Analysis of dynamical processes in solids

The purpose of this text, mostly inspired by the classical textbooks [1, 3, 5], is to collect some of the topics presented in a series of lectures at TU München in June–July 2014 with the intention to show how partial differential equations of mechanics and thermomechanics can be derived from a small number of basic physical principles. It is divided into two sections and deals exclusively with the modeling issues. Some comments on qualitative analysis of the resulting PDE systems will be included in a next iteration. For the moment, we assume that all functions describing the physical processes discussed here have sufficient regularity for the correctness of the mathematical developments.

1 Mechanics

We first specify the terminology and introduce the main concepts.

1.1 Space, mass, and motion

In a time interval $[0,T]$, consider a moving domain $\mathcal{B}(t) \subset \mathbb{R}^3$, (open, bounded, connected, smooth) for $t \in [0,T]$, filled with mass. In the space-time domain $\mathrm{Dom}(T) := \{(y,t) \in \mathbb{R}^3 \times [0,T]; y \in \mathcal{B}(t)\}$, we postulate the existence of a function $\rho : \mathrm{Dom}(T) \to [0,\infty)$, the *mass density*, such that the mass of any subdomain $\Omega(t) \subset \mathcal{B}(t)$ at time t is given by the integral

$$m(\Omega(t),t) = \int_{\Omega(t)} \rho(y,t)\,\mathrm{d}y. \tag{1.1}$$

We assume that points $y = (y_1,y_2,y_3) \in \mathcal{B}(t)$ correspond to particles in movement. The velocity of a particle which at time t occupies the point y is represented by the vector $v(y,t)$, $v = (v^1,v^2,v^3)$.

We further introduce a fixed reference body $\mathcal{B}$ with reference coordinates $x = (x_1,x_2,x_3) \in \mathcal{B}$ (the *Lagrange coordinates*), while the actual configuration will be equipped with actual coordinates $y = (y_1,y_2,y_3) \in \mathcal{B}(t)$ (the *Euler coordinates*).

Let now $\Omega \subset \mathcal{B}$ be an arbitrary subdomain (control volume) in the reference configuration, and let $u(x,t) = (u^1(x,t),u^2(x,t),u^3(x,t))$ be the displacement at time t of the particle with reference coordinate $x \in \Omega$. The actual position of this particle at time t will then be $y = x + u(x,t)$. Particles from a reference domain Ω occupy at time t the actual domain $\Omega(t)$ given as

$$\Omega(t) = \{y \in \mathcal{B}(t) : y = x + u(x,t), x \in \Omega\}, \tag{1.2}$$

see Figure 1. We denote by $D(u)$ the Jacobi matrix of u, that is,

$$(D(u))_{ij}(x,t) = \frac{\partial u^i}{\partial x_j}(x,t), \quad i,j = 1,2,3, \tag{1.3}$$

and adopt the following hypothesis.

Hypothesis 1.1 *The transformation* $x \mapsto x + u(x,t)$ *is for every* $t \in [0,T]$ *a diffeomorphism from* $\mathcal{B}$ *to* $\mathcal{B}(t)$, *and its Jacobian* $J(x,t) := \det\,(I + D(u)(x,t))$ *is positive for all* $x \in \mathcal{B}$ *and* $t \in [0,T]$.

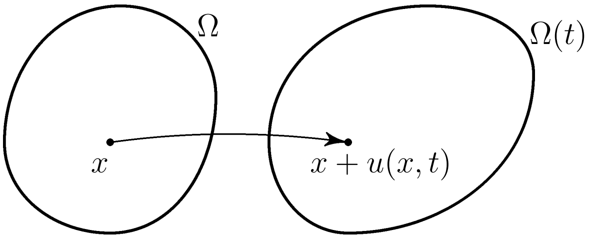

Figure 1: Deformation of a body

The velocity of the particle x in reference coordinates is

$$\frac{\partial u}{\partial t}(x,t) = v(x + u(x,t), t), \tag{1.4}$$

which is an ordinary differential equation for $u(x,\cdot)$ if $v(y,t)$ is known.

Our first physical principle is

F1. Mass conservation principle

Let $\rho_0(x)$ be the mass density in reference configuration. The deformation $x + u(x,t)$ leaves the mass of each control volume Ω invariant. In other words, by substitution,

$$\int_\Omega \rho_0(x)\,\mathrm{d}x = \int_{\Omega(t)} \rho(y,t)\,\mathrm{d}y = \int_\Omega \rho(x + u(x,t), t)\, J(x,t)\,\mathrm{d}x \tag{1.5}$$

for every $\Omega \subset \mathcal{B}$. This yields the mass conservation formula in Lagrange coordinates

$$\rho_0(x) = \rho(x + u(x,t), t)\, J(x,t) \tag{1.6}$$

for all x and t. To rewrite the mass conservation principle in Euler coordinates, we need the following Lemma.

Lemma 1.2 *For every* x *and* t *we have*

$$\frac{\partial J}{\partial t}(x,t) = \mathrm{div}_y v(x + u(x,t), t)\, J(x,t)\,, \tag{1.7}$$

where we denote

$$\mathrm{div}_y v(y,t) = \sum_{i=1}^{3} \frac{\partial v^i}{\partial y_i}(y,t).$$

Proof. Let P_3 be the permutation group of the set $\{1,2,3\}$. Then

$$J = \sum_{\pi \in P_3} \operatorname{sign} \pi \, J_{1\pi(1)} J_{2\pi(2)} J_{3\pi(3)},$$

where we denote by J_{ij} the entries of the matrix $I + D(u)$, that is, $J_{ij} = \delta_{ij} + \frac{\partial u^i}{\partial x_j}$ where δ_{ij} is Kronecker symbol $\delta_{ij} = 0$ if $i \neq j$, $\delta_{ij} = 1$ if $i = j$. Hence, by (1.4),

$$\frac{\partial}{\partial t} J_{i\pi(i)} = \sum_{k=1}^{3} \frac{\partial v^i}{\partial y_k} J_{k\pi(i)} \, .$$

For every $k \neq 1$, the sum

$$\sum_{\pi \in P_3} \operatorname{sign} \pi \, J_{k\pi(1)} J_{2\pi(2)} J_{3\pi(3)}$$

represents the determinant of a matrix with two identical rows, hence it vanishes. We conclude that

$$\sum_{\pi \in P_3} \operatorname{sign} \pi \, \frac{\partial J_{1\pi(1)}}{\partial t} J_{2\pi(2)} J_{3\pi(3)} = \frac{\partial v^1}{\partial y_1} J \, ,$$

and similarly for the other two terms in $\frac{\partial J}{\partial t}$, which yields the assertion. ■

We now differentiate the formula (1.6) in time and obtain, by virtue of (1.4) and (1.7), denoting by ∇_y the gradient with respect to y, that

$$0 = \left(\frac{\partial \rho}{\partial t} + \nabla_y \rho \cdot v + \rho \, \mathrm{div}_y v \right) (x + u(x,t), t) \, J(x,t),$$

which gives in terms of the Euler coordinate y the so-called *continuity equation*

$$\frac{\partial \rho}{\partial t}(y,t) + \mathrm{div}_y(\rho v)(y,t) = 0 \, . \tag{1.8}$$

Note that the quantity $J(x,t) - 1$ physically represents local volume change. Indeed, if we denote by $|\Omega|$ the Lebesgue measure of a set Ω, then the volume difference between $\Omega(t)$ and Ω is given by

$$|\Omega(t)| - |\Omega| = \int_{\Omega(t)} \mathrm{d}y - \int_{\Omega} \mathrm{d}x = \int_{\Omega} (J(x,t) - 1) \, \mathrm{d}x \, . \tag{1.9}$$

In particular, $J(x,t) = 1$ means that the process is volume preserving. For *incompressible materials*, all processes are volume preserving. A material is called *homogeneous*, if the reference density ρ_0 does not depend on x. Hence, by (1.9), homogeneous incompressible materials are characterized by the relation

$$\rho(y,t) = \rho_0 \, . \tag{1.10}$$

1.2 Force and momentum

We start with the physical postulate of

F2. Existence of volume and contact forces

We assume that there exists a volume force density function $g : \mathrm{Dom}(T) \to \mathbb{R}^3$ such that the force $F_{\mathrm{vol}}(\Omega(t))$ acting on each moving control volume $\Omega(t)$ is given by the integral

$$F_{\mathrm{vol}}(\Omega(t)) = \int_{\Omega(t)} g(y,t)\,\mathrm{d}y\,. \tag{1.11}$$

Furthermore, for points y on the boundary $\partial\Omega(t)$ of $\Omega(t)$ we denote by $n(y)$ the unit outward normal, by $\partial B_1(0)$ the unit sphere in $\mathbb{R}^3$, and assume that there exists a function $T : \mathrm{Dom}(T) \times \partial B_1(0) \to \mathbb{R}^3$ such that the contact force vector $F_{\mathrm{cont}}(\Omega(t))$ acting on each moving control volume $\Omega(t)$ through its boundary is given by the surface integral

$$F_{\mathrm{cont}}(\Omega(t)) = \int_{\partial\Omega(t)} T(y,t,n(y))\,\mathrm{d}s(y)\,. \tag{1.12}$$

An example of a volume force is the gravity, a classical contact force has the form $T(y,t,n) = -p(y,t)n$, where p is a scalar-valued function (the *pressure*).

