{f} - \mathbf{K}\,\mathbf{u} - \mathbf{C}\,\mathbf{v}).$$

6.9.2 Dynamic nonlinear elasticity

Governing equations

$$\begin{cases} \delta W_{\text{int}}(\mathbf{u}, p) - \delta W_{\text{ext}}(\dot{\mathbf{v}}) = 0 \quad \forall\, \delta\mathbf{u}, \\ \dot{\mathbf{u}} = \mathbf{v}, \\ D_{\delta p}\Pi_L(\mathbf{u}) = 0 \qquad\qquad\qquad \forall\, \delta p \end{cases} \tag{62}$$

where

$$\begin{aligned}
\delta W_{\text{int}}(\mathbf{u}, p) &= \int_\Omega \frac{1}{2}\, S_{AB}(\mathbf{u}, p)\, \left(F_{aB}\, \phi^M_{(a),A} + F_{aA}\, \phi^M_{(a),B} \right) \delta\hat{u}^M_a \,\mathrm{d}V \\
\delta W_{\text{ext}} &= \int_\Omega (B^L_{(a)} - \rho_0\, \dot{v}^L_{(a)})\, \phi^L_{(a)}\, \phi^M_{(a)}\, \delta\hat{u}^M_a \,\mathrm{d}V + \int_{\partial\Omega} \bar{T}^L_{(a)}\, \phi^L_{(a)}\, \phi^M_{(a)}\, \delta\hat{u}^M_a \,\mathrm{d}S \\
D_{\delta p}\Pi_L(\mathbf{u}) &= \int_\Omega \big(J(\mathbf{u}) - 1\big)\, \delta p \,\mathrm{d}V
\end{aligned} \tag{63}$$

We discretize it in time

$$\begin{aligned}
&\dot{\mathbf{u}} = \mathbf{v}: \quad \frac{1}{dt}\,(\mathbf{u}^{(n+1)} - \mathbf{u}^{(n)}) = \theta \mathbf{v}^{(n+1)} + (1-\theta)\mathbf{v}^{(n)}, \\
&\dot{\mathbf{v}} = \mathbf{a}: \quad \frac{1}{dt}\,(\mathbf{v}^{(n+1)} - \mathbf{v}^{(n)}) = \theta \mathbf{a}^{(n+1)} + (1-\theta)\mathbf{a}^{(n)},
\end{aligned}$$

For Crank-Nicolson method, $\theta = \frac{1}{2}$, for implicit Euler, $\theta = 1$. Plugging this into (62) yields the following three equations. Given values for $\mathbf{u}^{(n)}, \mathbf{v}^{(n)}, p^{(n)}$, solve the following to get $\mathbf{u}^{(n+1)}, \mathbf{v}^{(n+1)}, p^{(n+1)}$:

$$\delta W_{\text{int}}(\mathbf{u}, p)|_{\substack{\mathbf{u}=\theta\mathbf{u}^{(n+1)}+(1-\theta)\mathbf{u}^{(n)}, \\ p=\theta p^{(n+1)}+(1-\theta)p^{(n)}}} - \delta W_{\text{ext,dead}} + \int_\Omega \rho_0 \frac{v_{(a)}^{(n+1),L} - v_{(a)}^{(n),L}}{dt} \phi_{(a)}^L \phi_{(a)}^M \delta\hat{u}_a^M \, \mathrm{d}V = 0 \quad \forall\, \delta\mathbf{u},$$

$$\frac{1}{dt}(\mathbf{u}^{(n+1)} - \mathbf{u}^{(n)}) - \theta\mathbf{v}^{(n+1)} - (1-\theta)\mathbf{v}^{(n)} = 0.$$

$$D_{\delta p}\Pi_L(\mathbf{u}^{(n+1)}) = 0 \qquad \forall\, \delta p,$$

where

$$\begin{aligned}
\delta W_{\text{int}}(\mathbf{u}, p) &= \int_\Omega \frac{1}{2} S_{AB}(\mathbf{u}, p) \left(F_{aB} \phi_{(a),A}^M + F_{aA} \phi_{(a),B}^M \right) \delta\hat{u}_a^M \, \mathrm{d}V \\
\delta W_{\text{ext,dead}} &= \int_\Omega B_{(a)}^L \phi_{(a)}^L \phi_{(a)}^M \delta\hat{u}_a^M \, \mathrm{d}V + \int_{\partial\Omega} \bar{T}_{(a)}^L \phi_{(a)}^L \phi_{(a)}^M \delta\hat{u}_a^M \, \mathrm{d}S \\
D_{\delta p}\Pi_L(\mathbf{u}) &= \int_\Omega \left(J(\mathbf{u}) - 1 \right) \delta p \, \mathrm{d}V
\end{aligned} \tag{64}$$

This is a vectorial function, $F(\hat{\mathbf{u}}^{(n+1)}, \hat{\mathbf{v}}^{(n+1)}, \hat{p}^{(n+1)}) = -R = 0$ that can be solved by a Newton scheme.

The linear system for each Newton iteration takes the form

$$\begin{bmatrix} \mathbf{k}_{\delta\mathbf{u},\Delta\mathbf{u}} & \mathbf{l}_{\delta\mathbf{u},\Delta\mathbf{v}} & \mathbf{k}_{\delta p,\Delta\mathbf{u}}^\top \\ \mathbf{l}_{\delta\mathbf{v},\Delta\mathbf{u}} & \mathbf{l}_{\delta\mathbf{v},\Delta\mathbf{v}} & \mathbf{0} \\ \mathbf{k}_{\delta p,\Delta\mathbf{u}} & \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Delta\hat{\mathbf{u}} \\ \Delta\hat{\mathbf{v}} \\ \Delta\hat{p} \end{bmatrix} = \begin{bmatrix} \mathbf{R}_{\delta\mathbf{u}} \\ \mathbf{R}_{\delta\mathbf{v}} \\ \mathbf{R}_{\delta p} \end{bmatrix}.$$

with

$$-\mathbf{R}_{\delta\mathbf{u},(L,a)} = \delta W_{\text{int},(L,a)} - \delta W_{\text{ext},(L,a)} =: -\big(\mathbf{R}^{\text{int}}_{\delta\mathbf{u},(L,a)} + \mathbf{R}^{\text{ext,old}}_{\delta\mathbf{u},(L,a)} + \mathbf{R}^{\text{ext,new}}_{\delta\mathbf{u},(L,a)} + \mathbf{R}^{\text{ext,dead}}_{\delta\mathbf{u},(L,a)}\big) \text{ with}$$

$$-\mathbf{R}^{\text{int}}_{\delta\mathbf{u},(L,a)} = \int_\Omega \frac{1}{2}\, S_{AB}(\mathbf{u}^{(n+1/2)}(\mathbf{X}), p^{(n+1/2)}(\mathbf{X}))\, \Big(F_{aB}\phi^L_{(a),A} + F_{aA}\phi^L_{(a),B}\Big)\, \mathrm{d}V$$

$$\text{with } \mathbf{u}^{(n+1/2)}(\mathbf{X}) = \theta\mathbf{u}^{(n+1)}(\mathbf{X}) + (1-\theta)\mathbf{u}^{(n)}(\mathbf{X}),$$

$$p^{(n+1/2)}(\mathbf{X}) = \theta p^{(n+1)}(\mathbf{X}) + (1-\theta)p^{(n)}(\mathbf{X})$$

$$-\mathbf{R}^{\text{ext,new}}_{\delta\mathbf{u},(L,a)} = \frac{1}{dt}\int_\Omega \rho_0\, \hat{v}_a^{(n+1),M}\, \phi^M_{(a)}\phi^L_{(a)}\, \mathrm{d}V$$

$$-\mathbf{R}^{\text{ext,old}}_{\delta\mathbf{u},(L,a)} = -\frac{1}{dt}\int_\Omega \rho_0\, \hat{v}_a^{(n,M)}\, \phi^M_{(a)}\phi^L_{(a)}\, \mathrm{d}V$$

$$-\mathbf{R}^{\text{ext,dead}}_{\delta\mathbf{u},(L,a)} = -\int_\Omega B^M_a\, \phi^M_{(a)}\phi^L_{(a)}\, \mathrm{d}V - \int_{\partial\Omega} \bar{T}^M_a\, \phi^M_{(a)}\, \phi^L_{(a)}\, \mathrm{d}S$$

d blocks of subvectors with length u_{dofs}

$$-\mathbf{R}_{\delta\mathbf{v},(L,a)} = \frac{1}{dt}\,\hat{u}^{(n+1)}_{(L,a)} - \theta\hat{v}^{(n+1)}_{(L,a)} - \frac{1}{dt}\,\hat{u}^{(n)}_{(L,a)} + (\theta-1)\,\hat{v}^{(n)}_{(L,a)}$$

d blocks of subvectors with length u_{dofs}

$$-\mathbf{R}_{\delta p,L} = \int_\Omega \Big(J\big(\mathbf{u}^{(n+1)}(\mathbf{X})\big) - 1\Big)\, \psi^L\, \mathrm{d}V$$

1 subvector of length p_{dofs}

To reuse the derivation of the static case, we restrict to implicit Euler, $\theta = 1$. Then, $\mathbf{k}_{\delta\mathbf{u},\Delta\mathbf{u}}$ and $\mathbf{k}_{\delta p,\Delta\mathbf{u}}$ are the same as in (61).

$$\mathbf{l}_{\delta\mathbf{u},\Delta\mathbf{v},(L,a),(M,b)} = \frac{\partial}{\partial\hat{v}_b^{(n+1),M}}\left(\frac{1}{dt}\int_\Omega \rho_0\, \hat{v}_a^{(n+1),N}\, \phi^N_{(a)}\phi^L_{(a)}\, \mathrm{d}V\right) = \frac{1}{dt}\,\delta_{ab}\int_\Omega \rho_0\, \phi^M_{(b)}\,\phi^L_{(a)}\, \mathrm{d}V$$

$$\mathbf{l}_{\delta\mathbf{v},\Delta\mathbf{u},(L,a),(M,b)} = \frac{\partial}{\partial\hat{u}_b^{(n+1),M}}\left(-\mathbf{R}_{\delta\mathbf{v},(L,a)}\right) = \frac{1}{dt}\,\delta_{ab}\,\delta^{LM}$$

$$\mathbf{l}_{\delta\mathbf{v},\Delta\mathbf{v},(L,a),(M,b)} = \frac{\partial}{\partial\hat{v}_b^{(n+1),M}}\left(-\mathbf{R}_{\delta\mathbf{v},(L,a)}\right) = -\delta_{ab}\,\delta^{LM}$$

Note, the matrix is unsymmetric, it would be symmetric if $\mathbf{l}_{\delta\mathbf{u},\Delta\mathbf{v}} = \mathbf{l}^\top_{\delta\mathbf{v},\Delta\mathbf{u}}$ which is the case if $\rho_0 = 1$ and $\int_\Omega \phi^M_b\phi^L_a\, \mathrm{d}V = \delta_{ab}\delta^{LM}$, i.e. lumped mass matrix with row-sum.

