## CH.1. THERMODYNAMIC FOUNDATIONS OF CONSTITUTIVE MODELLING

Computational Solid Mechanics- Xavier Oliver-UPC
1.1 Dissipation approach for constitutive modelling

Ch.1. Thermodynamical foundations of constitutive modelling

## Power

$\square$ Power, $W(t)$, is the work done per unit of time.
$\square$ In some cases, the power is an exact differential of a field, which, then is termed energy $\mathcal{E}(t)$ :

$$
W(t)=\frac{d \mathcal{E}(t)}{d t}
$$

- It will be assumed that the continuous medium obtains power from the exterior through:
- Mechanical Power: the work performed by the mechanical actions (body and surface forces) acting on the medium.
- Thermal Power: the heat entering the medium.


## External Mechanical Power

$\square$ The external mechanical power is the work done by the body forces and surface forces per unit of time.

- In spatial form it is defined as:

$$
P_{e}(t)=\int_{V} \rho \mathbf{b} \cdot \mathbf{v} d V+\int_{\partial V} \mathbf{t} \cdot \mathbf{v} d S
$$



## Theorem of the expended mechanical

 power

## REMARK

The stress power is the mechanical power entering the system which is not spent in changing the kinetic energy. It can be interpreted as the work done, per unit of time, by the stresses in the deformation process of the medium. A rigid solid will have zero stress power.

## External Heat Power

$\square$ The external heat power is the incoming heat in the continuum medium per unit of time.
$\square$ The incoming heat can be due to:

- Non-convective heat transfer across the body surface (characterized by $\underbrace{\mathbf{q}(\mathbf{x}, t) \text { ) }}$
heat conduction flux vector
$\square$

- Internal heat sources (characterized by $\underbrace{r(\mathbf{x}, t)}$ ) heat source field

$$
\frac{\text { heat generated by internal sources }}{\text { unit of time }}=\int_{V} \rho r d V
$$

## External Heat Power

$\square$ The external heat power is the incoming heat in the continuum medium per unit of time.
$\square$ It is defined as:


Where:
$\mathbf{q}(\mathbf{x}, t)$ is the heat flux per unit of spatial surface area.
$r(\mathbf{x}, t)$ is an internal heat source rate per unit of mass.

## Total Incoming Power

- The total power entering the continuous medium is:



## Stored Mechanical Power Mechanical Dissipation

Stored mechanical power: is that part of the incoming mechanical power that can be eventually returned by the body:

$$
P_{\text {stored }}=\frac{d}{d t} \underbrace{2}_{\underbrace{\int_{V_{i=V}}}_{\text {Kinetic energy } \mathcal{K}} \frac{1}{2} \rho \mathrm{v}^{2} d V}+\frac{d}{d t} \underbrace{\int_{V} \rho \psi d V}_{\begin{array}{c}
\text { Stored mechanical } \\
\text { energy } \mathcal{V}
\end{array}}=\frac{d \mathcal{K}}{d t}+\frac{d \mathcal{V}}{d t}
$$

$$
\rho_{0} \psi(\mathbf{x}, t) \rightarrow\left\{\begin{array}{c}
\text { Density of free energy } \\
(\text { Helmholtz energy })
\end{array} \rightarrow \frac{\text { Stored mechancical energy }}{\text { unit of volume }}\right.
$$

Mechanical dissipation: is that part of the incoming mechanical power that is not stored (eventually can be lost)

$$
D_{\text {mech }}=\underbrace{P_{e}}_{\frac{d \mathcal{K}_{e}}{d t}+\mathcal{P}_{\sigma}}-\underbrace{\frac{P_{\text {stored }}}{d t}+\frac{d V}{d t}}_{P_{e}}=\underbrace{\frac{d \not \subset}{d t}+\int_{V} \sigma: \mathbf{d} d V}_{P_{V}}-(\frac{d \not \subset \not}{d t t}+\underbrace{\frac{d V}{d t}}_{\int_{V} \rho \dot{\psi} d V})=\int_{V} \sigma: \mathbf{d} d V-\int_{V} \rho \dot{\psi} d V
$$

