Continuum mechanics
V. Constitutive equations

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1. Constitutive equation: definition and basic axioms

Constitutive equation: relation between two physical quantities specific to a material, e.g.:

$$\tau^{ij} = \tau^{ij}(\mathbf{u}, \{e_{k\ell}\}, \{F^k_\ell\}, T)$$

Basic axioms

- Axiom of **causality**
- Axiom of **determinism**
- Axiom of **equipresence**
- Axiom of **neighbourhood**
- Axiom of **memory**
- Axiom of **objectivity**
- Axiom of **material invariance**
- Axiom of **admissibility**

1. Basic axioms: causality

Axiom of causality:

Independent variables in the constitutive laws are:

- Continuum position $y^i(\mathbf{x}, t)$
- Temperature T

Dependent variables (responses) are e.g.:

- Helmholtz free energy φ (thermodynamic potential, measure of the "useful" work obtainable from a closed thermodynamic system)
- Strain energy density Ψ
- Stress tensor τ^{ij}
- Heat flux q^i
- Internal energy ϵ
- Entropy S

1. Basic axioms: determinism and equipresence

Axiom of determinisim

Responses of the constitutive functions at a material point $\mathbf{x}$ at time t are determined by the **history of the motion** and **history of the temperature** of **all points** of the body.

Axiom of equipresence

If an independent variable enters in one function of response, it should be present in all constitutive laws (until the proof of the contrary)

1. Basic axioms: neighbourhood

Axiom of neighbourhood

Responses at a point $\mathbf{x}$ are not much influenced by values of **independent variables** (temperature and displacement) at a distant point $\bar{\mathbf{x}}$.

Hypothesis: functions $\mathbf{y}(\mathbf{x}, t)$ and $T(\mathbf{x}, t)$ are sufficiently smooth to be expanded into a Taylor series:

$$y^i(\bar{\mathbf{x}}, t) = y^i(\mathbf{x}, t) + \left.\frac{\partial y^i}{\partial x^j}\right|_{\mathbf{x},t} (\bar{x}^j - x^j) + \frac{1}{2}\left.\frac{\partial^2 y^i}{\partial x^j \partial x^k}\right|_{\mathbf{x},t} (\bar{x}^j - x^j)(\bar{x}^k - x^k) + \dots$$

with negligible higher-order terms.
Simple thermomechanical material: Taylor expansion terms with the second+higher derivatives are negligible:

$$\tau(\mathbf{x}, t) = \mathcal{T}\left[\mathbf{y}(\mathbf{x}, t'), \mathbf{y}_{,\mathbf{x}}(\mathbf{x}, t'), T(\mathbf{x}, t'), T_{,\mathbf{x}}(\mathbf{x}, t'); \mathbf{x}, t' \leq t\right]$$

This class of material also called **gradient continua**.

1. Basic axioms: memory

Axiom of memory

Values of constitutive variables from a distant past do not affect appreciably the values of constitutive laws now.

Smooth memory material: constitutive variables can be expanded to Taylor series in time with negligible higher order terms

Fading memory: response functionals must smooth possible discontinuities in memory

1. Basic axioms: objectivity

Axiom of objectivity

Invariance of constitutive laws with respect to rigid body motion of the **spatial frame of reference (spatial coordinates)**.

Simple consequence: constitutive laws depend of the deformation gradient (or strain tensor) rather than $\mathbf{y}(\mathbf{x})$.

1. Basic axioms: material invariance

Axiom of material invariance

Invariance of constitutive laws with respect to certain symmetries/transformations of the **material frame of reference (material coordinates)**.

Symmetries in material properties due to crystallographic orientation.

Hemitropic continuum: invariant w.r.t. all rotations
Isotropic continuum: hemitropic + invariance to reflection
Anisotropic continuum: otherwise (can have some invariance properties, but not all)
Homogeneous continuum: invariance w.r.t. shift of coord system

1. Basic axioms: admissibility

Axiom of admissibility

Consistence with respect to basic conservation laws (mass, momentum, energy), and the 2nd law of thermodynamics (entropy).

This axiom can also help to eliminate dependences on some constitutive variables.

2. Constitutive laws for simple thermo-mechanical continua

Thermo-elastic continua: simple thermo-mechanical continua with no memory.

By applying the basic axioms, all material properties depend only on the current values of deformation and temperature: hence also for Helmholtz free energy:

$$\varphi = \varphi(\{e_{ij})\}, T)$$

For simplicity, consider only small deformations (Cauchy strain tensor e_{ij}).