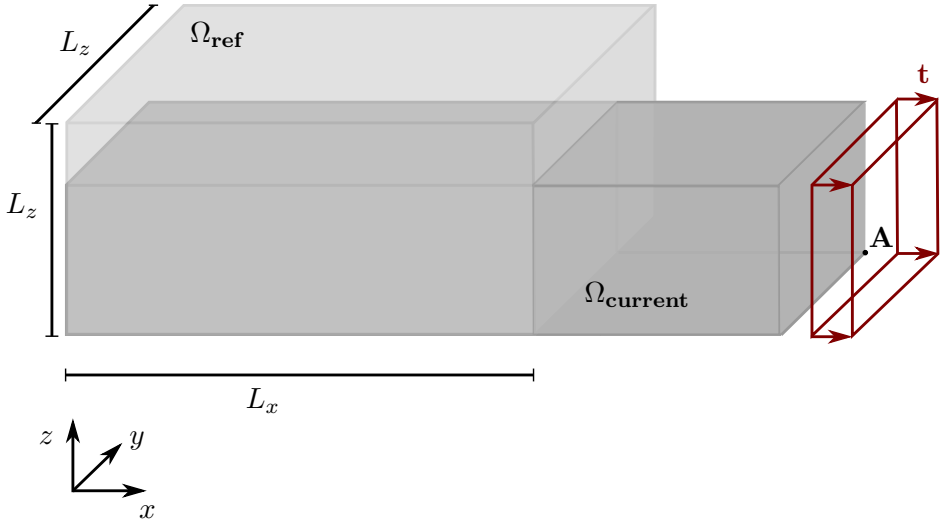


Abbildung 5: Uniaxial extension example

6.10 Examples with analytical solution

6.10.1 Uniaxial extension with constant total load

The domain in reference and current configuration is depicted in fig. 5) and defined as follows, symmetry between y and z-direction is assumed.

$$\Omega_{\text{ref}} = [0, L_x] \times [0, L_z]^2$$

$$\Omega_{\text{current}} = [0, \lambda\, L_x] \times [0, L_z/\sqrt{\lambda}]^2,$$

A load $t(\mathbf{x}) = t_{\max}/l_z^2$ is defined on the right surface area. In reference configuration it is

$$T(\mathbf{x}) = \frac{t_{\max}}{L_z^2}\,,$$

in current configuration

$$\begin{aligned} t(\mathbf{x}) \quad &= \frac{t_{\max}}{l_z^2} = \frac{t_{\max}}{\mathbf{L}_z \cdot \mathbf{C}\mathbf{L}_z} \quad \text{with } \mathbf{L}_z = (0,0,L_z), \quad l_z^2 = \frac{L_z^2}{\lambda} \\ &= t_{\max}\,\frac{\lambda}{L_z^2} \end{aligned}$$

Because the normal vector is the same, $\mathbf{n} = \mathbf{N}$, we have

$$T(\mathbf{x})\,\mathrm{d}S = \mathbf{t}\,\mathrm{d}s, \quad T(\mathbf{x}) = \mathbf{t}(\mathbf{x})\,\frac{\mathrm{d}s}{\mathrm{d}S} = \mathbf{t}(\mathbf{x})\,\frac{l_z^2}{L_z^2} = t(\mathbf{x})\frac{1}{\lambda} = \frac{t_{\max}}{L_z^2}$$

The geometric quantities can be computed to

$$\mathbf{x} = \begin{pmatrix} \lambda X_1 \\ X_2/\sqrt{\lambda} \\ X_3/\sqrt{\lambda} \end{pmatrix}, \quad \mathbf{F} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & 1/\sqrt{\lambda} & 0 \\ 0 & 0 & 1/\sqrt{\lambda} \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \lambda^2 & 0 & 0 \\ 0 & 1/\lambda & 0 \\ 0 & 0 & 1/\lambda \end{bmatrix},$$

$$\mathrm{tr}(\mathbf{C}) = \lambda^2 + 2/\sqrt{\lambda}, \quad \mathrm{tr}(\mathbf{C}^2) = \lambda^4 + 2/\lambda^2$$

$$I_1 = \mathrm{tr}(\mathbf{C}) = \lambda^2 + 2/\lambda$$

$$I_2 = \frac{1}{2}\left(\mathrm{tr}(\mathbf{C})^2 - \mathrm{tr}(\mathbf{C}^2)\right)$$

$$= \frac{1}{2}\left(\lambda^4 + \frac{4\,\lambda^2}{\sqrt{\lambda}} + \frac{4}{\lambda} - \lambda^4 - \frac{2}{\lambda^2}\right) = 2\,\lambda^{3/2} + 2\lambda^{-1} - \lambda^{-2}$$

$$I_3 = J = \det \mathbf{F} = 1, \quad \bar{\mathbf{C}} = \mathbf{C}$$

$$\mathbf{E} = \frac{1}{2}\begin{bmatrix} \lambda^2 - 1 & 0 & 0 \\ 0 & 1/\lambda - 1 & 0 \\ 0 & 0 & 1/\lambda - 1 \end{bmatrix}, \quad \mathbf{C}^{-1} = \begin{bmatrix} 1/\lambda^2 & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix}$$

Solution using penalty method

For the incompressible Mooney-Rivlin material with $\Psi(I_1, I_2) = c_1\,(I_1 - 3) + c_2\,(I_2 - 3), I_3 = 1$ we get the fictitious PK2 stress tensor as,

$$\bar{\mathbf{S}} = 2\,(c_1 + c_2\,I_1)\,\mathbf{I} - 2\,c_2\bar{\mathbf{C}} = \mathrm{diag}\left(2\,c_1 + 4\,c_2/\lambda, \quad 2\,c_1 - 2\,c_2/\lambda, \quad 2\,c_1 - 2\,c_2/\lambda\right)$$

The displacements at node A are given by

$$\hat{\mathbf{u}}^A = \left(\lambda\,L_x - L_x, \frac{L_z}{\sqrt{\lambda}} - L_z, 0\right) = \left((\lambda - 1)\,L_x, (\frac{1}{\sqrt{\lambda}} - 1)\,L_z, 0\right).$$

Computation of the fictitious stress tensor involves coefficients, $\bar{\gamma}_1, \bar{\gamma}_2$:

$$\bar{\gamma}_1 = 2\left(\frac{\partial \Psi_{\mathrm{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_1} + \bar{I}_1\,\frac{\partial \Psi_{\mathrm{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_2}\right)$$

$$\bar{\gamma}_2 = -2\frac{\partial \Psi_{\mathrm{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_2}$$

With $\Psi(\bar{I}_1, \bar{I}_2) = c_1\,(\bar{I}_1 - 3) + c_2\,(\bar{I}_2 - 3)$ we get

$$\frac{\partial \Psi_{\mathrm{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_1} = c_1, \quad \frac{\partial \Psi_{\mathrm{iso}}(\bar{I}_1, \bar{I}_2)}{\partial \bar{I}_2} = c_2$$

Now assume $c_2 = 0$.

$$\mathbf{C} : \bar{\mathbf{S}} = 2\,c_1\,\lambda^2 + 4\,c_1\,\lambda^{-1}$$

$$\begin{aligned}
\mathbf{S}_{\text{iso}} &= J^{-2/3}\,\mathbb{P} : \bar{\mathbf{S}} = \bar{\mathbf{S}} - \frac{1}{3}\,(\mathbf{C}^{-1} \otimes \mathbf{C}) : \bar{\mathbf{S}} \\
&= \bar{\mathbf{S}} - \frac{1}{3}\begin{bmatrix} 1/\lambda^2 \cdot (2\,c_1\,\lambda^2 + 4\,c_1\,\lambda^{-1}) & 0 & 0 \\ 0 & \lambda \cdot (2\,c_1\,\lambda^2 + 4\,c_1\,\lambda^{-1}) & 0 \\ 0 & 0 & \lambda \cdot (2\,c_1\,\lambda^2 + 4\,c_1\,\lambda^{-1}) \end{bmatrix} \\
&= \begin{bmatrix} 2\,c_1 & 0 & 0 \\ 0 & 2\,c_1 & 0 \\ 0 & 0 & 2\,c_1 \end{bmatrix} - \frac{1}{3}\begin{bmatrix} 2\,c_1 + 4\,c_1\,\lambda^{-3} & 0 & 0 \\ 0 & 2\,c_1\,\lambda^3 + 4\,c_1 & 0 \\ 0 & 0 & 2\,c_1\,\lambda^3 + 4\,c_1 \end{bmatrix} \\
&= \begin{bmatrix} \frac{4}{3}\,c_1\,(1 - \lambda^{-3}) & 0 & 0 \\ 0 & \frac{2}{3}\,c_1\,(1 - \lambda^3) & 0 \\ 0 & 0 & \frac{2}{3}\,c_1\,(1 - \lambda^3) \end{bmatrix}
\end{aligned}$$

$$\mathbf{S} = \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{vol}} = \mathbf{S}_{\text{iso}} + J\,p\,\mathbf{C}^{-1} = \begin{bmatrix} \frac{4}{3}\,c_1\,(1 - \lambda^{-3}) + p\,\lambda^{-2} & 0 & 0 \\ 0 & \frac{2}{3}\,c_1\,(1 - \lambda^3) + p\,\lambda & 0 \\ 0 & 0 & \frac{2}{3}\,c_1\,(1 - \lambda^3) + p\,\lambda \end{bmatrix}$$