F3. Conservation of momentum

This is a continuum mechanics variant of Newton's law of motion. We call

$$P(\Omega(t)) = \int_{\Omega(t)} \rho(y,t)\, v(y,t)\,\mathrm{d}y \tag{1.13}$$

the momentum associated with $\Omega(t)$. The conservation of momentum principle postulates that the total force acting on a body equals the time derivative of its momentum, that is,

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\Omega(t)) = F_{\mathrm{cont}}(\Omega(t)) + F_{\mathrm{vol}}(\Omega(t)). \tag{1.14}$$

Let $\Omega(t)$ be associated with a reference control volume Ω as in (1.2). By (1.4), (1.6), we have

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\Omega(t)) = \frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} \rho_0(x)\frac{\partial u}{\partial t}(x,t)\,\mathrm{d}x = \int_{\Omega} \rho_0(x)\frac{\partial^2 u}{\partial t^2}(x,t)\,\mathrm{d}x. \tag{1.15}$$

Differentiating Eq. (1.4) in time yields, for $i = 1,2,3$,

$$\begin{aligned}
\frac{\partial^2 u^i}{\partial t^2}(x,t) &= \left(\frac{\partial v^i}{\partial t}(x+u(x,t),t) + \sum_{k=1}^{3}\frac{\partial v^i}{\partial y_k}(x+u(x,t),t)\frac{\partial u^k}{\partial t}(x,t)\right)\\
&= \left(\frac{\partial v^i}{\partial t} + \sum_{k=1}^{3}\frac{\partial v^i}{\partial y_k}v^k\right)(x+u(x,t),t)\,.
\end{aligned}$$

Hence, by substitution and (1.6), we have in (1.15) that

$$\frac{\mathrm{d}}{\mathrm{d}t} P(\Omega(t)) = \int_{\Omega(t)} \rho(y,t)\left(\frac{\partial v}{\partial t} + (v\cdot\nabla_y)v\right)(y,t)\,\mathrm{d}y\,. \tag{1.16}$$

We now derive a representation formula for the contact force $F_{\mathrm{cont}}(\Omega(t))$.

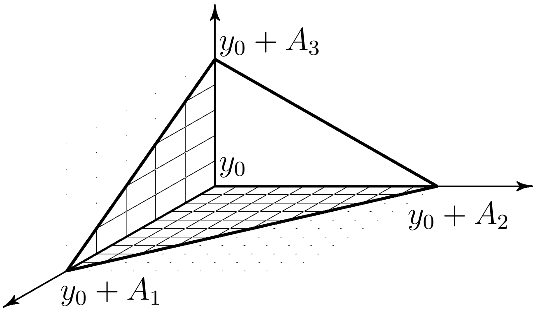

Figure 2: Balance of contact forces

Assume that $\Omega(t)$ is a simplex as on Figure 2, with vertices $y_0, y_0 + A_j$, $j = 1, 2, 3$. The vectors A_j are scalar multiples of the unit coordinate vectors $e_j = (e_j^1, e_j^2, e_j^3)$, with $e_j^i = \delta_{ij}$ (the Kronecker symbol). More precisely, we fix an arbitrary unit vector $n^* = \sum_{j=1}^3 n_j e_j$ with $n_j \neq 0$ and $n_1^2 + n_2^2 + n_3^2 = 1$, and and an arbitrary (small) $h > 0$, and set

$$A_j = \frac{h}{n_j} e_j \qquad \text{for } \ j = 1, 2, 3.$$

The equation of the plane S_0 determined by the three points $y_0 + A_j$, $j = 1, 2, 3$, reads

$$y \in S_0 \iff n^* \cdot (y - y_0) = h\,,$$

hence n^* is the unit outward normal vector to $\Omega(t)$ at each point of $\Gamma_0 := \partial\Omega(t) \cap S_0$. The remaining parts Γ_j of the boundary of $\Omega(t)$ are subsets of the coordinate planes $e_j \cdot (y - y_0) = 0$, with unit outward normal vectors $n_j^* = -\operatorname{sign}(n_j)\, e_j$, $j = 1, 2, 3$. There exists a subset $N \subset \partial\Omega(t)$ (the union of the edges) of 2D measure zero such that

$$\partial\Omega(t) = \Gamma_0 \cup \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \setminus N\,,$$

so that in (1.12) we have

$$\int_{\partial\Omega(t)} T(y, t, n(y))\,\mathrm{d}s(y) = \int_{\Gamma_0} T(y, t, n^*)\,\mathrm{d}s(y) + \sum_{j=1}^{3} \int_{\Gamma_j} T(y, t, n_j^*)\,\mathrm{d}s(y)\,. \tag{1.17}$$

To continue the developments, we need an additional physical principle, namely

F4. Principle of action and reaction

which states that if two bodies B_1, B_2 are in contact, and body B_1 acts on B_2 with contact force T, then B_2 acts on B_1 with contact force $-T$. In other words, exchanging the roles of $\Omega(t)$ and its exterior, we have for $y \in \Gamma_j$ that $T(y, t, -n_j^*) = -T(y, t, n_j^*)$. In view of this observation, we can rewrite (1.17) in the form

$$\int_{\partial\Omega(t)} T(y, t, n(y))\,\mathrm{d}s(y) = \int_{\Gamma_0} T(y, t, n^*)\,\mathrm{d}s(y) - \sum_{j=1}^{3} \operatorname{sign}(n_j) \int_{\Gamma_j} T(y, t, e_j)\,\mathrm{d}s(y)\,. \tag{1.18}$$

Let us denote

$$G(y,t) = \rho(y,t)\left(\frac{\partial v}{\partial t} + (v\cdot\nabla_y)v\right)(y,t) - g(y,t).$$

Then, by (1.16), Eq. (1.14) can be written in the form

$$\int_{\Omega(t)} G(y,t)\,\mathrm{d}y = \int_{\Gamma_0} T(y,t,n^*)\,\mathrm{d}s(y) - \sum_{j=1}^{3}\mathrm{sign}\,(n_j)\int_{\Gamma_j} T(y,t,e_j)\,\mathrm{d}s(y)\,. \tag{1.19}$$

The volume of $\Omega(t)$ equals

$$|\Omega(t)| = \frac{h^3}{6|n_1n_2n_3|}\,, \tag{1.20}$$

and the 2D area of Γ_j is

$$|\Gamma_j| = \frac{h^2|n_j|}{2|n_1n_2n_3|}\,. \tag{1.21}$$

To compute the area of Γ_0 let us recall that the area of the triangle with vertices A, B, C is $\frac{1}{2}|(A-C)\times(B-C)|$, where the symbol $\times$ denotes for vectors $a = (a_1,a_2,a_3)$, $b=(b_1,b_2,b_3)$ the vector product

$$(a\times b)_i = \sum_{j,k=1}^{3}\varepsilon_{ijk}a_jb_k\,,\quad i=1,2,3, \tag{1.22}$$

where ε_{ijk} is the Levi-Cività symbol

$$\varepsilon_{ijk} = \frac{1}{2}(i-j)(j-k)(k-i)\,. \tag{1.23}$$

The vector product is antisymmetric, that is, $a\times b = -b\times a$ and, in particular, we have $e_1\times e_2 = e_3$, $e_2\times e_3 = e_1$, $e_3\times e_1 = e_2$. Thus, the area of Γ_0 is given by the formula

$$|\Gamma_0| = \frac{1}{2}\left|\left(\frac{h}{n_2}e_2 - \frac{h}{n_1}e_1\right)\times\left(\frac{h}{n_3}e_3 - \frac{h}{n_1}e_1\right)\right| = \frac{h^2}{2|n_1n_2n_3|}|n^*| = \frac{h^2}{2|n_1n_2n_3|}\,. \tag{1.24}$$

This enables us to rewrite (1.19) as

$$\frac{h}{3|\Omega(t)|}\int_{\Omega(t)} G(y,t)\,\mathrm{d}y = \frac{1}{|\Gamma_0|}\int_{\Gamma_0} T(y,t,n^*)\,\mathrm{d}s(y) - \sum_{j=1}^{3} n_j\frac{1}{|\Gamma_j|}\int_{\Gamma_j} T(y,t,e_j)\,\mathrm{d}s(y)\,, \tag{1.25}$$

and letting h tend to 0 yields

$$T(y,t,n^*) = \sum_{j=1}^{3} n_jT(y,t,e_j) \tag{1.26}$$

for all arguments, the cases that $n_j = 0$ for some j being obtained by continuity. In other words, T is linear in n^*, and if we denote by $\boldsymbol{\sigma}$ the matrix with entries

$$\boldsymbol{\sigma}_{ij} = T^i(y,t,e_j)\,, \tag{1.27}$$

then

$$T(y,t,n^*) = \boldsymbol{\sigma}\,n^* \tag{1.28}$$

for all vectors n^*. Invoking the Gauss formula

$$\int_{\partial\tilde{\Omega}} f \cdot n(y)\,\mathrm{d}s(y) = \int_{\tilde{\Omega}} \mathrm{div}_y f\,\mathrm{d}y \tag{1.29}$$

for every regular vector function f and every regular domain $\tilde{\Omega}$, we obtain from (1.14) the pointwise equation

$$\rho\left(\frac{\partial v}{\partial t} + (v\cdot\nabla_y)v\right) = \mathrm{div}_y\boldsymbol{\sigma} + g\,. \tag{1.30}$$

A more standard form of Eq. (1.30) is obtained when it is added to the continuity equation (1.7), which yields

$$\frac{\partial\rho v}{\partial t} + \mathrm{div}_y(\rho v v^T) = \mathrm{div}_y\boldsymbol{\sigma} + g\,, \tag{1.31}$$

where vv^T is the matrix $(vv^T)_{ij} = v^i v^j$.

