Finite deformation linear viscoelasticity.

Main references: J. Simo, CMAME vol 60 : 153 - 173, 1987

G. Holzapfel & J. Simo, IJSS vol 33 : 3019-3034, 1996

J. Liu, et al. CMAME vol 385 : 114059, 2021.

$$\psi = \psi^{\infty}_{ich}(\bar{C}) + \psi^{\infty}_{vol}(J) + \sum_{\alpha=1}^{m} \Upsilon_\alpha(\bar{C}, \Gamma_\alpha)$$

non-equilibrium or configurational free energy

Clausius - Plank:

$$\frac{1}{2} S : \dot{C} - \dot{\psi} \geq 0$$

$$\parallel$$

$$\left(\frac{1}{2} S - \frac{\partial \psi^{\infty}_{ich}}{\partial \bar{C}} \frac{\partial \bar{C}}{\partial C} - \frac{\partial \psi^{\infty}_{vol}}{\partial J} \frac{\partial J}{\partial C} - \sum_{\alpha=1}^{m} \frac{\partial \Upsilon_\alpha}{\partial \bar{C}} \frac{\partial \bar{C}}{\partial C} \right) : \dot{C} - \sum_{\alpha=1}^{m} \frac{\partial \Upsilon_\alpha}{\partial \Gamma_\alpha} : \dot{\Gamma}_\alpha$$

$$S = S^{\infty}_{ich} + S^{\infty}_{vol} + \sum_{\alpha=1}^{m} S^{\alpha}_{neq}$$

$$S^{\infty}_{ich} = J^{-2/3} \mathbb{P} : \tilde{S}^{\infty}_{ich} \qquad S^{\infty}_{vol} = -J P C^{-1} \qquad S^{\alpha}_{neq} = J^{-\frac{2}{3}} \mathbb{P} : \tilde{S}^{\alpha}_{neq}$$

$$\tilde{S}^{\infty}_{ich} = 2 \frac{\partial \psi^{\infty}_{ich}}{\partial \bar{C}} \qquad P = - \frac{\partial \psi^{\infty}_{vol}}{\partial J} \qquad \tilde{S}^{\alpha}_{neq} = 2 \frac{\partial \Upsilon^{\alpha}}{\partial \bar{C}}.$$

$$\Rightarrow \quad -\sum_{\alpha=1}^{m} \frac{\partial \Upsilon_\alpha}{\partial \Gamma_\alpha} : \dot{\Gamma}_\alpha \geq 0$$

Define $Q_\alpha := -2\frac{\partial \psi}{\partial \Gamma_\alpha} = -2\frac{\partial \Upsilon_\alpha}{\partial \Gamma_\alpha}$ as the conjugate variable of Γ_α w.r.t. ψ.

$$\Rightarrow \quad \sum_{\alpha=1}^{m} Q_\alpha : \frac{1}{2}\dot{\Gamma}_\alpha \geq 0$$

constitutive model : $Q_\alpha = \mathbb{V}^\alpha : \left(\frac{1}{2}\dot{\Gamma}_\alpha\right)$

rank-4 tensor, positive semi-definite.

viscosity tensor.

Then the dissipation is $\sum_{\alpha=1}^{m} \frac{1}{2}\dot{\Gamma}_\alpha : \mathbb{V}^\alpha : \frac{1}{2}\dot{\Gamma}_\alpha \geq 0$

Now we give an explicit definition of Υ_α following Holzapfel-Simo :

$$\Upsilon^\alpha = \mu^\alpha \left| \frac{\Gamma^\alpha - I}{2} \right|^2 + \left(\hat{S}_0^\alpha - 2\frac{\partial G^\alpha}{\partial \tilde{C}} \right) : \frac{\Gamma^\alpha - I}{2} + F^\alpha(\tilde{C}).$$

$\hat{S}_0^\alpha := 2\frac{\partial G^\alpha}{\partial \tilde{C}}\Big|_{t=0} - Q^\alpha\Big|_{t=0}$

Issue : In the thermodynamic limit,

$$\dot{\Gamma}^\alpha\Big|_{eq} = 0 \quad \text{for } \alpha = 1, \cdots, m$$

or equivalently $Q^\alpha \big|_{eq} = 0$

The above Υ_α cannot guarantee $S^\alpha_{neq}\big|_{eq} = 0$ in general.

Several models take $\tilde{S}^\alpha_{neq} = Q^\alpha$ e.g. Simo & Hughes 2006.
which suffers from thermodynamic inconsistency.

