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Continuum thermodynamics of open / growing systems

Refs: Goriely ; Ericksen; Gurtin

(I) Conservation laws

(II) Model of the growth process (volumetric)

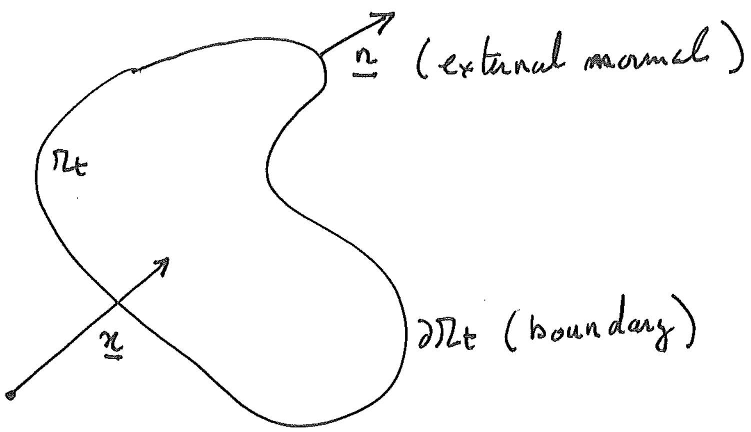
(III) Dissipation inequality

(IV) Examples

(I) Conservation laws

We consider the material domain Ω_t (where $t>0$ is the time)

The domain is open : it can exchange mass with a reservoir and this mass carries a certain amount of energy. This connection operates at any point $\underline{x}$ of the system



(1) Mass conservation

$$\partial_t \rho + \mathrm{div}_{\underline{x}} (\rho \underline{v}) = S(\underline{x},t)$$

$\rho(\underline{x},t)$ is the mass density
$v(\underline{x},t)$ — velocity field of material points
$S(\underline{x},t)$ — source term

We consider volumetric growth only such that the flux at the surface is zero:

$$\rho(\underline{v}-\underline{v}_f)\cdot\underline{n}\Big|_{x\in\partial\Omega_t} = 0 \quad ; \; v_f \text{ is the boundary velocity.}$$

(2) Momentum balance

$$\mathrm{div}_{\underline{x}} (\underline{\underline{\sigma}}) = \underline{0}$$

$$\underline{\underline{\sigma}}\,\underline{n} = \underline{f}_{ext}\Big|_{x\in\partial\Omega_t}$$

$\underline{\underline{\sigma}}(\underline{x},t)$ is the Cauchy stress
external applied tractions.

Balance of couples: $\underline{\underline{\sigma}}$ is symmetric for simplicity we not consider bulk forces and inertia (but we could)

$\underline{\underline{\sigma}}$ is considered to be symmetric and we do not consider the balance of torques

3 Energy balance

$T = \text{cte}$

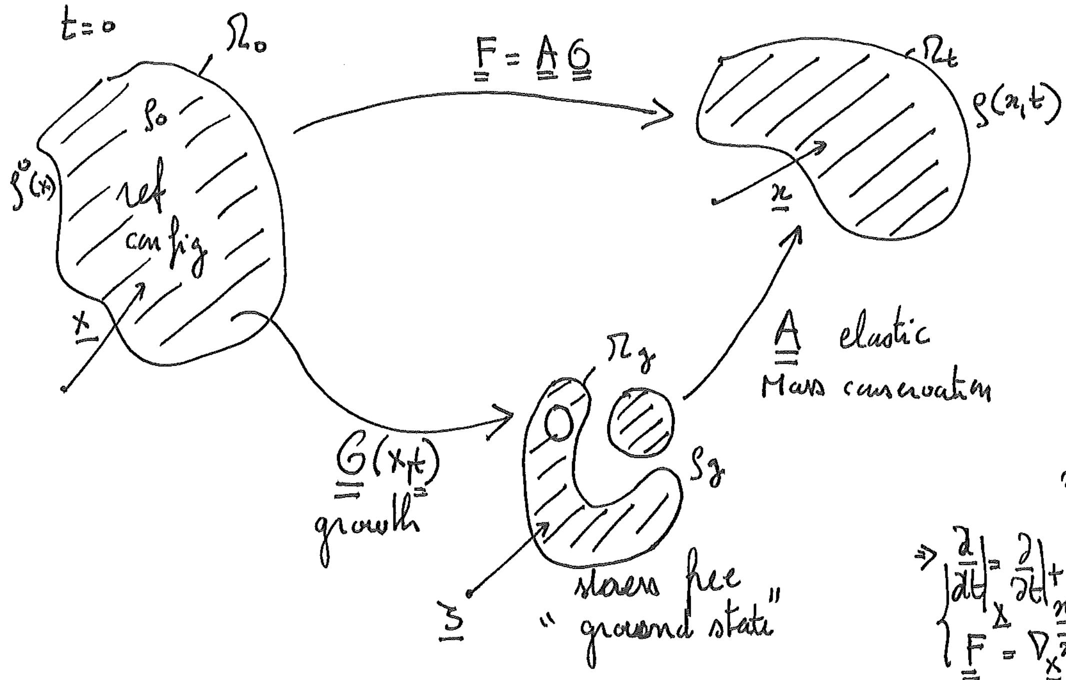
1st principle : $\underbrace{\frac{dU}{dt}}_{\text{internal energy}} = \overbrace{\frac{dQ}{dt}}^{\text{heat}} + \underbrace{\frac{dW}{dt}}_{\text{work}} + \overbrace{\frac{dU_e}{dt}}^{\text{exchange with a reservoir}}$; 2nd principle : $\underbrace{\frac{dS}{dt}}_{\text{entropy}} = \frac{1}{T}\frac{dQ}{dt} + \underbrace{\frac{dS_e}{dt}}_{\text{exchange}} + \underset{\geq 0}{\sigma}$ entropy creation rate.

