Coarse-scale stress and elasticity (tangent) tensors: Multiscale implementation

1 TKD resultant tensors: Averaging over TKD elements

1.1 Principal directions

First step consists on, for a non-diagonal deformation state, look for the principal directions. Let $\check{\boldsymbol{F}}^c$ to be a non-diagonal coarse deformation state. Then the deformation gradient in principal coordinates is obtained as,

$$
\begin{aligned}
\check{\boldsymbol{C}}^c &= \check{\boldsymbol{F}}^{c^T} \check{\boldsymbol{F}}^c \\
\check{\boldsymbol{b}}^c &= \check{\boldsymbol{F}}^c \check{\boldsymbol{F}}^{c^T} \\
\det\left(\check{\boldsymbol{C}}^c - \lambda_i^{c^2} \boldsymbol{I}\right) &= 0 \quad \forall i \in \{1,2,3\} \\
\det\left(\check{\boldsymbol{b}}^c - \lambda_i^{c^2} \boldsymbol{I}\right) &= 0 \quad \forall i \in \{1,2,3\} \\
\check{\boldsymbol{C}}^c \lambda_i^{c^2} &= \lambda_i^{c^2} \hat{\boldsymbol{N}}_i^c \quad \forall i \in \{1,2,3\} \\
\check{\boldsymbol{b}}^c \lambda_i^{c^2} &= \lambda_i^{c^2} \hat{\boldsymbol{n}}_i^c \quad \forall i \in \{1,2,3\} \\
\boldsymbol{F}^c &= \begin{bmatrix} \lambda_1^c & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}
\end{aligned}
$$

Likewise, the coarse-scale stress state can be obtained from the principal coordinates in the following way:

$$
\check{\boldsymbol{S}}^c = \sum_{a=1}^{3} S_a^c \; \hat{\boldsymbol{N}}_a^c \otimes \hat{\boldsymbol{N}}_a^c \tag{1}
$$

$$
\check{\boldsymbol{\sigma}}^c = \sum_{a=1}^{3} \sigma_a^c \; \hat{\boldsymbol{n}}_a^c \otimes \hat{\boldsymbol{n}}_a^c \tag{2}
$$

1.2 Material stress tensor for the purely hyperelastic TKD model

From the hyperelastic TKD model, we have that:

$$
\boldsymbol{\sigma}^c(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c) = \frac{2}{|\Theta_y|} \left(\boldsymbol{f}_7 \otimes \boldsymbol{F}^c \boldsymbol{b}_x + \boldsymbol{f}_{10} \otimes \boldsymbol{F}^c \boldsymbol{b}_y + \boldsymbol{f}_{15} \otimes \boldsymbol{F}^c \boldsymbol{b}_z\right) \tag{3}
$$

where it has been considered that:

$$
\begin{aligned}
|\Theta_y| &= |\Theta_y\ (\boldsymbol{F}^c)| = J^c(\boldsymbol{F}^c)|\Theta_Y| \\
\boldsymbol{f}_7 &= \boldsymbol{f}_7(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c) \\
\boldsymbol{f}_{10} &= \boldsymbol{f}_{10}(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c) \\
\boldsymbol{f}_{15} &= \boldsymbol{f}_{15}(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c)
\end{aligned}
$$

because they are functions of strut elongations, which are functions of nodal displacements and thus, functions of $\boldsymbol{r}^*$. For the sake of clarity, dependence of $\boldsymbol{r}^*$ on $\boldsymbol{F}^c$ will be omitted. To later compute the coarse-scale material elasticity tensor $\mathbb{C}_s^c$, the coarse-scale second Piola-Kirchhoff stress tensor $\boldsymbol{S}^c$ has to be obtained. For this purpose,

$$
\begin{aligned}
\boldsymbol{S}^c &= J^c \boldsymbol{F}^{c^{-1}} \boldsymbol{\sigma}^c \boldsymbol{F}^{c^{-T}} && (4) \\
S_{ij}^c &= J^c F_{ik}^{c^{-1}} \sigma_{kl}^c F_{lj}^{c^{-T}} \quad i, j \in \{1, 2, 3\} && (5)
\end{aligned}
$$