The requirement for fully relaxed S_{neq} is discussed in Liu 2021,
and we consider a special case :

$$G^\alpha = F^\alpha = \mu^\alpha \left| \frac{\tilde{C} - I}{2} \right|^2 .$$

$$\Rightarrow \Upsilon^\alpha = \frac{1}{4\mu^\alpha} \left| \mu^\alpha (\tilde{C} - \Gamma^\alpha) - \hat{S}^\alpha_0 \right|^2 .$$

$$Q^\alpha := -2 \frac{\partial \Upsilon^\alpha}{\partial \Gamma^\alpha} = \mu^\alpha (\tilde{C} - \Gamma^\alpha) + Q^\alpha_0$$

$$= \underbrace{\tilde{S}^\alpha_{iso}}_{= 2\frac{\partial G^\alpha}{\partial \tilde{C}} = \mu^\alpha (\tilde{C} - I)} - \hat{S}^\alpha_0 - \mu^\alpha (\Gamma^\alpha - I)$$

$$Q^\alpha_0 = \tilde{S}^\alpha_{iso}\big|_{t=0} = \hat{S}^\alpha_0$$

$$\tilde{S}^\alpha_{neq} = Q^\alpha .$$

To further simplify the theory, we take $\mathbb{V}^\alpha = 2\eta^\alpha \mathbb{I}$.

Then we have $\quad Q^\alpha = \mathbb{V}^\alpha : \frac{1}{2}\dot{\Gamma}^\alpha$

$$= \eta^\alpha \dot{\Gamma}^\alpha$$

$$\stackrel{\text{def.}}{=} \mu^\alpha(\overset{\smile}{C} - \Gamma^\alpha) + Q_0^\alpha$$

$\tau^\alpha := \eta^\alpha / \mu^\alpha \quad$ relaxation time of the α-th process

We have. $\quad \eta^\alpha \frac{d}{dt}\left(\frac{\Gamma^\alpha - I}{2}\right) + \mu^\alpha\left(\frac{\Gamma^\alpha - I}{2}\right) = \frac{1}{2}(\overset{\smile}{S}{}^\alpha_{iso} - \hat{S}_0^\alpha)$

or simply

$$\underbrace{\eta^\alpha \frac{d}{dt}\Gamma^\alpha}_{\parallel\; Q^\alpha} + \mu^\alpha \Gamma^\alpha = \mu^\alpha \overset{\smile}{C} + Q_0^\alpha$$

$$\Rightarrow \quad \dot{Q}^\alpha + \underbrace{\mu^\alpha \dot{\Gamma}^\alpha}_{Q^\alpha/\tau^\alpha} = \frac{d}{dt}(\mu^\alpha \overset{\smile}{C})$$

The most frequently used eqn.

$$\dot{Q}^\alpha + \frac{Q^\alpha}{\tau^\alpha} = \frac{d}{dt}(\mu^\alpha \overset{\smile}{C})$$

Remark: Many authors put wrong terms on the RHS.

The evolution eqns are <u>derived</u> rather than proposed heuristically.

Remark: For thermo-viscoelastic models, there will be $\frac{d}{dt}\mu^\alpha$ appearing on the RHS.

also JMPS 1991

Remark: The identical polymer chain model (Govindjee and Simo, IJSS 1992) can be incorported.

$$\Upsilon^\alpha = \mu^\alpha \left| \frac{\Gamma^\alpha - I}{2} \right|^2 + \left(\hat{S}_0^\alpha - 2\frac{\partial G^\alpha}{\partial \tilde{C}} \right) : \frac{\Gamma^\alpha - I}{2} + \frac{1}{4\mu^\alpha} \left| 2\frac{\partial G^\alpha}{\partial \tilde{C}} - \hat{S}_0^\alpha \right|^2$$

$$= \frac{1}{4\mu^\alpha} \left| \tilde{S}_{iso}^\alpha - \hat{S}_0^\alpha - \mu^\alpha (\Gamma^\alpha - I) \right|^2$$

$$= \frac{1}{4\mu^\alpha} \left| Q^\alpha \right|^2$$

$$\tilde{S}_{iso}^\alpha := 2\frac{\partial G^\alpha}{\partial \tilde{C}} = \beta_\alpha^\infty \, 2\frac{\partial G_{iso}^\infty}{\partial \tilde{C}} = \beta_\alpha^\infty \tilde{S}_{iso}^\infty$$

