BALANCE EQUATIONS FOR 3D SOLIDS

- The partial differential equations (PDE) governing the thermoelastic response of a 3D continuum are now derived by adopting an axiomatic approach where:

    1. Conservation of mass

    2. Conservation of the momentum

    3. Conservation of the angular momentum

    4. Conservation of energy
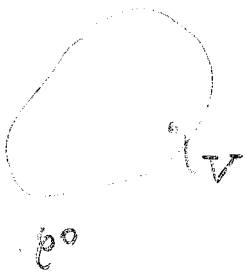
are retained valid a priori.

- The governing PDE are obtained in the context of the Lagrangian description

Conservation of mass

The balance equation is written by observing that the total mass of the body - before and after the application of the loads (thermal and/or mechanical) - does not change:

$$\int_{v} \rho(x,t) \, dv = \text{Const}$$

where

ρ^0: initial configuration

ρ^1: generic deformed configuration

Recalling that a generic quantity ϕ can be expressed as function of the lagrangian coordinates by performing a change of coordinates in the form

$$\phi = \phi(\underline{x}, t) = \phi(\underline{x}(\underline{X}, t), t)$$

and recalling that:

$$dv = J \, dV$$

the balance of mass is written as:

$$\int_v \rho(\underline{x}, t) \, dv = \int_V \rho(\underline{X}, t) J \, dV$$

$$= \int_V \rho_0(\underline{X}) \, dV$$

Note:
- $\rho_0(\underline{X})$ is the density of the configuration C^0, before the deformation process.

  It does not depend on time as it is the density associated with a specific time $t = t_0$.

The lagrangian form of the conservation of mass is then:

$$\boxed{\rho(\underline{X}, t) \, J = \rho_0(\underline{X})}$$

Balance of momentum

Recall the conservation of momentum

$$\frac{d}{dt}\left(mV\right) = F$$

meaning that the time derivative of the momentum is equal to the applied forces F.

Specializing this equation to the case of a 3D continuum, it is

$$\frac{d}{dt}\int_{v} \rho(x,t)\,\underline{v}\,dv \quad \int_{v} \rho(x,t)\,\underline{B}(x,t)\,dv + \int_{a}\underline{t}(x,t)\,da$$

with arrows labeling "body forces" and "surface forces"

By operating the change of coordinates, from Eulerian to Lagrangian, the three contributions read:

$$\frac{D}{Dt}\int_{v}\rho(x,t)v\,dv = \frac{D}{Dt}\int_{V}\rho(\underline{X},t)v\,J\,dV$$

$$= \frac{D}{Dt}\int_{V}\rho_0(\underline{X})\,\underline{v}\,dV$$

$$= \int_{V}\rho_0(\underline{X})\,a\,dV$$

having observed that $\frac{D}{Dt}\rho_0(\underline{X}) = 0$ as ρ_0 is time-independent.

Similarly:

$$\int_{v}\rho(x,t)\,\underline{B}(x,t)\,dv = \int_{V}\rho(\underline{X},t)\,\underline{B}(\underline{X},t)\,J\,dV$$

$$= \int_{V}\rho_0(\underline{X})\,\underline{B}(\underline{X},t)\,dV$$

The third contribution — the one associated with the surface forces — reads:

$$\int_{\partial} \underline{t}(\underline{x}, t)\, da = \int_{\partial} \underline{\sigma} \cdot \underline{n}\, da \qquad \left(\text{using the Cauchy relation } \underline{\sigma} \cdot \underline{n} = \underline{t} \right)$$

$$= \int_{A} \underline{\sigma}\, J \underline{F}^{-T} \underline{N}\, dA \qquad \left(\text{using the Nanson's formula} \right)$$

$$= \int_{A} \underline{P}\, \underline{N}\, dA$$

$$= \int_{V} \text{Div}\left(\underline{P} \right) dV$$

Concluding, the balance of momentum, in Lagrangian form, is

$$\boxed{ \rho_0\, \underline{a} = \rho_0\, \underline{B} + \text{Div}\, \underline{P} }$$

Conservation of angular momentum

The conservation of angular momentum can be written as:

$$\frac{D}{Dt} \int_v \rho(\underline{x},t) \, \underline{x} \times \underline{v} \, dv = \int_v \rho(\underline{x},t) \, \underline{x} \times \underline{b} \, dv + \int_a \underline{x} \times \underline{t} \, da$$

- This balance equation is here used to demonstrate the simmetry of the Cauchy stress tensor $\underline{\underline{\sigma}}$.

- As seen in the conservation of linear momentum, the transformation to the reference configuration ρ^0 (characterized by volume V and area A) determines the need for introducing the stress measure $\underline{\underline{P}}$ (First Piola-Kirchhoff).

  Having now in mind of demonstrating the simmetry of $\underline{\underline{\sigma}}$ the balance is written on the deformed configuration.

- Before manipulating the expressions, it is useful to note that:

$$\frac{D}{Dt} \int_v \rho \, \underline{\underline{A}} \, dv = \frac{D}{Dt} \int_V \rho \, \underline{\underline{A}} \, J \, dV \qquad \underline{\underline{A}} \text{ generic tensor}$$

$$= \frac{D}{Dt} \int_V \rho_0(\underline{X}) \, \underline{\underline{A}} \, dV$$

$$= \int_V \rho_0(\underline{X}) \, \frac{D\underline{\underline{A}}}{Dt} \, dV \qquad (\text{Lagrangian})$$

It is now possible to go back to the Eulerian description

$$= \int_V \rho_0(\underline{X}) \, \frac{D\underline{\underline{A}}}{Dt} \, J \, dv$$

$$= \int_v \rho(\underline{x},t) \, \frac{D\underline{\underline{A}}}{Dt} \, dv \qquad (\text{Eulerian})$$