As known, previous equation is valid for any state, principal or non-principal, accordint to tensor properties. Replacing expression for $\boldsymbol{\sigma}^c$ from equation (3), it yields

$$
S_{ij}^c = \frac{2J^c}{|\Theta_y|} \left[F_{ik}^{c^{-1}} f_{7_k} F_{lp}^c b_{x_p} F_{lj}^{c^{-T}} + F_{ik}^{c^{-1}} f_{10_k} F_{lp}^c b_{y_p} F_{lj}^{c^{-T}} + F_{ik}^{c^{-1}} f_{15_k} F_{lp}^c b_{z_p} F_{lj}^{c^{-T}} \right] \tag{6}
$$

which, rearranging terms

$$
S_{ij}^c = \frac{2J^c}{|\Theta_y|} \left[F_{ik}^{c^{-1}} f_{7_k} F_{jl}^{c^{-1}} F_{lp}^c b_{x_p} + F_{ik}^{c^{-1}} f_{10_k} F_{jl}^{c^{-1}} F_{lp}^c b_{y_p} + F_{ik}^{c^{-1}} f_{15_k} F_{jl}^{c^{-1}} F_{lp}^c b_{z_p} \right] \tag{7}
$$

Simplifying

$$
\begin{aligned}
S_{ij}^c &= \frac{2J^c}{|\Theta_y|} \left[F_{ik}^{c^{-1}} f_{7_k} \delta_{jp} b_{x_p} + F_{ik}^{c^{-1}} f_{10_k} \delta_{jp} b_{y_p} + F_{ik}^{c^{-1}} f_{15_k} \delta_{jp} b_{z_p} \right] && (8) \\
S_{ij}^c &= \frac{2J^c}{|\Theta_y|} \left[F_{ik}^{c^{-1}} f_{7_k} b_{x_j} + F_{ik}^{c^{-1}} f_{10_k} b_{y_j} + F_{ik}^{c^{-1}} f_{15_k} b_{z_j} \right] && (9)
\end{aligned}
$$

In tensorial notation last expression leads to

$$
\boldsymbol{S}^c = \frac{2J^c}{|\Theta_y|} \boldsymbol{F}^{c^{-1}} \left[\boldsymbol{f}_7 \otimes \boldsymbol{b}_x + \boldsymbol{f}_{10} \otimes \boldsymbol{b}_y + \boldsymbol{f}_{15} \otimes \boldsymbol{b}_z \right] \tag{10}
$$

Using that $|\Theta_y| = J^c|\Theta_Y|$, we have that:

$$
\boldsymbol{S}^c = \frac{2}{|\Theta_Y|} \boldsymbol{F}^{c^{-1}} \left[\boldsymbol{f}_7 \otimes \boldsymbol{b}_x + \boldsymbol{f}_{10} \otimes \boldsymbol{b}_y + \boldsymbol{f}_{15} \otimes \boldsymbol{b}_z \right] \tag{11}
$$

1.3 Material stress tensor for the finite-deformations poroelastic TKD model

$$
\begin{aligned}
\boldsymbol{\sigma}^c(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c) = \frac{2}{|\Theta_y|} \left(\boldsymbol{f}_7 \otimes \boldsymbol{F}^c \boldsymbol{b}_x + \boldsymbol{f}_{10} \otimes \boldsymbol{F}^c \boldsymbol{b}_y + \boldsymbol{f}_{15} \otimes \boldsymbol{F}^c \boldsymbol{b}_z \right) + \\
\frac{1}{|\Theta_y|} \sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} \left(\boldsymbol{a}_{e_1} \otimes \boldsymbol{a}_{e_1} + \boldsymbol{a}_{e_2} \otimes \boldsymbol{a}_{e_2} \right)
\end{aligned} \tag{12}
$$

with

$$\sigma_e^T = -p_{alv}^c \left(2 - \sqrt{\lambda_e}\right) \tag{13}$$

where, in addition to considerations taken for $\boldsymbol{f}_7, \boldsymbol{f}_{10}, \boldsymbol{f}_{15}$, it has been considered that:

$$\begin{aligned}
\lambda_e &= \lambda_e(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c) \\
\boldsymbol{a}_{e_1} &= \boldsymbol{a}_{e_1}(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c) \\
\boldsymbol{a}_{e_2} &= \boldsymbol{a}_{e_2}(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c)
\end{aligned}$$

