Weak formulation of mechano-electro-chemical cartilage model

Discretization and non-linear equations system

For the temporal discretization of the governing equations, we consider the partition $\cup_{\mathrm{n=1}}^{\mathrm{n_{step}-1}} [t_{\mathrm{n}}, t_{\mathrm{n+1}}]$ of the time interval of interest T, and focus on the typical time subinterval $[\mathrm{t_n}, \mathrm{t_{n+1}}]$ with $\Delta t = t_{\mathrm{n+1}} - t_{\mathrm{n}} \geq 0$ denoting the corresponding increment of time. It is assumed that the primary unknowns and all derivable quantities are known at time t_{n}. The generalized trapezoidal method is applied (Crank and Nicolson 1947), with $\alpha\epsilon(0,1]$, such that $t_{\mathrm{n+\alpha}} = t_{\mathrm{n}} + \alpha\, \Delta t$. In this method the following scheme is used for the temporal discretization of primary variables (here only ε^{w} is shown, while ε^{+} and ε^{-} and $\mathbf{u}$ have the same discretization):

$$\varepsilon_{n+1}^{w} = \varepsilon_{n}^{w} + \Delta t\, \dot{\varepsilon}_{n+\alpha}^{w} \,, \tag{A.1}$$

$$\dot{\varepsilon}_{n+\alpha}^{w} = \dot{\varepsilon}_{n}^{w}(1-\alpha) + \dot{\varepsilon}_{n+1}^{w}\alpha \,, \tag{A.2}$$

where ε_{n+1}^{w}, $\dot{\varepsilon}_{n+\alpha}^{w}$ and $\dot{\varepsilon}_{n+1}^{w}$ are approximations of $\varepsilon^{w}(t_{n+1})$, $(\frac{\partial \varepsilon^{w}}{\partial t})(t_{n+\alpha})$ and $(\frac{\partial \varepsilon^{w}}{\partial t})(t_{n+1})$, respectively. From a practical standpoint $\tilde{\varepsilon}_{n+1}^{w}$ is introduced as a predictor value of $\varepsilon_{n+1}^{\mathrm{w}}$, which only depends on magnitudes at time t_n:

$$\tilde{\varepsilon}_{n+1}^{w} = \varepsilon_{n}^{w} + (1-\alpha)\Delta t \cdot \dot{\varepsilon}_{n}^{w} \,, \tag{A.3}$$

$\dot{\varepsilon}_{n+1}^{w}$ can be computed by

$$\dot{\varepsilon}_{n+1}^{\mathrm{w}} = \frac{\varepsilon^{\mathrm{w}}{}_{\mathrm{n+1}} - \tilde{\varepsilon}_{n+1}^{\mathrm{w}}}{\alpha \Delta t} \,, \tag{A.4}$$

Substitution of equations (A.3) and (A.4) in the weak form of the problem yields a semi-discrete set of equations that are discretized in time.

Spatial discretization of the problem

The semi-discrete system is discretized in space using the finite element method. The domain Ω is discretized into n_{el} elements Ω^e, with $\Omega = \cup_{e=1}^{n_{\mathrm{el}}} \Omega^e$. The primary unknown fields are interpolated within a generic element Ω^{e} in terms of the nodal values through shape functions, that is,

$$\varepsilon^{wh}|_{\Omega^e} = \mathbf{N}_{\varepsilon^w} \boldsymbol{\varepsilon}^{w\mathrm{e}} ,$$

$$\varepsilon^{+h}|_{\Omega^e} = \mathbf{N}_{\varepsilon^+} \boldsymbol{\varepsilon}^{+\mathrm{e}} , \qquad \text{(A.5)}$$

$$\varepsilon^{-h}|_{\Omega^e} = \mathbf{N}_{\varepsilon^-} \boldsymbol{\varepsilon}^{-\mathrm{e}} ,$$