Thus, summarizing:

$$\frac{D}{Dt}\int_V \rho\, A\, dv = \int_V \rho_0(X)\, \frac{DA}{Dt}\, dv$$

$$= \int_V \rho(x,t)\, \frac{DA}{Dt}\, dv$$

- Rearrange now the three contribution of the angular momentum expression:

1) $\dfrac{D}{Dt}\displaystyle\int_V \rho(x,t)\, x \times v\; dv = \int_V \rho(x,t)\, \dfrac{D}{Dt}(x \times v)\, dv$

$$= \int_V \rho(x,t)\left[\frac{Dx}{Dt} \times v + x \times \frac{Dv}{Dt}\right] dv$$

$$= \int_V \rho(x,t)\left[v \times v + x \times a\right] dv$$

$$\boxed{= \int_V x \times (\rho a)\, dv}$$

Having observed that:
- $\underline{v} \times \underline{v} = \underline{0}$
- the density is a scalar field, so it can be freely "moved" inside the expression

2) $\displaystyle\int_V \rho(x,t)\, \underline{x} \times \underline{b}\, dv \;\boxed{= \int_V \underline{x} \times (\rho\underline{b})\, dv}$

3) $\displaystyle\int_{\partial a} \underline{x} \times \underline{t}\, da = \int_{\partial} \underline{x} \times \underline{\sigma}\cdot\underline{n}\, da$

$$= \int_V \operatorname{div}(\underline{x} \times \underline{\sigma})\, dv \qquad \text{(divergence theorem)}$$

$$= \int_v (\underline{x} \times \underline{\underline{\sigma}})_{ik/k} \, dv$$

(denoting with $(\cdot)_{ik}$ the ik component of the tensor. and recalling that $\text{div} \, \underline{\underline{A}} = A_{ik/k}$)

$$= \int_v \left[(\underline{x} \times)_{ir} (\underline{\underline{\sigma}})_{rk} \right]_{/k} \, dv$$

$$= \int_v \left[(\underline{x} \times)_{ir/k} \, \underline{\sigma}_{rk} + (\underline{x} \times)_{ir} \, \underline{\sigma}_{rk/k} \right] \, dv$$

$$\boxed{= \int_v \left[\underline{a} + (\underline{x} \times) \, \text{div} \, \underline{\underline{\sigma}} \right] \, dv} ; \quad \left(\text{discussion on } \underline{a} \atop \text{later} \right)$$

A few remarks:

1. What does $\underline{x} \times$ mean?

   It is a second order tensor, constructed in a specific way starting from the vector $\underline{x}$. How?

   Consider the vector product $\underline{x} \times \underline{y} = \underline{z}$

   We can imagine that a tensor $\underline{\underline{A}}$ exists such that:

   $$\underline{\underline{A}} \, \underline{y} = \underline{z}$$

   In other words, the vector product between two vectors can be seen as the scalar product between a tensor $\underline{\underline{A}}$, function of $\underline{x}$, and a vector $\underline{y}$

   $$\underline{x} \times \underline{y} = \underline{z}$$

   $$\underline{\underline{A}} \, \underline{y} = \underline{z} \qquad \text{with} \quad \underline{\underline{A}} = \underline{x} \times$$

If the components of $\underline{x}$ are $\underline{x} = \{x_1, x_2, x_3\}$, then:

$$(\underline{\underline{A}})_{ik} = \begin{bmatrix} 0 & -x_3 & x_2 \\ x_3 & 0 & -x_1 \\ -x_2 & x_1 & 0 \end{bmatrix}$$

2. We have used, the notation

$(\underline{\underline{A}})_{ik}$ to denote the component ik of the tensor $\underline{\underline{A}}$

The expression of the conservation of angular momentum is so obtained as:

$$\int_v \underline{x} \times (\rho \underline{a}) \, dv = \int_v \underline{x} \times (\rho \underline{b}) \, dv + \int_v \left[\underline{q} + (\underline{x} \times) \operatorname{div} \underline{\underline{\sigma}} \right] dv$$

$$\int_v \underline{x} \times \underbrace{\left(\rho \underline{a} - \rho \underline{b} - \operatorname{div} \underline{\underline{\sigma}} \right)}_{= 0} dv = \int_v \underline{q} \, dv$$

$= 0$ (Eulerian form of the conservation of linear momentum)

$$\Rightarrow \int_v \underline{q} \, dv = \underline{0}$$

Recall the definition of $\underline{q}$:

$$\underline{q} = (\underline{x} \times)_{ir/k} \, \underline{\underline{\sigma}}_{rk} = \underline{0}$$

but $(\underline{x} \times)_{/i} = \underline{e}_i \times$, so:

$$\alpha_i = \left(\underline{e}_k \times\right)_{ir} \sigma_{rk}$$

(The indexes r and k are repeated, while i is a free index $\Rightarrow$ the result is a vector)

To evaluate the components α_i of the vector $\underline{\alpha}$ consider now $i = 1, 2$ and 3. Recall also that

$$\underline{e}_1 = \{1 \ 0 \ 0\} \qquad \underline{e}_2 = \{0 \ 1 \ 0\} \qquad \underline{e}_3 = \{0 \ 0 \ 1\}$$

and so:

$$\underline{e}_1 \times = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \qquad \underline{e}_2 \times = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \qquad \underline{e}_3 \times = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- $\underline{i=1}$

$$\left(\underline{e}_k \times\right)_{1r} \sigma_{rk} = \qquad \text{expand now the summatory over } k$$

$$= \left(\underline{e}_1 \times\right)_{1r} \sigma_{r1} + \left(\underline{e}_2 \times\right)_{1r} \sigma_{r2} + \left(\underline{e}_3 \times\right)_{1r} \sigma_{r3}$$

element of the row 1, column r

$$= 0 + \underbrace{\left(\underline{e}_2 \times\right)_{13} \sigma_{32}}_{} + \underbrace{\left(\underline{e}_3 \times\right)_{12} \sigma_{23}}_{}$$