The artifical pressure, p is different from the real hydrostatic pressure. It is given by

$$p = \frac{\mathrm{d}\Psi_{\text{vol}}(J)}{\mathrm{d}J} = \frac{\mathrm{d}}{\mathrm{d}J}\left(\frac{\kappa}{2}\,(J-1)^2\right) = \kappa\,(J-1)$$

An incompressible solution has $J \approx 1$ but because $\kappa \to \infty$ it has a $p \neq 0$. To satisfy the force equilibrium we get

y-direction:

$$S_{22} = 0 \quad \Rightarrow \quad \frac{2}{3}\,c_1\,(1 - \lambda^3) + p\,\lambda = 0 \quad \Rightarrow \quad p = \frac{2}{3}\,c_1\,(\lambda^3 - 1)\lambda^{-1}$$

x-direction:

$$-\sigma_{11}\,l_z^2 + t_{\max}\,\frac{\lambda}{L_z^2}\,l_z^2 = 0, \quad \Rightarrow \quad \sigma_{11} = t_{\max}\frac{\lambda}{L_z^2}$$

$$\mathbf{S} = J\,\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-\top}, \quad S_{11} = \lambda^{-1}\sigma_{11}\lambda^{-1}$$

$$\begin{aligned}
&\Rightarrow \quad S_{11} \stackrel{!}{=} \frac{t_{\max}}{L_z^2\,\lambda} \\
&\Leftrightarrow \quad \frac{4}{3}\,c_1\,(1 - \lambda^{-3}) + \left(\frac{2}{3}\,c_1\,(\lambda^3 - 1)\lambda^{-1}\right)\lambda^{-2} \stackrel{!}{=} \frac{t_{\max}}{L_z^2\,\lambda} \\
&\Leftrightarrow \quad \frac{4}{3}\,c_1\,(1 - \lambda^{-3}) + \frac{2}{3}\,c_1\,(1 - \lambda^{-3}) = \frac{t_{\max}}{L_z^2\,\lambda} \\
&\Leftrightarrow \quad 2\,c_1\,(1 - \lambda^{-3}) = \frac{t_{\max}}{L_z^2\,\lambda} \quad \Leftrightarrow \quad 2\,L_z^2\,c_1\,(\lambda - \lambda^{-2}) = t_{\max} \\
&\Leftrightarrow \quad 2\,c_1\,L_z^2\,(\lambda^3 - 1) - t_{\max}\,\lambda^2 = 0
\end{aligned}$$

```
>>> solve(2./3*c0*lz*lz*(lambdaValue**3 - 1) - tmax*lambdaValue**2,
 lambdaValue, simplify=True, positive=True)[2]
0.5*tmax**2/(c0*lz**2*(4.0*c0**3*lz**6 + tmax**3 + (-tmax**6 + (4.0*
c0**3*lz**6 + tmax**3)**2)**0.5)**(1/3)) + 0.5*tmax/(c0*lz**2) + 0.5
*(4.0*c0**3*lz**6 + tmax**3 + (-tmax**6 + (4.0*c0**3*lz**6 + tmax**3
)**2)**0.5)**(1/3)/(c0*lz**2)
```

Direct solution using pressure from equilibrium

Analytical approach (p.224). Assuming Mooney-Rivlin with $c_2 = 0$ (Neo-Hookean),

$$\begin{aligned}\mathbf{S} &= -p\mathbf{C}^{-1} + 2\left(\frac{\partial\Psi}{\partial I_1} + I_1\frac{\partial\Psi}{\partial I_2}\right)\mathbf{I} - 2\,\frac{\partial\Psi}{\partial I_2}\,\mathbf{C} \\ &= -p\mathbf{C}^{-1} + 2\,c_1\,\mathbf{I} = \begin{bmatrix} -p/\lambda^2 + 2\,c_1 & 0 & 0 \\ 0 & -p\,\lambda + 2\,c_1 & 0 \\ 0 & 0 & -p\,\lambda + 2\,c_1 \end{bmatrix}\end{aligned}$$

From equilibrium we get

y-direction:

$$S_{22} = 0 \quad \Rightarrow \quad -p\,\lambda + 2\,c_1 = 0 \quad \Rightarrow \quad p = \frac{2\,c_1}{\lambda}$$

x-direction:

$$-\sigma_{11}\,l_z^2 + t_{\max}\,\frac{\lambda}{L_z^2}\,l_z^2 = 0, \quad \Rightarrow \quad \sigma_{11} = t_{\max}\frac{\lambda}{L_z^2}$$

$$\mathbf{S} = J\,\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-\top}, \quad S_{11} = \lambda^{-1}\sigma_{11}\lambda^{-1}$$

$$\Rightarrow \quad S_{11} \overset{!}{=} \frac{t_{\max}}{L_z^2\,\lambda}$$

$$\Rightarrow \quad -p\,\lambda^{-2} + 2\,c_1 = -2\,c_1\,\lambda^{-3} + 2\,c_1 = \frac{t_{\max}}{L_z^2\,\lambda}$$

$$\Rightarrow \quad 2\,c_1\,\lambda^3 - \frac{t_{\max}}{L_z^2}\,\lambda^2 - 2\,c_1 = 0 \quad \Rightarrow \quad \lambda = \text{nonlinear}(t_{\max})$$

```
>>> solve(2*c1*l**3 -t*l**2 -2*c1, l, simplify=True, positive=True)[2]
-t**2/(6*c1*(-108*c1**3 - t**3 + sqrt(-t**6 + (108*c1**3 + t**3)**2)
)**(1/3)) + t/(6*c1) - (-108*c1**3 - t**3 + sqrt(-t**6 + (108*c1**3
 + t**3)**2))**(1/3)/(6*c1)
```

Internal energy:

$$\delta W_{\text{int}} = \int_\Omega \frac{1}{2}\,S_{AB}(\hat{\mathbf{u}})\,\delta u_a^L\left(F_{aB}(\hat{\mathbf{u}})\,\frac{\partial\phi_L}{\partial X_A} + F_{aA}(\hat{\mathbf{u}})\,\frac{\partial\phi_L}{\partial X_B}\right)\mathrm{d}V$$

Now we assume a virtual displacement at node $\mathcal{A}$, $\delta u_a(\mathbf{X}) = \delta u_a^{\mathcal{A}}\phi^{\mathcal{A}}(\mathbf{X})$.

$$\delta W_{\text{int}} = \int_\Omega \frac{1}{2}\,S_{AB}\,\delta u_a^{\mathcal{A}}\left(F_{aB}\,\frac{\partial\phi^{\mathcal{A}}}{\partial X_A} + F_{aA}\,\frac{\partial\phi^{\mathcal{A}}}{\partial X_B}\right)\mathrm{d}V,$$

The ansatz function $\phi^{\mathcal{A}}$ and their derivatives are:

$$\begin{aligned}
\phi^{\mathcal{A}}(\mathbf{X}) &= \frac{X_1}{L_x}\,\frac{X_2}{L_z}\,\left(1-\frac{X_3}{L_z}\right),\\
\frac{\partial\phi^{\mathcal{A}}}{\partial X_1} &= \frac{1}{L_x}\,\frac{X_2}{L_z}\,\left(1-\frac{X_3}{L_z}\right),\\
\frac{\partial\phi^{\mathcal{A}}}{\partial X_2} &= \frac{1}{L_z}\,\frac{X_1}{L_x}\,\left(1-\frac{X_3}{L_z}\right),\\
\frac{\partial\phi^{\mathcal{A}}}{\partial X_3} &= -\frac{X_1}{L_x}\,\frac{X_2}{L_z}\,\frac{1}{L_z},
\end{aligned}$$

For $\delta\mathbf{u}(\mathbf{X}) = (\phi^{\mathcal{A}}(\mathbf{X}),0,0)^\top$, i.e. $\delta u_1^{\mathcal{A}} = 1, \delta u_2^{\mathcal{A}} = \delta u_3^{\mathcal{A}} = 0$ we compute the virtual internal energy:

$$\begin{aligned}
\delta W_{\text{int}} &= \int_\Omega \frac{1}{2}\,S_{AB}\left(F_{1B}\,\frac{\partial\phi^{\mathcal{A}}}{\partial X_A} + F_{1A}\,\frac{\partial\phi^{\mathcal{A}}}{\partial X_B}\right)\mathrm{d}V = \int_\Omega \frac{1}{2}\,S_{11}\left(F_{11}\frac{\partial\phi^{\mathcal{A}}}{\partial X_1} + F_{11}\frac{\partial\phi^{\mathcal{A}}}{\partial X_1}\right)\mathrm{d}V\\
&= S_{11}\int_\Omega \lambda\frac{1}{L_x}\,\frac{X_2}{L_z}\,\left(1-\frac{X_3}{L_z}\right)\mathrm{d}V = S_{11}\,\lambda\,\frac{L_x}{L_x}\,\frac{1}{2}\,\frac{L_z^2}{L_z}\int_0^{L_z}\left(1-\frac{X_3}{L_z}\right)\mathrm{d}X_3\\
&= S_{11}\,\lambda\,\frac{1}{2}\,L_z\left(L_z-\frac{1}{2}\,\frac{L_z^2}{L_z}\right)\\
&= \frac{1}{4}\;L_z^2\,S_{11}\,\lambda = \frac{1}{4}\;L_z^2\,F_{11}\,S_{11}
\end{aligned}$$