$$\mathbf{u}^h|_{\Omega^e} = \mathbf{N}_{\mathbf{u}} \mathbf{u}^e ,$$

where $\boldsymbol{\varepsilon}^{w\mathrm{e}}$, $\boldsymbol{\varepsilon}^{+\mathrm{e}}$, $\boldsymbol{\varepsilon}^{-\mathrm{e}}$ and $\mathbf{u}^{\mathrm{e}}$ are column vectors of nodal values of the primary unknowns at element e and $\mathbf{N}_{\varepsilon^{\mathrm{w}}}$, $\mathbf{N}_{\varepsilon^+}$, $\mathbf{N}_{\varepsilon^-}$ and $\mathbf{N}_{\mathbf{u}}$ are matrices of element shape functions, that is,

$$\mathbf{N}_{\varepsilon^{\mathrm{w}}} = [N_{\varepsilon^w}^1, \dots, N_{\varepsilon^w}^{n_{en}}] ,$$

$$\mathbf{N}_{\varepsilon^+} = [N_{\varepsilon^+}^1, \dots, N_{\varepsilon^+}^{n_{en}}] , \qquad \text{(A.6)}$$

$$\mathbf{N}_{\varepsilon^-} = [N_{\varepsilon^-}^1, \dots, N_{\varepsilon^-}^{n_{en}}] ,$$

$$\mathbf{N}_{\mathbf{u}} = \begin{bmatrix} N_u^1 & 0 & 0 \\ 0 & N_u^1 & 0 \\ 0 & 0 & N_u^1 \end{bmatrix} \cdots \begin{bmatrix} N_u^{n_{en}} & 0 & 0 \\ 0 & N_u^{n_{en}} & 0 \\ 0 & 0 & N_u^{n_{en}} \end{bmatrix} ,$$

where $\mathbf{N}^{\mathrm{i}}$ is the shape function associated with element node i and n_{en} is the number of element nodes. Following a Bubnov-Galerkin scheme, the same shape functions are also applied to interpolate the test functions:

$$\delta\varepsilon^{wh}|_{\Omega^e} = \mathbf{N}_{\varepsilon^w}\boldsymbol{\delta\varepsilon}^{we} \ ,$$

$$\delta\varepsilon^{+\mathrm{h}}|_{\Omega^e} = \mathbf{N}_{\varepsilon^+}\boldsymbol{\delta\varepsilon}^{+e} \ , \qquad (A.7)$$

$$\delta\varepsilon^{-h}|_{\Omega^e} = \mathbf{N}_{\varepsilon^-}\boldsymbol{\delta\varepsilon}^{-e},$$

$$\delta\mathbf{u}^h|_{\Omega^e} = \mathbf{N}_{\mathbf{u}}\delta\mathbf{u}^e \ .$$

Likewise, the discretization of the related gradients of the test functions and the primary unknowns take the following element wise format:

$$\nabla\varepsilon^{wh}|_{\Omega^e} = \nabla\cdot\mathbf{N}_{\varepsilon^w}\boldsymbol{\varepsilon}^{w\mathrm{e}} \xrightarrow{yields} \nabla\delta\varepsilon_h|_{\Omega^e} = \nabla\cdot\mathbf{N}_{\varepsilon^w}\delta\boldsymbol{\varepsilon}^{w\mathrm{e}} \ , \qquad (A.8)$$

$$\nabla\varepsilon^{+h}|_{\Omega^e} = \nabla\cdot\mathbf{N}_{\varepsilon^+}\boldsymbol{\varepsilon}^{+\mathrm{e}} \xrightarrow{yields} \nabla\delta\varepsilon^{+}{}_h|_{\Omega^e} = \nabla\cdot\mathbf{N}_{\varepsilon^+}\delta\boldsymbol{\varepsilon}^{+\mathrm{e}},$$

$$\nabla\varepsilon^{-h}|_{\Omega^e} = \nabla\cdot\mathbf{N}_{\varepsilon^-}\boldsymbol{\varepsilon}^{-\mathrm{e}} \xrightarrow{yields} \nabla\delta\varepsilon^{-}{}_h|_{\Omega^e} = \nabla\cdot\mathbf{N}_{\varepsilon^-}\delta\boldsymbol{\varepsilon}^{-\mathrm{e}} \ .$$