This system has to be complemented with material assumptions. If the material is assumed incompressible, then, in agreement with (1.10) the momentum balance and mass balance equations are reduced to the system

$$\begin{aligned} \rho_0\left(\frac{\partial v}{\partial t} + (v\cdot\nabla_y)v\right) &= \mathrm{div}_y\boldsymbol{\sigma} + g\,, & (1.32)\\ \mathrm{div}_y v &= 0\,. & (1.33)\end{aligned}$$

which, in the case that the particles do not interact with each other, so that the only contact force is due to the pressure, and $\boldsymbol{\sigma}$ is reduced to $\boldsymbol{\sigma}_{ij} = -p\delta_{ij}$, is called the *incompressible Euler system*

$$\begin{aligned} \rho_0\left(\frac{\partial v}{\partial t} + (v\cdot\nabla_y)v\right) &= -\nabla_y p + g\,, & (1.34)\\ \mathrm{div}_y v &= 0\,. & (1.35)\end{aligned}$$

Viscous behavior, where the friction force between particles is proportional to the velocity with a proportionality factor $\nu > 0$, can also be taken into account by considering

$$\boldsymbol{\sigma}_{ij} = \nu\left(\frac{\partial v^i}{\partial y_j} + \frac{\partial v^j}{\partial y_i}\right) - p\delta_{ij}$$

(cf. (2.20) below; note that here, $dive_y v = 0$). The corresponding counterpart of (1.34)–(1.35) then has the form

$$\begin{aligned} \rho_0\left(\frac{\partial v}{\partial t} + (v\cdot\nabla_y)v\right) &= \gamma\Delta_y v - \nabla_y p + g & (1.36)\\ \mathrm{div}_y v &= 0\,. & (1.37)\end{aligned}$$

with the Laplace operator $\Delta_y = \mathrm{div}_y\nabla_y$, and is called the *Navier-Stokes system.*

We conclude this subsection by proving that under the additional physical principle of

F5. Conservation of angular momentum

the stress $\boldsymbol{\sigma}$ is symmetric, that is, $\boldsymbol{\sigma}_{ij} = \boldsymbol{\sigma}_{ji}$ for all $i, j = 1, 2, 3$. To this end, we fix again a bounded domain $\Omega(t) \subset \mathcal{B}(t)$ and a point $y_0 \in \Omega(t)$, and for $h > 0$ denote

$$\Omega^h(t) = \left\{ y \in \mathcal{B}(t) : \frac{1}{h}(y - y_0) \in \Omega(t) \right\}.$$

Clearly, each $y \in \Omega^h(t)$ can be written as $y = y_0 + h(\hat{y} - y_0)$ for some $\hat{y} \in \Omega(t)$, hence,

$$|y - y_0| \le h \,\mathrm{diam}\, \Omega(t) \quad \forall y \in \Omega^h(t), \tag{1.38}$$

where diam denotes the diameter of a set.

The angular momentum of the part $\Omega^h(t)$ of the body $\mathcal{B}(t)$ with respect to the point y_0 is given by a formula analogous to (1.13), namely

$$\int_{\Omega^h(t)} (y - y_0) \times (\rho(y, t)\, v(y, t))\, \mathrm{d}y, \tag{1.39}$$

and its time derivative equals the total torque associated with both volume and contact forces

$$\int_{\Omega^h(t)} (y - y_0) \times g(y, t)\, \mathrm{d}y + \int_{\partial\Omega^h(t)} (y - y_0) \times \boldsymbol{\sigma} n(y)\, \mathrm{d}s(y). \tag{1.40}$$

Similar computation as above yields

$$\int_{\Omega^h(t)} (y - y_0) \times \left(\rho(y, t) \left(\frac{\partial v}{\partial t} + (v \cdot \nabla_y) v \right) - g \right) (y, t)\, \mathrm{d}y = \int_{\partial\Omega^h(t)} (y - y_0) \times \boldsymbol{\sigma} n(y)\, \mathrm{d}s(y). \tag{1.41}$$

The i-th component of the right hand side of (1.41) reads

$$\int_{\partial\Omega^h(t)} \sum_{j,k,l=1}^{3} \varepsilon_{ijk} (y_j - (y_0)_j) \boldsymbol{\sigma}_{kl} n_l(y)\, \mathrm{d}s(y)$$

and equals, by Gauss formula (1.29), to the volume integral

$$\int_{\Omega^h(t)} \sum_{j,k,l=1}^{3} \varepsilon_{ijk} \frac{\partial}{\partial y_l} \big((y_j - (y_0)_j) \boldsymbol{\sigma}_{kl} \big)\, \mathrm{d}y$$

which equals in turn

$$\int_{\Omega^h(t)} \left(\big((y - y_0) \times \mathrm{div}_y \boldsymbol{\sigma} \big)_i + \sum_{j,k=1}^{3} \varepsilon_{ijk} \boldsymbol{\sigma}_{kj} \right) \mathrm{d}y.$$

All terms in (1.41) are of the order h^4 by virtue of (1.38) except for

$$\int_{\Omega^h(t)} \sum_{j,k=1}^{3} \varepsilon_{ijk} \boldsymbol{\sigma}_{kj}\, \mathrm{d}y$$

which is of the order h^3, Hence, letting h tend to 0 we obtain

$$\sum_{j,k=1}^{3} \varepsilon_{ijk} \boldsymbol{\sigma}_{kj}(y_0, t) = 0 \qquad \text{for } i = 1, 2, 3,$$

which is equivalent to the identity $\boldsymbol{\sigma}_{ij}(y_0, t) = \boldsymbol{\sigma}_{ji}(y_0, t)$ for all i, j, y_0, and t, which we wanted to prove.

1.3 Deformation

In this section we study how forces acting on the body change its shape. We first try to answer the question how displacements $u(x,t)$ of particles transform directions and angles in the body, see Figure 3.

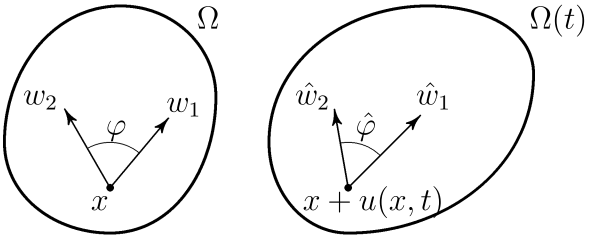

Figure 3: Deformation of angles

Consider unit vectors w_1, w_2, and three points $x, x+hw_1, x+hw_2$ in the reference configuration for small $h>0$. We define the transformed directions $\hat{w}_1, \hat{w}_2$ as

$$\hat{w}_i = \lim_{h\to 0} \frac{1}{h}(x+hw_i+u(x+hw_i,t)-x-u(x,t)) = w_i + D(u)w_i\,,\ i=1,2, \tag{1.42}$$

where $D(u)$ is as in (1.3). If we denote by φ the angle between w_1 and w_2, then $\cos\varphi$ is given by the scalar product $w_1\cdot w_2$, and the angle $\hat{\varphi}$ between $\hat{w}_1$ and $\hat{w}_2$ is given by

$$\cos\hat{\varphi} = \frac{\hat{w}_1\cdot\hat{w}_2}{|\hat{w}_1|\,|\hat{w}_2|}\,. \tag{1.43}$$

We have

$$\hat{w}_1\cdot\hat{w}_2 = (w_1+D(u)w_1)\cdot(w_2+D(u)w_2) = \big((I+D(u)+D^T(u)+D^T(u)D(u))w_1\big)\cdot w_2,$$

and we call the matrix

$$\boldsymbol{\varepsilon}^* = \frac{1}{2}(D(u)+D^T(u)+D^T(u)D(u))\,,\quad \boldsymbol{\varepsilon}^*_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}+\sum_{k=1}^{3}\frac{\partial u_k}{\partial x_j}\frac{\partial u_k}{\partial x_i}\right) \tag{1.44}$$

the *strain*. The geometric meaning of $\boldsymbol{\varepsilon}^*_{ij}$ can easily be interpreted if we choose w_1, w_2 to be the unit orthonormal coordinate vectors e_n, e_m, $n,m=1,2,3$. Then, for $n\neq m$, we have

$$\hat{e}_n\cdot\hat{e}_m = \sum_{i,j=1}^{3} 2\boldsymbol{\varepsilon}^*_{ij}e_n^i e_m^j = 2\boldsymbol{\varepsilon}^*_{nm}\,, \tag{1.45}$$

and

$$|\hat{e}_n|^2 = 1+\sum_{i,j=1}^{3} 2\boldsymbol{\varepsilon}^*_{ij}e_n^i e_n^j = 1+2\boldsymbol{\varepsilon}^*_{nn}\,. \tag{1.46}$$

We now make a step out of physics and out of mathematics, and postulate an “engineering principle” which will have to be a posteriori justified in each particular case, namely

E1. Terms of higher order of smallness can be neglected

The idea is that there exists a smallness parameter $0 < \alpha \ll 1$ such that $|\frac{\partial u_i}{\partial x_j}| < \alpha$ with the goal to declare terms of the order 2 and higher as negligible.