Virtual external energy

$$\begin{aligned}
\delta W_{\text{ext}} &= \int_\Omega (\mathbf{B}-\rho_0\,\ddot{\mathbf{u}})\cdot\delta\mathbf{u}\,\mathrm{d}V + \int_{\partial\Omega}\bar{\mathbf{T}}\cdot\delta\mathbf{u}\,\mathrm{d}S\\
&= \int_{\partial\Omega}(T(\mathbf{X}),0,0)^\top\cdot\big(\delta u_1(\mathbf{X}),\delta u_2(\mathbf{X}),\delta u_3(\mathbf{X})\big)^\top\,\mathrm{d}S\\
&= \int_0^{L_z}\int_0^{L_z}\frac{t_{\max}}{L_z^2}\;\phi^{\mathcal{A}}(L_x,X_2,X_3)\,\mathrm{d}X_2\,\mathrm{d}X_3\\
&= \frac{t_{\max}}{L_z^2}\int_0^{L_z}\int_0^{L_z}\frac{L_x}{L_x}\,\frac{X_2}{L_z}\,\left(1-\frac{X_3}{L_z}\right)\mathrm{d}X_2\,\mathrm{d}X_3\\
&= \frac{t_{\max}}{L_z^2}\,\frac{1}{2}\,\frac{L_z^2}{L_z}\left(L_z-\frac{1}{2}\,\frac{L_z^2}{L_z}\right) = \frac{1}{4}\;L_z^2\,t_{\max}\frac{1}{L_z^2}\;=\frac{1}{4}\;t_{\max} = \frac{1}{4}\;L_z^2\,T(\mathbf{x})
\end{aligned}$$

From principle of virtual work we should get the correct stress.

$$\begin{aligned}
&\delta W_{\text{int}} - \delta W_{\text{ext}} = 0 \quad\Leftrightarrow\quad \frac{1}{4}\;L_z^2\,S_{11}\,\lambda - \frac{1}{4}\;t_{\max} = 0\\
&\Leftrightarrow\quad \frac{1}{4}\;(L_z^2\,S_{11}\,\lambda - t_{\max}) = 0\\
&\Leftrightarrow\quad L_z^2\,S_{11}\,\lambda = t_{\max}\quad\Leftrightarrow\quad S_{11} = \frac{t_{\max}}{\lambda\,L_z^2} = \frac{1}{\lambda^2}\,t(\mathbf{X}) = \frac{1}{\lambda}\,T(\mathbf{X})\quad\checkmark
\end{aligned}$$

Note: we do not get any further information from the principle of virtual work further than the equilibrium conditions. This is because the stress was preserved as variable and not replaced by the constitutive equations, that relate them to strain and stretch λ.

Assume Mooney-Rivlin with $c_2 \neq 0$,

$$\begin{aligned}
\mathbf{S} &= -p\mathbf{C}^{-1} + 2\left(\frac{\partial \Psi}{\partial I_1} + I_1 \frac{\partial \Psi}{\partial I_2}\right)\mathbf{I} - 2\,\frac{\partial \Psi}{\partial I_2}\,\mathbf{C} \\
&= -p\mathbf{C}^{-1} + (2\,c_1 + \mathrm{tr}\mathbf{C} c_2)\,\mathbf{I} - 2\,c_2\,\mathbf{C} \\
&= \mathrm{diag}\big(-p\,\lambda^{-2} + 2\,c_1 + 2\,c_2\,\lambda^2 + 4\,c_2\,\lambda^{-1} - 2\,c_2\,\lambda^2, \\
&\qquad -p\,\lambda + 2\,c_1 + 2\,c_2\,\lambda^2 + 4\,c_2\,\lambda^{-1} - 2\,c_2\,\lambda^{-1}, \\
&\qquad -p\,\lambda + 2\,c_1 + 2\,c_2\,\lambda^2 + 4\,c_2\,\lambda^{-1} - 2\,c_2\,\lambda^{-1}\big) \\
&= \mathrm{diag}\big(-p\,\lambda^{-2} + 2\,c_1 + 4\,c_2\,\lambda^{-1}, \\
&\qquad -p\,\lambda + 2\,c_1 + 2\,c_2\,\lambda^2 + 2\,c_2\,\lambda^{-1}, \\
&\qquad -p\,\lambda + 2\,c_1 + 2\,c_2\,\lambda^2 + 2\,c_2\,\lambda^{-1}\big)
\end{aligned}$$

6.10.2 Uniaxial extension with constant load per surface area

This is the same example as the previous one except now with load constant per surface area, but total load varying, $t(\mathbf{x}) = \hat{t} = t_{\max}/L_z^2, T = \hat{t}/\lambda$. For Neo-Hookean we have the equilibrium conditions,

y-direction:

$S_{22} = 0 \quad \Rightarrow \quad -p\,\lambda + 2\,c_1 = 0 \quad \Rightarrow \quad p = \dfrac{2\,c_1}{\lambda}$

x-direction:

$\sigma_{11} = \hat{t} \quad \Leftrightarrow \quad \mathbf{S} = J\,\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-\top}, \quad S_{11} = \lambda^{-1}\sigma_{11}\lambda^{-1}$

$\Rightarrow \quad S_{11} = \hat{t}\,\lambda^{-2} \quad \Rightarrow \quad -p\,\lambda^{-2} + 2\,c_1 = -2\,c_1\,\lambda^{-3} + 2\,c_1 = \hat{t}\,\lambda^{-2}$

$\Rightarrow \quad 2\,c_1\,\lambda^3 - \hat{t}\,\lambda - 2\,c_1 = 0$

```
>>> solve(2*c1*l**(3) -t*l**2 -2*c1, l, simplify=True, positive=True)[0].eval
0.30285343213869*(1.81712059283214*that + (18.0*c0**1.5 + 2.44948974278318*(5
```

Internal virtual energy:

$$\delta W_{\mathrm{int}} = \frac{1}{4}\,L_z^2\,F_{11}\,S_{11}$$

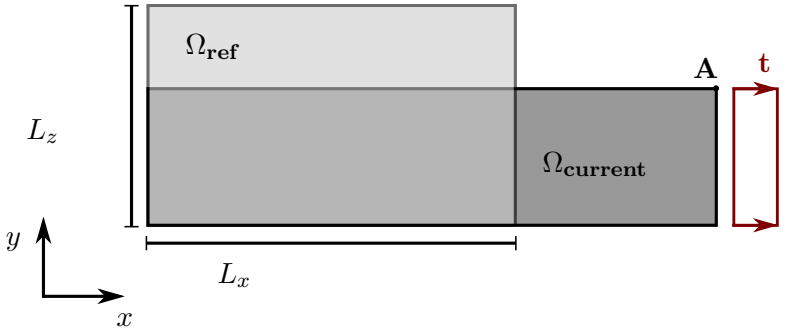


Abbildung 6: Uniaxial extension example

External virtual energy:

$$\begin{aligned}
\delta W_{\text{ext}} &= \int_\Omega (\mathbf{B} - \rho_0\, \ddot{\mathbf{u}}) \cdot \delta\mathbf{u}\, \mathrm{d}V + \int_{\partial\Omega} \bar{\mathbf{T}} \cdot \delta\mathbf{u}\, \mathrm{d}S \\
&= \int_{\partial\Omega} (T(\mathbf{X}), 0, 0)^\top \cdot \delta\mathbf{u}\, \mathrm{d}S = \int_0^{L_z}\int_0^{L_z} \frac{\hat{t}}{\lambda}\, \phi^{\mathcal{A}}(L_x, X_2, X_3)\, \mathrm{d}X_2\, \mathrm{d}X_3 \\
&= \frac{\hat{t}}{\lambda} \int_0^{L_z}\int_0^{L_z} \frac{L_x}{L_x}\, \frac{X_2}{L_z} \left(1 - \frac{X_3}{L_z}\right) \mathrm{d}X_2\, \mathrm{d}X_3 \\
&= \frac{\hat{t}}{\lambda}\, \frac{1}{2}\, \frac{L_z^2}{L_z} \left(L_z - \frac{1}{2}\, \frac{L_z^2}{L_z}\right) = \frac{1}{4}\, L_z^2\, \frac{\hat{t}}{\lambda}
\end{aligned}$$

We get

$$\delta W_{\text{int}} - \delta W_{\text{ext}} = \frac{1}{4}\, L_z^2 \left(F_{11}\, S_{11} - \frac{\hat{t}}{\lambda}\right) \quad \Leftrightarrow \quad S_{11} = \hat{t}\, \lambda^{-2} \quad \checkmark$$

6.11 2D uniaxial extension with constant total load

The domain in reference and current configuration is depicted in fig. 6) and defined as follows,

$$\Omega_{\text{ref}} = [0, L_x] \times [0, L_y]$$

$$\Omega_{\text{current}} = [0, \lambda\, L_x] \times [0, L_y\, \lambda^{-1}],$$

A load $t(\mathbf{x}) = t_{\max}/l_y$ is defined on the right border. In reference configuration it is

$$T(\mathbf{x}) = \frac{t_{\max}}{L_y}\,,$$

in current configuration

$$t(\mathbf{x}) \;\; = \frac{t_{\max}}{l_y} \; = t_{\max}\, \frac{\lambda}{L_y}\,.$$

Because the normal vector is the same, $\mathbf{n} = \mathbf{N}$, we have

$$T(\mathbf{x})\,\mathrm{d}S = \mathbf{t}\,\mathrm{d}s, \quad T(\mathbf{x}) = \mathbf{t}(\mathbf{x})\,\frac{\mathrm{d}s}{\mathrm{d}S} = \mathbf{t}(\mathbf{x})\,\frac{l_y}{L_y} = t(\mathbf{x})\frac{1}{\lambda}, \quad \text{i.e.} \qquad T(\mathbf{x}) = t(\mathbf{x})\,\lambda^{-1}$$

