# 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

**D** Power, W(t), is the work done per unit of time.

In some cases, the power is an exact differential of a field, which, then is termed **energy**  $\mathcal{E}(t)$ :

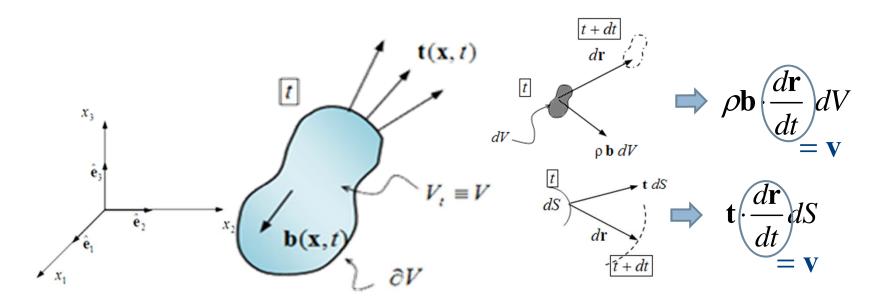
$$W(t) = \frac{d\mathcal{E}(t)}{dt}$$

- 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**

- 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:

$$P_{e}(t) = \int_{V} \rho \mathbf{b} \cdot \mathbf{v} \, dV + \int_{\partial V} \mathbf{t} \cdot \mathbf{v} \, dS$$



## Theorem of the expended mechanical

#### power

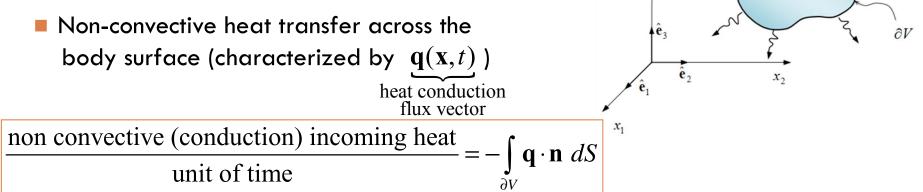
$$P_{e}(t) = \int_{V} \rho \mathbf{b} \cdot \mathbf{v} \, dV + \int_{\partial V} \mathbf{t} \cdot \mathbf{v} \, dS = \frac{d}{dt} \int_{V_{i}=V} \frac{1}{2} \rho v^{2} dV + \int_{V} \sigma : \mathbf{d} \, dV$$
  
External mechanical power Entering the medium External medium 
$$P_{e}(t) = \frac{d}{dt} \mathcal{K}(t) + \mathcal{P}_{\sigma}$$

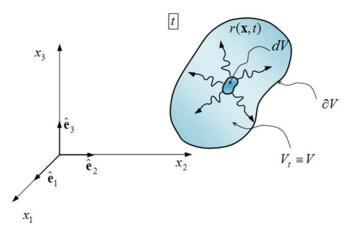
#### REMARK

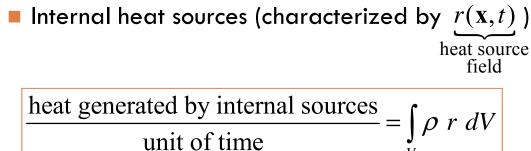
The **stress power** is the mechanical power entering the system which is not spent in changing the kinetic energy. It can be interpreted as the work done, per unit of time, by the stresses in the deformation process of the medium. A rigid solid will have zero stress power.

# **External Heat Power**

- The external heat power is the incoming heat in the continuum medium per unit of time.  $v_t = v$
- The incoming heat can be due to:







 $\mathbf{q}(\mathbf{x},t)$ 

# **External Heat Power**

The external heat power is the incoming heat in the continuum medium per unit of time.

