Continuum mechanics
IV. Thermodynamics

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0. Time-derivative of volume integral in Euler formulation

Scalar field $\Phi(\mathbf{y}, t)$ (eg. density, concentration)
Volume integral: over current (deformed) domain Ω_t:

$$\mathcal{I} = \int_{\Omega_t} \Phi(\mathbf{y}, t) dy$$

Time-derivative of volume integral: (as we saw earlier)

$$\frac{D\mathcal{I}}{Dt} = \int_{\Omega_t} \left[\frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial y^i} \left(\Phi\, v^i \right) \right] dy = \int_{\Omega_t} \left[\frac{\partial \Phi}{\partial t} + v^i \frac{\partial \Phi}{\partial y^i} + \Phi \frac{\partial v^i}{\partial y^i} \right] dy$$

$$= \int_{\Omega_t} \left[\frac{D\Phi}{Dt} + \Phi \frac{\partial v^i}{\partial y^i} \right] dy$$

Application for $\Phi \equiv \rho$: mass-conservation (continuity eqn.)

$$0 = \frac{D\rho}{Dt} + \rho \frac{\partial v^i}{\partial y^i} = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial y^i} (\rho v^i)$$

1. Thermodynamical variables

Basic state variables:

- **temperature** T: intensive quantity, ie. there is no "specific temperature" or "temperature per unit mass",
- **internal energy** U and **thermodynamical entropy** S: extensive quantities, one defines specific internal energy ϵ and specific entropy η so that:

$$U = \int_{\Omega_t} \rho\, \epsilon\, dy \qquad , \qquad S = \int_{\Omega_t} \rho\, \eta\, dy$$

Remark: the physical nature of these quantities is linked to statistical mechanics beyond the scope of this lecture. We can consider them as certain averaged characteristics of the particle nature of the continuum.

2. First law of thermodynamics: conservation of energy

Theorem: The change of the kinetic and internal energy $\delta(E_k + U)$ of a body Ω_t is equal to the work δW of mechanical forces and heat δQ.

$$\frac{DE_k}{Dt} + \frac{DU}{Dt} = \frac{DW}{Dt} + \frac{DQ}{Dt}$$

Kinetic energy E_k**:**

$$E_k = \frac{1}{2} \int_{\Omega_t} \rho\, |\mathbf{v}|^2\, dy = \frac{1}{2} \int_{\Omega_t} \rho\, v^i\, v_i\, dy$$

Internal energy U**:**

$$U = \int_{\Omega_t} \rho\, \epsilon\, dy$$

Volume integrals in Euler formulation $\rightarrow$ apply formula for time-derivatives.

2.1. Time-derivative of kinetic energy E_k

Time-derivative of E_k: (volume integral in Euler formulation):

$$\frac{DE_k}{Dt} = \frac{1}{2}\int_{\Omega_t} \frac{D(\rho\,\mathbf{v}^2)}{Dt}\,dy + \frac{1}{2}\int_{\Omega_t} \rho\,\mathbf{v}^2\,\frac{\partial v^i}{\partial y^i}\,dy$$

$$= \frac{1}{2}\int_{\Omega_t} \rho\,\frac{D(\mathbf{v}^2)}{Dt}\,dy + \frac{1}{2}\int_{\Omega_t} \mathbf{v}^2\,\frac{D\rho}{Dt}\,dy + \frac{1}{2}\int_{\Omega_t} \rho\,\mathbf{v}^2\,\frac{\partial v^i}{\partial y^i}\,dy$$

$$= \frac{1}{2}\int_{\Omega_t} \rho\,\frac{D(\mathbf{v}^2)}{Dt}\,dy + \frac{1}{2}\int_{\Omega_t} \underbrace{\mathbf{v}^2\left(\frac{D\rho}{Dt} + \rho\,\frac{\partial v^i}{\partial y^i}\right)dy}_{=0\text{ by continuity eqn.}}$$

$$= \frac{1}{2}\int_{\Omega_t} \rho\,\frac{D(\mathbf{v}^2)}{Dt}\,dy$$

2.2. Time-derivative of internal energy U

Time-derivative of U: (volume integral in Euler formulation):

$$\frac{DU}{Dt} = \int_{\Omega_t} \frac{D(\rho\,\epsilon)}{Dt}\,dy + \int_{\Omega_t} \rho\,\epsilon\,\frac{\partial v^i}{\partial y^i}\,dy$$