The geometric quantities can be computed to

$$\mathbf{x} = \begin{pmatrix} \lambda\, X_1 \\ \lambda^{-1}\, X_2 \end{pmatrix}, \quad \mathbf{F} = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{bmatrix}, \quad \mathbf{C} = \begin{bmatrix} \lambda^2 & 0 \\ 0 & \lambda^{-2} \end{bmatrix},$$

$$\mathrm{tr}(\mathbf{C}) = \lambda^2 + \lambda^{-2}, \quad \mathrm{tr}(\mathbf{C}^2) = \lambda^4 + \lambda^{-4}$$

$$I_1 = \mathrm{tr}(\mathbf{C}) = \lambda^2 + \lambda^{-2}$$

$$I_2 = \frac{1}{2}\left(\mathrm{tr}(\mathbf{C})^2 - \mathrm{tr}(\mathbf{C}^2)\right) = \frac{1}{2}\left(\lambda^4 + 2 + \lambda^{-4} - \lambda^4 - \lambda^{-4}\right) = 1$$

$$I_3 = J = \det \mathbf{F} = 1, \quad \bar{\mathbf{C}} = \mathbf{C}$$

$$\mathbf{E} = \frac{1}{2}\begin{bmatrix} \lambda^2 - 1 & 0 \\ 0 & \lambda^{-2} - 1 \end{bmatrix}, \quad \mathbf{C}^{-1} = \begin{bmatrix} \lambda^{-2} & 0 \\ 0 & \lambda^2 \end{bmatrix}$$

Solution using penalty method

For the incompressible Mooney-Rivlin material with $\Psi(I_1, I_2) = c_1\,(I_1 - 3) + c_2\,(I_2 - 3), I_3 = 1$ we get the fictitious PK2 stress tensor as, The displacements at node A are given by

$$\hat{\mathbf{u}}^A = \left(\lambda\, L_x - L_x, L_y\,\lambda^{-1} - L_y\right) = \left((\lambda - 1)\, L_x, (\lambda^{-1} - 1)\, L_y\right).$$

Assuming Neo-Hookean material law, $\Psi(I_1) = c_1\,(I_1 - 2)$ the fictitious PK2 stress tensor yields

$$\bar{\mathbf{S}} = 2\,c_1\,\mathbf{I}.$$

and the stress tensor

$$\begin{aligned}
\mathbf{C} : \bar{\mathbf{S}} &= 2\,c_1\,(\lambda^2 + \lambda^{-2}) \\
\mathbf{S}_{\text{iso}} &= J^{-1}\,\mathbb{P} : \bar{\mathbf{S}} = \bar{\mathbf{S}} - \frac{1}{2}\,(\mathbf{C}^{-1} \otimes \mathbf{C}) : \bar{\mathbf{S}} \\
&= \bar{\mathbf{S}} - \frac{1}{2}\begin{bmatrix} \lambda^{-2} \cdot \left(2\,c_1\,(\lambda^2 + \lambda^{-2})\right) & 0 \\ 0 & \lambda^2 \cdot \left(2\,c_1\,(\lambda^2 + \lambda^{-2})\right) \end{bmatrix} \\
&= \begin{bmatrix} 2\,c_1 & 0 \\ 0 & 2\,c_1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 2\,c_1\,(1 + \lambda^{-4}) & 0 \\ 0 & 2\,c_1\,(\lambda^4 + 1) \end{bmatrix} \\
&= \begin{bmatrix} c_1\,(1 - \lambda^{-4}) & 0 \\ 0 & c_1\,(1 - \lambda^4) \end{bmatrix}
\end{aligned}$$

$$\mathbf{S} = \mathbf{S}_{\text{iso}} + \mathbf{S}_{\text{vol}} = \mathbf{S}_{\text{iso}} + J\,p\,\mathbf{C}^{-1} = \begin{bmatrix} c_1\,(1 - \lambda^{-4}) + p\,\lambda^{-2} & 0 \\ 0 & c_1\,(1 - \lambda^4) + p\,\lambda^2 \end{bmatrix}$$

The artifical pressure, p is different from the real hydrostatic pressure. It is given by

$$p = \frac{\mathrm{d}\Psi_{\mathrm{vol}}(J)}{\mathrm{d}J} = \frac{\mathrm{d}}{\mathrm{d}J}\left(\frac{\kappa}{2}(J-1)^2\right) = \kappa\,(J-1)$$

An incompressible solution has $J \approx 1$ but because $\kappa \to \infty$ it has a $p \neq 0$. To satisfy the force equilibrium we get

y-direction:
$S_{22} = 0 \quad \Rightarrow \quad c_1\,(1-\lambda^4) + p\,\lambda^2 = 0 \quad \Rightarrow \quad p = \big(c_1\,(\lambda^4-1)\big)\lambda^{-2} = c_1\,(\lambda^2 - \lambda^{-2})$

x-direction:
$-\sigma_{11}\,l_y + t_{\max}\,\dfrac{\lambda}{L_y}\,l_y = 0, \quad \Rightarrow \quad \sigma_{11} = t_{\max}\dfrac{\lambda}{L_y}$
$\mathbf{S} = J\,\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-\top}, \quad S_{11} = \lambda^{-1}\sigma_{11}\lambda^{-1}$

$$\Rightarrow \quad S_{11} \overset{!}{=} \frac{t_{\max}}{L_y\,\lambda}$$

$$\Leftrightarrow \quad c_1\,(1-\lambda^{-4}) + \big(c_1\,(\lambda^2-\lambda^{-2})\big)\,\lambda^{-2} \overset{!}{=} \frac{t_{\max}}{L_y\,\lambda}$$

$$\Leftrightarrow \quad c_1\,(1-\lambda^{-4}) + c_1\,(1-\lambda^{-4}) = \frac{t_{\max}}{L_y\,\lambda}$$

$$\Leftrightarrow \quad 2\,c_1\,(1-\lambda^{-4}) = \frac{t_{\max}}{L_y\,\lambda} \quad \Leftrightarrow \quad 2\,L_y\,c_1\,(\lambda - \lambda^{-3}) = t_{\max}$$

$$\Leftrightarrow \quad 2\,c_1\,L_y\,(\lambda^4 - 1) - t_{\max}\,\lambda^3 = 0$$

```
>>> solve(2*c0*ly*(lambdaValue**4 - 1) - tmax*lambdaValue**3,
lambdaValue, simplify=True, positive=True)[2]
(tmax/8 + sqrt(-384*3**(2/3)*c0**(8/3)*ly**(8/3)/(-9*tmax**2
 + sqrt(3)*sqrt(4096*c0**4*ly**4 + 27*tmax**4))**(1/3)
 + 24*3**(1/3)*c0**(4/3)*ly**(4/3)*(-9*tmax**2 + sqrt(3)*
 sqrt(4096*c0**4*ly**4 + 27*tmax**4))**(1/3) + 9*tmax**2)/24
  - sqrt(384*3**(2/3)*c0**(8/3)*ly**(8/3)/(-9*tmax**2 +
  sqrt(3)*sqrt(4096*c0**4*ly**4 + 27*tmax**4))**(1/3)
  - 24*3**(1/3)*c0**(4/3)*ly**(4/3)*(-9*tmax**2 + sqrt(3)*
  sqrt(4096*c0**4*ly**4 + 27*tmax**4))**(1/3)
  + 18*sqrt(3)*tmax**3/sqrt(-128*3**(2/3)*c0**(8/3)*ly**(8/3)
  /(-9*tmax**2 + sqrt(3)*sqrt(4096*c0**4*ly**4 + 27*tmax**4))
  **(1/3) + 8*3**(1/3)*c0**(4/3)*ly**(4/3)*(-9*tmax**2
  + sqrt(3)*sqrt(4096*c0**4*ly**4 + 27*tmax**4))**(1/3)
  + 3*tmax**2) + 18*tmax**2)/24)/(c0*ly)
```

From the penalty parameter $p = c_1\,(\lambda^2 - \lambda^{-2})$ we can compute the amount by which the system violates incompressibility:

$$p = \kappa\,(J-1) \quad \Rightarrow \quad J = 1 + \frac{p}{\kappa}$$

Direct solution using pressure from equilibrium

Analytical approach (p.224). Assuming Incompressibility ($I_3 = 1$), Mooney-Rivlin with $c_2 = 0$

(Neo-Hookean),

$$\begin{aligned}\mathbf{S} &= -p\mathbf{C}^{-1} + 2\left(\frac{\partial\Psi}{\partial I_1} + I_1\frac{\partial\Psi}{\partial I_2}\right)\mathbf{I} - 2\,\frac{\partial\Psi}{\partial I_2}\,\mathbf{C} \\ &= -p\mathbf{C}^{-1} + 2\,c_1\,\mathbf{I} = \begin{bmatrix} -p\,\lambda^{-2} + 2\,c_1 & 0 \\ 0 & -p\,\lambda^2 + 2\,c_1 \end{bmatrix}\end{aligned} \tag{65}$$

From equilibrium we get

y-direction:

$S_{22} = 0 \quad \Rightarrow \quad -p\,\lambda^2 + 2\,c_1 = 0 \quad \Rightarrow \quad p = \dfrac{2\,c_1}{\lambda^2}$

x-direction:

$-\sigma_{11}\,l_y + t_{\max}\,\dfrac{\lambda}{L_y}\,l_y = 0, \quad \Rightarrow \quad \sigma_{11} = t_{\max}\dfrac{\lambda}{L_y}$

$\mathbf{S} = J\,\mathbf{F}^{-1}\boldsymbol{\sigma}\mathbf{F}^{-\top}, \quad S_{11} = \lambda^{-1}\sigma_{11}\lambda^{-1}$

$\Rightarrow \quad S_{11} \overset{!}{=} \dfrac{t_{\max}}{L_y\,\lambda}$

$\Rightarrow \quad -p\,\lambda^{-2} + 2\,c_1 = -2\,c_1\,\lambda^{-4} + 2\,c_1 = \dfrac{t_{\max}}{L_y\,\lambda}$

$\Rightarrow \quad 2\,c_1\,\lambda^4 - \dfrac{t_{\max}}{L_y}\,\lambda^3 - 2\,c_1 = 0 \quad \Rightarrow \quad \lambda = \text{nonlinear}(t_{\max})$

```
>>> solve(2.*c0*ly*(lambdaValue**4. - 1.) - tmax*lambdaValue**3.,
 lambdaValue, simplify=True, positive=True)[3]

(0.125*tmax + 0.0416666666666667*sqrt(34.6139896873778*
c0**1.33333333333333*ly**1.33333333333333*
(-9.0*tmax**2 + 1.73205080756888*(4096.0*
c0**4*ly**4 + 27.0*tmax**4)**0.5)**0.333333333333333
- 798.752188051931*c0**2.66666666666667*ly**2.66666666666667
*(-9.0*tmax**2 + 1.73205080756888*(4096.0*c0**4*ly**4 + 27.0*tmax**4)**0.5)**
```