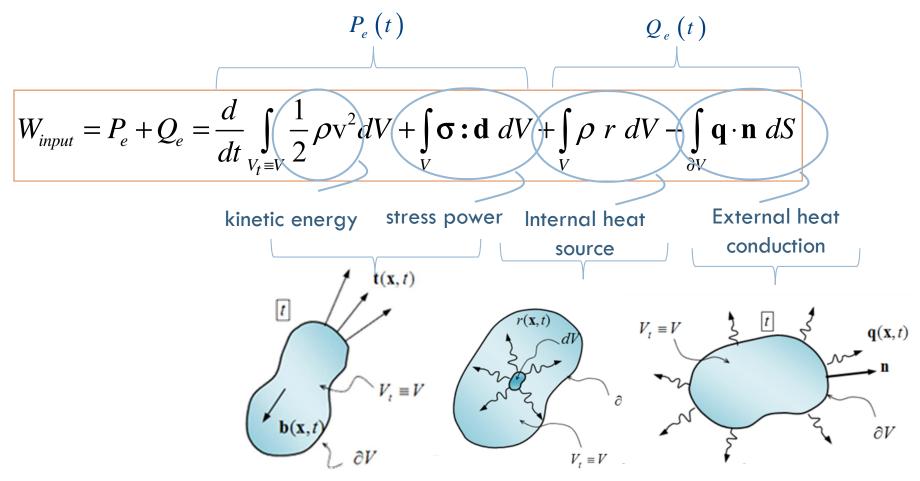
It is defined as:

Where:

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

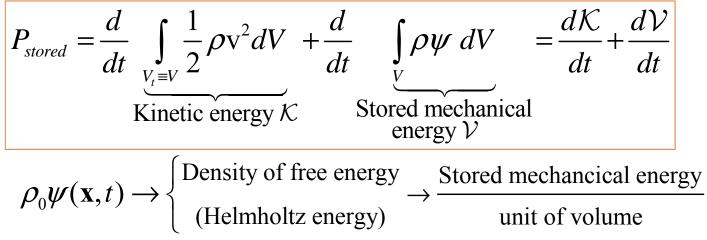
# **Total Incoming Power**

The total power entering the continuous medium is:



# Stored Mechanical Power Mechanical Dissipation

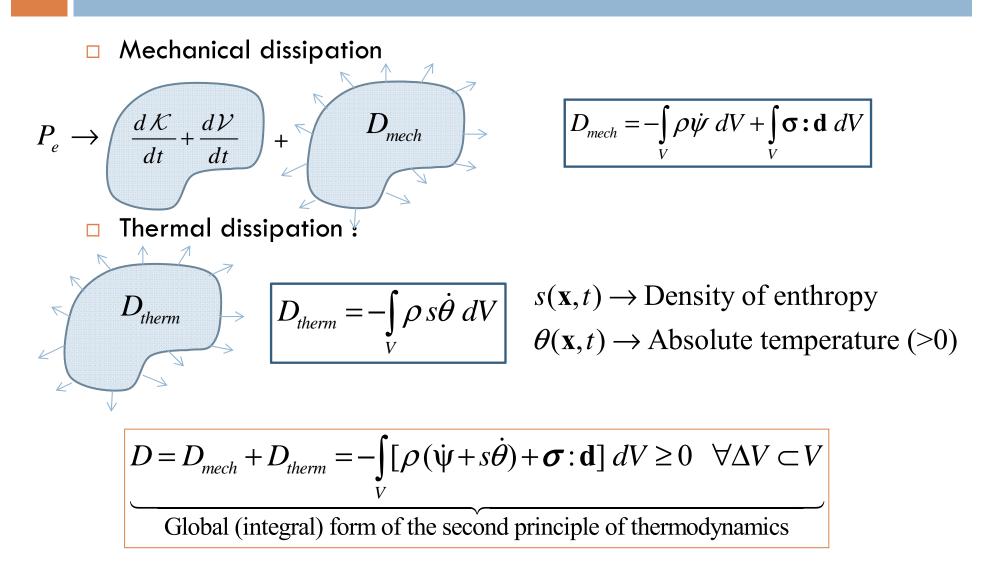
Stored mechanical power: is that part of the incoming mechanical power that can be eventually returned by the body:



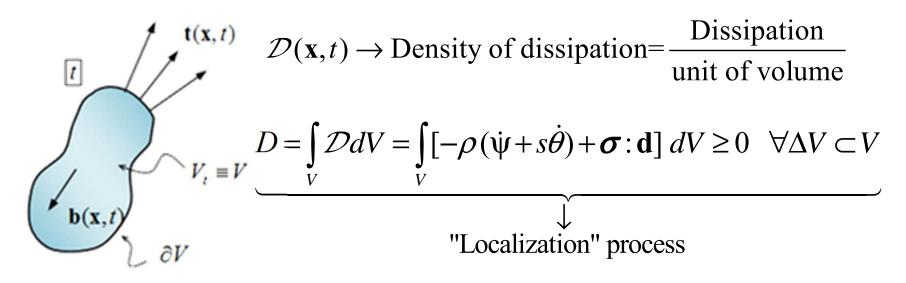
Mechanical dissipation: is that part of the incoming mechanical power that is not stored (eventually can be lost)

$$D_{mech} = \underbrace{P_{e}}_{\frac{d\mathcal{K}}{dt} + \mathcal{P}_{\sigma}} - \underbrace{P_{stored}}_{\frac{d\mathcal{K}}{dt} + \frac{d\mathcal{V}}{dt}} = \underbrace{\frac{d\mathcal{K}}{dt} + \int_{V} \mathbf{\sigma} : \mathbf{d} \, dV - \left(\frac{d\mathcal{K}}{dt} + \frac{d\mathcal{V}}{\frac{dt}{dt}}\right) = \int_{V} \mathbf{\sigma} : \mathbf{d} \, dV - \int_{V} \rho \dot{\psi} \, dV$$

# Second principle of the thermodynamics Dissipation



# Second principle of the thermodynamics Dissipation



$$\mathcal{D}(\mathbf{x},t) = -\rho(\dot{\psi} + s\dot{\theta}) + \boldsymbol{\sigma} : \mathbf{d} \ge 0 \quad \forall \mathbf{x} \ \forall t$$
  
Local (differential) form of the second principle of the thermodynamics

# Alternative forms of the Dissipation

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

 $u(\mathbf{x},t) := \psi + s\theta \rightarrow \begin{cases} u(\mathbf{x},t) \to \text{Total stored energy} \\ \psi(\mathbf{x},t) \to \text{Mechanical stored stored energy} \\ s\theta(\mathbf{x},t) \to \text{Thermal stored stored energy} \end{cases}$ 

Taking the material time derivative,

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

and introducing it into the Dissipation inequality

$$\mathcal{D} = -\rho(\dot{\psi} + s\dot{\theta}) + \boldsymbol{\sigma} : \mathbf{d} \ge 0 \qquad \Longrightarrow \qquad \mathcal{D} = -\rho(\dot{u} - \theta\dot{s}) + \boldsymbol{\sigma} : \mathbf{d} \ge 0$$

#### REMARK

For infinitessimal deformation,  $\mathbf{d} = \dot{\mathbf{\epsilon}}$ , the Clausius-Planck inequality becomes:  $-\rho(\dot{\psi} + s \dot{\theta}) + \mathbf{\sigma} : \dot{\mathbf{\epsilon}} \ge 0$  Clausius-Planck Inequality in terms of the **specific internal energy** 

## Dissipation in a continuum medium

□ The dissipation of a continuum medium is defined as:

$$\mathcal{D} \coloneqq -\rho(\dot{u} - \theta \dot{s}) + \boldsymbol{\sigma} \colon \mathbf{d} \ge 0$$

corresponding to the Clausius-Planck Inequality.

□ In terms of the Helmholtz free energy, dissipation may be written as:

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

Hypotheses assumed
Infinitesimal deformation:  $\begin{cases} \mathbf{d}(\mathbf{x},t) = \dot{\mathbf{\varepsilon}}(\mathbf{x},t) \\ \rho(\mathbf{x},t) = \rho_0 \end{cases}$ 

Hence, the dissipation may be written as:

$$\mathcal{D} = -\rho_0 \left( \dot{\boldsymbol{\psi}} + s \dot{\boldsymbol{\theta}} \right) + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} \ge 0$$

**Dissipation** of a continuum medium in terms of the Helmholtz free energy assuming infinitesimal deformation

# 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**:

$$\mathbb{V} \coloneqq \{\mathbf{v}_1, \mathbf{v}_2, ..., \mathbf{v}_{n_v}\} \quad \mathbf{v}_i(\mathbf{x}, t) \ i \in \{1, 2, ..., n_v\}$$

which will be classified into:

**Free variables:** 

$$\mathbb{F} := \left\{ \lambda_1, \lambda_2, \dots, \lambda_{n_F} \right\} \quad \lambda_i(\mathbf{x}, t) \ i \in \left\{ 1, 2, \dots, n_F \right\}$$