$\downarrow$

$\hookrightarrow$ this is the only not null contribution of the 1st row

$$= \sigma_{32} - \sigma_{23}$$

- $i = 2$

$$(\underline{e}_k \times)_{2r} \, \sigma_{rk} =$$

$$= (\underline{e}_1 \times)_{2r} \, \sigma_{r1} + (\underline{e}_2 \times)_{2r} \, \sigma_{r2} + (\underline{e}_3 \times)_{2r} \, \sigma_{r3}$$

$$= (\underline{e}_1 \times)_{23} \, \sigma_{31} + 0 + (\underline{e}_3 \times)_{21} \, \sigma_{13}$$

$$= -\sigma_{31} + \sigma_{13}$$

- $i = 3$

$$(\underline{e}_k \times)_{3r} \, \sigma_{rk} =$$

$$= (\underline{e}_1 \times)_{3r} \, \sigma_{r1} + (\underline{e}_2 \times)_{3r} \, \sigma_{r2} + (\underline{e}_3 \times)_{3r} \, \sigma_{r3}$$

$$= (\underline{e}_1 \times)_{32} \, \sigma_{21} + (\underline{e}_2 \times)_{31} \, \sigma_{12} + 0$$

$$= \sigma_{21} - \sigma_{12}$$

It is then concluded that:

$$\boxed{\underline{q} = (\sigma_{32} - \sigma_{23}) \underline{e}_1 + (-\sigma_{31} + \sigma_{13}) \underline{e}_2 + (\sigma_{21} - \sigma_{21}) \underline{e}_3}$$

It follows that $\underline{q} = 0$ iif

$$\begin{vmatrix} \sigma_{32} = \sigma_{23} \\ \sigma_{31} = \sigma_{13} \\ \sigma_{21} = \sigma_{12} \end{vmatrix}$$

Conservation of energy

The conservation of energy is written by recalling:

$$\frac{D}{Dt}(U+K) = W + H$$

where

U : internal energy

K : kinetic energy

W : power input (power due to the applied forces)

H : heat input (power due to heat sources and heat fluxes)

The contributions are written as:

1) $U = \int_v \rho(x,t)\, e(x,t)\, dv$

$\quad = \int_v \rho_0(\underline{X})\, E(\underline{X},t)\, dV$

$$\boxed{\frac{D}{Dt}U = \int_v \rho_0 \cdot \dot{E}\, dV}$$

2) $K = \frac{1}{2}\int_v \rho(x,t)\, \underline{v}\cdot\underline{v}\, dv$

$\quad = \frac{1}{2}\int_v \rho_0(\underline{X})\, \underline{v}\cdot\underline{v}\, dV$

$$\frac{D}{Dt} K = \frac{1}{2} \int_V \rho_0(\underline{X}) \frac{D}{Dt}(\underline{v} \cdot \underline{v}) dV$$

$$\boxed{= \int_V \rho_0(\underline{X}) \underline{v} \cdot \underline{a} \, dV}$$

3) $\quad W = \int_v \rho(\underline{x}, t) \, \underline{v} \cdot \underline{b}(\underline{x}, t) \, dv + \int_a \underline{v} \cdot \underline{t} \, da$

$$= \int_V \rho_0(\underline{X}) \underline{v} \cdot \underline{B}(\underline{X}, t) dV + \int_A \underline{v} \cdot \underline{\underline{\sigma}} \, J \underline{\underline{F}}^{-T} \underline{N} \, dA$$
$$(\text{Nanson})$$

$$= \int_V \underline{v} \cdot (\rho_0 \underline{B}) dV + \int_V \text{div}(\underline{v} \cdot \underline{P}) dV$$

The second term can be rearranged:

$$\text{div}(\underline{v} \cdot \underline{P}) = (v_i P_{iK})_{/K}$$

$$= v_{i/K} P_{iK} + v_i P_{iK/K}$$

$$\left[\text{but} \quad dx_i = F_{iK} dX_K \implies F_{iK} = x_{i/K} \implies v_{i/K} = \dot{F}_{iK} \right]$$

$$= \dot{F}_{iK} P_{iK} + v_i P_{iK/K}$$

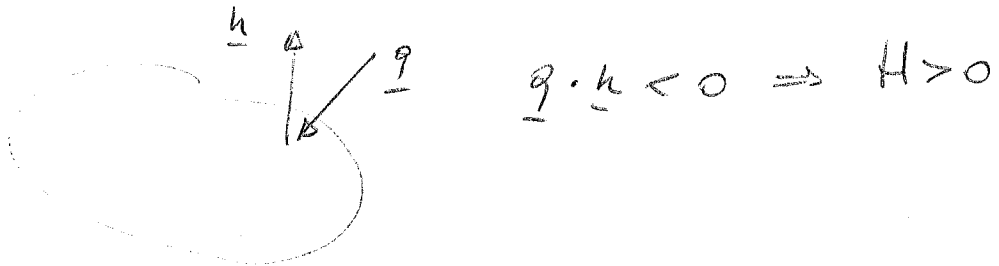$$= \dot{\underline{\underline{F}}} : \underline{P} + \underline{v} \cdot \text{Div} \, \underline{P}$$

finally:

$$\boxed{W = \int_V [\underline{v} \cdot (\rho_0 \underline{B}) + \dot{\underline{\underline{F}}} : \underline{P} + \underline{v} \cdot \text{Div} \, \underline{P}] dV}$$

4) $H = \int_V \rho(\underline{x},t)\, r(\underline{x},t)\, dv - \int_\partial \underline{q}(\underline{x},t) \cdot \underline{n}\, da$