$$= \int_{\Omega_t} \rho\,\frac{D\epsilon}{Dt}\,dy + \int_{\Omega_t} \epsilon\,\frac{D\rho}{Dt}\,dy + \int_{\Omega_t} \rho\,\epsilon\,\frac{\partial v^i}{\partial y^i}\,dy$$

$$= \int_{\Omega_t} \rho\,\frac{D\epsilon}{Dt}\,dy + \int_{\Omega_t} \underbrace{\epsilon\left(\frac{D\rho}{Dt} + \rho\,\frac{\partial v^i}{\partial y^i}\right)dy}_{=0\text{ by continuity eqn.}}$$

$$= \int_{\Omega_t} \rho\,\frac{D\epsilon}{Dt}\,dy$$

2.3. Time-derivative of heat

$$\frac{DQ}{Dt} = -\int_{\partial\Omega_t} \mathbf{q}\cdot\mathbf{n}\, d\Gamma + \int_{\Omega_t} \rho\, r\, dy = -\int_{\partial\Omega_t} q^i\, n_i\, d\Gamma + \int_{\Omega_t} \rho\, r\, dy$$

Here, $\mathbf{q} = q^i\, \mathbf{g}_i$ is the heat flux $[J\, m^{-2}\, s^{-1}]$ and r is the specific heat source intensity $[J\, kg^{-1}\, s^{-1}]$.
The minus sign appears because $\mathbf{n}$ is the *external* normal.

By the Divergence theorem:

$$\frac{DQ}{Dt} = -\int_{\Omega_t} \frac{\partial q^i}{\partial y^i}\, dy + \int_{\Omega_t} \rho\, r\, dy$$

2.4. Time-derivative of mechanical work = power

Power of surfacic traction forces and body-forces:

$$\frac{DW}{Dt} = \int_{\partial\Omega_t} \tau^{ij}\, n_j\, v_i\, d\Gamma + \int_{\Omega_t} \rho\, f^i\, v_i\, dy$$

By the Divergence theorem:

$$\frac{DW}{Dt} = \int_{\Omega_t} \frac{\partial(\tau^{ij}\, v_i)}{\partial y^j}\, dy + \int_{\Omega_t} \rho\, f^i\, v_i\, dy$$

2. First law of thermodynamics: conservation of energy

$$\frac{DE_k}{Dt} + \frac{DU}{Dt} = \frac{DW}{Dt} + \frac{DQ}{Dt}$$

For any $\omega_t \subset \Omega_t$, subdomain of the continuum:

$$\int_{\omega_t} \left(\frac{\rho}{2} \frac{D(\mathbf{v}^2)}{Dt} + \rho \frac{D\epsilon}{Dt} \right) dy = \int_{\omega_t} \left(\rho\, r - \frac{\partial q^i}{\partial y^i} + \frac{\partial (\tau^{ij}\, v_i)}{\partial y^j} + \rho\, f^i\, v_i \right) dy$$

Hence (pointwise formulation with worked-out derivatives):

$$\rho\, v_i \frac{Dv^i}{Dt} + \rho \frac{D\epsilon}{Dt} = \rho\, r - \frac{\partial q^i}{\partial y^i} + \frac{\partial \tau^{ij}}{\partial y^j} v_i + \tau^{ij} \frac{\partial v_i}{\partial y^j} + \rho\, f^i\, v_i$$

And

$$\rho \frac{D\epsilon}{Dt} = \rho\, r - \frac{\partial q^i}{\partial y^i} + \tau^{ij} \frac{\partial v_i}{\partial y^j} + \underbrace{v_i \left(-\rho \frac{Dv^i}{Dt} + \frac{\partial \tau^{ij}}{\partial y^j} + \rho\, f^i \right)}_{= 0 \text{ by force-equilibrium}}$$

2. First law of thermodynamics: energy equation

Energy equation: in cartesian coordinates:

$$\boxed{\rho \frac{D\epsilon}{Dt} = \rho\, r - \frac{\partial q^i}{\partial y^i} + \tau^{ij} \frac{\partial v_i}{\partial y^j}}$$

In curvilinear coordinates:

$$\boxed{\rho \frac{D\epsilon}{Dt} = \rho\, r - \nabla_i q^i + \tau^{ij}\, \nabla_j v_i}$$

3. Second law of thermodynamics: entropy

Theorem: The change of total entropy in the body Ω_t over time is greater or equal to the sum of entropy flow over the boundary $\partial\Omega_t$ from the exterior and the entropy produced by internal heat sources on Ω_t.