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

$$\dot{\lambda}_i(\mathbf{x},t) = \frac{\partial \lambda_i(\mathbf{x},t)}{\partial t} \to \text{any}$$

### Sets of thermo-mechanical variables

Internal/Hidden variables:

$$\mathbb{I} := \left\{ \alpha_1, \alpha_2, \dots, \alpha_{n_I} \right\} \quad \alpha_i(\mathbf{x}, t) \ i \in \{1, 2, \dots, n_I\}$$

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

$$\dot{\alpha}_{i} = \frac{\partial \alpha_{i}(\mathbf{x}, t)}{\partial t} = \xi_{i} \left( \underbrace{\lambda(\mathbf{x}, t), \boldsymbol{\alpha}(\mathbf{x}, t)}_{\text{instantaneous}} \right) \quad i \in \{1, 2, \dots, n_{I}\}$$

which account for micro-structural mechanisms.

**Dependent variables:**  $\mathbb{D} := \{d_1, d_2, ..., d_{n_D}\} \quad d_i(\mathbf{x}, t) \ i \in \{1, 2, ..., n_D\}$ are the remaining of the variables of the problem (depending on the previous ones):  $d_i = \gamma_i(\lambda, \alpha) \rightarrow \dot{d}_i = \varphi_i(\lambda, \alpha, \dot{\lambda}) \ i \in \{1, 2, ..., n_D\}$ 

 $\mathbb{V} = \mathbb{F} \cup \mathbb{I} \cup \mathbb{D} \qquad \mathbb{F} \cap \mathbb{I} = \mathbb{F} \cap \mathbb{D} = \mathbb{I} \cap \mathbb{D} = \emptyset$ 

### **Example:**

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

**Free** variables: 
$$\mathbb{F} := \{\rho, \varepsilon\}$$
  $\forall \dot{\rho}, \forall \dot{\varepsilon}$ 

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

$$\psi = \psi(\rho, \varepsilon, \alpha)$$

$$\dot{\psi} = \gamma(\rho, \varepsilon, \alpha, \dot{\rho}, \dot{\varepsilon}, \dot{\alpha}(\rho, \varepsilon, \alpha)) = \underbrace{\psi(\rho, \varepsilon, \alpha, \dot{\rho}, \dot{\varepsilon})}_{\text{not depending on the internal variable evolution, } \dot{\alpha}}_{\sigma = \sigma(\rho, \varepsilon, \alpha)}$$

$$\dot{\sigma} = \varphi(\rho, \varepsilon, \alpha, \dot{\rho}, \dot{\varepsilon}, \underbrace{\dot{\alpha}(\rho, \varepsilon, \alpha)}_{\text{provided by the evolution equation}}) = \dot{\sigma}(\rho, \varepsilon, \alpha, \dot{\rho}, \dot{\varepsilon})$$

## Elements of a constitutive model

□ 1) Definition of the free variables of the problem

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

□ 2) Choice of the internal variables of the problem

$$\mathbb{I} := \underbrace{\{\alpha_1, \alpha_2, \dots, \alpha_{n_l}\}}_{\boldsymbol{\alpha}}$$

□ 3) Definition of the corresponding evolution equations,

$$\dot{\alpha}_i = \dot{\alpha}_i(\lambda, \alpha) \quad i \in \{1, 2, \dots n_I\}$$

□ 4) Postulate a specific form of the free energy:

 $\psi = \psi(\lambda, \alpha, t) \rightarrow \begin{cases} \text{provides the constitutive equation} \\ \text{through the dissispation inequality} \end{cases}$ 

# **Example: Thermo-elastic material**

#### Linear elastic material

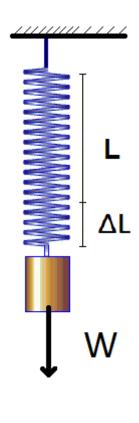
Linear relation stresses-strains

$$\Box 1D: \quad \frac{W}{A} = E \frac{\Delta L}{L} \quad \Box \quad \overline{\sigma} = E \varepsilon$$