This enables us to introduce the linearized strain

$$\boldsymbol{\varepsilon} = \frac{1}{2}(D(u) + D^T(u)) \tag{1.47}$$

In this approximation, formulas (1.45)–(1.46) yield the following expressions for the transformed coordinate vectors $\hat{e}_n$ and transformed angles $\hat{\varphi}_{nm}$ between $\hat{e}_n$ and $\hat{e}_m$:

$$|\hat{e}_n| \quad \approx \quad \sqrt{1 + 2\boldsymbol{\varepsilon}_{nn}} \approx 1 + \boldsymbol{\varepsilon}_{nn}\,, \tag{1.48}$$

$$\frac{\pi}{2} - \hat{\varphi}_{nm} \quad \approx \quad \sin\left(\frac{\pi}{2} - \hat{\varphi}_{nm}\right) = \cos\hat{\varphi}_{nm} \approx \frac{2\boldsymbol{\varepsilon}_{nm}}{(1+\boldsymbol{\varepsilon}_{nn})(1+\boldsymbol{\varepsilon}_{mm})} \approx 2\boldsymbol{\varepsilon}_{nm}\,. \tag{1.49}$$

We see that the diagonal elements $\boldsymbol{\varepsilon}_{nn}$ of the strain give the elongation in direction e_n, and the off-diagonal elements $\boldsymbol{\varepsilon}_{nm}$ describe the deviation from the right angle. Furthermore,

$$J(x,t) = \det(I + D(u)) \approx 1 + \boldsymbol{\varepsilon}_{11} + \boldsymbol{\varepsilon}_{22} + \boldsymbol{\varepsilon}_{33} = 1 + \operatorname{div}_x u(x,t)\,,$$

so that we can interpret $\operatorname{div}_x u$ as the volume change rate in agreement with (1.9).

We will see that it is convenient to separate volume deformations from volume preserving deformations, and introduce the following notation.

Let $\mathbb{T}$ be the space of symmetric matrices 3×3, $\dim\mathbb{T} = 6$. This is a Hilbert space endowed with the scalar product $\boldsymbol{\xi} : \boldsymbol{\eta} = \sum_{i,j=1}^{3} \boldsymbol{\xi}_{ij}\boldsymbol{\eta}_{ij}$ for $\boldsymbol{\xi}, \boldsymbol{\eta} \in \mathbb{T}$. We denote by $\mathbf{1}$ the unit matrix $\mathbf{1}_{ij} = \delta_{ij}$. Then the deformation given by $\boldsymbol{\varepsilon}$ is volume preserving if $\boldsymbol{\varepsilon} : \mathbf{1} = 0$. We define the subspace $\mathbb{T}_{\text{dev}}$ of volume preserving matrices, the so-called deviatoric space, and the orthogonal projection Dev of $\mathbb{T}$ onto $\mathbb{T}_{\text{dev}}$ by the formula

$$\operatorname{Dev}(\boldsymbol{\varepsilon}) = \boldsymbol{\varepsilon} - \frac{1}{3}(\boldsymbol{\varepsilon} : \mathbf{1})\,\mathbf{1}\,. \tag{1.50}$$

1.4 Linear elasticity

The main hypothesis in linear elasticity is

F6. The Hooke law

which postulates the existence of materials (the so-called *elastic materials*) in which strains and stresses are related to each other by a linear formula

$$\boldsymbol{\sigma}_{ij} = \sum_{k,l=1}^{3} A_{ijkl}\boldsymbol{\varepsilon}_{kl}\,, \tag{1.51}$$

and A_{ijkl} are constants characterizing the material response to multiaxial loading that may be different for different materials. Indeed, not all of these constants are independent. As both $\boldsymbol{\varepsilon}$

and $\boldsymbol{\sigma}$ are symmetric matrices, we necessary have $A_{ijkl} = A_{jikl} = A_{ijlk}$. In order to further reduce this number, we refer to a physical hypothesis that

F7. Elastic deformations are reversible

which states that the relation (1.51) is one-to-one, and there exists a potential energy functional $U : \mathbb{T} \to \mathbb{R}^+$ such that the work done by the stresses in any subdomain $\Omega \subset \mathcal{B}$ during any time interval $[t_1, t_2] \subset [0, T]$ is fully transformed into potential increase. In other words,

$$\int_{t_1}^{t_2} \int_\Omega \frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \boldsymbol{\sigma}(x,t)\,\mathrm{d}x\,\mathrm{d}t = \int_\Omega (U(\boldsymbol{\varepsilon}(x,t_2) - U(\boldsymbol{\varepsilon}(x,t_2))\,\mathrm{d}x$$

for all $\Omega \subset \mathcal{B}$ and $[t_1, t_2] \subset [0, T]$ and all strains $\boldsymbol{\varepsilon}$. Hence,

$$\sum_{i,j=1}^{3} \frac{\partial \boldsymbol{\varepsilon}_{ij}}{\partial t} \boldsymbol{\sigma}_{ij} = \frac{\partial U}{\partial t} = \sum_{i,j=1}^{3} \frac{\partial \boldsymbol{\varepsilon}_{ij}}{\partial t} \frac{\partial U}{\partial \boldsymbol{\varepsilon}_{ij}},$$

which is only possible if

$$\boldsymbol{\sigma}_{ij} = \frac{\partial U}{\partial \boldsymbol{\varepsilon}_{ij}} \tag{1.52}$$

for all $i, j = 1, 2, 3$. By (1.51) we have

$$\frac{\partial^2 U}{\partial \boldsymbol{\varepsilon}_{ij} \partial \boldsymbol{\varepsilon}_{kl}} = A_{ijkl} = \frac{\partial^2 U}{\partial \boldsymbol{\varepsilon}_{kl} \partial \boldsymbol{\varepsilon}_{ij}} = A_{klij}.$$

If we represent $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ as six-dimensional vectors $\boldsymbol{\varepsilon} = (\boldsymbol{\varepsilon}_{11}, \boldsymbol{\varepsilon}_{22}, \boldsymbol{\varepsilon}_{33}, \boldsymbol{\varepsilon}_{23}, \boldsymbol{\varepsilon}_{31}, \boldsymbol{\varepsilon}_{12})^T$ and similarly for $\boldsymbol{\sigma}$, we see that $A = (A_{ijkl})$ can be considered as a symmetric positive definite 6×6 matrix, and $\boldsymbol{\sigma}$ and U can be written in the form

$$\boldsymbol{\sigma} = A\boldsymbol{\varepsilon}\,, \quad U(\boldsymbol{\varepsilon}) = \frac{1}{2}(A\boldsymbol{\varepsilon}) : \boldsymbol{\varepsilon}\,. \tag{1.53}$$

Hence, elastic materials with no symmetries are characterized by 21 constants, which is the number of independent entries of a symmetric 6×6 matrix. Most common materials, however, possess a certain degree of invariance with respect to coordinate transformations, and often can be considered as fully invariant (*isotropic materials*).

The invariance with respect to coordinate transformations is an important issue and we devote the rest of this section to an introduction into this part of linear algebra.

As above, we denote by $E = \{e_1, e_2, e_3\}$ the canonical basis of $\mathbb{R}^3$, the vector e_j having components $e_j = (e_j^1, e_j^2, e_j^3)$, with $e_j^i = \delta_{ij}$. Let $W = \{w_1, w_2, w_3\}$ be any other orthonormal basis. Let M be the transition matrix from E to W, that is,

$$w_j = \sum_{i=1}^{3} M_{ij} e_i\,. \tag{1.54}$$

We have $w_i \cdot w_j = \delta_{ij}$ for $i, j = 1, 2, 3$, hence

$$\delta_{ij} = \sum_{k,l=1}^{3} M_{ki} M_{lj} e_k \cdot e_l = \sum_{k,l=1}^{3} M_{ki} M_{lj} \delta_{kl} = \sum_{k=1}^{3} M_{ki} M_{kj}.$$

In matrix multiplication formalism, this means $M\,M^T = I$, that is, $M^{-1} = M^T$, which characterizes *orthogonal matrices*.

