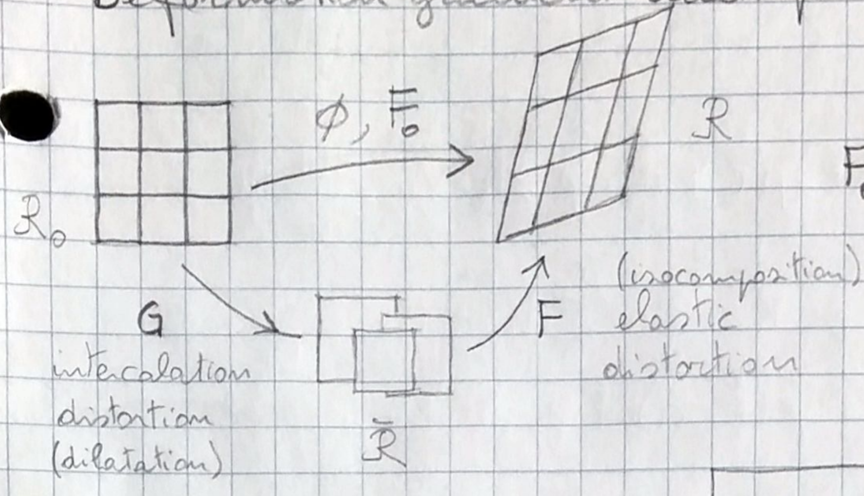
Deformation gradient decomposition



$F_0 \equiv \nabla \phi$

$\beta = \det G \qquad G = \beta^{1/3} I \qquad \boxed{F_0 = F\, G}$

$\det F_0 = \beta (\det F)$

stoichiometric constant

$\det G = (\rho_0 V_0 + \rho_{Li} V_{Li})/(\rho_0 V_0) = 1 + c \dfrac{V_{Li}}{V_0} = 1 + c\, \alpha$

$\dot\beta = \alpha \dot c \qquad \dfrac{d}{dt}(\det G) = (\det G)\, \mathrm{tr}(\dot G G^{-1}) = \dots = \alpha \dot c$

$\dot G G^{-1} = \dfrac{1}{3} \beta^{-\frac{2}{3}} \beta^{-\frac{1}{3}} \alpha \dot c\, I = \dfrac{1}{3} \dfrac{\alpha}{\beta} \dot c\, I$

$\dot F_0 F_0^{-1} = (\dot F G + F \dot G) G^{-1} F^{-1} = \dot F F^{-1} + \dfrac{1}{3} \dfrac{\alpha}{\beta} \dot c\, I$

$S_0 = T F_0^{-T} (\det F_0) \qquad S = T F^{-T} (\det F)$

$S_0 \cdot \dot F_0 = (\det F_0)\, T F_0^{-T} \cdot \dot F_0 = \beta (\det F)\, T \cdot \dot F_0 F_0^{-1}$

$= \beta (\det F)\, T \cdot \dot F F^{-1} + \dfrac{1}{3} \alpha (\det F)\, T \cdot I\, \dot c = \beta S \cdot \dot F - \alpha (\det F)\, p\, \dot c$

with $-p = \dfrac{1}{3} T \cdot I = \dfrac{1}{3} \mathrm{tr}\, T$

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Hence the energy imbalance takes the form

$$\beta S\cdot\dot{F} - \alpha(\det F)\,p\,\dot{c} + \mu_o \dot{c}\,\rho_o - h_o\cdot\nabla\mu_o - \frac{d}{dt}\psi \geq 0$$

If we choose for the free energy the expression

$$\hat{\psi}(F_o, c) = \beta\,\varphi(F)$$

while assuming

$$\frac{d}{dt}\varphi(F) = \hat{S}(F)\cdot\dot{F}$$

then

$$\frac{d}{dt}\psi = \dot{\beta}\,\varphi(F) + \beta\,\hat{S}(F)\cdot\dot{F} = \alpha\dot{c}\,\varphi(F) + \beta\,\hat{S}(F)\cdot\dot{F}$$

We finally get

$$\beta(S-\hat{S}(F))\cdot\dot{F} - \alpha\dot{c}\,\varphi(F) - (\det F)\,p\,\alpha\dot{c} + \mu_o\dot{c}\,\rho_o - h_o\cdot\nabla\mu_o \geq 0$$

which, rearranging terms, becomes

$$\beta\underbrace{(S-\hat{S}(F))}_{S^+} + \underbrace{\left(\frac{\rho_o}{\alpha}\mu_o - (\det F)\,p - \varphi(F)\right)}_{\mu^+}\alpha\dot{c} - h_o\cdot\nabla\mu_o \geq 0$$

$$\Rightarrow \begin{cases} S = \hat{S}(F) + S^+ & S^+\cdot\dot{F} \geq 0 \\ \mu_o = \dfrac{\alpha}{\rho_o}\left((\det F)\,p + \varphi(F)\right) + \mu^+ & \mu^+\cdot\dot{c} \geq 0 \\ -h_o\cdot\nabla\mu_o \geq 0 & \end{cases}$$

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Let us extend the free energy expression introducing an energy term depending just on the concentration

$$\hat{\psi}(F_o, c) = \varphi_{ch}(c) + \beta\, \varphi_e(F)$$

and setting
$$\frac{d}{dt}\varphi_{ch}(c) = \rho_o \hat{\mu}_{ch}(c)\, \dot{c}$$

We get

$$\frac{d}{dt}\hat{\psi}(F_o, c) = \rho_o \hat{\mu}_{ch}(c)\, \dot{c} + \dot{\beta}\, \varphi_e(F) + \beta\, \hat{S}(F) \cdot \dot{F}$$

$$= \left(\rho_o \hat{\mu}_{ch}(c) + \alpha\, \varphi_e(F)\right)\dot{c} + \beta\, \hat{S}(F) \cdot \dot{F}$$

From the energy imbalance expression we arrive at

$$\mu_o = \hat{\mu}_{ch}(c) + \frac{\alpha}{\rho_o}\left((\det F)\, p + \varphi_e(F)\right) + \mu^+$$

with
$$p = -\frac{1}{3}\,\mathrm{tr}\, T$$

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Summarizing

$$S = \hat{S}_e(F) + S^+ \qquad S^+ = (\det F)\, T^+ F^{-T}$$

$$T = \hat{T}_e(F) + T^+ \qquad T^+ = 2\mu \,\mathrm{sym}(\dot{F} F^{-1})$$

For an almost incompressible neo-Hookean material

$$\hat{T}_e(F) = \underbrace{2k_I\, J^{-\frac{5}{3}}\left(B - \frac{1}{3}\iota_1 I\right)}_{\text{deviatoric}} + \underbrace{2k_v (J-1)}_{\text{spherical}}$$

$$\hat{S}_e(F) = 2k_I\, J^{-\frac{2}{3}}\left(F - \frac{1}{3}\iota_1 F^{-T}\right) + 2k_v (J-1) J F^{-T}$$

[2018-06-06]

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