Total entropy: units $[J/K]$, defined up to a constant by

$$dS = \frac{dQ}{T}$$

Clausius-Duhem inequality: mathematical form of the 2nd law:

$$\frac{DS}{Dt} \geq \int_{\Omega_t} \frac{\rho\, r}{T} dy - \int_{\partial\Omega_t} \frac{1}{T} \mathbf{q} \cdot \mathbf{n}\, d\Gamma$$

For reversible processes we have the "$=$" sign,
for **irreversible** ones we have the "$>$" sign.

3.1. Clausius-Duhem inequality

Using the specific entropy η:

$$\frac{D}{Dt}\left(\int_{\Omega_t} \rho\, \eta\, dy\right) \geq \int_{\Omega_t} \frac{\rho\, r}{T} dy - \int_{\partial\Omega_t} \frac{1}{T} \mathbf{q} \cdot \mathbf{n}\, d\Gamma$$

Time-derivative of an integral formula and the Divergence theorem:

$$\int_{\Omega_t} \rho \frac{D\eta}{Dt}\, dy + \underbrace{\int_{\Omega_t} \eta \frac{D\rho}{Dt}\, dy + \int_{\Omega_t} \rho\, \eta \frac{\partial v^i}{\partial y^i}\, dy}_{=0 \text{ by the continuity eqn.}} - \int_{\Omega_t} \frac{\rho\, r}{T} dy + \int_{\Omega_t} \frac{\partial}{\partial y^i}\left(\frac{q^i}{T}\right) dy \geq 0$$

Clausius-Duhem inequality in the integral form:

$$\int_{\Omega_t} \rho \frac{D\eta}{Dt}\, dy - \int_{\Omega_t} \frac{\rho\, r}{T} dy + \int_{\Omega_t} \frac{\partial}{\partial y^i}\left(\frac{q^i}{T}\right) dy \geq 0$$

for any subdomain Ω_t of the continuum.

3.1. Clausius-Duhem inequality

Local (pointwise) form of Clausius-Duhem inequality:

$$\rho\,\dot{\eta} - \frac{\rho\,r}{T} + \frac{\partial}{\partial y^i}\left(\frac{q^i}{T}\right) \geq 0$$

In cartesian coordinates

$$\rho\,T\,\dot{\eta} - \rho\,r + \frac{\partial q^i}{\partial y^i} - \frac{q^i}{T}\frac{\partial T}{\partial y^i} \geq 0$$

In curvilinear coordinates:

$$\rho\,T\,\dot{\eta} - \rho\,r + \nabla_i q^i - \frac{q^i}{T}\nabla_i T \geq 0$$

3.2. Clausius-Duhem inequality with Helmholz free energy

Physical meaning of entropy: by itself S does not have any meaning. However, $dS\ T$ is the increase of the portion of internal energy which cannot be used to do work.

Specific Helmholz free energy φ: the density of mechanically exploitable internal energy:

$$\varphi = \epsilon - T\,\eta$$

Derive φ in time

$$\dot{\varphi} = \dot{\epsilon} - \dot{T}\,\eta - T\,\dot{\eta}$$

and substitute into the Clausius-Duhem inequality.

3.2. Clausius-Duhem inequality with Helmholz free-energy

Express $\nabla_i q^i$ from the **Energy equation**:

$$\nabla_i q^i = -\rho\,\dot{\epsilon} + \rho\,r + \tau^{ij}\,\nabla_j v_i$$

Plug it into Clausius-Duhem inequality:

$$\begin{aligned} 0 &\geq -\rho\,T\,\dot{\eta} + \rho\,r - \nabla_i q^i + \frac{q^i}{T}\,\nabla_i T \\ &= -\rho\,T\,\dot{\eta} + \rho\,r + \rho\,\dot{\epsilon} - \rho\,r - \tau^{ij}\,\nabla_j v_i + \frac{q^i}{T}\,\nabla_i T \\ &= \rho\,\dot{\varphi} + \rho\,\dot{T}\,\eta - \tau^{ij}\,\nabla_j v_i + \frac{q^i}{T}\,\nabla_i T \end{aligned}$$

Here we used $\dot{\varphi} = \dot{\epsilon} - \dot{T}\,\eta - T\,\dot{\eta}$.

Dissipation inequality:

$$\underbrace{\rho\,\dot{\varphi} + \rho\,\dot{T}\,\eta - \tau^{ij}\,\nabla_j v_i}_{\equiv -\delta \ldots \text{internal dissipation}} \quad + \frac{q^i}{T}\,\nabla_i T \leq 0$$