## Second principle of the thermodynamics Dissipation

$\square$ Mechanical dissipation


$$
D_{\text {mech }}=-\int_{V} \rho \dot{\psi} d V+\int_{V} \sigma: \mathbf{d} d V
$$

Thermal dissipation :


$$
D_{\text {therm }}=-\int_{V} \rho s \dot{\theta} d V
$$

$s(\mathbf{x}, t) \rightarrow$ Density of enthropy $\theta(\mathbf{x}, t) \rightarrow$ Absolute temperature $(>0)$

$$
D=D_{\text {mech }}+D_{\text {therm }}=-\int_{V}[\rho(\dot{\psi}+s \dot{\theta})+\sigma: \mathbf{d}] d V \geq 0 \quad \forall \Delta V \subset V
$$

Global (integral) form of the second principle of thermodynamics

## Second principle of the thermodynamics Dissipation



$$
\mathcal{D}(\mathbf{x}, t)=-\rho(\dot{\psi}+s \dot{\theta})+\boldsymbol{\sigma}: \mathbf{d} \geq 0 \quad \forall \mathbf{x} \quad \forall t
$$

Local (differential) form of the second principle of the thermodynamics

## Alternative forms of the Dissipation

$\square$ The internal energy per unit of mass (specific internal energy) is :

$$
u(\mathbf{x}, t):=\psi+s \theta \rightarrow\left\{\begin{array}{l}
u(\mathbf{x}, t) \rightarrow \text { Total stored energy } \\
\psi(\mathbf{x}, t) \rightarrow \text { Mechanical stored stored energy } \\
s \theta(\mathbf{x}, t) \rightarrow \text { Thermal stored stored energy }
\end{array}\right.
$$

$\square$ Taking the material time derivative,

$$
\dot{u}=\dot{\psi}+s \dot{\theta}+\dot{s} \theta \quad \square \quad \dot{\psi}+s \dot{\theta}=\dot{u}-\theta \dot{s}
$$

and introducing it into the Dissipation inequality

$$
\mathcal{D}=-\rho(\dot{\psi}+s \dot{\theta})+\sigma: \mathbf{d} \geq 0 \quad \Rightarrow \mathcal{D}=-\rho(\dot{u}-\theta \dot{s})+\sigma: \mathbf{d} \geq 0
$$

## REMARK

For infinitessimal deformation, $\mathbf{d}=\dot{\boldsymbol{\varepsilon}}$, the Clausius-Planck inequality becomes: $-\rho(\dot{\psi}+s \dot{\theta})+\sigma: \dot{\varepsilon} \geq 0$

Clausius-Planck Inequality
in terms of the
specific internal energy

## Dissipation in a continuum medium

$\square$ The dissipation of a continuum medium is defined as:

$$
\mathcal{D}:=-\rho(\dot{u}-\theta \dot{s})+\sigma: \mathbf{d} \geq 0
$$

corresponding to the Clausius-Planck Inequality.
$\square$ In terms of the Helmholtz free energy, dissipation may be written as:

$$
\mathcal{D}=-\rho(\dot{\psi}+s \dot{\theta})+\sigma: \mathbf{d} \geq 0
$$

$\square$ Hypotheses assumed
$\square$ Infinitesimal deformation: $\left\{\begin{array}{l}\mathbf{d}(\mathbf{x}, t)=\dot{\varepsilon}(\boldsymbol{x}, t) \\ \rho(\mathbf{x}, t)=\rho_{0}\end{array}\right.$
Hence, the dissipation may be written as:

$$
\mathcal{D}=-\rho_{0}(\dot{\psi}+s \dot{\theta})+\boldsymbol{\sigma}: \dot{\boldsymbol{\varepsilon}} \geq 0 \quad \begin{aligned}
& \text { Dissipation of a continuum medium in terms } \\
& \text { of the Helmholtz free energy assuming } \\
& \text { infinitesimal deformation }
\end{aligned}
$$