$$\mathcal{D} = T\sigma = \frac{dW}{dt} - \frac{d\mathcal{F}}{dt} + \frac{d\mathcal{F}_e}{dt} \geq 0 \quad \text{where } \mathcal{F} = U - TS \text{ Gibbs free energy.}$$

A constitutive behavior of the material has to be consistent with this requirement.

II Model of the growth process

We assume that there exists a configuration of the object that is stress free. This configuration can be obtained by an infinite number of cuts that release all the stress. Signorini. (This idea that living matter is "folded" on itself dynamically may be attributed to Leibniz: the concept of a Monade)
This ground state metric evolves with time which defines a certain volumetric growth process (a "swelling" in a hydrostatic symmetry)



rot $\underline{\underline{F}} = 0$
↑
$\underline{\underline{F}}$ is compatible
i.e.: the gradient of a deformation transformation
$x = \phi(X,t)$

$$\Rightarrow \begin{cases} \left.\frac{d}{dt}\right|_X = \left.\frac{\partial}{\partial t}\right|_x + v\cdot\nabla_{\underline{x}} \;;\; v = \left.\frac{d}{dt}\phi\right|_X \\ \underline{\underline{F}} = \nabla_X \underline{x} \end{cases}$$

How is $\underline{\underline{G}}$ linked to growth?

$\det \underline{\underline{A}} = \frac{\rho_g}{\rho}$ since for any volume in Ω_g ; $\int \rho_0 \, dy = \int \underbrace{\rho_0 \det A^{-1}}_{\rho} \, dx$

So $\frac{1}{\rho}\frac{d\rho}{dt} + |A|^{-1}\frac{d|A|}{dt} = 0$; but from mass balance $\frac{1}{\rho}\frac{d\rho}{dt} + \mathrm{div}_x v = \frac{S}{\rho}$

and $\mathrm{div}_{\underline{x}}(\underline{v}) = |F|^{-1}\frac{d|F|}{dt}$

dem :

$$\mathrm{div}_{\underline{x}}(\underline{v}) = \mathrm{div}_{\underline{x}}\left(\partial_t\big|_{\underline{X}} \phi(\underline{X},t)\right)$$

$$= \mathrm{tr}\left(\nabla_x \partial_t \phi\right) \underset{\text{change of variable.}}{=} \mathrm{tr}\left(\nabla_{\underline{X}} \partial_t \phi \, \underline{\underline{F}}^{-1}\right)$$

$$= \mathrm{tr}\left(\partial_t\big|_{\underline{X}} \underline{\underline{F}} \, \underline{\underline{F}}^{-1}\right) \underset{\text{Jacobi formula.}}{=} \frac{1}{|F|}\frac{d|F|}{dt}$$

So ; $\frac{1}{\rho}\frac{d\rho}{dt} + \frac{1}{|A||G|}\left(|G|\frac{d|A|}{dt} + |A|\frac{d|G|}{dt}\right) = \frac{S}{\rho}$

$$\underbrace{\cancel{\frac{1}{\rho}\frac{d\rho}{dt} + \frac{1}{|A|}\frac{d|A|}{dt}}}_{\text{mass conservation}}^{=0} + \boxed{\frac{1}{|G|}\frac{d|G|}{dt} = \frac{S}{\rho}}$$

The metric "swelling" is related to the mass source / sink.

