Problem Set 8

CIVIL-425: Continuum Mechanics and Applications

01 May 2025

Exercise 1: Thermodynamic potentials

Consider a thermoelastic material in the Lagrangian description, with internal energy per unit mass:

$$U(\boldsymbol{C}, N, \boldsymbol{Q}),$$

where:

- $\boldsymbol{C}$ is the right Cauchy-Green deformation tensor,
- N is the entropy per unit mass,
- $\boldsymbol{Q}$ is a vector of internal variables.

(a) Define the thermodynamic potentials: Helmholtz free energy $A(\boldsymbol{C}, T, \boldsymbol{Q})$, enthalpy $H(\boldsymbol{S}^e, N, \boldsymbol{Q})$, and Gibbs free energy $G(\boldsymbol{S}^e, T, \boldsymbol{Q})$ via Legendre transforms of the internal energy $U(\boldsymbol{C}, N, \boldsymbol{Q})$.

(b) Derive expressions for A, H, and G, and then compute H from G, and A from H.

(c) Let the internal variable be a scalar damage variable $d \in [0, 1]$. Let the Helmholtz free energy per unit mass be:

$$A(\boldsymbol{C}, T, d) = \frac{1}{2R}(1-d)^2 \boldsymbol{C} : \mathbb{C}_0 : \boldsymbol{C} - \left[c\,T \ln\left(\frac{T}{T_0}\right) - c(T - T_0) \right].$$

- Write the corresponding thermodynamic forces
- State the dissipation inequality for this material.

Solution

(a) Thermodynamic Potentials via Legendre Transform

Helmholtz free energy:

$$A(\boldsymbol{C}, T, \boldsymbol{Q}) = \inf_{N} \left\{ U(\boldsymbol{C}, N, \boldsymbol{Q}) - TN \right\}.$$

Enthalpy:

$$RH(\boldsymbol{S}^e, N, \boldsymbol{Q}) = \inf_{\boldsymbol{C}} \left\{ RU(\boldsymbol{C}, N, \boldsymbol{Q}) - \boldsymbol{S}^e : \tfrac{1}{2}\boldsymbol{C} \right\}.$$

Gibbs free energy:

$$RG(\boldsymbol{S}^e, T, \boldsymbol{Q}) = \inf_{\boldsymbol{C}} \left\{ RA(\boldsymbol{C}, T, \boldsymbol{Q}) - \tfrac{1}{2}\boldsymbol{C} : \boldsymbol{S}^e \right\}.$$

Note: All potentials are per unit mass. To convert derivatives to per unit volume, multiply by the reference mass density R.

(b) Derivation Between Potentials

From the definition of G and A, we get:

$$G(\boldsymbol{S}^e, T, \boldsymbol{Q}) = \inf_{\boldsymbol{C}} \left\{ \inf_{N} \left(U(\boldsymbol{C}, N, \boldsymbol{Q}) - TN \right) - \tfrac{1}{2R} \boldsymbol{C} : \boldsymbol{S}^e \right\}.$$

So, combining these steps:

$$G(\boldsymbol{S}^e, T, \boldsymbol{Q}) = \inf_{\boldsymbol{C}, N} \left\{ U(\boldsymbol{C}, N, \boldsymbol{Q}) - TN - \tfrac{1}{2R} \boldsymbol{C} : \boldsymbol{S}^e \right\}.$$

Recovering Enthalpy from Gibbs:

$$H(\boldsymbol{S}^e, N, \boldsymbol{Q}) = \inf_{T} \left\{ G(\boldsymbol{S}^e, T, \boldsymbol{Q}) + TN \right\}.$$

Recovering Helmholtz free energy from Enthalpy:

$$A(\boldsymbol{C}, T, \boldsymbol{Q}) = \inf_{\boldsymbol{S}^e, N} \left\{ H(\boldsymbol{S}^e, N, \boldsymbol{Q}) - \boldsymbol{S}^e : \tfrac{1}{2R} \boldsymbol{C} - TN \right\}$$

(c) Helmholtz Free Energy and Dissipation with Scalar Damage

Derived thermodynamic quantities:

$$\begin{aligned} \boldsymbol{S}^e &= 2R \frac{\partial A}{\partial \boldsymbol{C}} = 2(1-d)^2 \, \mathbb{C}_0 : \boldsymbol{C}, \\ N &= -\frac{\partial A}{\partial T} = c \ln \left(\frac{T}{T_0} \right), \\ Y &= -R \frac{\partial A}{\partial d} = 2(1-d) \, \boldsymbol{C} : \mathbb{C}_0 : \boldsymbol{C}. \end{aligned}$$

In the Lagrangian configuration, the Clausius-Duhem inequality (per unit reference volume) is:

$$\mathcal{D} = \boldsymbol{S} : \tfrac{1}{2} \dot{\boldsymbol{C}} - R\dot{U} + RT\dot{N} + \nabla \cdot \boldsymbol{h} \geq 0.$$

Substituting $dU = dA + TdN$, and using the chain rule:

$$\mathcal{D} = Y\dot{d} - \frac{1}{T} \boldsymbol{h} \cdot \nabla T \geq 0.$$

Thus, for admissible thermomechanical processes:

$$2(1-d) \left(\boldsymbol{C} : \mathbb{C}_0 : \boldsymbol{C} \right) \dot{d} \geq \frac{1}{T} \boldsymbol{h} \cdot \nabla T.$$

This ensures non-negative dissipation from damage and heat conduction.

This shows:

- If there is no heat flux, the damage evolution must satisfy $2(1-d)\dot{d} \left(\boldsymbol{C} : \mathbb{C}_0 : \boldsymbol{C} \right)$, which reduces to $\dot{d} \geq 0$, i. e. damage irreversibility
- If there is no damage, the heat flux must satisfy Fourier's law direction: $\boldsymbol{h} \cdot \nabla T \leq 0$.

These relations are consistent with the first and second laws of thermodynamics in the Lagrangian formulation.