1.2 A thermodynamic framework for constitutive modeling

Ch.1. Thermodynamical foundations of constitutive modelling

## Sets of thermo-mechanical variables

In a thermo-mechanical problem we will consider the set of all the variables of the problem:

$$
\mathbb{V}:=\left\{\mathrm{v}_{1}, \mathrm{v}_{2}, \ldots, \mathrm{v}_{\mathrm{n}_{\mathrm{v}}}\right\} \quad \mathrm{v}_{i}(\mathbf{x}, t) \quad i \in\left\{1,2, \ldots, n_{\mathrm{v}}\right\}
$$

which will be classified into:
$\square$ Free variables:

$$
F:=\left\{\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n_{F}}\right\} \quad \lambda_{i}(\mathbf{x}, t) \quad i \in\left\{1,2, \ldots, n_{F}\right\}
$$

which are physically observable variables, whose evolution along time is unrestricted

$$
\dot{\lambda}_{i}(\mathbf{x}, t)=\frac{\partial \lambda_{i}(\mathbf{x}, t)}{\partial t} \rightarrow \text { any }
$$

## Sets of thermo-mechanical variables

$\square$ Internal/Hidden variables:

$$
I:=\left\{\alpha_{1}, \alpha_{2}, \ldots, \alpha_{n_{I}}\right\} \quad \alpha_{i}(\mathbf{x}, t) \quad i \in\left\{1,2, \ldots, n_{I}\right\}
$$

are non-observable variables. Their evolution is limited along time in terms of specific evolution equations defined as:

$$
\dot{\alpha}_{i}=\frac{\partial \alpha_{i}(\mathbf{x}, t)}{\partial t}=\xi_{i}(\underbrace{\lambda(\mathbf{x}, t), \boldsymbol{\alpha}(\mathbf{x}, t)}_{\begin{array}{c}
\text { instantaneous } \\
\text { values (at time } t)
\end{array}}) i \in\left\{1,2, \ldots n_{I}\right\}
$$

which account for micro-structural mechanisms.
$\square$ Dependent variables: $\mathbb{D}:=\left\{d_{1}, d_{2}, \ldots, d_{n_{D}}\right\} \quad d_{i}(\mathbf{x}, t) i \in\left\{1,2, \ldots, n_{D}\right\}$ are the remaining of the variables of the problem (depending on the previous ones):

$$
d_{i}=\gamma_{i}(\lambda, \alpha) \rightarrow \dot{d}_{i}=\varphi_{i}(\lambda, \alpha, \dot{\lambda}) i \in\left\{1,2, \ldots n_{D}\right\}
$$

$$
\mathbb{V}=\mathbb{F} \cup \mathbb{I} \cup \mathbb{D} \quad \mathbb{F} \cap \mathbb{I}=\mathbb{F} \cap \mathbb{D}=\mathbb{I} \cap \mathbb{D}=\varnothing
$$

## Example:

$\square$ Problem variables: $\mathbb{V}:=\{\rho, \sigma, \varepsilon, u, \psi, s, \theta, \alpha\}$
$\square$ Free variables:

$$
\mathbb{F}:=\{\rho, \varepsilon\}
$$

$$
\forall \dot{\rho}, \forall \dot{\boldsymbol{\varepsilon}}
$$

$\square$ Internal/Hidden variable: $\quad I I:=\{\alpha\} \quad \dot{\alpha}=\gamma(\rho, \varepsilon, \alpha)$
$\square$ Dependent variables: $\mathbb{D}:=\{\not, \sigma, \not, \not, u, \psi, s, \theta, \not \alpha\}$

$$
\begin{gathered}
\psi=\psi(\rho, \boldsymbol{\varepsilon}, \alpha) \\
\dot{\psi}=\gamma(\rho, \boldsymbol{\varepsilon}, \alpha, \dot{\rho}, \dot{\varepsilon}, \dot{\alpha}(\rho, \boldsymbol{\varepsilon}, \alpha))=\underbrace{\dot{\psi}\left(\frac{\rho, \boldsymbol{\varepsilon}, \alpha, \dot{\rho}, \dot{\boldsymbol{\varepsilon}})}{}\right.}_{\begin{array}{c}
\text { not depending on } \\
\text { the internal variable } \\
\text { evolution, } \dot{\alpha}
\end{array}} \\
\dot{\boldsymbol{\sigma}}=\varphi(\rho, \boldsymbol{\varepsilon}, \alpha, \dot{\rho}, \dot{\boldsymbol{\varepsilon}}, \underbrace{\dot{\alpha}(\rho, \boldsymbol{\sigma}(\rho, \boldsymbol{\varepsilon}, \alpha)}_{\begin{array}{c}
\text { provided by the } \\
\text { evolution equation }
\end{array}})=\dot{\boldsymbol{\sigma}}(\rho, \boldsymbol{\varepsilon}, \alpha, \dot{\rho}, \dot{\boldsymbol{\varepsilon}})
\end{gathered}
$$