The strains are interpolated in the following form:

$$\epsilon^h|_{\Omega^e} = \mathbf{B}_{\mathbf{u}}\mathbf{u}^e \ , \qquad (A.9)$$

where $\mathbf{B}_{\mathbf{u}}$ is a matrix of derivatives of shape functions:

$$\mathbf{B}_{\mathbf{u}} = \mathbf{H}\mathbf{N}_{\mathbf{u}} \ ,$$

(A.10)

$$
\mathbf{H} = \begin{bmatrix} \frac{\partial}{\partial \mathrm{x}} & 0 & 0 \\ 0 & \frac{\partial}{\partial \mathrm{y}} & 0 \\ 0 & 0 & \frac{\partial}{\partial \mathrm{z}} \\ \frac{1}{2}\frac{\partial}{\partial \mathrm{y}} & \frac{1}{2}\frac{\partial}{\partial \mathrm{x}} & 0 \\ \frac{1}{2}\frac{\partial}{\partial \mathrm{y}} & 0 & \frac{1}{2}\frac{\partial}{\partial \mathrm{y}} \\ 0 & \frac{1}{2}\frac{\partial}{\partial \mathrm{z}} & \frac{1}{2}\frac{\partial}{\partial \mathrm{y}} \end{bmatrix}. \tag{A.11}
$$

Substituting the equations (A.5), (A.7) and (A.10) into the semi-discrete system and choosing appropriately arbitrary coefficients $\delta\boldsymbol{\varepsilon}^{we}$, $\delta\boldsymbol{\varepsilon}^{+e}$, $\delta\boldsymbol{\varepsilon}^{-e}$ and $\delta\mathbf{u}^{e}$ of the test functions, one can finally arrive at a set of non-linear algebraic equations which is sufficient to determine the nodal values of the primary unknowns that can be written in the form:

$$
\mathbf{F}^{\text{int}} = \left(\mathbb{Z}_{n+1}, \frac{\mathbb{Z}_{n+1} - \widetilde{\mathbb{Z}}_{n+1}}{\alpha \Delta t}\right) = \mathbf{F}^{\text{ext}}(\mathbb{Z}_{n+1}), \tag{A.12}
$$

where $\mathbb{Z}_{n+1}$ and $\widetilde{\mathbb{Z}}_{n+1}$ are the global column vector of nodal values of the primary unknown fields at time $t_{\mathrm{n+1}}$ and the corresponding predictor value, respectively. This vector can be obtained as follow:

$$
\mathbb{Z}_{n+1} = \mathcal{R}_{e=1}^{n_{\text{en}}} \mathbf{d}_{n+1}^{e}, \tag{A.13}
$$

$$
\widetilde{\mathbb{Z}}_{n+1} = \mathcal{R}_{e=1}^{n_{\text{en}}} \tilde{\mathbf{d}}_{n+1}^{e}, \tag{A.14}
$$

where $\mathcal{R}$ denotes the standard finite element assembly operator and $\mathbf{d}_{n+1}^{e}$ and $\tilde{\mathbf{d}}_{n+1}^{e}$ can be defined by

$$
\mathbf{d}_{n+1}^{e} = [\boldsymbol{\varepsilon}_{n+1}^{w^e}, \boldsymbol{\varepsilon}_{n+1}^{+^e}, \boldsymbol{\varepsilon}_{n+1}^{-^e}, \mathbf{u}_{n+1}^{e}]^{\mathrm{T}}, \tag{A.15}
$$

$$
\tilde{\mathbf{d}}_{n+1}^{e} = [\tilde{\boldsymbol{\varepsilon}}_{n+1}^{w^e}, \tilde{\boldsymbol{\varepsilon}}_{n+1}^{+^e}, \tilde{\boldsymbol{\varepsilon}}_{n+1}^{-^e}, \tilde{\mathbf{u}}_{n+1}^{e}]^{\mathrm{T}}. \tag{A.16}
$$