$r = $ internal heat generation

$\underline{q} = $ heat flux $\rightarrow$ $H > 0$ when q is directed in the inward direction

$\underline{q} \cdot \underline{n} < 0 \implies H > 0$

$H = \int_V \rho_0(\underline{X})\, R(\underline{X},t)\, dV - \int_A \underline{q}(\underline{X},t)\, J\, F^{-T}\, \underline{N}\, dA$

$= \int_V \rho_0 R\, dV - \int_A \underline{Q} \cdot \underline{N}\, dA$ with $\underline{Q} = J\underline{q}F^{-T}$

$\boxed{= \int_V \left(\rho_0 R - \mathrm{Div}\, \underline{Q} \right) dV}$

The conservation of energy is thus:

$\dfrac{\Delta}{\Delta t}(U + k) = W + H$

$\int_V \left[\rho_0 \dot{E} + \underline{v} \cdot (\rho_0 \underline{a}) \right] dV = \int_V \left[\underline{v} \cdot (\rho_0 \underline{B} + \mathrm{Div}\,\underline{P}) + \dot{F} : \underline{P} \right.$

$\left. + \rho_0 R - \mathrm{Div}\,\underline{Q} \right] dV$

or, collecting the terms pre-multiplied by $\underline{v}$:

$\int_V \underline{v} \cdot \left(\rho_0 \underline{a} - \rho_0 \underline{B} - \mathrm{Div}\,\underline{P} \right) dV + \underbrace{\qquad}_{= 0}$ due to the linear momentum eq.

$+ \int_V \rho_0 \dot{E}\, dV = \int_V \left[\dot{F} : \underline{P} + \rho_0 R - \mathrm{Div}\,\underline{Q} \right] dV$

and so:

$$\boxed{\rho_0 \dot{E} = \dot{F} : P + \rho_0 R - \text{Div } Q}$$

Lagrangian form of the energy equation

Note

- $\dot{F} : P$ is denoted as stress power. It is an energy contributions associated with the internal stress (P) and the time derivative of F.

- $\dot{F} : P$ is responsible for the coupling between the energy and the linear momentum equations. (it is a form of thermoelastic coupling)

  If $\dot{F} : P$ is dropped out (neglected) the energy equation can be solved alone; on the contrary a thermoelastic coupling still exists in the linear momentum equation via the constitutive law (which depends over the temperature)

Energy Conjugacy

The energy equation includes a contribution in the form

$$\dot{\underline{F}} : \underline{P} = S_p$$ S_p = stress power

— stress-related

— strain-related

- Note that, in order to obtain an _energy_, the stress-related quantity should be contracted with a precise strain-related quantity.

  In other words S_p cannot be obtained by taking two "randomly" chosen stress/strain quantities.

- IF $\underline{A} : \underline{B} = S_p \implies \underline{A}$ and $\underline{B}$ are in a

  energy conjugacy relation

- Generally it is useful to re-write S_p in terms of the strain tensor $\underline{\underline{\epsilon}}$, which is an objective tensor well suited for expressing the constitutive relation

$$\dot{\underline{\underline{\epsilon}}} : \boxed{?} = S_p$$

Which is the stress measure energetically conjugate to $\underline{\underline{\epsilon}}$?

It is possible to demonstrate that

$$\dot{\underline{\underline{\epsilon}}} : \underline{S} = \dot{\underline{F}} : \underline{P} = \underline{d} : \underline{\sigma} = S_p$$

velocity gradient $\underline{\underline{d}} = \frac{1}{2}\left(\text{grad}\,\underline{v} + \text{grad}\,\underline{v}^T \right)$

To illustrate that $\boxed{S_\rho = \dot{\underline{\underline{\epsilon}}} : \underline{\underline{S}} = \dot{\underline{\underline{F}}} : \underline{\underline{P}}}$, recall that

$$\underline{\underline{\epsilon}} = \frac{1}{2}\left(\underline{\underline{F}}^T \underline{\underline{F}} - \underline{\underline{I}}\right) \quad \Rightarrow \quad \dot{\underline{\underline{\epsilon}}} = \frac{1}{2}\left(\dot{\underline{\underline{F}}}^T \underline{\underline{F}} + \underline{\underline{F}}^T \dot{\underline{\underline{F}}}\right)$$

So

$$\dot{\underline{\underline{\epsilon}}} : \underline{\underline{S}} = \frac{1}{2}\left(\dot{\underline{\underline{F}}}^T \underline{\underline{F}} + \underline{\underline{F}}^T \dot{\underline{\underline{F}}}\right) : \underline{\underline{S}}$$

$$= \frac{1}{2}\left(\dot{F}_{ir}^T F_{rk} + F_{ir}^T \dot{F}_{rk}\right) S_{ik}$$

$$= \frac{1}{2}\left(\dot{F}_{ri} F_{rk} + F_{ri} \dot{F}_{rk}\right) S_{ik}$$

$$= \frac{1}{2}\dot{F}_{ri} F_{rk} S_{ki} + \frac{1}{2}\dot{F}_{rk} F_{ri} S_{ik}$$

$$\underset{\text{symmetry of } S}{\Big\uparrow}$$

$$= \frac{1}{2}\dot{\underline{\underline{F}}} : \left(\underline{\underline{F}}\,\underline{\underline{S}}\right) + \frac{1}{2}\dot{\underline{\underline{F}}} : \left(\underline{\underline{F}}\,\underline{\underline{S}}\right)$$

$$= \dot{\underline{\underline{F}}} : \underline{\underline{P}} \qquad \left(\text{having recalled that } \underline{\underline{P}} = \underline{\underline{F}}\,\underline{\underline{S}}\right)$$