Consider now the representation of a point x and displacement vector u with respect to the two bases E and W

$$\begin{aligned} x &= \sum_{i=1}^{3} x_i e_i = \sum_{j=1}^{3} x'_j w_j = \sum_{i,j=1}^{3} x'_j M_{ij} e_i \,, \\ u &= \sum_{k=1}^{3} u_k e_k = \sum_{l=1}^{3} u'_l w_l = \sum_{k,l=1}^{3} u'_l M_{kl} e_k \,. \end{aligned}$$

Hence,

$$x_i = \sum_{j=1}^{3} x'_j M_{ij} \,, \quad u_k = \sum_{l=1}^{3} u'_l M_{kl} \,, \quad u'_l = \sum_{k=1}^{3} u_k M_{kl} \,,$$

so that

$$\frac{\partial u'_l}{\partial x'_j} = \sum_{k=1}^{3} \frac{\partial u_k}{\partial x'_j} M_{kl} = \sum_{k,i=1}^{3} \frac{\partial u_k}{\partial x_i}\frac{\partial x_i}{\partial x'_j} M_{kl} = \sum_{k,i=1}^{3} \frac{\partial u_k}{\partial x_i} M_{ij} M_{kl},$$

and similarly

$$\frac{\partial u'_l}{\partial x'_j} = \sum_{k,i=1}^{3} \frac{\partial u_i}{\partial x_k} M_{ij} M_{kl},$$

and we conclude that

$$\boldsymbol{\varepsilon}'_{jl} = \frac{1}{2}\left(\frac{\partial u'_l}{\partial x'_j} + \frac{\partial u'_j}{\partial x'_l}\right) = \sum_{k,i=1}^{3} \boldsymbol{\varepsilon}_{ik} M_{ij} M_{kl} \,. \tag{1.55}$$

In physics, a quantity which is transformed according to the recipe in (1.55) is called a *second order tensor*.

We now show that $\boldsymbol{\sigma}$ is transformed in the same way, so that both $\boldsymbol{\varepsilon}$ and $\boldsymbol{\sigma}$ are second order tensors. Indeed, if $n = \sum_{j=1} n_j e_j$ is a normal vector and $T = \sum_{i,j=1} \boldsymbol{\sigma}_{ij} n_j e_i$ is a contact force, then

$$n = \sum_{j,k=1}^{3} n_j M_{jk} w_k = \sum_{k=1}^{3} n'_k w_k \,, \quad T = \sum_{i,j=1} \boldsymbol{\sigma}'_{kl} n'_k w_l = \sum_{i,j,k,l=1} \boldsymbol{\sigma}'_{kl} M_{jk} M_{il} n_j e_i \,.$$

We thus have $\boldsymbol{\sigma}_{ij} = \sum_{k,l=1} \boldsymbol{\sigma}'_{kl} M_{jk} M_{il}$, or, equivalently,

$$\boldsymbol{\sigma}'_{kl} = \sum_{i,j=1} \boldsymbol{\sigma}_{ij} M_{jk} M_{il} \,, \tag{1.56}$$

which we wanted to prove.

The transformation formula $\boldsymbol{\sigma}'_{mn} = \sum_{q,r=1}^{3} A'_{mnqr} \boldsymbol{\varepsilon}'_{qr}$ for the elastic constitutive law is easily derived from (1.55)–(1.56), and reads

$$A'_{mnqr} = \sum_{i,j,k,l=1}^{3} A_{ijkl} M_{im} M_{jn} M_{kq} M_{lr} \,. \tag{1.57}$$

In physical terminology, A is a *fourth order tensor*.

We say that the elastic constitutive law is *invariant with respect to the transformation* M_{ij} if in (1.57) we have $A'_{mnqr} = A_{mnqr}$ for all indices. We say that the material is *isotropic* if it is invariant with respect to all rotations about coordinate axes.

Proposition 1.3 *If the elastic material is isotropic, then there exist two constants* μ, λ *such that matrix* A *in the constitutive relation* $\boldsymbol{\sigma} = A\boldsymbol{\varepsilon}$ *has the form*

$$\boldsymbol{\sigma} = 2\mu\boldsymbol{\varepsilon} + \lambda(\boldsymbol{\varepsilon} : \mathbf{1})\mathbf{1}\,. \tag{1.58}$$

In terms of the deviator (1.50), we can rewrite the constitutive equation in the form

$$\boldsymbol{\sigma} = 2\mu\mathrm{Dev}(\boldsymbol{\varepsilon}) + \left(\lambda + \frac{2}{3}\mu\right)(\boldsymbol{\varepsilon} : \mathbf{1})\mathbf{1}\,. \tag{1.59}$$

We see that the matrix A is positive definite if and only the numbers μ and $3\lambda + 2\mu$ are positive. In classical terminology, μ, λ are called the Lamé constants; μ is the shear modulus characterizing volume preserving shape deformations, $\lambda + (2/3)\mu$ is the bulk elasticity modulus characterizing volume deformations.

Proof of Proposition 1.3. The matrix of rotation by angle φ about the axis x_3 has the form

$$M = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Consider first $\varphi = \pi$, that is, $-M_{11} = -M_{22} = M_{33} = 1$, $M_{ij} = 0$ for $i \neq j$. Then $A'_{mnqr} = A_{mnqr}(-1)^{N(3)}$, where $N(3)$ is the number of occurrences of the number 3 in the sequence $\{m, n, q, r\}$. A similar formula with the number of occurrences of 1 and 2 holds for rotations about the axes x_1 and x_2. Hence, for isotropic materials, all coefficients A_{mnqr} containing an odd number of 1, 2, or 3, necessarily vanish. The only possible nonzero coefficients are therefore $A_{1111}, A_{2222}, A_{3333}, A_{1122}, A_{2233}, A_{3311}, A_{2323}, A_{3131}, A_{1212}$.

Next, consider $\varphi = \pi/2$. This corresponds to interchanging all occurrences of 1 and 2 in the indices $mnqr$, and similarly for rotations about the other axes. Hence, only three independent constants μ, λ, γ remain, namely

$$\begin{aligned} A_{1111} = A_{2222} = A_{3333} &= \gamma\,, \\ A_{1122} = A_{2233} = A_{3311} &= \lambda\,, \\ A_{2323} = A_{3131} = A_{1212} &= \mu\,. \end{aligned}$$

Finally, we take an arbitrary φ and compute

$$\gamma = A_{1111} = \sum_{i,j,k,l=1}^{3} A_{ijkl} M_{i1} M_{j1} M_{k1} M_{l1} = \gamma(\cos^4\!\varphi + \sin^4\!\varphi) + (2\lambda + 4\mu)\cos^2\!\varphi\,\sin^2\!\varphi\,.$$

Using the formula $1 = (\cos^2\!\varphi + \sin^2\!\varphi)^2 = \cos^4\!\varphi + \sin^4\!\varphi + 2\cos^2\!\varphi\,\sin^2\!\varphi$ we conclude that

$$\gamma = \lambda + 2\mu\,, \tag{1.60}$$

which is exactly the statement that we wanted to prove. ■

We now can state the equations of motion for elastic solids in Lagrange coordinates. We denote $\tilde{\boldsymbol{\sigma}}_{ij}(x,t) = \boldsymbol{\sigma}_{ij}(x+u(x,t),t)$, $\tilde{g}(x,t) = g(x+u(x,t),t)$. Using Hypothesis 1.1 and Eqs. (1.11), (1.12), (1.15), (1.28), (1.29), we rewrite the equation of motion as

$$\rho_0(x)\frac{\partial^2 u^i}{\partial t^2}(x,t) = \sum_{j=1}^{3}\frac{\partial\tilde{\boldsymbol{\sigma}}_{ij}}{\partial y_j}(x+u(x,t),t)J(x,t) + \tilde{g}^i(x,t)J(x,t)$$

By the engineering principle E1 about negligible quantities, we neglect the discrepancies between Euler and Lagrange coordinates, identify $\tilde{\boldsymbol{\sigma}}$ with $\boldsymbol{\sigma}$ and $\tilde{g}$ with g, and write the equation of motion in the form

$$\rho_0(x)\frac{\partial^2 u^i}{\partial t^2}(x,t) = \sum_{j=1}^{3}\frac{\partial\boldsymbol{\sigma}_{ij}}{\partial x_j}(x,t) + g^i(x,t)\,, \tag{1.61}$$

which, for isotropic elastic material with constitutive law (1.58) can be written in compact form

$$\rho_0(x)\frac{\partial^2 u}{\partial t^2} = \mu\Delta u + (\lambda+\mu)\nabla\mathrm{div}\,u = g\,, \tag{1.62}$$

where Δ denotes the Laplace operator

$$\Delta u = \sum_{j=1}^{3}\frac{\partial^2 u}{\partial x_j^2}\,.$$

2 An introduction to thermodynamics

This introduction is indeed very short. For a deep explanation of the concepts and principles of thermodynamics, we refer to [5].

The basic concept of continuum thermodynamics is the *state space*. Elements z of the state space Z are called the *states*. Physically, they may consist of scalar, vectorial or tensorial components $z = (z_1,\dots,z_n)$ (the *state variables*) of different physical nature (e.g. strain, temperature, magnetic field, phase fraction, various internal variables etc.). Functions $f : Z \to \mathbb{R}$ are called *state functions*.

If $\mathcal{B} \subset \mathbb{R}^3$ is a body and $[0,T]$ a given time interval, then a function $z : \bar{\mathcal{B}} \times [0,T]$ is called a *process* if it satisfies thermodynamic balance equations as well as empirical constitutive equations.

The thermodynamic balance equations are based on the following

F8. Three principles of thermodynamics

Zeroth principle. There exists a state variable $\theta > 0$, called the *absolute temperature*.

First principle. There exists a state function $U : Z \to [0,\infty)$ called the *internal energy* which is conserved in the following sense: On every subdomain $\Omega \subset \mathcal{B}$, the increase rate of the internal energy equals the sum of the power supplied to the system and the heat flux through the boundary of Ω.