The internal and external global force vector represented by F^{int} and F^{ext} also come from the assembly of element contributions:

$$F_{n+1}^{int} = \mathcal{R}_{e=1}^{n_{en}} \mathbf{f}_{n+1}^{int,e} , \tag{A.17}$$

$$F_{n+1}^{ext} = \mathcal{R}_{e=1}^{n_{en}} \mathbf{f}_{n+1}^{ext,e} , \tag{A.18}$$

where

$$\mathbf{f}_{n+1}^{int,e} = [\mathbf{f}_{\varepsilon^w,n+1}^{int,e}; \mathbf{f}_{\varepsilon^+,n+1}^{int,e}; \mathbf{f}_{\varepsilon^-,n+1}^{int,e}; \mathbf{f}_{\mathbf{u},n+1}^{int,e}]^T , \tag{A.19}$$

$$\mathbf{f}_{n+1}^{ext,e} = [\mathbf{f}_{\varepsilon^w,n+1}^{ext,e}; \mathbf{f}_{\varepsilon^+,n+1}^{ext,e}; \mathbf{f}_{\varepsilon^-,n+1}^{ext,e}; \mathbf{f}_{u,n+1}^{ext,e}]^T . \tag{A.20}$$

The element contributions to the internal force reads as:

$$\mathbf{f}_{\boldsymbol{\varepsilon}^w,n+1}^{int,e} =$$

$$\int \nabla \cdot \mathbf{N}_{\boldsymbol{\varepsilon}^w}^T \left[\frac{\mathbf{u}_{n+1}^h - \tilde{\mathbf{u}}_{n+1}^h}{\alpha \Delta t} + \frac{RT}{\alpha} \Phi^w \nabla \varepsilon^{wh} + \frac{RT}{\alpha} \Phi^w \frac{c^+}{\varepsilon^{+h}} \nabla \varepsilon^{+h} + \frac{RT}{\alpha} \Phi^w \frac{c^-}{\varepsilon^{-h}} \nabla \varepsilon^{-h}\right]_{n+1} dV ,$$

$$\mathbf{f}_{\varepsilon^+,n+1}^{int,e} =$$

$$\int_\Omega \nabla \cdot \mathbf{N}_{\varepsilon^+}^T \left[-\frac{RT}{\alpha} \Phi^w c^F \nabla \cdot \mathbf{N}_{\boldsymbol{\varepsilon}^w} \varepsilon^w - \left(\frac{\Phi^w c^+ D^+}{\varepsilon^{+h}} + \frac{RT}{\alpha} \Phi^w \frac{(c^+)^2}{\varepsilon^{+h}} - \frac{RT}{\alpha} \Phi^w \frac{c^+ c^-}{\varepsilon^{+h}}\right) \nabla \varepsilon^{+h} + \right.$$

$$\left. \left(\frac{\Phi^w c^- D^-}{\varepsilon^{-h}} + \frac{RT}{\alpha} \Phi^w \frac{(c^-)^2}{\varepsilon^{-h}} - \frac{RT}{\alpha} \Phi^w \frac{c^+ c^-}{\varepsilon^{-h}}\right) \nabla \varepsilon^{+h}\right]_{n+1} dV,$$