III Dissipation inequality

1 Work

$$\frac{dW}{dt} = \int_{\partial\Omega_t} f_{ext} \cdot v_f = \int_{\partial\Omega_t} \underline{\underline{\sigma}} \cdot \underline{n} \cdot \underline{v} = \int_{\Omega_t} \underbrace{\mathrm{div}(\underline{\underline{\sigma}}\,\underline{v})}_{\cancel{\mathrm{div}(\underline{\underline{\sigma}})}^{=0} \cdot \underline{v} + \underline{\underline{\sigma}} : \nabla \underline{v}} = \int_{\Omega_t} \underline{\underline{\sigma}} : \nabla \underline{v} = \int_{\Omega_t} \underline{\underline{\sigma}} : \frac{d\underline{\underline{F}}}{dt}\underline{\underline{F}}^{-1}$$

$$\underline{\underline{A}} : \underline{\underline{B}} = \mathrm{tr}\left(\underline{\underline{A}}\,\underline{\underline{B}}^T\right)$$

2 Exchange

$$\frac{d\mathcal{F}_e}{dt} = \int_{\Omega_t} \rho \underbrace{\frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1}}_{\text{mass delivery in each direction}} : \underline{\underline{Q}}_0$$

potential to deliver mass in the associated direction

Exp: The scalar case where $\underline{\underline{Q}}_0 = \mu_0 \underline{\underline{I}}$ $\quad \mu_0$ fixed

$$\frac{dF_e}{dt} = \int_{\Omega_t} \mu_0 \,\mathrm{tr}\Big(\rho \frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1}\Big) = \int_{\Omega_t} \mu_0 S = \int_{\Omega_t} \mu_0 \big\{ \partial_t \rho + \mathrm{div}(\rho \underline{v}) \big\}$$

$$= \mu_0 \int_{\Omega_t} \partial_t \rho + \int_{\partial\Omega_t} \overbrace{\rho \underline{v}\cdot\underline{n}}^{\rho \underline{v}_f\cdot\underline{n}} = \overbrace{\mu_0 \frac{d}{dt}\int_{\Omega_t} \rho \, dx}^{\overset{\text{def}}{=} M(t)}$$

Reynolds thm

$$\Rightarrow \frac{dF_e}{dt} = \mu_0 \dot{M}$$: This is the grand canonical ensemble in statistical mechanics.

3 Free energy

free energy per unit mass

We assume that: $\mathcal{F} = \int_{\Omega_t} \rho f(\underline{\underline{A}}, \underline{\underline{G}})$

stored elastic energy ($\underline{\underline{A}}$) — stored "chemical" energy ($\underline{\underline{G}}$).

$$\frac{d\mathcal{F}}{dt} = \int_{\Omega_t} \partial_t(\rho f) + \int_{\partial\Omega_t} \underline{v}_f\cdot\underline{n}\,\rho f = \int_{\Omega_t} \underbrace{\partial_t \rho}_{-\mathrm{div}(\rho\underline{v}) + S} f + \int_{\Omega_t} \rho \,\partial_t f + \int_{\partial\Omega_t} \underline{v}_f\cdot\underline{n}\,\rho f$$

$$= \int_{\Omega_t} S f + \int_{\Omega_t} \rho\,\underline{v}\cdot\nabla_x f + \rho\,\partial_t f = \int_{\Omega_t} S f + \rho \frac{df}{dt}$$

$$\Rightarrow \frac{d\mathcal{F}}{dt} = \int_{\Omega_t} \rho\Big(\frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1} : f\underline{\underline{I}} + \frac{\partial f}{\partial \underline{\underline{A}}} : \frac{d\underline{\underline{A}}}{dt} + \frac{\partial f}{\partial \underline{\underline{G}}} : \frac{d\underline{\underline{G}}}{dt} \Big)$$

$$\frac{d\underline{\underline{A}}}{dt} = \frac{d\underline{\underline{F}}}{dt}\underline{\underline{G}}^{-1} + \underline{\underline{F}}\frac{d\underline{\underline{G}}^{-1}}{dt} \qquad \text{since } \underline{\underline{G}}\,\underline{\underline{G}}^{-1} = \underline{\underline{I}} \qquad \frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1} = -\underline{\underline{G}}\frac{d\underline{\underline{G}}^{-1}}{dt}$$

$$= \frac{dF}{dt}G^{-1} - \underbrace{F G^{-1}}_{A}\frac{dG}{dt}G^{-1} = \frac{dF}{dt}F^{-1}A - A\frac{dG}{dt}G^{-1}$$