Now, developing the term associated to the alveolar pressure, we have that

$$\begin{aligned}
\boldsymbol{S}^c_{pressure} &= \frac{1}{|\Theta_y|} \sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} J^c \left(\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_1} \otimes \boldsymbol{a}_{e_1} \boldsymbol{F}^{c^{-T}} + \boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_2} \otimes \boldsymbol{a}_{e_2} \boldsymbol{F}^{c^{-T}} \right) &\quad (14) \\
&= \frac{1}{|\Theta_y|} \sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} J^c \left[(\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_1}) \otimes (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_1}) + (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_2}) \otimes (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_2}) \right] &\quad (15)
\end{aligned}$$

Using that $|\Theta_y| = J^c |\Theta_Y|$, we have that:

$$\boldsymbol{S}^c_{pressure} = \frac{1}{|\Theta_Y|} \sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} \left[(\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_1}) \otimes (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_1}) + (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_2}) \otimes (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_2}) \right] \tag{16}$$

Then, the material stress state is:

$$\begin{aligned}
\boldsymbol{S}^c(\boldsymbol{r}^*(\boldsymbol{F}^c), \boldsymbol{F}^c) = \frac{2}{|\Theta_Y|} \boldsymbol{F}^{c^{-1}} \left[\boldsymbol{f}_7 \otimes \boldsymbol{b}_x + \boldsymbol{f}_{10} \otimes \boldsymbol{b}_y + \boldsymbol{f}_{15} \otimes \boldsymbol{b}_z \right] + \\
\frac{1}{|\Theta_Y|} \sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} \left[(\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_1}) \otimes (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_1}) + (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_2}) \otimes (\boldsymbol{F}^{c^{-1}} \boldsymbol{a}_{e_2}) \right]
\end{aligned} \tag{17}$$

From the previous material stress tensor, we will just take the terms in the diagonal, then we can consider this tensor as a diagonal one, such that its principal values are:

Finally, we have to rotate back the material stress state in principal directions $\boldsymbol{S}^c$ to non-principal directions $\check{\boldsymbol{S}}^c$.

$$\check{\boldsymbol{S}}^c = \sum_{a=1}^{3} S_a^c \, \hat{\boldsymbol{N}}_a \otimes \hat{\boldsymbol{N}}_a \tag{18}$$

At this point we note that tensor $\boldsymbol{S}^c$ is not exactly diagonal. In fact, it has non-zero components outside diagonal. This components are up to a couple of orders of magnitud smaller than terms in diagonal. However, this could be a controversial point because according to equation (18) we should use only principal (in-diagonal) stresses.

1.4 Stress tensor in principal coordinates

From the Cauchy stress tensor we have (no sum):

$$\sigma_a^c = \frac{2}{|\Theta_y|} \left(\boldsymbol{f}_{7_a} \lambda_a^c \boldsymbol{b}_{x_a} + \boldsymbol{f}_{10_a} \lambda_a^c \boldsymbol{b}_{y_a} + \boldsymbol{f}_{15_a} \lambda_a^c \boldsymbol{b}_{z_a} \right) + \frac{1}{|\Theta_y|} \sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} \left(\boldsymbol{a}_{e_{1_a}} \boldsymbol{a}_{e_{1_a}} + \boldsymbol{a}_{e_{2_a}} \boldsymbol{a}_{e_{2_a}} \right) \tag{19}$$

And, for the material stress tensor:

$$S_a^c = J^c \lambda_a^{c^{-2}} \sigma_a \tag{20}$$

$$S_a^c = \frac{2}{|\Theta_Y|}\lambda_a^{c^{-1}}\left(f_{7_a} b_{x_a} + f_{10_a} b_{y_a} + f_{15_a} b_{z_a}\right) + \frac{1}{|\Theta_Y|}\sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} \lambda_a^{c^{-2}} \left(a_{e_{1_a}} a_{e_{1_a}} + a_{e_{2_a}} a_{e_{2_a}}\right) \tag{21}$$

1.5 Tangent (Stress-stretch) calculation

According to Holzapfel 6.180, le elasticity tensor in terms of principal stretches (in material configuration) reads:

$$\mathbb{C} = \sum_{a,b=1}^{3} \frac{1}{\lambda_b^c}\frac{\partial S_a^c}{\partial \lambda_b^c} \hat{\boldsymbol{N}}_a \otimes \hat{\boldsymbol{N}}_a \otimes \hat{\boldsymbol{N}}_b \otimes \hat{\boldsymbol{N}}_b + \sum_{\substack{a,b=1\\ a\neq b}}^{3} \frac{S_b^c - S_a^c}{\lambda_b^{c^2} - \lambda_a^{c^2}} \left(\hat{\boldsymbol{N}}_a \otimes \hat{\boldsymbol{N}}_b \otimes \hat{\boldsymbol{N}}_a \otimes \hat{\boldsymbol{N}}_b + \hat{\boldsymbol{N}}_a \otimes \hat{\boldsymbol{N}}_b \otimes \hat{\boldsymbol{N}}_b \otimes \hat{\boldsymbol{N}}_a\right) \tag{22}$$