It is useful to observe that the same equation can be easily verified by adopting the "leg-wise" interpretation of the tensor products

$$\dot{\underline{\underline{\epsilon}}} : \underline{\underline{S}} = \frac{1}{2}\dot{\underline{\underline{F}}}^T \underline{\underline{F}} : \underline{\underline{S}} + \frac{1}{2}\underline{\underline{F}}^T \dot{\underline{\underline{F}}} : \underline{\underline{S}}$$

$$= \frac{1}{2}\dot{\underline{\underline{F}}} : \underline{\underline{F}}\,\underline{\underline{S}} + \frac{1}{2}\dot{\underline{\underline{F}}} : \underline{\underline{F}}\,\underline{\underline{S}}$$

viz. the way the symbols $\circ, \square, \oslash, \boxtimes$ and $\times$ are connected does not change

Energy Conjugacy between $\underline{\underline{\sigma}}$ and $\underline{\underline{d}}$ (velocity gradient)

To demonstrate that $\underline{\underline{\sigma}}$ and $\underline{\underline{d}}$ are in energy-conjugacy relation, it is easier (and useful) to write the energy equation in Eulerian form.

Briefly:

$$\frac{\Delta}{\Delta t} \int_v \left[\rho(\underline{x},t) e(\underline{x},t) + \frac{1}{2} \rho(\underline{x},t) \underline{v} \cdot \underline{v} \right] dv =$$

$$= \int_v \rho(\underline{x},t) \underline{v} \cdot \underline{b}(\underline{x},t) dv + \boxed{\int_a \underline{v} \cdot \underline{t} \, da}$$

In analogy with the Lagrangian case, the contribution associated with the stress power S_ρ is the <u>last one</u>, which can be re-arranged as:

$$\int_a \underline{v} \cdot \underline{t} \, da = \int_a \underline{v} \cdot \underline{\underline{\sigma}} \, \underline{n} \, da$$

$$= \int_v \text{div}(\underline{v} \cdot \underline{\underline{\sigma}}) dv \qquad \left(\text{Note: Eulerian divergence} \right)$$

$$= \int_v \left(v_i \sigma_{ik/k} + v_{i/k} \sigma_{ik} \right) dv$$

$$= \int_v \left[\underline{v} \cdot \text{div} \, \underline{\underline{\sigma}} + \boxed{\underline{\underline{d}} : \underline{\underline{\sigma}}} \right] dv$$

$$\uparrow$$

while $\underline{\underline{d}} = \frac{1}{2} \left(\text{grad} \, \underline{v} + \text{grad} \, \underline{v}^T \right)$

• Entropy balance

In order to guarantee the thermodynamic consistency of the formulation, it is necessary to satisfy the second principle of thermodynamics (the energy equation is insensitive to the direction of the energy transfer)

$$\underbrace{\frac{D}{Dt} \int_v \rho s \, dv}_{} \geq \underbrace{\int_v \frac{\rho r}{T} \, dv - \int_a \frac{q \cdot n}{T} \, da}_{}$$

rate of entropy
increase

entropy input rate

The equation can be written in Lagrangian form with the usual procedure:

$$\int_V \rho_o \dot{S} \, dV \geq \int_V \left[\frac{\rho_o R}{T} - Div\left(\frac{Q}{T}\right) \right] dV$$

but $Div \dfrac{Q}{T} = \dfrac{Q_{i,i}}{T} - \dfrac{Q_i T_{,i}}{T^2} = \dfrac{1}{T}\left(Div\, Q - Q \cdot \dfrac{Grad\, T}{T} \right)$

So:

$$\rho_o \dot{S} \geq \frac{\rho_o R}{T} - \frac{1}{T}\left(Div\, Q - Q\, \frac{Grad\, T}{T} \right)$$

$$\rightarrow \boxed{\rho_o T \dot{S} \geq \underbrace{\rho_o R - Div\, Q}_{} + Q \cdot \frac{Grad\, T}{T}}$$ entropy equation (Lagrangian)

$$\downarrow$$

Recall now the energy equation

$$\rho_o R - Div\, Q = \rho_o \dot{E} - \underline{S} : \underline{\dot{e}}$$

The entropy equation is then,

$$\rho_0 T \mathring{S} \geq \rho_0 \mathring{E} - \underline{S} : \mathring{\underline{e}} + \underline{Q} \cdot \frac{Grad\, T}{T}$$

$$\rho_0 (T \mathring{S} - \mathring{E}) \geq \underline{Q} \cdot \frac{Grad\, T}{T} - \underline{S} : \mathring{\underline{e}}$$

It is now useful to introduce a potential function. More specifically, given the expression of the entropy equation here derived, a natural choice is given by the <u>Helmholtz free energy function</u> ψ

$$\psi = E - TS \qquad \Rightarrow \mathring{\psi} = \mathring{E} - \mathring{T}S - T\mathring{S}$$

$$\Rightarrow T\mathring{S} - \mathring{E} = -\mathring{\psi} - \mathring{T}S$$

Assume also that the thermodynamical state can be described by two different <u>state variables</u>, viz. $\underline{e}$ and T

$$\psi = \psi(\underline{e}, T) \qquad \Rightarrow \mathring{\psi} = \psi_{/\underline{e}} : \mathring{\underline{e}} + \psi_{/T} \cdot \mathring{T}$$

The entropy equation is then;

$$\rho_0 (\mathring{\psi} + \mathring{T}S) \leq \underline{S} : \mathring{\underline{e}} - \underline{Q} \cdot \frac{Grad\, T}{T}$$

$$\boxed{\rho_0 \left(\psi_{/\underline{e}} : \mathring{\underline{e}} + \psi_{/T} \cdot \mathring{T} + \mathring{T}S \right) \leq \underline{S} : \mathring{\underline{e}} - \underline{Q} \cdot \frac{Grad\, T}{T}}$$