**3D:** 
$$\boldsymbol{\sigma} = \mathbb{C} : \boldsymbol{\varepsilon}$$
 or  $\boldsymbol{\sigma}_{ij} = \mathbb{C}_{ijkl} \boldsymbol{\varepsilon}_{kl}$ 

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

$$\begin{cases} \boldsymbol{\sigma} = \lambda tr(\boldsymbol{\varepsilon}) + 2\mu\boldsymbol{\varepsilon} \\ \boldsymbol{\sigma}_{ij} = \lambda \varepsilon_{kk} \delta_{ij} + 2\mu \varepsilon_{ij} & i, j \in \{1, 2, 3\} \end{cases}$$



# Tensor Notation (reminder)

- Open product
  - Of two first-order tensors:

$$\begin{bmatrix} \mathbf{a} \otimes \mathbf{b} \end{bmatrix}_{i,j} = a_i b_j$$
  
r: 
$$\begin{bmatrix} \mathbf{A} \otimes \mathbf{B} \end{bmatrix}_{ijkl} = A_{ij} B_{kl}$$

- Between two second order tensor:
- Identity tensors
  - First order identity tensor

$$\begin{bmatrix} \mathbf{1} \end{bmatrix}_{ij} = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \quad i, j \in \{1, 2, 3\}$$

Second order tensor identity tensor

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

#### REMARK

**Einstein notation** (summation of repeated indices) is considered

# Thermo-elastic material (reminder)

#### Linear thermo-elastic material

□ Adding the thermal effects (thermoelasticity)

$$\begin{cases} \boldsymbol{\sigma} = \lambda tr(\boldsymbol{\varepsilon}) + 2\mu\boldsymbol{\varepsilon} - \boldsymbol{\beta}\Delta\boldsymbol{\theta}\mathbf{1} \\ \boldsymbol{\sigma}_{ij} = \lambda\boldsymbol{\varepsilon}_{kk}\boldsymbol{\delta}_{ij} + 2\mu\boldsymbol{\varepsilon}_{ij} - (\boldsymbol{\beta}\Delta\boldsymbol{\theta})\boldsymbol{\delta}_{ij} & i, j \in \{1, 2, 3\} \end{cases}$$

 $\beta = \rightarrow$  Thermal property  $\alpha = \frac{1-2\nu}{\beta} \rightarrow$  Thermal expansion coefficient

# **Coleman's Method**

□ Theorem

$$\mathcal{D}(x, y, \dot{x}, \dot{y}) = f(x, y)\dot{x} + g(x, y)\dot{y} \ge 0 \quad \forall \dot{x}, \dot{y} \Longrightarrow \begin{cases} f(x, y) = 0\\ g(x, y) = 0 \end{cases}$$

□ Proof:

■ Taking 
$$\dot{y} = 0$$
  $\longrightarrow$   $\mathcal{D} = f(x, y)\dot{x} \ge 0$   $\forall \dot{x}$   
If  $f(x, y) < 0$  taking  $\dot{x} > 0$   $\longrightarrow$   $\mathcal{D} = f(x, y)\dot{x} < 0$  NOT POSSIBLE  
If  $f(x, y) > 0$  taking  $\dot{x} < 0$   $\longrightarrow$   $\mathcal{D} = f(x, y)\dot{x} < 0$   $f(x, y) = 0$   
■ Taking  $\dot{x} = 0$   $\longrightarrow$   $\mathcal{D} = g(x, y)\dot{y} \ge 0$   $\forall \dot{y}$ 

If 
$$g(x, y) < 0$$
 taking  $\dot{y} > 0 \implies \mathcal{D} = g(x, y)\dot{y} < 0$   
If  $g(x, y) > 0$  taking  $\dot{y} < 0 \implies \mathcal{D} = g(x, y)\dot{y} < 0$   
 $f(x, y) = 0$ 

## **Elastic Material formulation**

- Variable sets definition
  - Free variables:  $\mathbb{F} := \{ \epsilon \}$
  - Internal variables:  $I := \{ \emptyset \} \rightarrow \text{No evolution equation}$