At this point we only have to compute $\frac{\partial S_a^c}{\partial \lambda_b^c}$. Then,

$$\frac{\partial S_a^c}{\partial \lambda_b^c} = \left(\frac{\partial S_a^c}{\partial \boldsymbol{r}^*} : \frac{\partial \boldsymbol{r}^*}{\partial \lambda_b^c} + \frac{\partial S_a^c}{\partial \lambda_b^c}_{\mathrm{EQ}}\right) + \frac{\partial S_a^c}{\partial \lambda_b^c}_{\mathrm{AVG}} \tag{23}$$

1.5.1 First term

For the first term, $\frac{\partial S_a^c}{\partial \boldsymbol{r}^*}$, we have:

$$\begin{aligned}\frac{\partial S_a^c}{\partial \boldsymbol{r}^*} = \frac{2}{|\Theta_Y|}\lambda_a^{c^{-1}}\left[\frac{\partial f_{7_a}}{\partial \boldsymbol{r}^*} b_{x_a} + \frac{\partial f_{10_a}}{\partial \boldsymbol{r}^*} b_{y_a} + \frac{\partial f_{15_a}}{\partial \boldsymbol{r}^*} b_{z_a}\right] + \frac{1}{|\Theta_Y|}\sum_{e=1}^{18} \frac{p_{alv}^c}{2\sqrt{\lambda_e}}\frac{\partial \lambda_e}{\partial \boldsymbol{r}^*} A_o L_{eo_{eff}} \lambda_a^{c^{-2}} \left(a_{e_{1_a}}^2 + a_{e_{2_a}}^2\right) +\\ \frac{1}{|\Theta_Y|}\sum_{e=1}^{18} \sigma_e^T A_o L_{eo_{eff}} \lambda_a^{c^{-2}} \left(2a_{e_{1_a}}\frac{\partial a_{e_{1_a}}}{\partial \boldsymbol{r}^*} + 2a_{e_{2_a}}\frac{\partial a_{e_{2_a}}}{\partial \boldsymbol{r}^*}\right)\end{aligned} \tag{24}$$

So, we have to compute: $\frac{\partial f_{7_a}}{\partial \boldsymbol{r}^*}, \frac{\partial f_{10_a}}{\partial \boldsymbol{r}^*}, \frac{\partial f_{15_a}}{\partial \boldsymbol{r}^*}, \frac{\partial a_{e_{1_a}}}{\partial \boldsymbol{r}^*}, \frac{\partial a_{e_{2_a}}}{\partial \boldsymbol{r}^*}$.

1.5.2 Second term

For the second term, we know that in the TKD problem, we solved

$$\min_{\boldsymbol{r}} \Pi^{eff}(\boldsymbol{r}; \boldsymbol{F}^c, p_{alv}^c) \iff \frac{\partial \Pi^{eff}}{\partial \boldsymbol{r}}(\boldsymbol{r}^*; \boldsymbol{F}^c, p_{alv}^c) = \boldsymbol{0} \tag{25}$$

Now, deriving equation (25), right, with respect to $\boldsymbol{F}^c$, it is obtained that

$$\frac{\partial^2 \Pi^{eff}(\boldsymbol{r}; \boldsymbol{F}^c, p_{alv}^c)}{\partial \boldsymbol{r}\partial \boldsymbol{r}} : \frac{\partial \boldsymbol{r}^*}{\partial \boldsymbol{F}^c} + \frac{\partial^2 \Pi^{eff}(\boldsymbol{r}; \boldsymbol{F}^c, p_{alv}^c)}{\partial \boldsymbol{F}^c \partial \boldsymbol{r}} = \boldsymbol{0} \tag{26}$$