The previous equation should be always verified, for any choice of the state variables, so:

$$\rho_0 \Psi_{/\epsilon} = \underline{S}$$

$$S = - \Psi_{/T}$$

$$- \underline{Q} \cdot \text{Grad } T \geqslant 0 \qquad \Rightarrow \qquad + \underline{\underline{k}} \text{ Grad } T \cdot \text{Grad } T \geqslant 0$$

$$\Rightarrow \qquad \underline{\underline{k}} \text{ positive defined}$$

Summarizing, the entropy equation leads to:

$$\boxed{\begin{array}{l} \underline{\underline{S}} = \rho_0 \Psi_{/\underline{\underline{\epsilon}}} \\[2mm] S = - \Psi_{/T} \\[2mm] \underline{\underline{k}} \text{ positive defined} \end{array}} \qquad \leftarrow \text{ thermodynamic definition of stresses}$$

Constitutive law

The energy equation was obtained in the form:

$$\rho_0 \dot{E} = \rho_0 R - \text{Div} \underline{Q} + \underline{\underline{S}} : \underline{\underline{\dot{E}}}$$

In terms of Helmholtz free energy:

$$\psi = E + TS \quad \Rightarrow \quad \dot{E} = \dot{\psi} + \dot{T}S + T\dot{S}$$

and recalling that:

$$\dot{\psi} = \psi_{/\underline{\underline{E}}} : \underline{\underline{\dot{E}}} + \psi_{/T} \dot{T} \quad ; \quad \psi_{/\underline{\underline{E}}} = \frac{1}{\rho_0} \underline{\underline{S}} \quad ; \quad \psi_{/T} = -S$$

it is:

$$\dot{E} = \frac{1}{\rho_0} \underline{\underline{S}} : \underline{\underline{\dot{E}}} - S\dot{T} + \cancel{\dot{T}S} + T\dot{S}$$

So the energy equation reads:

$$\underline{\underline{S}} : \underline{\underline{\dot{E}}} + \rho_0 \dot{T}S = \rho_0 R - \text{Div} \underline{Q} + \underline{\underline{S}} : \underline{\underline{\dot{E}}}$$

$$\boxed{\rho_0 T\dot{S} = \rho_0 R - \text{Div} \underline{Q}}$$

The entropy S is a state function, which can be described by means of two state variables; consider now T and $\underline{\underline{E}}$

$$S = S(T, \underline{\underline{E}})$$

$$\dot{S} = S_{/T} \dot{T} + S_{/\underline{\underline{E}}} : \underline{\underline{\dot{E}}}$$

From the entropy equation : $S = -\psi_{/T}$ and $\frac{1}{\rho_0} \underline{\underline{S}} = \psi_{/\underline{\underline{E}}}$

So

$$\dot{S} = -\psi_{/TT} \dot{T} - \psi_{/TE} : \dot{\underline{e}}$$

$$= -\psi_{/TT} \dot{T} - \frac{1}{\rho_0} S_{/T} : \dot{\underline{e}}$$

Assume now a constitutive law in the form:

$$\underline{S} = \underline{\underline{C}} \underline{e} - \underline{\beta}(T - T_0) \quad \Rightarrow \quad \underline{S}_{/T} = -\underline{\beta}$$

$$\Rightarrow \quad \dot{S} = -\psi_{/TT} \dot{T} + \frac{1}{\rho_0} \underline{\beta} : \dot{\underline{e}}$$

The energy equation is thus:

$$\rho_0 T \dot{S} = \rho_0 R - \text{Div} \underline{Q}$$

$$= \rho_0 \boxed{-T \psi_{/TT}} \dot{T} + T \underline{\beta} : \dot{\underline{e}} = \rho_0 R - \text{Div} \underline{Q}$$

$$\boxed{\rho_0 C_v \dot{T} \left(1 + \frac{T \underline{\beta} : \dot{\underline{e}}}{\rho_0 C_v \dot{T}}\right) = \rho_0 R - \text{Div} \underline{Q}}$$

thermoelectric
coupling

whenever the thermoelectric coupling contribution can be neglected, the energy equation reads:

$$\boxed{\rho_0 C_v \dot{T} = \rho_0 R - \text{Div} \underline{Q}}$$

Engineering energy
equation

Consider now the case of an __adiabatic transformation__, viz.

$R = 0$ and $\underline{Q} = 0$ (note that sometimes is intended as

$\underline{Q} = 0$ but $R \neq 0$).

The energy equation is then:

$$\rho_0 C_v \dot{T} + T \underline{\beta} : \underline{\dot{\varepsilon}} = 0$$

and linearize around a reference configuration

$$T = T_0 + \Delta T \qquad \dot{T} = \Delta \dot{T}$$
$$\underline{\varepsilon} = \underline{\varepsilon}_0 + \Delta \underline{\varepsilon} \qquad \underline{\dot{\varepsilon}} = \Delta \underline{\dot{\varepsilon}}$$

The equation becomes:

$$\rho_0 C_v \Delta \dot{T} + (T_0 + \Delta T) \underline{\beta} : \Delta \underline{\dot{\varepsilon}} = 0$$

$$\rho_0 C_v \Delta \dot{T} + T_0 \underline{\beta} : \Delta \underline{\dot{\varepsilon}} + \underbrace{\Delta T \underline{\beta} : \Delta \underline{\dot{\varepsilon}}}_{\text{higher order contribution } (\Delta T, \Delta \underline{\dot{\varepsilon}})} = 0$$

$$\rho_0 C_v \Delta \dot{T} + T_0 \underline{\beta} : \Delta \underline{\dot{\varepsilon}} = 0$$

and integrating:

$$\rho_0 C_v \Delta T + T_0 \underline{\beta} : \Delta \underline{\varepsilon} = 0 \implies \Delta T = - \frac{T_0}{\rho_0 C_v} \underline{\beta} : \Delta \underline{\varepsilon}$$