Internal energy:

$$\delta W_{\text{int}} = \int_\Omega \frac{1}{2}\,S_{AB}(\hat{\mathbf{u}})\,\delta u_a^L\left(F_{aB}(\hat{\mathbf{u}})\,\frac{\partial\phi_L}{\partial X_A} + F_{aA}(\hat{\mathbf{u}})\,\frac{\partial\phi_L}{\partial X_B}\right)\mathrm{d}V$$

Now we assume a virtual displacement at node $\mathcal{A}$, $\delta u_a(\mathbf{X}) = \delta u_a^{\mathcal{A}}\phi^{\mathcal{A}}(\mathbf{X})$.

$$\delta W_{\text{int}} = \int_\Omega \frac{1}{2}\,S_{AB}\,\delta u_a^{\mathcal{A}}\left(F_{aB}\,\frac{\partial\phi^{\mathcal{A}}}{\partial X_A} + F_{aA}\,\frac{\partial\phi^{\mathcal{A}}}{\partial X_B}\right)\mathrm{d}V,$$

The ansatz function $\phi^{\mathcal{A}}$ and their derivatives are given by:

$$\phi^{\mathcal{A}}(\mathbf{X}) = \frac{X_1}{L_x}\,\frac{X_2}{L_y}, \quad \frac{\partial\phi^{\mathcal{A}}}{\partial X_1} = \frac{1}{L_x}\,\frac{X_2}{L_y}, \quad \frac{\partial\phi^{\mathcal{A}}}{\partial X_2} = \frac{1}{L_y}\,\frac{X_1}{L_x}$$

For $\delta\mathbf{u}(\mathbf{X}) = (\phi^{\mathcal{A}}(\mathbf{X}), 0)^\top$, i.e. $\delta u_1^{\mathcal{A}} = 1, \delta u_2^{\mathcal{A}} = 0$ we compute the virtual internal energy:

$$\begin{aligned}
\delta W_{\text{int}} &= \int_\Omega \frac{1}{2}\, S_{AB} \left(F_{1B}\, \frac{\partial \phi^{\mathcal{A}}}{\partial X_A} + F_{1A}\, \frac{\partial \phi^{\mathcal{A}}}{\partial X_B} \right) \mathrm{d}V = \int_\Omega \frac{1}{2}\, S_{11} \left(F_{11} \frac{\partial \phi^{\mathcal{A}}}{\partial X_1} + F_{11} \frac{\partial \phi^{\mathcal{A}}}{\partial X_1} \right) \mathrm{d}V \\
&= S_{11} \int_\Omega \lambda \frac{1}{L_x}\, \frac{X_2}{L_y}\, \mathrm{d}V = S_{11}\, \lambda\, \frac{L_x}{L_x}\, \frac{1}{2}\, \frac{L_y^2}{L_y} \\
&= \frac{1}{2}\, L_y\, S_{11}\, \lambda = \frac{1}{2}\, L_y\, F_{11}\, S_{11}
\end{aligned}$$

Virtual external energy

$$\begin{aligned}
\delta W_{\text{ext}} &= \int_\Omega (\mathbf{B} - \rho_0\, \ddot{\mathbf{u}}) \cdot \delta\mathbf{u}\, \mathrm{d}V + \int_{\partial\Omega} \bar{\mathbf{T}} \cdot \delta\mathbf{u}\, \mathrm{d}S \\
&= \int_{\partial\Omega} (T(\mathbf{X}), 0)^\top \cdot \big(\delta u_1(\mathbf{X}), \delta u_2(\mathbf{X})\big)^\top \mathrm{d}S \\
&= \int_0^{L_y} \frac{t_{\max}}{L_y}\, \phi^{\mathcal{A}}(L_x, X_2)\, \mathrm{d}X_2 \\
&= \frac{t_{\max}}{L_y} \int_0^{L_y} \frac{L_x}{L_x}\, \frac{X_2}{L_y}\, \mathrm{d}X_2 \\
&= \frac{t_{\max}}{L_y}\, \frac{1}{2}\, \frac{L_y^2}{L_y} = \frac{1}{2}\, t_{\max} = \frac{1}{2}\, L_y\, T(\mathbf{x})
\end{aligned}$$

From principle of virtual work we should get the correct stress.

$$\begin{aligned}
&\delta W_{\text{int}} - \delta W_{\text{ext}} = 0 \quad \Leftrightarrow \quad \frac{1}{4}\, L_z^2\, S_{11}\, \lambda - \frac{1}{4}\, t_{\max} = 0 \\
&\Leftrightarrow \quad \frac{1}{2}\, (L_y\, S_{11}\, \lambda - t_{\max}) = 0 \\
&\Leftrightarrow \quad L_y\, S_{11}\, \lambda = t_{\max} \quad \Leftrightarrow \quad S_{11} = \frac{t_{\max}}{\lambda\, L_y} = \frac{1}{\lambda^2}\, t(\mathbf{X}) = \frac{1}{\lambda}\, T(\mathbf{X}) \quad \checkmark
\end{aligned}$$

Note: we do not get any further information from the principle of virtual work further than the equilibrium conditions. This is because the stress was preserved as variable and not replaced by the constitutive equations, that relate them to strain and stretch λ.

6.12 2D uniaxial extension with constant total load, 2 elements

This is the same example as before, now considering a discretization with 2 linear-quadratic elements.

Computation of δW_{int} for a virtual displacement at node $\mathcal{B}$, $\delta u_a(\mathbf{X}) = \delta u_a^{\mathcal{B}} \phi^{\mathcal{B}}(\mathbf{X})$. We have

$$\delta W_{\text{int}} = \int_\Omega \frac{1}{2}\, S_{AB}\, \delta u_a^{\mathcal{B}} \left(F_{aB}\, \frac{\partial \phi^{\mathcal{B}}}{\partial X_A} + F_{aA}\, \frac{\partial \phi^{\mathcal{B}}}{\partial X_B} \right) \mathrm{d}V,$$

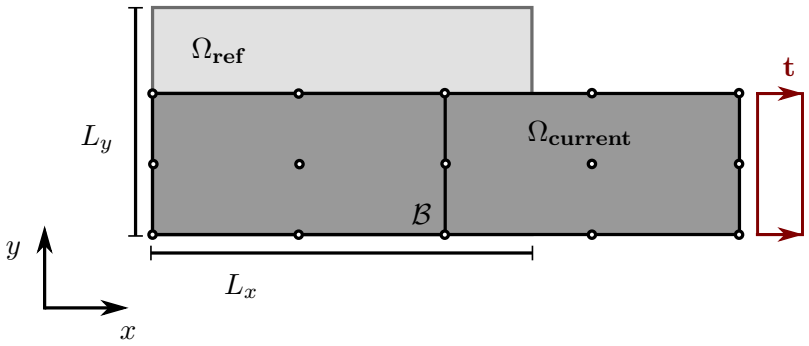


Abbildung 7: Uniaxial extension example with two quadratic elements, mixed formulation

The ansatz function $\phi^{\mathcal{B}}$ and their derivatives are given by:

$$\phi^{\mathcal{B}}(\mathbf{X}) = \left(1 - \left|\frac{2\,X_1}{L_x} - 1\right|\right)\frac{L_y - X_2}{L_y} = \begin{cases} \dfrac{2\,X_1}{L_x}\,\dfrac{L_y - X_2}{L_y} & \text{for } 0 < X_1 \leq L_x/2 \\ \left(2 - \dfrac{2\,X_1}{L_x}\right)\dfrac{L_y - X_2}{L_y} & \text{for } L_x/2 < X_1 \leq L_x \end{cases}$$

$$\frac{\partial \phi^{\mathcal{B}}}{\partial X_1} = \begin{cases} \dfrac{2}{L_x}\,\dfrac{L_y - X_2}{L_y} & \text{for } 0 < X_1 \leq L_x/2 \\ -\dfrac{2}{L_x}\,\dfrac{L_y - X_2}{L_y} & \text{for } L_x/2 < X_1 \leq L_x \end{cases}$$

$$\frac{\partial \phi^{\mathcal{B}}}{\partial X_2} = \begin{cases} -\dfrac{2\,X_1}{L_x}\,\dfrac{1}{L_y} & \text{for } 0 < X_1 \leq L_x/2 \\ -\left(2 - \dfrac{2\,X_1}{L_x}\right)\dfrac{1}{L_y} & \text{for } L_x/2 < X_1 \leq L_x \end{cases}$$

For $\delta\mathbf{u}(\mathbf{X}) = (\phi^{\mathcal{B}}(\mathbf{X}), 0)^{\top}$, i.e. $\delta u_1^{\mathcal{B}} = 1, \delta u_2^{\mathcal{B}} = 0$ we compute the virtual internal energy. The

deformation gradient, F, is constant over the domain, therefore $F_{11} = \lambda$.