• Dependent: 
$$\mathbb{D} := \{\sigma, \psi\}$$
  
Potential  $\rho_0 \psi(\varepsilon) = \frac{1}{2}\varepsilon : \mathbb{C} : \varepsilon$ 

$$\begin{cases} \sigma(\varepsilon) \to \dot{\sigma} = \frac{\partial \sigma(\varepsilon)}{\partial \varepsilon} : \dot{\varepsilon} \\ \rho_0 \psi(\varepsilon) \to \rho_0 \dot{\psi} = \frac{\partial \rho_0 \psi(\varepsilon)}{\partial \varepsilon} : \dot{\varepsilon} \end{cases}$$

- Helmholtz free energy:
- Dissipation Isothermal case  $\mathcal{D} = -\rho_0 (\dot{\psi} + s\dot{\theta}) + \sigma : \dot{\epsilon} \ge 0 \quad \Rightarrow \quad \mathcal{D} = (\sigma - \frac{\partial \rho_0 \psi(\epsilon)}{\partial \epsilon}) : \dot{\epsilon} \ge 0 \quad \forall \dot{\epsilon} \Rightarrow f(\epsilon) = 0$   $\underbrace{\sigma = \frac{\partial \rho_0 \psi(\epsilon)}{\partial \epsilon} = \mathbb{C} : \epsilon}_{f(\epsilon)} \quad \Rightarrow \quad \mathcal{D} = 0$ Constitute equation  $\sigma = \Sigma(\epsilon)$

## **Thermo-elastic Material formulation**

Variable sets definition

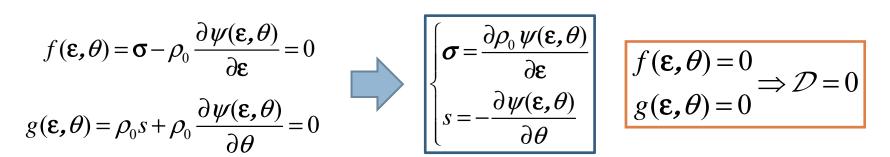
Free variables:  $\mathbb{F} := \{ \boldsymbol{\varepsilon}, \boldsymbol{\theta} \}$ Internal variables:  $\mathbb{I} := \{ \boldsymbol{\varnothing} \}$ Dependent:  $\mathbb{D} := \{ \boldsymbol{\sigma}, \boldsymbol{\psi} \} \rightarrow \begin{cases} \dot{\boldsymbol{\sigma}} = \frac{\partial \boldsymbol{\sigma}(\boldsymbol{\varepsilon}, \boldsymbol{\theta})}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \frac{\partial \boldsymbol{\sigma}(\boldsymbol{\varepsilon}, \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} : \dot{\boldsymbol{\theta}} \\ \rho_0 \dot{\boldsymbol{\psi}} = \frac{\partial \rho_0 \boldsymbol{\psi}(\boldsymbol{\varepsilon}, \boldsymbol{\theta})}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} + \frac{\partial \rho_0 \boldsymbol{\psi}(\boldsymbol{\varepsilon}, \boldsymbol{\theta})}{\partial \boldsymbol{\theta}} : \dot{\boldsymbol{\theta}} \end{cases}$ Potential definition

• Helmholtz free energy: 
$$\rho_0 \Psi(\varepsilon, \theta) = \frac{1}{2}\varepsilon : \mathbb{C} : \varepsilon - \beta \underbrace{(\theta - \theta_0)}_{\Delta \theta} \mathbf{I}$$

**Dissipation**  $\mathcal{D} = -\rho_0 \left( \dot{\psi} + s\dot{\theta} \right) + \sigma : \dot{\varepsilon} \ge 0$  $\mathcal{D} = \left( \sigma - \frac{\partial \rho_0 \psi(\varepsilon, \theta)}{\partial \varepsilon} \right) : \dot{\varepsilon} - \left( \rho_0 s + \frac{\partial \rho_0 \psi(\varepsilon, \theta)}{\partial \theta} \right) : \dot{\theta} \ge 0 \quad \forall \dot{\varepsilon}, \dot{\theta}$  $\underbrace{f(\varepsilon, \theta)}_{f(\varepsilon, \theta)} = \underbrace{f(\varepsilon, \theta)}_{g(\varepsilon, \theta)} : \dot{\theta} \ge 0 \quad \forall \dot{\varepsilon}, \dot{\theta}$ 

## **Thermo-elastic Material formulation**

Using the Coleman's method:



and differentiating the Helmholtz free energy:

# END OF LECTURE 1

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