Using the approach of principal values, indicial notation is used an $\boldsymbol{F}^c$ changes to λ_b^c. Then,

$$\frac{\partial^2\Pi^{eff}(\boldsymbol{r};\lambda_b^c,p_{alv}^c)}{\partial\boldsymbol{r}\partial\boldsymbol{r}}\frac{\partial\boldsymbol{r}^*}{\partial\lambda_b^c}+\frac{\partial^2\Pi^{eff}(\boldsymbol{r};\lambda_b^c,p_{alv}^c)}{\partial\lambda_b^c\partial\boldsymbol{r}} \quad = \quad \boldsymbol{0} \tag{27}$$

Hence, solving for $\frac{\partial\boldsymbol{r}^*}{\partial\lambda_b^c}$,

$$\frac{\partial\boldsymbol{r}^*}{\partial\lambda_b^c} \quad = \quad -\left(\frac{\partial^2\Pi^{eff}(\boldsymbol{r};\lambda_b^c,p_{alv}^c)}{\partial\boldsymbol{r}\partial\boldsymbol{r}}\right)^{-1}\frac{\partial^2\Pi^{eff}(\boldsymbol{r};\boldsymbol{F}^c,p_{alv}^c)}{\partial\lambda_b^c\partial\boldsymbol{r}} \tag{28}$$

1.5.3 Third term

$$\frac{\partial S_a^c}{\partial\lambda_b}_{\text{EQ}}=\frac{2}{|\Theta_Y|}\lambda_a^{c^{-1}}\left[\frac{\partial f_{7_a}}{\partial\lambda_b}b_{x_a}+\frac{\partial f_{10_a}}{\partial\lambda_b}b_{y_a}+\frac{\partial f_{15_a}}{\partial\lambda_b}b_{z_a}\right] \tag{29}$$

1.5.4 Fourth term

$$\frac{\partial S_a^c}{\partial\lambda_b^c}_{\text{AVG}}=\frac{-2}{|\Theta_Y|}\frac{\delta_{ab}}{\lambda_a^{c^2}}\left(f_{7_a}b_{x_a}+f_{10_a}b_{y_a}+f_{15_a}b_{z_a}\right)-\frac{2}{|\Theta_Y|}\sum_{e=1}^{18}\sigma_e^T A_o L_{eo_{eff}}\frac{\delta_{ab}}{\lambda_a^{c^3}}\left(a_{e_{1_a}}^2+a_{e_{2_a}}^2\right) \tag{30}$$

1.6 Voigt notation

1.6.1 Material stress tensor $\check{\boldsymbol{S}}^c$

$$\check{\boldsymbol{S}}^c=\left[\begin{array}{cccccc}\check{S}_{11}^c & \check{S}_{22}^c & \check{S}_{33}^c & \check{S}_{12}^c & \check{S}_{23}^c & \check{S}_{31}^c\end{array}\right]^T \tag{31}$$

1.6.2 Material elasticity tensor $\mathbb{C}^c$

$$\mathbb{C}^c=\left[\begin{array}{cccccc}
\mathbb{C}_{1111}^c & \mathbb{C}_{1122}^c & \mathbb{C}_{1133}^c & \mathbb{C}_{1112}^c & \mathbb{C}_{1123}^c & \mathbb{C}_{1131}^c\\
\mathbb{C}_{2211}^c & \mathbb{C}_{2222}^c & \mathbb{C}_{2233}^c & \mathbb{C}_{2212}^c & \mathbb{C}_{2223}^c & \mathbb{C}_{2231}^c\\
\mathbb{C}_{3311}^c & \mathbb{C}_{3322}^c & \mathbb{C}_{3333}^c & \mathbb{C}_{3312}^c & \mathbb{C}_{3323}^c & \mathbb{C}_{3331}^c\\
\mathbb{C}_{1211}^c & \mathbb{C}_{1222}^c & \mathbb{C}_{1233}^c & \mathbb{C}_{1212}^c & \mathbb{C}_{1223}^c & \mathbb{C}_{1231}^c\\
\mathbb{C}_{2311}^c & \mathbb{C}_{2322}^c & \mathbb{C}_{2333}^c & \mathbb{C}_{2312}^c & \mathbb{C}_{2323}^c & \mathbb{C}_{2331}^c\\
\mathbb{C}_{3111}^c & \mathbb{C}_{3122}^c & \mathbb{C}_{3133}^c & \mathbb{C}_{3112}^c & \mathbb{C}_{3123}^c & \mathbb{C}_{3131}^c
\end{array}\right] \tag{32}$$