Second principle. There exists a state function $S : Z \to \mathbb{R}$ called the *entropy* which is nondecreasing in the following sense: On every subdomain $\Omega \subset \mathcal{B}$, the increase rate of the entropy is greater than or equal to the sum of the external entropy sources and the entropy flux through the boundary of Ω.

Example 2.1 Thermoelasticity. The state variables are chosen to be the strain $\boldsymbol{\varepsilon}$ and the absolute temperature θ. We consider the state function $\boldsymbol{\sigma}$ to be given by the empirical constitutive law

$$\boldsymbol{\sigma} = A\boldsymbol{\varepsilon} - \beta(\theta - \theta_c)\mathbf{1}\,, \tag{2.1}$$

where A is the elasticity matrix as, e.g., in Proposition 1.3, $\theta_c > 0$ is a given reference temperature, and $\beta \in \mathbb{R}$ is the *thermal expansion coefficient, all determined from experimental data.*

We will see that the other state functions U (the internal energy) and S (the entropy) cannot be chosen independently, if the thermodynamic principles are supposed to hold.

For any regular domain $\Omega \subset \mathcal{B}$ we have by virtue of the First principle

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega U\,\mathrm{d}x + \int_{\partial\Omega} q\cdot n(x)\,\mathrm{d}x = \int_\Omega \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}}{\partial t}\,\mathrm{d}x + \int_\Omega \psi\,\mathrm{d}x\,, \tag{2.2}$$

where q is the heat flux vector, $n(x)$ is the unit outward normal vector, $\int_{\partial\Omega} q\cdot n(x)\,\mathrm{d}x$ is the amount of heat flowing out of Ω, $\int_\Omega \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}}{\partial t}\,\mathrm{d}x$ is the mechanical power supplied to the system, and ψ is the heat source density. By the Gauss formula (1.29), we have

$$\frac{\partial U}{\partial t} + \operatorname{div} q = \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}}{\partial t} + \psi\,. \tag{2.3}$$

The entropy flux is defined as q/θ, and the entropy sources as ψ/θ. The Second principle then has the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega S\,\mathrm{d}x + \int_{\partial\Omega} \frac{q}{\theta}\cdot n(x)\,\mathrm{d}x \ge \int_\Omega \frac{\psi}{\theta}\,\mathrm{d}x\,, \tag{2.4}$$

In differential form, we obtain the *Clausius-Duhem inequality*

$$\frac{\partial S}{\partial t} + \operatorname{div}\frac{q}{\theta} \ge \frac{\psi}{\theta}\,. \tag{2.5}$$

To find U and S, we first eliminate ψ from the thermodynamic principles by multiplying (2.5) by $-\theta$, and adding the result to (2.3). This yields

$$\frac{\partial U}{\partial t} - \theta\frac{\partial S}{\partial t} + \frac{q\cdot\nabla\theta}{\theta} \le \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}}{\partial t}\,. \tag{2.6}$$

This inequality has to hold for all processes, in particular, for spatially homogeneous ones, for which $\nabla\theta = 0$. Hence, we must have

$$\frac{\partial U}{\partial t} - \theta\frac{\partial S}{\partial t} \le \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}}{\partial t}\,. \tag{2.7}$$

On the other hand, for stationary (or very slow) processes the time derivatives vanish (or almost vanish), so that, necessarily,

$$\frac{q \cdot \nabla\theta}{\theta} \le 0\,. \tag{2.8}$$

In other words, heat has the tendency to flow from hot domains to cold ones. We assume here for simplicity the empirical

F9. Fourier law

$$q = -\kappa \nabla\theta\,, \tag{2.9}$$

with a positive constant κ called the *heat conductivity*. It is indeed in agreement with (2.8).

We introduce the *free energy* F by the formula

$$F = U - \theta S\,. \tag{2.10}$$

Notice that both U and S are state functions, and thus depend only on $\boldsymbol{\varepsilon}$ and θ. Hence, F is a state function, too, and satisfies for all processes, by virtue of (2.7), the inequality

$$\frac{\partial F}{\partial t} + S\frac{\partial\theta}{\partial t} \le \boldsymbol{\sigma} : \frac{\partial\boldsymbol{\varepsilon}}{\partial t}\,. \tag{2.11}$$

By the chain rule, we obtain

$$\left(\frac{\partial F}{\partial\theta} + S\right)\frac{\partial\theta}{\partial t} + \left(\frac{\partial F}{\partial\boldsymbol{\varepsilon}} - \boldsymbol{\sigma}\right) : \frac{\partial\boldsymbol{\varepsilon}}{\partial t} \le 0 \tag{2.12}$$

for all processes. Then, necessarily,

$$\frac{\partial F}{\partial\theta} = -S\,, \quad \frac{\partial F}{\partial\boldsymbol{\varepsilon}} = \boldsymbol{\sigma}\,. \tag{2.13}$$

Hence, F can be computed by integrating the constitutive equation (2.1) with respect to $\boldsymbol{\varepsilon}$, that is,

$$F(\theta,\boldsymbol{\varepsilon}) = \frac{1}{2}A\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} - \beta(\theta-\theta_c)\boldsymbol{\varepsilon} : \mathbf{1} + F_0(\theta) \tag{2.14}$$

with an integration “constant” $F_0(\theta)$ which is to be identified. By (2.13), we have

$$S(\theta,\boldsymbol{\varepsilon}) = \beta\theta - F_0'(\theta)\,, \tag{2.15}$$

hence,

$$U(\theta,\boldsymbol{\varepsilon}) = F(\theta,\boldsymbol{\varepsilon}) + \theta S(\theta,\boldsymbol{\varepsilon}) = \frac{1}{2}A\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} + \beta\theta_c\boldsymbol{\varepsilon} : \mathbf{1} + F_0(\theta) - \theta F_0'(\theta)\,. \tag{2.16}$$

The function $c_V(\theta) := \frac{F_0(\theta)}{\theta} - F_0'(\theta)$ is a material quantity that can be measured, and is called the *specific heat capacity*. It determines the amount of heat that has to be supplied to a unit volume of the body to increase the temperature by 1 Kelvin. It is easy then to compute F_0 as the solution of the differential equation

$$F_0(\theta) - \theta F_0'(\theta) = \theta c_V(\theta)\,.$$

For example, if c_V is assumed constant and we choose the "initial condition" $F_0(\theta_c) = 0$, then

$$F_0(\theta) = -c_V \theta \log\left(\frac{\theta}{\theta_c}\right) . \tag{2.17}$$

Inserting the formulas (2.1), (1.58) for $\boldsymbol{\sigma}$, (2.16) for U, and (2.9) for q into the momentum balance equation (1.61) and the energy balance equation (2.3), we obtain the following system of partial differential equations for the unknown functions u and θ

$$\varrho_0 \frac{\partial^2 u}{\partial t^2} = \mu \Delta u + (\mu + \lambda) \nabla \mathrm{div}\, u - \beta \nabla \theta + g \,, \tag{2.18}$$

$$c_V \frac{\partial \theta}{\partial t} = \kappa \Delta \theta - \beta \theta \frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \mathbf{1} + \psi \,. \tag{2.19}$$

Note that for this system, no existence theory is known. The quadratic energy exchange term $\beta\theta\frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \mathbf{1}$ on the right hand side of (2.19) makes the problem too difficult for the existing techniques in the theory of partial differential equations. If dissipation mechanisms are taken into account, however, the situation is more favorable, and we will comment on that below.

Example 2.2 Thermo-visco-elasticity. In addition to the situation considered in Example 2.1, we assume that $\boldsymbol{\sigma}$ is split into the sum $\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{rev}} + \boldsymbol{\sigma}^{\mathrm{v}}$ of a reversible component $\boldsymbol{\sigma}^{\mathrm{rev}}$ given by (2.1), and an irreversible dissipative viscous component $\boldsymbol{\sigma}^{\mathrm{v}}$ proportional to the strain rate

$$\boldsymbol{\sigma}^{\mathrm{v}} = 2\nu \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + \eta \left(\frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \mathbf{1}\right) \mathbf{1} \tag{2.20}$$

with positive viscosity coefficients ν, η, so that

$$\boldsymbol{\sigma} = A\boldsymbol{\varepsilon} - \beta(\theta - \theta_c)\mathbf{1} + B\frac{\partial \boldsymbol{\varepsilon}}{\partial t} \,, \tag{2.21}$$

where B is the viscosity matrix corresponding to (2.20). As no energy can be stored in purely dissipative terms, we take the same free energy an in (2.14), and easily check that the Second principle in the form (2.11) still holds.

Viscosity then appears in both balance equations, and the corresponding counterpart of (2.18)–(2.19) then reads

$$\varrho_0 \frac{\partial^2 u}{\partial t^2} = \mu \Delta u + (\mu + \lambda) \nabla \mathrm{div}\, u + \nu \Delta \frac{\partial u}{\partial t} + (\nu + \eta) \nabla \mathrm{div}\, \frac{\partial u}{\partial t} - \beta \nabla \theta + g \,, \tag{2.22}$$

$$c_V \frac{\partial \theta}{\partial t} = \kappa \Delta \theta - \beta \theta \frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \mathbf{1} + B \frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + \psi \,. \tag{2.23}$$

We see that the viscous dissipation rate $B\frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t}$ appears as an additional positive heat source in the energy balance (2.23). This system is more accessible to mathematical analysis, see [4].