Are we able to say more about the form of the constitutive laws in this case?

Axiom of admissibility: we need to be consistent with thermodynamical laws and basic equilibria.

Let us derive φ with respect to time

$$\dot{\varphi} = \frac{\partial \varphi}{\partial e_{ij}} \dot{e}_{ij} + \frac{\partial \varphi}{\partial T} \dot{T}$$

and substitute it into the dissipation inequality

$$\rho\, \dot{\varphi} + \rho\, \dot{T}\, \eta - \tau^{ij}\, \nabla_j v_i + \frac{q^i}{T} \nabla_i T \leq 0.$$

We get

$$\rho\, \frac{\partial \varphi}{\partial e_{ij}} \dot{e}_{ij} + \rho\, \frac{\partial \varphi}{\partial T} \dot{T} + \rho\, \dot{T}\, \eta - \tau^{ij}\, \nabla_j v_i + \frac{q^i}{T} \nabla_i T \leq 0.$$

NB. Due to the symmetry of $\tau^{ij} = \tau^{ji}$, we have

$$\tau^{ij}\, \nabla_j v_i = \frac{1}{2} \left(\tau^{ij}\, \nabla_j v_i + \tau^{ij}\, \nabla_i v_j \right) = \tau^{ij}\, \dot{e}_{ij}$$

2. Constitutive laws for simple thermo-mechanical continua

Hence, the dissipation inequality looks now like:

$$\dot{e}_{ij} \left(\rho\, \frac{\partial \varphi}{\partial e_{ij}} - \tau^{ij} \right) + \dot{T}\, \rho \left(\eta + \frac{\partial \varphi}{\partial T} \right) + \frac{q^i}{T} \nabla_i T \leq 0.$$

This inequality must hold for any time-dependent process, ie. **for any** $\dot{e}_{ij}$ **and** $\dot{T}$!

Hence there **must be**:

$$\rho\, \frac{\partial \varphi}{\partial e_{ij}} - \tau^{ij} = 0 \qquad \Rightarrow \qquad \tau^{ij} = \rho\, \frac{\partial \varphi}{\partial e_{ij}},$$

$$\eta + \frac{\partial \varphi}{\partial T} \qquad \Rightarrow \qquad \eta = -\frac{\partial \varphi}{\partial T},$$

$$\frac{q^i}{T} \nabla_i T \leq 0.$$

3. Simple thermo-mechanical continuum: large deformation

Small deformations: (Cauchy stress tensor)

$$\tau^{ij} = \rho \frac{\partial \varphi}{\partial e_{ij}} \quad , \quad \eta = -\frac{\partial \varphi}{\partial T} \quad , \quad \frac{q^i}{T} \nabla_i T \leq 0$$

Large deformations: (2nd Piola-Kirchhoff)

$$T^{ij} = \rho_0 \frac{\partial \varphi}{\partial \varepsilon_{ij}} \quad , \quad \eta = -\frac{\partial \varphi}{\partial T} \quad , \quad \frac{q^i}{T} \nabla_i T \leq 0$$

Define **strain (or stored) energy density** $\Psi = \rho_0 \, \varphi$, then:

$$\boxed{T^{ij} = \frac{\partial \Psi}{\partial \varepsilon_{ij}} \quad , \quad \eta = -\frac{1}{\rho_0} \frac{\partial \Psi}{\partial T} \quad , \quad \frac{q^i}{T} \nabla_i T \leq 0}$$

NB: $\underline{\underline{T}} = \frac{\partial \Psi}{\partial \underline{\underline{\varepsilon}}}$ is a derivative of a scalar function with respect to a tensor, see M2, Section 2.

Hyperelastic material: material for which $T^{ij} = \dfrac{\partial \Psi}{\partial \varepsilon_{ij}}$

4. Hooke's law (Robert Hooke 1635–1703)

Neglect temperature: Taylor expansion of strain energy density:

$$\Psi(e) = \Psi_0 + E^{ij} \, e_{ij} + \frac{1}{2} E^{ijk\ell} \, e_{ij} \, e_{k\ell} + \dots$$

with material coefficients E^{ij}, $E^{ijk\ell}$ called **elastic tensors**.