## Elements of a constitutive model

$\square$ 1) Definition of the free variables of the problem

$$
\mathbb{F}:=\underbrace{\left\{\lambda_{1}, \lambda_{2}, \ldots, \lambda_{n_{F}}\right\}}_{\lambda}
$$

$\square$ 2) Choice of the internal variables of the problem

$$
I:=\underbrace{\left\{\alpha_{1}, \alpha_{2}, \ldots, \alpha_{n_{I}}\right\}}_{\alpha}
$$

$\square$ 3) Definition of the corresponding evolution equations,

$$
\dot{\alpha}_{i}=\dot{\alpha}_{i}(\lambda, \alpha) \quad i \in\left\{1,2, \ldots n_{I}\right\}
$$

$\square$ 4) Postulate a specific form of the free energy:

$$
\psi=\psi(\boldsymbol{\lambda}, \boldsymbol{\alpha}, \mathrm{t}) \rightarrow\left\{\begin{array}{l}
\text { provides the constitutive equation } \\
\text { through the dissispation inequality }
\end{array}\right.
$$

## Example: Thermo-elastic material

## Linear elastic material

$\square$ Linear relation stresses-strains

$$
\square 1 \mathrm{D}: \quad \frac{W}{A}=E \frac{\Delta L}{L} \square \sigma=E \boldsymbol{\varepsilon}
$$

$\square 3 \mathrm{D}: \quad \boldsymbol{\sigma}=\mathbb{C}: \boldsymbol{\varepsilon} \quad$ or $\quad \sigma_{i j}=\mathbb{C}_{i j k l} \varepsilon_{k l}$

Isotropic elastic material: $\quad \mathbb{C}_{i j k l}=\lambda \mathbf{1} \otimes \mathbf{1}+2 \mu \mathrm{I}$ being $\mathbb{C}_{i j k l}$ a second order tensor, and $\lambda$ and $\mu$ the Lamé constants.


$$
\left\{\begin{array}{l}
\boldsymbol{\sigma}=\lambda \operatorname{tr}(\boldsymbol{\varepsilon})+2 \mu \boldsymbol{\varepsilon} \\
\sigma_{i j}=\lambda \varepsilon_{k k} \delta_{i j}+2 \mu \varepsilon_{i j} \quad i, j \in\{1,2,3\}
\end{array}\right.
$$

## Tensor Notation (reminder)

$\square$ Open product

- Of two first-order tensors: $\quad[\mathbf{a} \otimes \mathbf{b}]_{i, j}=a_{i} b_{j}$
$\square$ Between two second order tensor: $[\mathbf{A} \otimes \mathbf{B}]_{i j k l}=A_{i j} B_{k l}$
$\square$ Identity tensors
- First order identity tensor

$$
[1]_{i j}=\delta_{i j}=\left\{\begin{array}{ll}
1 & i=j \\
0 & i \neq j
\end{array} \quad i, j \in\{1,2,3\}\right.
$$

$\square$ Second order tensor identity tensor

$$
[I]_{i j k l}=\frac{1}{2}\left[\delta_{i k} \delta_{j l}+\delta_{i l} \delta_{j k}\right] \quad i, j, k, l \in\{1,2,3\}
$$

## REMARK

Einstein notation (summation of repeated indices) is considered

## Thermo-elastic material (reminder)

## Linear thermo-elastic material

$\square$ Adding the thermal effects (thermoelasticity)

$$
\begin{aligned}
& \left\{\begin{array}{l}
\boldsymbol{\sigma}=\lambda \operatorname{tr}(\boldsymbol{\varepsilon})+2 \mu \boldsymbol{\varepsilon}-\beta \Delta \theta \mathbf{1} \\
\sigma_{i j}=\lambda \varepsilon_{k k} \delta_{i j}+2 \mu \varepsilon_{i j}-(\beta \Delta \theta) \delta_{i j} \quad i, j \in\{1,2,3\}
\end{array}\right. \\
& \beta=\rightarrow \text { Thermal property } \\
& \alpha=\frac{1-2 v}{\beta} \rightarrow \text { Thermal expansion coefficient }
\end{aligned}
$$