Consider now a linear thermoelastic constitutive law:

$$\underline{S} = \underline{\underline{C}} : \underline{\varepsilon} - \underline{\beta} \Delta T$$

$$\implies \Delta \underline{S} = \underline{\underline{C}} : \Delta \underline{\varepsilon} - \underline{\beta} \Delta T$$

$$\Delta S = \underline{\underline{C}} : \left(\Delta \varepsilon + \beta \frac{T_0}{\rho_0 C_v} \beta : \Delta \varepsilon \right)$$

$$= \underline{\underline{C}} : \left(\Delta \varepsilon + \frac{T_0}{\rho_0 C_v} \beta \otimes \beta : \Delta \varepsilon \right)$$

$$\Rightarrow \boxed{\Delta S = \left(\underline{\underline{C}} + \frac{T_0}{\rho_0 C_v} \beta \otimes \beta \right) : \Delta \varepsilon}$$

⇧ Constitutive law
for adiabatic transformation

Remarks

1. Why considering the adiabatic case?
It is an "extreme condition": the material is deformed so fast that it cannot even exchange heat with the surrounding media.
This is in contrast with the more "classical" condition of isothermal transformation: the material is deformed relatively slow and, at any time frame, the heat transfer with the external is possible.

So what happens in the extreme adiabatic case (limit condition)?

The isothermal constitutive law modifies, and an additional contribution, providing additional stiffness is obtained

$$\Delta \underline{\underline{S}} = \left(\underline{\underline{\underline{C}}} + \frac{T_0}{\rho_0 C_v} \underline{\beta} \otimes \underline{\beta} \right) : \Delta \underline{\underline{E}}$$

        └ isothermal   └ extra contribution

For typical metallic materials it is observed that the extra contribution is negligible with respect to the isothermal one, so:

1. The isothermal constitutive law can be used even for studying non isothermal conditions with a good degree of accuracy.

2. The small role played by the "extra-contribution" highlights that the thermoelastic coupling effect in the energy equation can be assumed to be negligible, thus <u>justifying the use of the engineering energy equation</u>.

Summarizing

The energy equation has been expressed in the form

$$\rho_0 \, C_v \, \dot{T} \left(1 + \underbrace{\frac{T \, \underline{\underline{\beta}} : \dot{\underline{\underline{\epsilon}}}}{\rho_0 \, C_v \, \dot{T}}}_{} \right) = \rho_0 \, R - \operatorname{div} \underline{Q}$$

$$\quad \quad \quad \quad \quad \quad \quad \hookrightarrow \text{thermoelastic coupling contribution}$$

① If $\dot{\underline{\underline{\epsilon}}}$ is "high", the coupling contribution (S_p) cannot be neglected. Example: impact problems

② If T is "high", S_p cannot be neglected ($\Rightarrow$ high temperatures are responsible for coupling)

③ The effect of the stress-power in terms of constitutive law is the presence of an additional contribution with respect to the isothermal constitutive law.

$$\Delta \underline{\underline{S}} = \underbrace{\left(\underbrace{\underline{\underline{C}}}_{} + \underbrace{\frac{T_0}{\rho_0 \, C_v} \, \underline{\underline{\beta}} \otimes \underline{\underline{\beta}}}_{} \right) : \Delta \underline{\underline{\epsilon}}}_{}$$

$$\quad \quad \quad \uparrow \text{isothermal} \quad \quad \uparrow \text{adiabatic}$$
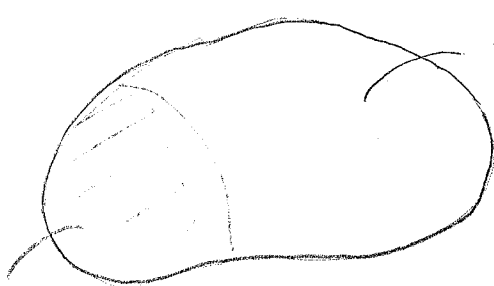
The fact that $\underline{\underline{C}}_{\text{isothermal}} \simeq \underline{\underline{C}}_{\text{adiabatic}}$ justifies the possibility of simplifying the energy equation and neglecting S_p.

Governing equations in Lagrangian form — summary

$$
\left(
\begin{cases}
\rho_0 = \rho J & \left(\text{* it is enforced by substitution} \atop \text{of } \rho_0 = \rho J \text{ in the other equations}\right) ; \quad \text{mass conservation} \\[4mm]
\rho_0 \, \underline{a} = \rho_0 \, \underline{B} + \text{Div} \, \underline{P} & \text{momentum conservation} \\[4mm]
\rho_0 \, C_v \, \dot{T} \left(1 + \dfrac{T \, \underline{\underline{\beta}} : \underline{\underline{\dot{\varepsilon}}}}{\rho_0 \, C_v \, T} \right) = \rho_0 \, R - \text{Div} \, \underline{Q} & \text{energy} \\[6mm]
\underline{\underline{\varepsilon}} = \dfrac{1}{2} \left(\underline{\underline{F}}^T \underline{\underline{F}} - \underline{\underline{I}} \right) & \begin{array}{l}\text{G-L. strain} \\ (\text{compatibility})\end{array} \\[5mm]
\underline{\underline{S}} = \psi(\underline{\underline{\varepsilon}}, T) & \text{constitutive law}
\end{cases}
\right.
$$

$+$

$$
\begin{cases}
\underline{u} = \hat{\underline{u}} & \text{on } S_u \\[3mm]
\underline{\underline{\sigma}} \cdot \underline{n} = \underline{t} & \text{on } S_F \\[3mm]
T = \hat{T} & \text{on } S_T \\[3mm]
\underline{q} \cdot \underline{n} = q_S & \text{on } S_Q
\end{cases}
\qquad \longleftarrow \quad \text{Boundary conditions}
$$

S_F = imposed forces

S_u = imposed displacements

$$S_u \cup S_F = S$$
$$S_u \cap S_F = \emptyset$$

Similarly : $\quad S_T \cup S_Q = S \; ; \quad S_T \cap S_Q = \emptyset$

From the previous, general form of the equations,
it is possible to derive the governing equation for
some "special" cases.