(A.21)

$$\mathbf{f}_{\boldsymbol{\varepsilon}^-,n+1}^{int,e} =$$

$$\int_\Omega \nabla \cdot \mathbf{N}_{\boldsymbol{\varepsilon}^-}^T \left[-\frac{RT}{\alpha} \Phi^w c^F \nabla \cdot \mathbf{N}_{\boldsymbol{\varepsilon}^w} \varepsilon^w + \left(\frac{\Phi^w c^+ D^+}{\varepsilon^{+h}} + \frac{RT}{\alpha} \Phi^w \frac{(c^+)^2}{\varepsilon^{+h}} + \frac{RT}{\alpha} \Phi^w \frac{c^+ c^-}{\varepsilon^{+h}}\right) \nabla \varepsilon^{+h} + \right.$$

$$\left(\frac{\Phi^{w} c^{-} D^{-}}{\varepsilon^{-h}} + \frac{RT}{\alpha}\Phi^{w}\frac{(c^{-})^{2}}{\varepsilon^{-h}} + \frac{RT}{\alpha}\Phi^{w}\frac{c^{+}c^{-}}{\varepsilon^{-h}}\right)\nabla\varepsilon^{-h}\bigg]_{n+1} dV +$$

$$\int \nabla\cdot\mathbf{N}_{\boldsymbol{\varepsilon}^{-}}^{T}\left(\Phi^{w} c^{k^{h}}\frac{\mathbf{u}_{n+1}^{h}-\tilde{\mathbf{u}}_{n+1}^{h}}{\alpha\Delta t}\right) dV + \int \mathbf{N}_{\boldsymbol{\varepsilon}^{-}}^{T}\left(\Phi^{w}\frac{c_{n+1}^{k^{h}}-\tilde{c}^{k^{h}}_{n+1}}{\alpha\Delta t}\right) dV,$$

$$\mathbf{f}_{\mathbf{u},n+1}^{int,e} = \int \mathbf{B}_{\mathbf{u}}^{T}\left[\mathbf{D}_{elas}\mathbf{H}\mathbf{u}^{h} - RT\varepsilon^{w^{h}}\mathbf{I} + RT\Phi c^{k^{h}}\mathbf{I} - B_{w}\mathbf{H}\mathbf{u}^{h}\right]_{n+1} dV,$$

where $\mathbf{D}_{elas}$ is the elastic constitutive matrix:

$$D_{elas} = \xi\begin{bmatrix} 1-\nu & \nu & \nu & & & \\ \nu & 1-\nu & \nu & & \tilde{0} & \\ \nu & \nu & 1-\nu & & & \\ & & & \frac{1-2\nu}{2} & 0 & 0 \\ & \tilde{0} & & 0 & \frac{1-2\nu}{2} & 0 \\ & & & 0 & 0 & \frac{1-2\nu}{2} \end{bmatrix}, \qquad \text{(A.22)}$$

with $\xi = \frac{E}{(1+\nu)(1-2\nu)}$.

In the case of the external force vector the element contributions have the following expressions:

$$\mathbf{f}_{\mathbf{u},n+1}^{ext,e} = \int \mathbf{N}_{\mathbf{u}}^{T}\boldsymbol{\sigma}^{*h}_{n+1}\, dV\,,$$

$$\mathbf{f}_{\boldsymbol{\varepsilon}^{w},n+1}^{ext,e} = -\int \mathbf{N}_{\boldsymbol{\varepsilon}^{wh}}^{T}\mathbf{J}^{w*h}_{n+1}\, dV\,, \qquad \text{(A.23)}$$

$$\mathbf{f}_{\boldsymbol{\varepsilon}^{+},n+1}^{ext,e} = \int \mathbf{N}_{\boldsymbol{\varepsilon}^{+}}^{T}(\mathbf{J}^{+*h}_{n+1} - \mathbf{J}^{-*h}_{n+1})\, dV\,,$$

$$\mathbf{f}_{\boldsymbol{\varepsilon}^{-},n+1}^{ext,e} = -\int \mathbf{N}_{\boldsymbol{\varepsilon}^{+}}^{T}\left(\mathbf{J}^{+*h}_{n+1} + \mathbf{J}^{-*h}_{n+1}\right) dV.$$