Example 2.3 Thermo-visco-elasto-plasticity. In addition to the situation considered in Example 2.2, we assume that $\boldsymbol{\sigma}$ is the sum of a reversible component $\boldsymbol{\sigma}^{\mathrm{rev}}$ given by (2.1), and an irreversible dissipative component $\boldsymbol{\sigma}^{\mathrm{irr}} = \boldsymbol{\sigma}^{\mathrm{v}} + \boldsymbol{\sigma}^{\mathrm{p}}$ consisting of the viscous part $\boldsymbol{\sigma}^{\mathrm{v}}$ as in (2.20) and the plastic part $\boldsymbol{\sigma}^{\mathrm{p}}$ which we now describe in more detail.

The main modeling assumption is that $\boldsymbol{\sigma}^{\mathrm{p}}$ cannot reach arbitrarily large values, and is restricted to a convex closed set $K \subset \mathbb{T}$, under natural restriction $0 \in K$. As soon as the plastic stress component reaches the boundary of K (the so-called *yield surface*), plastic yielding starts, while in the interior of K, the behavior is elastic. We decompose the strain $\boldsymbol{\varepsilon}$ into the sum of $\boldsymbol{\varepsilon}^{\mathrm{e}} + \boldsymbol{\varepsilon}^{\mathrm{p}}$, and consider $\boldsymbol{\varepsilon}^{\mathrm{e}}$ as a new state variable (also called *internal variable*). We model the linear elastic relation between $\boldsymbol{\varepsilon}^{\mathrm{e}}$ $\boldsymbol{\sigma}^{\mathrm{p}}$ similarly as in Proposition 1.3 in the form $\boldsymbol{\sigma}^{\mathrm{p}} = A_p\boldsymbol{\varepsilon}^{\mathrm{e}}$ with a matrix A_p as in (1.58) with Lamé constants μ_p, λ_p. The evolution of $\boldsymbol{\varepsilon}^{\mathrm{e}}$ is governed by the

F10. Principle of maximal plastic dissipation rate

which states that the process chooses the maximally dissipative path with respect to all admissible plastic stress values. We refer again to the Second principle in the form (2.11), taking into account the additional dependence of F on $\boldsymbol{\varepsilon}^{\mathrm{e}}$. By the chain rule, we obtain similarly as in (2.12) that

$$\left(\frac{\partial F}{\partial \theta} + S\right)\frac{\partial \theta}{\partial t} + \left(\frac{\partial F}{\partial \boldsymbol{\varepsilon}} - \boldsymbol{\sigma}\right) : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + \frac{\partial F}{\partial \boldsymbol{\varepsilon}^{\mathrm{e}}} \cdot \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{e}}}{\partial t} \le 0 \tag{2.24}$$

for all processes. We have

$$\boldsymbol{\sigma} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} = \boldsymbol{\sigma}^{\mathrm{rev}} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + B\frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + A_p\boldsymbol{\varepsilon}^{\mathrm{e}} : \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{e}}}{\partial t} + \boldsymbol{\sigma}^{\mathrm{p}} : \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{p}}}{\partial t}.$$

Then, invoking (2.13),

$$\frac{\partial F}{\partial \theta} = -S\,, \quad \frac{\partial F}{\partial \boldsymbol{\varepsilon}} = \boldsymbol{\sigma}^{\mathrm{rev}}\,, \quad \frac{\partial F}{\partial \boldsymbol{\varepsilon}^{\mathrm{e}}} = A_p\boldsymbol{\varepsilon}^{\mathrm{e}}\,, \quad \boldsymbol{\sigma}^{\mathrm{p}} : \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{p}}}{\partial t} \ge 0\,, \tag{2.25}$$

hence

$$F(\theta, \boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\mathrm{e}}) = \frac{1}{2}A\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} + \frac{1}{2}A_p\boldsymbol{\varepsilon}^{\mathrm{e}} : \boldsymbol{\varepsilon}^{\mathrm{e}} - \beta(\theta - \theta_c)\boldsymbol{\varepsilon} : \mathbf{1} + F_0(\theta) \tag{2.26}$$

as in (2.14), and the term $\boldsymbol{\sigma}^{\mathrm{p}} : \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{p}}}{\partial t}$ represents the plastic dissipation. In agreement with F10, we require more, namely that this dissipation has to be maximal with respect to all admissible plastic stress values, that is,

$$(\boldsymbol{\sigma}^{\mathrm{p}} - \tilde{\boldsymbol{\sigma}}) : \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{p}}}{\partial t} \ge 0 \quad \forall \tilde{\boldsymbol{\sigma}} \in K\,. \tag{2.27}$$

In terms of the state variables, we rewrite (2.27) as a variational inequality

$$\left\{\begin{array}{l} \boldsymbol{\varepsilon}^{\mathrm{e}} \in A_p^{-1}(K)\,, \\ A_p(\boldsymbol{\varepsilon}^{\mathrm{e}} - \tilde{\boldsymbol{\varepsilon}})\left(\dfrac{\partial \boldsymbol{\varepsilon}}{\partial t} - \dfrac{\partial \boldsymbol{\varepsilon}^{\mathrm{e}}}{\partial t}\right) \ge 0 \quad \forall \tilde{\boldsymbol{\varepsilon}} \in A_p^{-1}(K)\,. \end{array}\right. \tag{2.28}$$

The corresponding counterpart of (2.22)–(2.23) has the following form

$$\varrho_0\frac{\partial^2 u}{\partial t^2} = \mu\Delta u + (\mu + \lambda)\nabla\mathrm{div}\, u + \nu\Delta\frac{\partial u}{\partial t} + (\nu + \eta)\nabla\mathrm{div}\,\frac{\partial u}{\partial t} + \mathrm{div}\, A_p\boldsymbol{\varepsilon}^{\mathrm{e}} - \beta\nabla\theta + g\,, \tag{2.29}$$

$$c_V\frac{\partial \theta}{\partial t} = \kappa\Delta\theta - \beta\theta\frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \mathbf{1} + B\frac{\partial \boldsymbol{\varepsilon}}{\partial t} : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + A_p\boldsymbol{\varepsilon}^{\mathrm{e}} : \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{p}}}{\partial t} + \psi\,. \tag{2.30}$$

Again, the plastic dissipation rate $A_p\boldsymbol{\varepsilon}^{\mathrm{e}} : \frac{\partial \boldsymbol{\varepsilon}^{\mathrm{p}}}{\partial t}$ appears as an additional heat source in the energy balance (2.30). Indeed, system (2.28)–(2.30) is to be complemented with the small strain formula $\boldsymbol{\varepsilon} = \frac{1}{2}(D(u) + D^T(u))$.

Example 2.4 Phase transitions. Imagine a two-phase body, the phases can be both solid, or for instance one solid and one liquid, and the two phases may coexist. We introduce a new state variable $\chi \in [0,1]$, where $\chi = 1$ corresponds to the hot phase, $\chi = 0$ is to the cold phase, and intermediate values describe the hot phase fraction.

As before, we first propose an empirical constitutive equation for $\boldsymbol{\sigma}$. Let the reference temperature $\theta_c > 0$ be the phase transition temperature at standard pressure 10^5 Pa, at let V_c, V_h be the specific volumes of the cold and the hot phase, respectively. We denote by

$$\alpha = \frac{V_c - V_h}{V_h} \tag{2.31}$$

the relative volume increment of the cold phase with respect to the hot phase. In most materials, it is negative, in water it is positive and relatively high (about 0.09). Recall that we stay in Lagrangian coordinates, so that the mass density is constant.

As in Example 2.2, we decompose $\boldsymbol{\sigma}$ into the sum $\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathrm{v}} + \boldsymbol{\sigma}^{\mathrm{rev}}$ of an irreversible dissipative viscous component $\boldsymbol{\sigma}^{\mathrm{v}}$ as in (2.20), and a reversible component $\boldsymbol{\sigma}^{\mathrm{rev}}$

$$\boldsymbol{\sigma}^{\mathrm{rev}} = 2\mu \mathrm{Dev}(\boldsymbol{\varepsilon}) + \left(\lambda + \frac{2}{3}\mu\right)(\boldsymbol{\varepsilon} : \mathbf{1} - \alpha(1-\chi))\mathbf{1} - \beta(\theta - \theta_c)\mathbf{1} \tag{2.32}$$

containing the additional term $\alpha(1-\chi)$ with respect to (2.1), namely the phase volume increment. It is convenient here to use the deviator formalism for the elastic component as in (1.59).

In reality, the Lamé constants may depend on the phase χ, see [2]. Here, for simplicity, this dependence is neglected.