Dynamics

The dynamics is generally studied with a displacement-based
approach. (as far as the inertial forces depend upon the
derivative of the displacements, it follows that the
displacement formulation is the most "natural" one).

In this case:

1. $\underline{\underline{E}} = \frac{1}{2}\left(\underline{\underline{F}}^T\underline{\underline{F}} - \underline{\underline{I}}\right)$ is imposed a priori

2. $\underline{\underline{S}} = \Psi(\underline{\underline{E}}, T)$ is given

It is possible to distinguish between two cases:

1. <u>Fully coupled problem</u> (two-way)

$$\begin{cases} \rho_0\, \underline{a} = \rho_0\, \underline{B} + Div\, \underline{\underline{P}} & \text{3 eqs} \\ \rho_0 C_v T \left(1 + \dfrac{T\, \underline{\underline{\beta}} : \dot{\underline{\underline{E}}}}{\rho_0 C_v T}\right) = \rho_0 R - Div\, \underline{Q} & \text{1 eq} \end{cases}$$

+

BCs

→ The unknowns are taken as $\underline{u}$ and T

→ The two equations can be expressed as function
of the unknowns $\underline{u}, T$ (4 eqs, 4 unknowns)

2. Coupled problem (_one-way_)

$$\begin{cases} \rho_0 \, \underline{a} = \rho_0 \, \underline{B} + \text{Div} \, \underline{P} \\ \rho_0 \, C_v \dot{T} = \rho_0 \, R - \text{Div} \, \underline{Q} \end{cases}$$

$+$

BCs

- The Sp contribution is neglected. This is an acceptable assumption in those cases previously discussed

- It is called "_one way_" problem because the coupling will exists, although it is such that the energy equation can be solved first and the linear momentum later on. The two equations do not need to be solved together. Consider the solution of the problem in terms of displacement $\underline{u}$ and temperature T.

  Recalling the Fourier's law $\underline{Q} = - \underline{k} \, \text{Grad} \, T$, it is possible to write the two equations as:

$$\boxed{\begin{cases} \rho_0 \, \underline{a} = \rho_0 \, \underline{B} + \text{Div} \, \underline{P} \\ \rho_0 \, C_v \dot{T} + \text{Div}(- \underline{k} \, \text{Grad} \, T) = \rho_0 R \end{cases}}$$

  $\leftarrow$ Function of T and $\underline{u}$

  $\leftarrow$ Function of T

  So:

1. The temperature field can be obtained by solving the energy equation.

2. Once the temperature field is available, it can be substituted into the linear momentum equation as a forcing term, and the displacement field determined.

$$\left(\text{Note that } \underline{\underline{S}} = \underline{\underline{C}} : \left(\underline{\underline{\epsilon}} - \underline{\beta}\, \Delta T \right), \text{ so} \right.$$

$$\left. \text{div } \underline{P} \quad \text{depends on } T \right)$$

Statics

The statics is sometimes analyzed with a force-based approach, sometimes with a displacement-based approach.

For generality the equilibrium and the compatibility equations are both reported:

$$\begin{cases} \rho_0 \underline{B} + \text{div } \underline{P} = 0 \\[2mm] \text{div}\left(- \underline{\underline{K}} \,\text{Grad}\, T \right) = \rho_0 R \\[2mm] \underline{\underline{\epsilon}} - \frac{1}{2}\left(\underline{\underline{F}}^{\top} \underline{\underline{F}} - \underline{\underline{I}} \right) = \underline{\underline{0}} \end{cases}$$

← equilibrium

← energy

← compatibility

- In statics the problem is intrinsically "one-way", as far as

$$S_p = 0;$$

Again, the steady-state thermal problem can be solved from the energy equation to determine T. Then, in a second step, the equilibrium condition can be imposed by taking the temperature field as a forcing contribution

Secondary effects of thermoellastic coupling

While the discussion regarding the coupling between the elastic and the thermal response has regarded the analysis of the governing equations (i.e. the possibility of neglecting S_P), it is worth noting that the coupling can be due to the boundary conditions.

Consider the one-way problem:

$$\begin{cases} \rho_o c_v \dot{T} = \rho_o R - \text{Div}\left(-\underline{\underline{k}}\,\text{Grad}\,T\right) \\ \rho_o \underline{a} = \rho_o \underline{B} + \text{Div}\,\underline{\underline{P}} \end{cases}$$

and assume that a boundary condition exists regarding the imposed heat flux

$$\underline{Q} = \overline{\underline{Q}} \qquad \text{on} \quad S_Q$$
$$= -\underline{\underline{k}}\,\text{Grad}\,T$$

Recall, as observed when deriving the energy equation, that:

$$\underline{Q} = J\,\underline{q}\,\underline{\underline{F}}^{-T}$$

$$\uparrow \underline{\underline{F}} \text{ depends on the deformation and so does } \underline{Q}$$

For instance, in the presence of <u>solar radiation</u> $\underline{q}$ is given

$$\Rightarrow \quad \overline{\underline{Q}} = J\,\underline{q}_{solar}\,\underline{\underline{F}}^{-T} \quad \Rightarrow \quad \underline{\text{the boundary condition}}$$

$$\underline{\text{is function of the deformed configuration}}$$

$$\Rightarrow \underline{\text{the thermoellastic coupling is retrieved via BCs}}$$