## Coleman's Method

$\square$ Theorem
$\square$ Proof:

$$
\mathcal{D}(x, y, \dot{x}, \dot{y})=f(x, y) \dot{x}+g(x, y) \dot{y} \geq 0 \quad \forall \dot{x}, \dot{y} \Rightarrow\left\{\begin{array}{l}
f(x, y)=0 \\
g(x, y)=0
\end{array}\right.
$$

- Taking $\dot{y}=0 \quad \square \mathcal{D}=f(x, y) \dot{x} \geq 0 \quad \forall \dot{x}$

$$
\begin{array}{lll}
\text { If } f(x, y)<0 & \text { taking } & \dot{x}>0 \\
\text { If } f(x, y)>0 & \text { taking } & \dot{x}<0
\end{array} \quad \mathcal{D}=f(x, y) \dot{x}<0 \quad \text { NOT POSSIBLE }
$$

- Taking $\dot{x}=0 \quad \Longrightarrow \mathcal{D}=g(x, y) \dot{y} \geq 0 \quad \forall \dot{y}$

$$
\begin{array}{rll}
\text { If } g(x, y)<0 & \text { taking } \quad \dot{y}>0 & \Longrightarrow \mathcal{D}=g(x, y) \dot{y}<0 \\
\text { If } g(x, y)>0 & \text { taking } & \dot{y}<0
\end{array} \quad \text { NOT POSSIBLE }
$$

## Elastic Material formulation

- Variable sets definition
- Free variables: $\mathbb{F}:=\{\varepsilon\}$
- Internal variables: II $:=\{\varnothing\} \rightarrow$ No evolution equation

Dependent: $\mathbb{D}:=\{\sigma, \psi\} \longrightarrow\left\{\begin{array}{l}\sigma(\varepsilon) \rightarrow \dot{\sigma}=\frac{\partial \sigma(\varepsilon)}{\partial \varepsilon}: \dot{\varepsilon} \\ \text { Potential } \rho_{0} \psi(\boldsymbol{\varepsilon})=\frac{1}{2} \boldsymbol{\varepsilon}: \mathbb{C}: \boldsymbol{\varepsilon} \\ \rho_{0} \psi(\varepsilon) \rightarrow \rho_{0} \dot{\psi}=\frac{\partial \rho_{0} \psi(\varepsilon)}{\partial \varepsilon}: \dot{\varepsilon}\end{array}\right.$

- Helmholtz free energy:
$\square$ Dissipation Isothermal case

$$
\mathcal{D}=-\rho_{0}(\dot{\psi}+\delta \dot{\theta})+\sigma: \dot{\varepsilon} \geq 0 \rightarrow \mathcal{D}=\underbrace{\left(\sigma-\frac{\partial \rho_{0} \psi(\varepsilon)}{\partial \varepsilon}\right.}_{f(\boldsymbol{\varepsilon})}): \dot{\varepsilon} \geq 0 \quad \forall \dot{\varepsilon} \Rightarrow f(\boldsymbol{\varepsilon})=0
$$

$$
\underbrace{\sigma=\frac{\partial \rho_{0} \psi(\varepsilon)}{\partial \varepsilon}=\mathbb{C}: \varepsilon}
$$

$$
\mathcal{D}=0
$$

## Thermo-elastic Material formulation

$\square$ Variable sets definition
$\square$ Free variables: $\mathbb{F}:=\{\varepsilon, \theta\}$