$$\frac{d\mathcal{F}}{dt} = \int_{\Omega_t} \rho\Big[\frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1} : f\underline{\underline{I}} + \mathrm{tr}\Big(\underline{\underline{A}}\frac{\partial f}{\partial \underline{\underline{A}}}^{T}\frac{d\underline{\underline{F}}}{dt}\underline{\underline{F}}^{-1}\Big) - \mathrm{tr}\Big(\Big(\frac{\partial f}{\partial \underline{\underline{A}}}\Big)^{T}\underline{\underline{A}}\frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1}\Big) + \mathrm{tr}\Big(\underline{\underline{G}}\frac{\partial f}{\partial \underline{\underline{G}}}^{T}\frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1}\Big)\Big]$$

Hence :

$$\boxed{\mathcal{D} = \int_\Omega \Big(\underbrace{\underline{\underline{\sigma}} - \frac{\rho_g}{\det A}\frac{\partial f}{\partial \underline{\underline{A}}}\underline{\underline{A}}^T}_{\text{sym}}\Big) : \underbrace{\frac{d\underline{\underline{F}}}{dt}\underline{\underline{F}}^{-1}} + \rho\Big(\underline{\underline{Q}}_0 - \underbrace{f\underline{\underline{I}} + \underline{\underline{A}}^T\frac{\partial f}{\partial \underline{\underline{A}}} - \frac{\partial f}{\partial \underline{\underline{G}}}\underline{\underline{G}}^T}\Big) : \frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1} \geq 0}$$

can be symetrized
$\underline{\underline{D}} = \frac{1}{2}\left(\underline{\underline{F}}^{-T}\frac{d\underline{\underline{F}}^T}{dt} + \frac{d\underline{\underline{F}}}{dt}\underline{\underline{F}}^{-1}\right)$

$\underline{\underline{\mu}}$: general chemical potential (tensorial)

IV Examples

1 Classical non-linear viscoelasticity $\sim f = f(A)$

$$\underline{\underline{G}} = \underline{\underline{I}} \Rightarrow \sigma = \frac{\rho_g}{\det \underline{A}}\frac{\partial f}{\partial \underline{\underline{A}}}\underline{\underline{A}}^T + \underbrace{\underline{\underline{\underline{\underline{\eta}}}}}_{\text{sym} +}\underline{\underline{D}} \Rightarrow \mathcal{D} = \int \underline{\underline{\underline{\underline{\eta}}}}\|\underline{\underline{D}}\|^2 \geq 0$$

2 Equilibrium pre-stress (passive) $f = f(A)$

$\underline{\underline{G}} = \underline{\underline{G}}_0(X)$ (indep of time)

$$\underline{\underline{\sigma}} = \frac{\rho_g}{|A|}\frac{\partial f}{\partial \underline{\underline{A}}}\underline{\underline{A}}^T \quad ; \quad \underline{\underline{F}} = \underline{\underline{A}}\,\underline{\underline{G}}_0 \Rightarrow \underline{\underline{F}}\,\underline{\underline{G}}_0^{-1} = \underline{\underline{A}}$$

$$\operatorname{div}(\underline{\underline{\sigma}}) = 0 \quad ; \quad \underline{\underline{\sigma}}\cdot\underline{n} = f_{ext} \qquad \underline{\underline{F}} = \nabla_X\phi = I + \nabla_X u$$

small def : $\|\nabla_X u\| \ll 1 \Rightarrow \underline{\underline{A}} = \underline{\underline{G}}_0^{-1} + \nabla_X u\, G_0^{-1}$ + Taylor expansion.

$$\underline{\underline{\sigma}} = \underbrace{\sigma_0[G_0^{-1}]}_{\text{prestress}} + \text{elasticity (coefficients renormed by } G_0)$$

non-dissipative.

4 Non equilibrium pre stress (active) $f = f(\underline{\underline{G}})$

$$\sigma - \cancel{\frac{\rho_g}{|A|}\frac{\partial f}{\partial \underline{\underline{A}}}\underline{\underline{A}}^T}^{=0} = \eta \quad \mathbb{D} + \lambda_{12}(\mu_0 - \mu)$$

$$\rho\frac{d\underline{\underline{G}}}{dt}\underline{\underline{G}}^{-1} = -\lambda_{12}\underline{\underline{\mathbb{D}}} + \lambda(\mu_0 - \mu)$$

$$\mathcal{D} = \int \eta\|\mathbb{D}\|^2 + \lambda\|\mu - \mu_0\|^2 \geq 0$$

Close to equilibrium Onsager framework
The symmetry of coefficients depends on the time reversal symmetry.