$$
\begin{aligned}
\delta W_{\text{int}} &= \int_\Omega \frac{1}{2}\, S_{AB} \left(F_{1B}\, \frac{\partial \phi^{\mathcal{B}}}{\partial X_A} + F_{1A}\, \frac{\partial \phi^{\mathcal{B}}}{\partial X_B} \right) \mathrm{d}V = \int_\Omega \frac{1}{2}\, S_{11} \left(F_{11} \frac{\partial \phi^{\mathcal{B}}}{\partial X_1} + F_{11} \frac{\partial \phi^{\mathcal{B}}}{\partial X_1} \right) \mathrm{d}V \\
&= S_{11}\, \lambda \int_\Omega \frac{\partial \phi^{\mathcal{B}}}{\partial X_1}\, \mathrm{d}V = S_{11}\, \lambda \left(\int_{X_1=0}^{L_x/2} \int_{X_2=0}^{L_y} \frac{\partial \phi^{\mathcal{B}}}{\partial X_1}\, \mathrm{d}X_2\, \mathrm{d}X_1 + \int_{X_1=L_x/2}^{L_x} \int_{X_2=0}^{L_y} \frac{\partial \phi^{\mathcal{B}}}{\partial X_1}\, \mathrm{d}X_2\, \mathrm{d}X_1 \right) \\
&= S_{11}\, \lambda \left(\int_{X_1=0}^{L_x/2} \int_{X_2=0}^{L_y} \frac{2}{L_x}\, \frac{L_y - X_2}{L_y}\, \mathrm{d}X_2\, \mathrm{d}X_1 + \int_{X_1=L_x/2}^{L_x} \int_{X_2=0}^{L_y} -\frac{2}{L_x}\, \frac{L_y - X_2}{L_y}\, \mathrm{d}X_2\, \mathrm{d}X_1 \right) \\
&= S_{11}\, \lambda \left(\int_{X_1=0}^{L_x/2} \frac{2}{L_x}\, \frac{L_y^2 - L_y^2/2}{L_y}\, \mathrm{d}X_1 + \int_{X_1=0}^{L_x/2} -\frac{2}{L_x}\, \frac{L_y^2 - L_y^2/2}{L_y}\, \mathrm{d}X_1 \right) \\
&= S_{11}\, \lambda \left(\int_{X_1=0}^{L_x/2} \frac{2}{L_x}\, \frac{L_y}{2}\, \mathrm{d}X_1 + \int_{X_1=0}^{L_x/2} -\frac{2}{L_x}\, \frac{L_y}{2}\, \mathrm{d}X_1 \right) \\
&= S_{11}\, \lambda \left(\int_{X_1=0}^{L_x/2} \frac{L_y}{L_x}\, \mathrm{d}X_1 + \int_{X_1=0}^{L_x/2} -\frac{L_y}{L_x}\, \mathrm{d}X_1 \right) \\
&= S_{11}\, \lambda \left(\frac{L_y}{2} - \frac{L_y}{2} \right) = 0 \quad \checkmark
\end{aligned}
$$

For $\delta \mathbf{u}(\mathbf{X}) = (0, \phi^{\mathcal{B}}(\mathbf{X}))^\top$, i.e. $\delta u_1^{\mathcal{B}} = 0, \delta u_2^{\mathcal{B}} = 1$ we get:

$$
\delta W_{\text{int}} = \int_\Omega \frac{1}{2}\, S_{AB} \left(F_{2B}\, \frac{\partial \phi^{\mathcal{B}}}{\partial X_A} + F_{2A}\, \frac{\partial \phi^{\mathcal{B}}}{\partial X_B} \right) \mathrm{d}V = 0 \qquad \text{because } S_{ij} = 0 \quad \forall\, (i,j) \neq (1,1), \quad F_{21} = 0
$$

Problem: $S_{22} \neq 0$ in code

From the analytical approach eq. (65) (p.224) we have:

$$
p = \frac{2\, c_1}{\lambda^2}, \qquad \mathbf{S} = \begin{bmatrix} -p\, \lambda^{-2} + 2\, c_1 & 0 \\ 0 & -p\, \lambda^2 + 2\, c_1 \end{bmatrix}, \quad \text{i.e.}
$$

$$
\mathbf{S} = \begin{bmatrix} 2\, c_1\, (1 - \lambda^{-4}) & 0 \\ 0 & 0 \end{bmatrix}
$$

The solution from mixed formulation gives, using $J = 1$, $\Psi = c_1\,(I_1 - 2)$:

$$\bar{\mathbf{C}} = J^{-1}\,\mathbf{C} = \mathbf{C} = \begin{bmatrix} \lambda^2 & 0 \\ 0 & \lambda^{-2} \end{bmatrix}, \quad \mathbf{C}^{-1} = \begin{bmatrix} \lambda^{-2} & 0 \\ 0 & \lambda^2 \end{bmatrix}$$

$$\bar{\gamma}_1 = 2\,\frac{\partial \Psi_{\text{iso}}(\bar{I}_1)}{\partial \bar{I}_1} = 2\,c_1, \qquad \bar{\gamma}_2 = 0$$

$$\bar{\mathbf{S}} = \bar{\gamma}_1\,\mathbf{I} + \bar{\gamma}_2\,\bar{\mathbf{C}} = \begin{bmatrix} 2\,c_1 & 0 \\ 0 & 2\,c_1 \end{bmatrix}.$$

$$\mathbf{S}_{\text{iso}} = J^{-2/2}\,\mathbb{P} : \bar{\mathbf{S}} = \bar{\mathbf{S}} - \frac{1}{2}\,\mathbf{C}^{-1}\,(\mathbf{C} : \bar{\mathbf{S}}) = \begin{bmatrix} 2\,c_1 & 0 \\ 0 & 2\,c_1 \end{bmatrix} - \frac{1}{2}\,\begin{bmatrix} \lambda^{-2} & 0 \\ 0 & \lambda^2 \end{bmatrix}\left(2\,c_1\,\lambda^2 + 2\,c_1\,\lambda^{-2}\right)$$

$$= \begin{bmatrix} 2\,c_1 & 0 \\ 0 & 2\,c_1 \end{bmatrix} - \frac{1}{2}\,\begin{bmatrix} 2\,c_1 + 2\,c_1\,\lambda^{-4} & 0 \\ 0 & 2\,c_1\,\lambda^4 + 2\,c_1 \end{bmatrix}$$

$$= \begin{bmatrix} c_1\,(1 - \lambda^{-4}) & 0 \\ 0 & c_1\,(1 - \lambda^4) \end{bmatrix}$$

From $S_{22} \overset{!}{=} 0$ we get $p = c_1\,(\lambda^2 - \lambda^{-2})$. Then,

$$\mathbf{S}_{\text{vol}} = J\,p\,\mathbf{C}^{-1} = \begin{bmatrix} c_1\,(1 - \lambda^{-4}) & 0 \\ 0 & c_1\,(\lambda^4 - 1) \end{bmatrix}$$

$$\mathbf{S} = \mathbf{S}_{\text{vol}} + \mathbf{S}_{\text{iso}} = \begin{bmatrix} 2\,c_1\,(1 - \lambda^{-4}) & 0 \\ 0 & 0 \end{bmatrix}$$

Transformation in current configaration yields the Cauchy stress, $\boldsymbol{\sigma}$,

$$\boldsymbol{\sigma} = J^{-1}\mathbf{F}\mathbf{S}\,\mathbf{F}^{\top} = \begin{bmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{bmatrix}\begin{bmatrix} 2\,c_1\,(1 - \lambda^{-4}) & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} \lambda & 0 \\ 0 & \lambda^{-1} \end{bmatrix} = \begin{bmatrix} 2\,c_1\,(\lambda^2 - \lambda^{-2}) & 0 \\ 0 & 0 \end{bmatrix}$$

$$\Rightarrow \quad p = -\frac{1}{2}\,\text{tr}\boldsymbol{\sigma} = -c_1\,(\lambda^2 - \lambda^{-2})$$

7 Model Order Reduction

Considering the total reduction, we get the system to be solved for the fully reduced state $\tilde{\mathbf{z}}$:

$$\tilde{\mathbf{z}}^* = \tilde{\mathbf{z}}^{(t)} + \mathbf{V}_k^{\mathrm{T}} \mathbf{FG}(\mathbf{v}_{\mathrm{m}}^{(t)}, \mathbf{y}^{(t)}),$$
$$\tilde{\mathbf{z}}^{(t+1)} = \tilde{\mathbf{z}}^* + \mathbf{V}_k^{\mathrm{T}} \mathbf{A}_{\mathrm{enh}} \mathbf{V}_k \tilde{\mathbf{z}}^{(t+1)},$$

where $\mathbf{FG}(\mathbf{v}_{\mathrm{m}}, \mathbf{y})$ and $\mathbf{A}_{\mathrm{enh}}$ as well as the full state recovery are defined by

$$\mathbf{FG}(\mathbf{v}_{\mathrm{m}}, \mathbf{y}) := \begin{bmatrix} \mathbf{F}_1(\mathbf{v}_{\mathrm{m}}, \mathbf{y}) \\ \mathbf{F}_2(\mathbf{v}_{\mathrm{m}}, \mathbf{y}) \\ \vdots \\ \mathbf{F}_n(\mathbf{v}_{\mathrm{m}}, \mathbf{y}) \\ \mathbf{G}_1(\mathbf{v}_{\mathrm{m}}, \mathbf{y}) \\ \mathbf{G}_2(\mathbf{v}_{\mathrm{m}}, \mathbf{y}) \\ \vdots \\ \mathbf{G}_n(\mathbf{v}_{\mathrm{m}}, \mathbf{y}) \end{bmatrix}, \quad \mathbf{A}_{\mathrm{enh}} := \begin{bmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \\ \mathbf{A}_n \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \quad \mathbf{V}_k \tilde{\mathbf{z}} = \begin{bmatrix} \mathbf{v}_{\mathrm{m},1} \\ \mathbf{v}_{\mathrm{m},2} \\ \vdots \\ \mathbf{v}_{\mathrm{m},n} \\ \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_n \end{bmatrix}.$$

8 Quadrature

The aim is to compute a good approximation for the integral

$$I := \int_0^1 f(\xi)\,\mathrm{d}\xi$$

with a low number of function evaluations $f(\xi)$.

8.1 Gaussian quadrature

The Gaussian quadrature rule approximates the integral by

$$I \approx \sum_{i=1}^{n} f(\xi_i)\, w_i$$

with appropriate *Gauss points* ξ_i and weights $w_i, i = 1, \ldots, n$. The sampling points and weights are chosen such that the rule approximates polynomials of degree $p_{\mathrm{exact}} = 2\,n - 1$ exactly. Some values are listed below.