and $G^\alpha = \beta_\alpha^\infty G_{iso}^\infty(\tilde{C})$

The evolution equation is

$$Q^\alpha = \eta^\alpha \dot{\Gamma}^\alpha = -2\frac{\partial \Upsilon^\alpha}{\partial \Gamma^\alpha}$$

$$= \tilde{S}_{iso}^\alpha - \hat{S}_0^\alpha - \mu^\alpha (\Gamma^\alpha - I)$$

Re-organize: $$\eta^\alpha \frac{d}{dt}\left(\frac{\Gamma^\alpha - I}{2} \right) + \mu^\alpha \left(\frac{\Gamma^\alpha - I}{2} \right) = \frac{1}{2}\left(\tilde{S}_{iso}^\alpha - \hat{S}_0^\alpha \right)$$

Take time derivative: $$\frac{d}{dt} Q^\alpha = \frac{d}{dt}\tilde{S}_{iso}^\alpha - \mu^\alpha \frac{d}{dt}\Gamma^\alpha$$

$$\Rightarrow \frac{d}{dt} Q^\alpha + \frac{\mu^\alpha}{\eta^\alpha} Q^\alpha = \frac{d}{dt}\tilde{S}_{iso}^\alpha .$$

$$\begin{cases} \dfrac{d}{dt} Q^{\alpha} + \dfrac{1}{\tau^{\alpha}} Q^{\alpha} = \dfrac{d}{dt} \tilde{S}_{iso}^{\alpha} \\ Q^{\alpha}\Big|_{t=0} = Q_0^{\alpha} \end{cases}$$

$$Q^{\alpha} = \exp\left(-\frac{t}{\tau^{\alpha}}\right) Q_0^{\alpha} + \int_{0^+}^{t} \exp\left(-\frac{t-s}{\tau^{\alpha}}\right) \frac{d}{ds} \tilde{S}_{iso}^{\alpha}(s)\, ds.$$

$\rightarrow$ known as the Hereditary integral.

Numerical Design

Consider a time interval $(t_n \quad t_{n+1})$

U_n

$U_{n+1,(\ell)}$ given by a predictor or the previous iteration

$$S_{n+1} = S_{iso\, n+1} + S_{vol\, n+1}$$

$$S_{vol\, n+1} = -J_{n+1} P_{n+1} C_{n+1}^{-1}$$

$$S_{iso\, n+1} = J_{n+1}^{-2/3} \mathbb{P}_{n+1} : \tilde{S}_{n+1}$$

$$\tilde{S}_{n+1} = \tilde{S}_{iso\, n+1}^{\infty} + \sum_{\alpha=1}^{m} \tilde{S}_{neq\, n+1}^{\alpha}$$

$$\tilde{S}_{iso\, n+1}^{\infty} = 2 \frac{\partial G_{iso}^{\infty}}{\partial \tilde{C}}(\tilde{C}_{n+1})$$

$$\tilde{S}_{neq\, n+1}^{\alpha} = Q_{n+1}^{\alpha} \qquad \text{HS}$$

$$= \frac{J^{\frac{4}{3}} \beta_{\alpha}^{\infty}}{2\mu^{\alpha}} \bar{\mathbb{C}}_{iso\, n+1}^{\infty} : Q_{n+1}^{\alpha} \qquad \text{MIPC}$$

$$\bar{\mathbb{C}}_{iso\, n+1}^{\infty} := 4 J_{n+1}^{-\frac{4}{3}} \frac{\partial^2 G_{iso}^{\infty}}{\partial \tilde{C}\, \partial \tilde{C}}(\tilde{C}_{n+1})$$

$$Q^\alpha_{n+1} = \exp\left(-\frac{t_{n+1}}{\tau^\alpha}\right) Q^\alpha_0 + \int_{0^+}^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{\tau^\alpha}\right) \frac{d}{ds} \tilde{S}^\alpha_{iso}(s)\, ds$$

$$= \exp\left(-\frac{\Delta t_n}{\tau^\alpha}\right) \exp\left(-\frac{t_n}{\tau^\alpha}\right) Q^\alpha_0$$

$$+ \exp\left(-\frac{\Delta t_n}{\tau^\alpha}\right) \int_{0^+}^{t_n} \exp\left(-\frac{t_n - s}{\tau^\alpha}\right) \frac{d}{ds} \tilde{S}^\alpha_{iso}(s)\, ds$$

$$+ \int_{t_n}^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{\tau^\alpha}\right) \frac{d}{ds} \tilde{S}^\alpha_{iso}(s)\, ds$$