- Internal variables:

$$
\mathbb{I}:=\{\varnothing\}
$$

- Dependent:
$\square$ Potential definition

$$
\mathbb{D}:=\{\sigma, \psi\} \rightarrow\left\{\begin{array}{l}
\dot{\sigma}=\frac{\partial \sigma(\varepsilon, \theta)}{\partial \varepsilon}: \dot{\varepsilon}+\frac{\partial \sigma(\varepsilon, \theta)}{\partial \theta}: \dot{\theta} \\
\rho_{0} \dot{\psi}=\frac{\partial \rho_{0} \psi(\varepsilon, \theta)}{\partial \varepsilon}: \dot{\varepsilon}+\frac{\partial \rho_{0} \psi(\varepsilon, \theta)}{\partial \theta}: \dot{\theta}
\end{array}\right.
$$

$\square$ Helmholtz free energy: $\rho_{0} \psi(\boldsymbol{\varepsilon}, \theta)=\frac{1}{2} \boldsymbol{\varepsilon}: \mathbb{C}: \boldsymbol{\varepsilon}-\beta \underbrace{\left(\theta-\theta_{0}\right)}_{\Delta \theta} \mathbf{I}$
Dissipation

$$
\mathcal{D}=-\rho_{0}(\dot{\psi}+s \dot{\theta})+\sigma: \dot{\varepsilon} \geq 0
$$

$$
\rightarrow \mathcal{D}=\underbrace{\left(\sigma-\frac{\partial \rho_{0} \psi(\varepsilon, \theta)}{\partial \varepsilon}\right)}_{f(\varepsilon, \theta)}: \dot{\varepsilon}-\underbrace{\left(\rho_{0} s+\frac{\partial \rho_{0} \psi(\varepsilon, \theta)}{\partial \theta}\right)}_{g(\varepsilon, \theta)}: \dot{\theta} \geq 0 \quad \forall \dot{\varepsilon}, \dot{\theta}
$$

## Thermo-elastic Material formulation

$\square$ Using the Coleman's method:

$$
\begin{gathered}
f(\varepsilon, \theta)=\sigma-\rho_{0} \frac{\partial \psi(\varepsilon, \theta)}{\partial \varepsilon}=0 \\
g(\varepsilon, \theta)=\rho_{0} s+\rho_{0} \frac{\partial \psi(\varepsilon, \theta)}{\partial \theta}=0
\end{gathered} \quad \square\left\{\begin{array}{l}
=\frac{\partial \rho_{0} \psi(\varepsilon, \theta)}{\partial \varepsilon} \\
s=-\frac{\partial \psi(\varepsilon, \theta)}{\partial \theta}
\end{array} \quad \begin{array}{l}
f(\varepsilon, \theta)=0 \\
g(\varepsilon, \theta)=0
\end{array} \Rightarrow \mathcal{D}=0\right.
$$

and differentiating the Helmholtz free energy:

$$
\rho_{0} \psi(\varepsilon, \theta)=\frac{1}{2} \varepsilon: \mathbb{C}: \varepsilon-\beta \underbrace{\left(\theta-\theta_{0}\right)}_{\Delta \theta} \underbrace{\mathbf{1} \boldsymbol{\varepsilon}}_{\operatorname{Tr}(\boldsymbol{\varepsilon})} \rightarrow
$$

Constitutive
equations

$$
\left\{\begin{array}{l}
\frac{\partial \rho_{0} \psi}{\partial \varepsilon}=\frac{1}{2} \underbrace{\varepsilon: \mathbb{C}}_{=\mathbb{C}: \varepsilon}+\frac{1}{2} \mathbb{C}: \varepsilon-(\beta \Delta \theta) \mathbf{1}=\mathbb{C}: \varepsilon-(\beta \Delta \theta) \mathbf{1} \\
\frac{\partial \psi}{\partial \theta}=-\frac{1}{\rho_{0}} \beta \operatorname{Tr}(\boldsymbol{\varepsilon})
\end{array}\right.
$$

$$
\left\{\begin{array}{l}
\sigma=\rho_{0} \frac{\partial \psi(\varepsilon, \theta)}{\partial \varepsilon}=\mathbb{C}: \boldsymbol{\varepsilon}-\beta \Delta \theta \mathbf{1} \\
s=-\frac{\partial \psi(\varepsilon, \theta)}{\partial \theta}=\frac{1}{\rho_{0}} \beta \operatorname{Tr}(\boldsymbol{\varepsilon})
\end{array}\right.
$$

## END OF LECTURE 1