2 TKD resultant tensors: Using Hill's lema

2.1 Principal directions

First step consist on, for a non-diagonal deformation state, look for the principal directions. Let $\check{\boldsymbol{F}}^c$ to be a non-diagonal coarse deformation state. Then the deformation gradient in principal coordinates is obtained as,

$$\begin{aligned}
\check{\boldsymbol{C}}^c &= \check{\boldsymbol{F}}^{c^T}\check{\boldsymbol{F}}^c \\
\check{\boldsymbol{b}}^c &= \check{\boldsymbol{F}}^c\check{\boldsymbol{F}}^{c^T} \\
\det\left(\check{\boldsymbol{C}}^c - \lambda_i^{c^2}\boldsymbol{I}\right) &= 0 \quad \forall i \in \{1,2,3\} \\
\det\left(\check{\boldsymbol{b}}^c - \lambda_i^{c^2}\boldsymbol{I}\right) &= 0 \quad \forall i \in \{1,2,3\} \\
\check{\boldsymbol{C}}^c\lambda_i^{c^2} &= \lambda_i^{c^2}\hat{\boldsymbol{N}}_i^c \quad \forall i \in \{1,2,3\} \\
\check{\boldsymbol{b}}^c\lambda_i^{c^2} &= \lambda_i^{c^2}\hat{\boldsymbol{n}}_i^c \quad \forall i \in \{1,2,3\} \\
\boldsymbol{U}^c &= \begin{bmatrix} \lambda_1^c & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}
\end{aligned}$$

2.2 First Piola-Kirchhoff stress tensor

We know that

$$\Pi^{eff} = \Pi^{eff}(\boldsymbol{r}(\boldsymbol{U}^c, p^c); \boldsymbol{U}^c, p^c) \tag{33}$$

Then, using Hill's lema for large deformations

$$\boldsymbol{P}^c = \frac{\partial \Pi^{eff}}{\partial \boldsymbol{r}} : \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{U}^c} + \frac{\partial \Pi^{eff}}{\partial \boldsymbol{U}^c} \tag{34}$$

or using indicial notation

$$P_{ij}^c = \frac{\partial \Pi^{eff}}{\partial r_p}\frac{\partial r_p}{\partial U_{ij}^c} + \frac{\partial \Pi^{eff}}{\partial U_{ij}^c} \tag{35}$$

where the first term corresponds to the TKD problem's residual

$$\boldsymbol{R} = \frac{\partial \Pi^{eff}}{\partial \boldsymbol{r}} \Rightarrow R_p = \frac{\partial \Pi^{eff}}{\partial r_p} \tag{36}$$

For the second term in equation (34) (i.e., $\partial r_p/\partial U_{ij}^c$), we note that the TKD problem is solved when $\boldsymbol{R} = \boldsymbol{0}$, so

$$\frac{\partial \Pi^{eff}}{\partial \boldsymbol{r}}(\boldsymbol{r}^*; \boldsymbol{U}^c, p_{alv}^c) = \boldsymbol{0} \tag{37}$$

Now, deriving last equation with respect to $\boldsymbol{U}^c$,

$$\frac{\partial^2 \Pi^{eff}}{\partial \boldsymbol{r}\partial \boldsymbol{r}} : \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{U}^c} + \frac{\partial^2 \Pi^{eff}}{\partial \boldsymbol{U}^c \partial \boldsymbol{r}} = \boldsymbol{0} \tag{38}$$

Which, in indicial notation leads to

$$\frac{\partial^2 \Pi^{eff}}{\partial r_p \partial r_m} \frac{\partial r_p}{\partial U_{ij}^c} + \frac{\partial^2 \Pi^{eff}}{\partial U_{ij}^c \partial r_m} = \mathbf{0} \tag{39}$$

Now, solving for $\partial \boldsymbol{r} / \partial \boldsymbol{U}^c$,

$$\frac{\partial r_p}{\partial U_{ij}^c} = -\left(\frac{\partial^2 \Pi^{eff}}{\partial r_p \partial r_m} \right)^{-1} \frac{\partial^2 \Pi^{eff}}{\partial U_{ij}^c \partial r_m} \tag{40}$$

Here we see that the TKD problem uses a jacobian which is defined by:

$$\boldsymbol{K} = \frac{\partial^2 W}{\partial \boldsymbol{r} \partial \boldsymbol{r}} \quad \Rightarrow \quad K_{mp} = \frac{\partial^2 W}{\partial r_p \partial r_m} \tag{41}$$