$\xi^\alpha := -\frac{\Delta t_n}{2\tau^\alpha}$

$$= \exp(2\xi^\alpha)\, Q^\alpha_n + \int_{t_n}^{t_{n+1}} \exp\left(-\frac{t_{n+1}-s}{\tau^\alpha}\right) \frac{d}{ds} \tilde{S}^\alpha_{iso}(s)\, ds$$

$$\approx \exp(2\xi^\alpha)\, Q^\alpha_n + \exp\left(-\frac{t_{n+1}-s}{\tau^\alpha}\right)\Big|_{s=\frac{t_{n+1}+t_n}{2}} \int_{t_n}^{t_{n+1}} \frac{d}{ds} \tilde{S}^\alpha_{iso}(s)\, ds$$

$$= \exp(2\xi^\alpha)\, Q^\alpha_n + \exp(\xi^\alpha) \left(\tilde{S}^\alpha_{iso\, n+1} - \tilde{S}^\alpha_n \right)$$

$\to \mu^\alpha (\tilde{C}_{n+1} - \tilde{C}_n)$ for $G^\alpha \hat{=} \mu^\alpha \left| \frac{\tilde{C} - I}{2} \right|^2$

$\beta^\infty_\alpha (\tilde{S}_{iso\, n+1} - \tilde{S}_{iso\, n})$ for $G^\alpha \hat{=} \beta^\infty_\alpha G^\infty_{iso}$

Alternatively.

$$\int_{t_n}^{t_{n+1}} \exp\left(\frac{t_{n+1}-s}{-\tau^\alpha}\right) \frac{d}{ds} \tilde{S}^\alpha_{iso}(s)\, ds \approx \frac{\tilde{S}^\alpha_{iso\, n+1} - \tilde{S}^\alpha_{iso\, n}}{\Delta t_n} \int_{t_n}^{t_{n+1}} \exp\left(\frac{t_{n+1}-s}{-\tau^\alpha}\right) ds$$

$$= \frac{\tilde{S}^{\alpha}_{iso\,n+1} - \tilde{S}^{\alpha}_{iso\,n}}{\Delta t_n} (+\tau^{\alpha}) \exp\left(\frac{t_{n+1}-s}{\tau^{\alpha}}\right)\Big|_{t_n}^{t_{n+1}}$$

$$= \frac{\tilde{S}^{\alpha}_{iso\,n+1} - \tilde{S}^{\alpha}_{iso\,n}}{\Delta t_n} \left(1 - \exp(2\xi^{\alpha})\right) \tau^{\alpha}$$

$$\Rightarrow \quad Q^{\alpha}_{n+1} \simeq \exp(2\xi^{\alpha})\, Q^{\alpha}_{n} - \frac{1-\exp(2\xi^{\alpha})}{2\xi^{\alpha}} \left(\tilde{S}^{\alpha}_{iso\,n+1} - \tilde{S}^{\alpha}_{iso\,n}\right).$$

Elasticity tensor:

Only consider the case of $G^{\alpha} = \mu^{\alpha} \left| \frac{\tilde{C}-I}{2} \right|^2$:

$$\tilde{S}^{\alpha}_{neq\,n+1} = Q^{\alpha}_{n+1}.$$

Recall the def. of $\mathbb{C}_{ich}$ on page 95.

$$\mathbb{C}_{ich} = \mathbb{P} : \bar{\mathbb{C}} : \mathbb{P}^T + \cdots\cdots$$

$$\bar{\mathbb{C}} := 4J^{-4/3} \frac{\partial \phi_{ich}}{\partial \tilde{C}\, \partial \bar{C}} \quad \leftarrow \quad \psi^{\infty}_{ich} + \sum_{\alpha=1}^{m} \Upsilon_{\alpha}$$

$$= \bar{\mathbb{C}}^{\infty} + \bar{\mathbb{C}}^{vis}$$

$$4J^{-4/3} \frac{\partial \Upsilon_{\alpha}}{\partial \bar{C}\, \partial \bar{C}}$$

$$\parallel$$

$$2J^{-4/3} \frac{\partial \tilde{S}^{\alpha}_{neq}}{\partial \bar{C}}$$

$$\frac{\partial \tilde{S}^{\alpha}_{neq}}{\partial \bar{C}_{n+1}} = \frac{\partial Q^{\alpha}_{n+1}}{\partial \bar{C}_{n+1}} = \exp(\xi^{\alpha})\, \mu^{\alpha} \mathbb{I}$$

depend on your integration formula for the constitutive equations.