In the Second principle (2.11), F is a state function, and thus depends on $\boldsymbol{\varepsilon}, \theta$, and χ. The counterparts of (2.12) has the form

$$\left(\frac{\partial F}{\partial \theta} + S\right)\frac{\partial \theta}{\partial t} + \left(\frac{\partial F}{\partial \boldsymbol{\varepsilon}} - \boldsymbol{\sigma}\right) : \frac{\partial \boldsymbol{\varepsilon}}{\partial t} + \frac{\partial F}{\partial \chi}\frac{\partial \chi}{\partial t} \le 0\,, \tag{2.33}$$

for all processes, and we conclude as in (2.25) that

$$\frac{\partial F}{\partial \theta} = -S\,, \quad \frac{\partial F}{\partial \boldsymbol{\varepsilon}} = \boldsymbol{\sigma}^{\mathrm{rev}}\,, \quad \frac{\partial F}{\partial \chi}\frac{\partial \chi}{\partial t} \le 0\,, \tag{2.34}$$

and integrating (2.32) with respect to $\boldsymbol{\varepsilon}$ we obtain

$$F(\theta, \boldsymbol{\varepsilon}, \chi) = \mu \mathrm{Dev}(\boldsymbol{\varepsilon}) : \mathrm{Dev}(\boldsymbol{\varepsilon}) + \frac{1}{2}\left(\lambda + \frac{2}{3}\mu\right)(\boldsymbol{\varepsilon} : \mathbf{1} - \alpha(1-\chi))^2 - \beta(\theta - \theta_c)\boldsymbol{\varepsilon} : \mathbf{1} + F_1(\theta, \chi)\,, \tag{2.35}$$

where $F_1(\theta, \chi)$ is the "integration constant" which is to be identified. To motivate the choice of $F_1(\theta, \chi)$, consider first $\alpha = 0$, that is, no volume change takes place during phase transition. Then no extra pressure due to phase change arises, and the process remains at standard pressure, that is, the implications hold

$$(\chi < 1, \theta > \theta_c) \implies \frac{\partial \chi}{\partial t} > 0\,, \quad (\chi > 0, \theta < \theta_c) \implies \frac{\partial \chi}{\partial t} < 0\,. \tag{2.36}$$

In other words, for temperatures higher than θ_c, χ moves towards the hot phase $\chi = 1$, for temperatures lower than θ_c, χ moves towards the cold phase $\chi = 0$. Furthermore, we have

$$\frac{\partial F}{\partial \chi}\frac{\partial \chi}{\partial t} = \frac{\partial F_1}{\partial \chi}\frac{\partial \chi}{\partial t} \leq 0\,.$$

Assuming linear dependence of $\frac{\partial F_1}{\partial \chi}$ on θ leads to the hypothesis that there exists a constant L such that

$$\frac{\partial F_1}{\partial \chi} = L\left(1 - \frac{\theta}{\theta_c}\right) + \partial I_{[0,1]}(\chi)\,. \tag{2.37}$$

Here, $\partial I_{[0,1]}(\chi)$ denotes the subdifferential of the indicator function $I_{[0,1]}(\chi)$, where

$$I_{[0,1]}(\chi) = \begin{cases} 0 & \text{for } \chi \in [0,1]\,, \\ +\infty & \text{for } \chi \notin [0,1]\,, \end{cases} \qquad \partial I_{[0,1]}(\chi) = \begin{cases} \{0\} & \text{for } \chi \in (0,1)\,, \\ (-\infty, 0] & \text{for } \chi = 0\,, \\ [0, +\infty) & \text{for } \chi = 1\,, \\ \emptyset & \text{for } \chi \notin [0,1]\,, \end{cases}$$

see Figure 4.

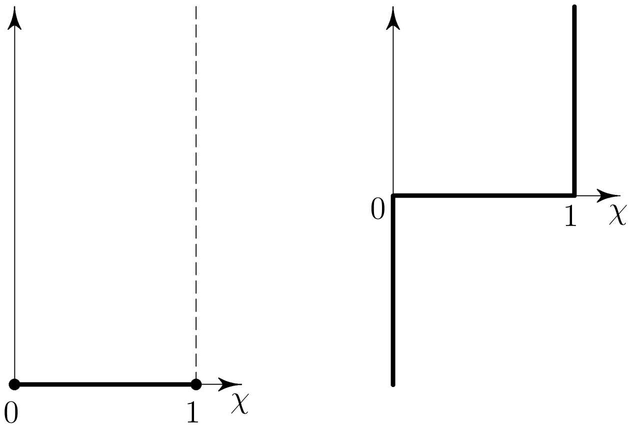

Figure 4: Graphs of $I_{[0,1]}$ (left) and $\partial I_{[0,1]}$ (right).

We conclude that

$$F_1(\theta, \chi) = L\left(1 - \frac{\theta}{\theta_c}\right)\chi + I_{[0,1]}(\chi) + F_0(\theta) \tag{2.38}$$

with F_0 as in (2.17). We then find easily the expressions for the entropy S and the internal energy U as

$$\begin{aligned} S &= -\frac{\partial F}{\partial \theta} = \beta \boldsymbol{\varepsilon} : \mathbf{1} + \frac{L\chi}{\theta_c} + c_V \log\left(\frac{\theta}{\theta_c}\right) + c_V\,, && (2.39) \\ U &= F + \theta S && (2.40) \\ &= \mu \mathrm{Dev}(\boldsymbol{\varepsilon}) : \mathrm{Dev}(\boldsymbol{\varepsilon}) + \frac{1}{2}\left(\lambda + \frac{2}{3}\mu\right)(\boldsymbol{\varepsilon} : \mathbf{1} - \alpha(1-\chi))^2 + \beta\theta_c \boldsymbol{\varepsilon} : \mathbf{1} + L\chi + c_V\theta + I_{[0,1]}(\chi)\,. \end{aligned}$$

Now, we can interpret the meaning of the constant L: This is the *latent heat*, that is, the amount of heat which has to be supplied to a unit volume of the body to perform the phase transition from cold phase to hot phase, and the value of this constant is known for most materials.

It remains to define an evolution law for $\frac{\partial\chi}{\partial t}$. In order to satisfy the inequality in (2.34), we assume that it is proportional to $-\frac{\partial F}{\partial\chi}$ with a proportionality constant γ (the *relaxation time*. Hence,

$$-\gamma\frac{\partial\chi}{\partial t} \in L\left(1-\frac{\theta}{\theta_c}\right) + \alpha\left(\lambda+\frac{2}{3}\mu\right)(\boldsymbol{\varepsilon}:\mathbf{1}-\alpha(1-\chi)) + \partial I_{[0,1]}(\chi)\,. \tag{2.41}$$

From (1.61) and (2.3) we derive PDEs for u and θ which turn out to be similar to (2.22)–(2.23) with an additional phase contribution, namely

$$\begin{aligned}
\varrho_0\frac{\partial^2 u}{\partial t^2} &= \mu\Delta u + (\mu+\lambda)\nabla\mathrm{div}\, u + \nu\Delta\frac{\partial u}{\partial t} + (\nu+\eta)\nabla\mathrm{div}\,\frac{\partial u}{\partial t} - \beta\nabla\theta \qquad (2.42)\\
&\quad + \alpha\left(\lambda+\frac{2}{3}\mu\right)\nabla\chi + g\,,\\
c_V\frac{\partial\theta}{\partial t} &= \kappa\Delta\theta - \beta\theta\frac{\partial\boldsymbol{\varepsilon}}{\partial t}:\mathbf{1} + B\frac{\partial\boldsymbol{\varepsilon}}{\partial t}:\frac{\partial\boldsymbol{\varepsilon}}{\partial t} \qquad (2.43)\\
&\quad - \left(L + \alpha\left(\lambda+\frac{2}{3}\mu\right)(\boldsymbol{\varepsilon}:\mathbf{1}-\alpha(1-\chi))\right)\frac{\partial\chi}{\partial t} + \psi\,.
\end{aligned}$$

Let us have a closer look at the equilibria of the system (2.41)–(2.43), that is, solutions which do not depend on time. Assuming for example a thermally insulated body with vanishing heat sources ψ and with no heat flux on the boundary $q\cdot n(x) = 0$ for $x\in\partial\mathcal{B}$, we obtain from (2.43) for the equilibrium temperature θ^* the equation $\Delta\theta^* = 0$, hence $\theta^* =$ const. Furthermore, by (2.41), phases can coexist (that is, $\chi\in(0,1)$) only if

$$L\left(1-\frac{\theta}{\theta_c}\right) + \alpha\left(\lambda+\frac{2}{3}\mu\right)(\boldsymbol{\varepsilon}:\mathbf{1}-\alpha(1-\chi)) = 0\,. \tag{2.44}$$

By (2.32), the equilibrium mechanical pressure p^* is given by (note that $\boldsymbol{\sigma}^v = 0$ in equilibrium)

$$p^* = -\frac{1}{3}\boldsymbol{\sigma}:\mathbf{1} = -\left(\lambda+\frac{2}{3}\mu\right)(\boldsymbol{\varepsilon}:\mathbf{1}-\alpha(1-\chi)) + \beta(\theta^*-\theta_c)\,, \tag{2.45}$$

hence (2.44)–(2.45) can be rewritten as

$$p^* = \left(\frac{L}{\alpha\theta_c} - \beta\right)(\theta_c - \theta^*)\,. \tag{2.46}$$

For water, the approximate values of the physical constants are $L = 3\cdot 10^8 J/m^3$, $\beta = 4\cdot 10^5 J/m^3K$, $\theta_c = 273K$, $\alpha = 9\cdot 10^{-2}$, hence $\frac{L}{\alpha\theta_c} - \beta > 0$. We conclude in agreement with experimental observation that the melting temperature θ^* of ice is smaller than θ_c if the body is subject to positive mechanical pressure. In physical literature, Eq. (2.46) is called the *Clausius-Clapeyron equation.*

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