Additionally, we will call:

$$\mathbb{G} = \frac{\partial^2 \Pi^{eff}}{\partial \boldsymbol{U}^c \partial \boldsymbol{r}} \quad \Rightarrow \quad G_{mij} = \frac{\partial^2 \Pi^{eff}}{\partial U_{ij}^c \partial r_m} \tag{42}$$

Then

$$\frac{\partial r_p}{\partial U_{ij}^c} = -K_{mp}^{-1} G_{mij} \tag{43}$$

which in vectorial notation:

$$\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{U}^c} = -\boldsymbol{K}^{-T} : \mathbb{G} \quad \Rightarrow \quad \frac{\partial r_p}{\partial U_{ij}^c} = -K_{pm}^{-T} G_{mij} \tag{44}$$

Finally, the term $\partial \Pi^{eff} / \partial \boldsymbol{U}^c$ in equation (34) is obtained just by direct differentiation.

2.3 Elasticity tensor

The elasticity tensor is obtained according to

$$\mathcal{C}_{ijkl}^c = \frac{\partial \boldsymbol{P}^c}{\partial \boldsymbol{F}^c} \tag{45}$$

where we note

$$\frac{\partial \boldsymbol{P}^c}{\partial \boldsymbol{U}^c} = \frac{1}{V_o} \frac{\partial}{\partial \boldsymbol{U}^c} \left[\frac{\partial \Pi^{eff}}{\partial \boldsymbol{r}} : \frac{\partial \boldsymbol{r}}{\partial \boldsymbol{U}^c} + \frac{\partial \Pi^{eff}}{\partial \boldsymbol{U}^c} \right] \tag{46}$$

Using indicial notation, it becomes

$$\frac{\partial \boldsymbol{P}^c}{\partial \boldsymbol{U}^c} = \frac{1}{V_o} \frac{\partial}{\partial U_{kl}^c} \left[\frac{\partial \Pi^{eff}}{\partial r_p} \frac{\partial r_p}{\partial U_{ij}^c} + \frac{\partial \Pi^{eff}}{\partial U_{ij}^c} \right] \tag{47}$$

which can be rewritten as

$$V_o \frac{\partial \boldsymbol{P}^c}{\partial \boldsymbol{U}^c} = \left(\frac{\partial^2 \Pi^{eff}}{\partial r_q \partial r_p} \frac{\partial r_q}{\partial U_{kl}^c} + \frac{\partial^2 \Pi^{eff}}{\partial U_{kl}^c \partial r_p} \right) \frac{\partial r_p}{\partial U_{ij}^c} \quad + \quad \frac{\partial \Pi^{eff}}{\partial r_p} \frac{\partial^2 r_p}{\partial U_{kl}^c \partial U_{ij}^c} \quad + \quad \left(\frac{\partial^2 \Pi^{eff}}{\partial r_p \partial U_{ij}^c} \frac{\partial r_p}{\partial U_{kl}^c} + \frac{\partial^2 \Pi^{eff}}{\partial U_{kl}^c \partial U_{ij}^c} \right) \tag{48}$$

but using the terms we defined before, we see that the first term in brackets is zero

$$
\begin{aligned}
\frac{\partial^2 W^c}{\partial r_q \partial r_p}\frac{\partial r_q}{\partial U^c_{kl}} + \frac{\partial^2 W^c}{\partial U^c_{kl}\partial r_p} &= -K_{qp}K^{-1}_{qm}G_{klm} + G_{klp} &(49)\\
&= -K_{pq}K^{-1}_{qm}G_{klm} + G_{klp} &(50)\\
&= -\delta_{pm}G_{klm} + G_{klp} &(51)\\
&= -G_{klp} + G_{klp} &(52)\\
&= 0 &(53)
\end{aligned}
$$

while the second term in (46) is zero because it contains the residual expression evaluated at the solution of the degrees of freedom ($\partial\Pi^{eff}/\partial r_p = 0$). So, finally we have

$$
\mathcal{C}^c_{ijkl} = \frac{\partial \boldsymbol{P}^c}{\partial \boldsymbol{F}^c} = \frac{1}{V_o}\left(\frac{\partial^2\Pi^{eff}}{\partial r_p \partial U^c_{ij}}\frac{\partial r_p}{\partial U^c_{kl}} + \frac{\partial^2 \Pi^{eff}}{\partial U^c_{kl}\partial U^c_{ij}}\right) \tag{54}
$$