Note: Literature on Gauss quadrature often describes the case of an integral $\int_{-1}^{1} f(x)\,\mathrm{d}x$. The transformation is given by:

$$\int_0^1 f(\xi)\,\mathrm{d}\xi = \frac{1}{2} \int_{-1}^{1} f\big(1/2 + x/2\big)\,\mathrm{d}x.$$

n	ξ_i	w_i	p_{exact}
1	$\frac{1}{2}$	1	1
2	$\pm\frac{1+\sqrt{3}}{2\sqrt{3}}$	$\frac{1}{2}$	3
3	$\frac{1}{2}$	$\frac{4}{9}$	5
	$\pm\frac{\sqrt{3}+\sqrt{5}}{2\sqrt{5}}$	$\frac{5}{18}$	

Tabelle 3: Gauss points and weights

8.2 Clenshaw-Curtis quadrature

Clenshaw-Curtis quadrature approximates the function by a number of Chebyshev polynomials for which the exact integral is known. The function f is evaluated at the $n+1$ roots of the Chebyshev polynomial T_{n+1}, which are:

$$\xi_i = \cos(i\pi/n), \quad i = 0, \ldots, n,\ n \text{ even.}$$

The function can be written as Chebyshev series

$$f(\xi) = \frac{a_0}{2}\, T_0(\xi) + \sum_{i=1}^{\infty} a_i\, T_i(x)$$

where the coefficients result from discrete cosine transform. The approximated integral is computed by

$$I \approx a_0 + \sum_{i=1}^{n/2-1} \frac{2\, a_{2\,i}}{1-(2\,i)^2} + \frac{a_n}{1-n^2}\,.$$

The coefficients are

$$a_{2\,i} = \frac{2}{n}\left(\frac{f(1)+f(-1)}{2} + f(0)\,(-1)^i + \sum_{i=1}^{n/2-1} \big(f(\xi_i)+f(-\xi_i)\big)\cos(k/2\,\xi_i)\right)$$

This quadrature rule approximates polynomials with degree $p_{\text{exact}} = m-1$ exactly when using m sampling points. However for some non-polynomial functions its accuracy may be better than the respective Gauss quadrature.

9 Propositions

In this section some propositions are collected such that they can be referenced when needed.

9.1 Divergence theorem

Also called Gauss's theorem. Let $U \subset \mathbb{R}^d$ be a compact set with a piecewise smooth boundary ∂U, $\mathbf{F} : U \to \mathbb{R}^d$ a continuously differentiable vector field. Then:

$$\int_U \nabla \cdot \mathbf{F}(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_{\partial U} \mathbf{F}(\mathbf{x}) \cdot \mathbf{n} \, \mathrm{d}\mathbf{x}. \tag{66}$$

For $d = 2$ one gets *Stoke's theorem*.

9.1.1 Corollary

Replacing $\mathbf{F}$ of (66) by $f\,\mathbf{F}$ yields the following proposition:

For a differentable function $f : U \to \mathbb{R}$ and a vector field $\mathbf{F} : U \to \mathbb{R}^d$ the following holds:

$$\int_U f(\nabla \cdot \mathbf{F}) \, \mathrm{d}\mathbf{x} = \int_{\partial U} (f\,\mathbf{F}) \cdot \mathbf{n} \, \mathrm{d}\mathbf{x} - \int_U \mathbf{F} \cdot \nabla f \, \mathrm{d}\mathbf{x} \tag{67}$$

Now set $\mathbf{F} \equiv (1, 0, \dots), (0, 1, \dots), \dots$ to get the following vector-valued identity:

For a differentable function $f : U \to \mathbb{R}$ the following holds:

$$\int_U \nabla f(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_{\partial U} f(\mathbf{x}) \, \mathbf{n} \, \mathrm{d}\mathbf{x} \tag{68}$$

9.2 Classical Stoke's theorem

Let $U \subset \mathbb{R}^3$ be an open set, V a 2-manifold in U with boundary ∂V and $\mathbf{F} : U \to \mathbb{R}^3$ a continuously differentiable vector field. Then:

$$\oint_{\partial V} \mathbf{F} \cdot \mathrm{d}s = \int_V \big(\nabla \times \mathbf{F}\big) \cdot \mathbf{n} \, \mathrm{d}\mathbf{x}, \tag{69}$$

where $\mathbf{n}$ is the normal on the surface V.

9.3 Integration on manifolds

In the following it is outlined how to integrate on 1D and 2D domains that are embedded in $\mathbb{R}^d$. The formalism of manifolds is omitted for simplicity.

9.3.1 1D curve integrals

Let $U \subset \mathbb{R}$ be an open set (the parameter space) and $\Phi : U \to \mathbb{R}^d$ a smooth mapping that defines a curve $\Omega = \Phi(U)$ embedded in $\mathbb{R}^d$. An integrable function $g : \Omega \to \mathbb{R}$ can then be integrated as follows:

$$\int_{\Phi(U)} g(\mathbf{x}) \, \mathrm{d}\mathbf{x} = \int_U g\big(\Phi(\xi)\big) \, \|\Phi'(\xi)\|_2 \, \mathrm{d}\xi \tag{70}$$

9.3.2 2D surface integrals

Let $U \subset \mathbb{R}^2$ be an open set (parameter space), $\Phi : U \to \Phi(U) =: \Omega \subset \mathbb{R}^3$ a diffeomorphism, Φ maps parameters $\boldsymbol{\xi} = (\xi_1, \xi_2) \in U$ to points in world space $\mathbf{x} \in \Omega$. The inverse map $\Phi^{-1} : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^2$ assigns coordinates (ξ_1, ξ_2) to each point $\mathbf{x} \in \Omega$. We name $\Phi^{-1}(\mathbf{x}) = (x(\mathbf{x}), y(\mathbf{x}))$ in the following formula. The integration of a 2-dimensional function $g : \Omega \to \mathbb{R}$ is performed as follows.

$$\begin{aligned}
\int_{\Phi(U)} g(\mathbf{x})\,\mathrm{d}\mathbf{x} &= \int_U g\big(\Phi(\boldsymbol{\xi})\big)\sqrt{\det\left(J_\Phi(\boldsymbol{\xi})^\top J_\Phi(\boldsymbol{\xi})\right)}\,\mathrm{d}\boldsymbol{\xi} \\
&= \int_U g\big(\Phi(\boldsymbol{\xi})\big)\sqrt{\det\begin{pmatrix} \frac{\mathrm{d}\Phi}{\mathrm{d}\xi_1}\cdot\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_1} & \frac{\mathrm{d}\Phi}{\mathrm{d}\xi_1}\cdot\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_2} \\ \frac{\mathrm{d}\Phi}{\mathrm{d}\xi_1}\cdot\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_2} & \frac{\mathrm{d}\Phi}{\mathrm{d}\xi_2}\cdot\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_2} \end{pmatrix}}\,\mathrm{d}\boldsymbol{\xi} \\
&= \int_U g\big(\Phi(\boldsymbol{\xi})\big)\sqrt{\left\|\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_1}\right\|_2^2\left\|\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_2}\right\|_2^2 - \left(\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_1}\cdot\frac{\mathrm{d}\Phi}{\mathrm{d}\xi_2}\right)^2}\,\mathrm{d}\boldsymbol{\xi}
\end{aligned} \tag{71}$$

9.3.3 Substitution on domains with same dimensionality

Integration by substitution, *German "Transformationssatz"*, also *change of variables rule*. Let $U \subset \mathbb{R}^d$ be an open set, $\Phi : U \to \Phi(U) \subset \mathbb{R}^d$ a diffeomorphism (Φ bijective and continuously differentiable, inverse map Φ^{-1} also continuously differentiable).

Then $g : \Phi(U) \to \mathbb{R}$ is integrable on $\Phi(U)$ if and only if the function $\boldsymbol{\xi} \mapsto g(\Phi(\boldsymbol{\xi}))\,|\det(J_\Phi(\boldsymbol{\xi}))|$ is integrable on U. The following holds:

$$\int_{\Phi(U)} g(\mathbf{x})\,\mathrm{d}\mathbf{x} = \int_U g(\Phi(\boldsymbol{\xi}))\,|\det(J_\Phi(\boldsymbol{\xi}))|\,\mathrm{d}\boldsymbol{\xi}, \tag{72}$$

where J_Φ is the Jacobian of Φ.

9.3.4 Summary

The transformation rules eqs. (70) to (72) can be summarized in a unified form as follows.

Let $U \subset \mathbb{R}^d, d \in \{1, 2, 3\}$ be an open set (parameter space), $\Phi : U \to \Phi(U) =: \Omega \subset \mathbb{R}^d$ a diffeomorphism that maps parameters $\boldsymbol{\xi} \in U$ to points in world space $\mathbf{x} \in \Omega$. A function defined in parameter space, $f : U \to \mathbb{R}$, can then be integrated as follows in world space.

$$\int_{\Phi(U)} f\big(\Phi^{-1}(\mathbf{x})\big)\,\mathrm{d}\mathbf{x} = \int_U f(\boldsymbol{\xi})\,\mathcal{J}_d(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}, \tag{73}$$

where the definition of $\mathcal{J}_d(\boldsymbol{\xi})$ depends on the dimension d as follows:

$$\begin{aligned}
\mathcal{J}_1(\xi) &= \|\Phi'(\xi)\|_2 && \text{for } d = 1, \boldsymbol{\xi} = \xi \in U \subset \mathbb{R}, \\
\mathcal{J}_2(\boldsymbol{\xi}) &= \sqrt{\det\left(J_\Phi(\boldsymbol{\xi})^\top J_\Phi(\boldsymbol{\xi})\right)} && \text{for } d = 2, \boldsymbol{\xi} \in U \subset \mathbb{R}^2, \phi^{-1}(\mathbf{x}) =: \big(x(\mathbf{x}), y(\mathbf{x})\big), \\
\mathcal{J}_3(\boldsymbol{\xi}) &= |\det(J_\Phi(\boldsymbol{\xi}))| && \text{for } d = 3, \boldsymbol{\xi} \in U \subset \mathbb{R}^3.
\end{aligned}$$

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