then $$\bar{\mathbb{C}} = \bar{\mathbb{C}}^{\infty} + \sum_{\alpha=1}^{m} 2 J_{n+1}^{-4/3} \exp(\xi^{\alpha})\, \mu^{\alpha} \mathbb{I}.$$

Remark: For $G^{\alpha} = \beta^{\infty}_{\alpha} G^{\infty}_{iso}$, the $\tilde{S}^{\alpha}_{neq} = \cdots$ and the tensor $\bar{\mathbb{C}}^{vis}$ is more involved. Refer to Liu, et al. CMAME 385: 114059. 2021 for more details.

An outline of constitutive integration using $G^{\alpha} = \mu^{\alpha} \left| \frac{\tilde{C} - I}{2} \right|^2$.

Step 1: $F_{n+1} = I + \nabla_X U_{n+1}$; $J_{n+1} = \det(F_{n+1})$;

$C_{n+1} = F_{n+1}^{T} F_{n+1}$; $\tilde{C}_{n+1} = J_{n+1}^{-2/3} C_{n+1}$.

Step 2: $$\tilde{S}^{\infty}_{iso\, n+1} = 2 \frac{\partial G^{\infty}_{iso}}{\partial \bar{C}} (\bar{C}_{n+1})$$

Step 3: For $\alpha = 1, \cdots, m$, calculate

$$Q^{\alpha}_{n+1} = \exp(2\xi^{\alpha})\, Q^{\alpha}_{n} + \mu^{\alpha} \exp(\xi^{\alpha}) \left(\bar{C}^{\alpha}_{n+1} - \bar{C}^{\alpha}_{n} \right)$$

Step 4: $$\tilde{S}_{n+1} = \tilde{S}^{\infty}_{iso\, n+1} + \sum_{\alpha=1}^{m} Q^{\alpha}_{n+1}$$

Step 5: Calculate the projection tensor $\mathbb{P}_{n+1} = \mathbb{I} - \frac{1}{3} C_{n+1}^{-1} \otimes C_{n+1}$

Step 6: $$S_{iso\; n+1} = J_{n+1}^{-\frac{2}{3}} \mathbb{P}_{n+1} : \hat{S}_{n+1}$$

Step 7: $$\bar{\mathbb{C}}^{\infty} = 4 J_{n+1}^{-4/3} \left(\frac{\partial^2 G_{iso}^{\infty}}{\partial \bar{C} \partial \bar{C}} \right) (\bar{C}_{n+1})$$

$$\bar{\mathbb{C}}^{vis} = \left(\sum_{\alpha=1}^{m} 2\mu^{\alpha} \exp(\xi^{\alpha}) J_{n+1}^{-4/3} \right) \mathbb{I}$$

Step 8: $$\bar{\mathbb{C}} = \bar{\mathbb{C}}^{\infty} + \bar{\mathbb{C}}^{vis}$$

Step 9: $$\hat{\mathbb{P}}_{n+1} = C_{n+1}^{-1} \odot C_{n+1}^{-1} - \frac{1}{3} C_{n+1}^{-1} \otimes C_{n+1}^{-1}$$

Step 10: $$\mathbb{C}_{iso\; n+1} = \mathbb{P}_{n+1} : \bar{\mathbb{C}} : \mathbb{P}_{n+1}^{T} + \frac{2}{3} Tr\left(J_{n+1}^{-2/3} \hat{S}_{n+1} \right) \hat{\mathbb{P}}_{n+1} - \frac{2}{3} \left(C_{n+1}^{-1} \otimes S_{iso\; n+1} + S_{iso\; n+1} \otimes C_{n+1}^{-1} \right)$$

Step 11. $$S_{vol\; n+1} = - J_{n+1} P_{n+1} C_{n+1}^{-1} \qquad P_{n+1} = - \frac{\partial \psi_{vol}}{\partial J} (J_{n+1})$$

Step 12. $$\mathbb{C}_{vol\; n+1} = J_{n+1} \left(P_{n+1} + J_{n+1} \frac{dP}{dJ} (J_{n+1}) \right) C_{n+1}^{-1} \otimes C_{n+1}^{-1} - 2 J_{n+1} P_{n+1} C_{n+1}^{-1} \odot C_{n+1}^{-1} .$$