Suppose small deformations: take only the 3 first terms of the expansion: then from $\tau^{ij} = \frac{\partial \Psi}{\partial e_{ij}}$ we obtain the **Hooke's law** (1660):

$$\boxed{\tau^{ij} = E^{ij} + E^{ijk\ell} e_{k\ell}}$$

with the **pre-stress** E^{ij} at initial configuration.
If no pre-stress:

$$\tau^{ij} = E^{ijk\ell} e_{k\ell}$$

4.1. Hooke's law: elastic tensor $E^{ijk\ell}$

Elastic tensor $E^{ijk\ell}$: $3^4 = 81$ components depending only on material coordinates

Possible reduction of degrees of freedom:

- Symmetry of τ^{ij} and $e_{k\ell}$ $\Rightarrow$ symmetry of $E^{ijk\ell}$ within ij and $k\ell$:

$$E^{ijk\ell} = E^{jik\ell} = E^{ij\ell k} = E^{ji\ell k}$$

  no. of components reduced to 36.
- Taylor expansion of $\Psi(e)$ $\Rightarrow$ symmetry in pairs ij and $k\ell$:

$$E^{ijk\ell} = E^{k\ell ij}$$

  no. of components thus reduced to 21.

4.2. Hooke's law in deviator-form

Consider only small deformations. Physical meaning of Cauchy strain $\underline{\underline{e}}$:

Relative volume change: $\dfrac{dV - dV_0}{dV_0} = e^1_1 + e^2_2 + e^3_3 = \mathrm{tr}(\underline{\underline{e}}) = e^\ell_\ell$

(cf. "1. Kinematics", section 4.)

Define:

Volumic dilatation e: volume-changing deformation component:

$$e = \frac{1}{3}\mathrm{tr}(\underline{\underline{e}}) = \frac{1}{3} e^\ell_\ell$$

Strain deviator $\underline{\underline{\tilde{e}}}$: volume-preserving deformation component

$$\tilde{e}_{ij} = e_{ij} - e\, g_{ij} \qquad \tilde{e}^i_j = e^i_j - e\, \delta^i_j$$

changes only shape, not the volume, $\mathrm{tr}(\underline{\underline{\tilde{e}}}) = 0$.

Hydrostatic tension s: forces opposed to volume change

$$s = \frac{1}{3}\mathrm{tr}(\underline{\underline{\tau}}) = \frac{1}{3}\tau^j_j$$

Stress deviator $\underline{\underline{\tilde{\tau}}}$: forces opposed to shape change:

$$\tilde{\tau}^{ij} = \tau^{ij} - s\, g^{ij} \qquad \tilde{\tau}^i_j = \tau^i_j - s\, \delta^i_j$$

4.2. Hooke's law in deviator-form, shear and bulk moduli

Hooke's law for isotropic materials (in deviator form):

$$\tilde{\tau}^i_j = 2\,\mu\,\tilde{e}^i_j \qquad \text{volume-preserving deformations}$$
$$s = 3\,K\,e \qquad \text{volume-change}$$

Material properties characterized only by 2 constants

- **shear modulus** μ characterizes genuine shear
- **bulk modulus** K characterizes (in)compressibility (incompressible material for $K \to \infty$)

Total strain tensor:

$$\begin{aligned}
\tau^i_j &= \tilde{\tau}^i_j + s\,\delta^i_j = 2\,\mu\tilde{e}^i_j + 3\,K\,e\,\delta^i_j \\
&= 2\,\mu\left(e^i_j - \frac{1}{3}\,e^\ell_\ell\,\delta^i_j\right) + K\,e^\ell_\ell\,\delta^i_j \\
&= 2\,\mu\,e^i_j + \left(K - \frac{2\,\mu}{3}\right)\,e^\ell_\ell\,\delta^i_j
\end{aligned}$$

4.3. Hooke's law for isotropic materials: elastic tensor $E^{ijk\ell}$

Total strain tensor:

$$\begin{aligned}
\tau^{ij} &= 2\,\mu\,e^{ij} + \left(K - \frac{2\,\mu}{3}\right)\,e^\ell_\ell\,g^{ij} \\
&= 2\,\mu\,g^{ik}\,g^{j\ell}\,e_{k\ell} + \underbrace{\left(K - \frac{2\,\mu}{3}\right)}_{=\lambda}\,g^{ij}\,g^{k\ell}\,e_{k\ell} \\
&= \mu\left(g^{ik}\,g^{j\ell} + g^{i\ell}\,g^{jk}\right)\,e_{k\ell} + \lambda\,g^{ij}\,g^{k\ell}\,e_{k\ell}
\end{aligned}$$

Here, λ and μ are the so called **Lamé coefficients**, $K = \dfrac{2\,\mu + 3\,\lambda}{3}$.

The corresponding elastic tensor $E^{ijk\ell}$ is thus ($\tau^{ij} = E^{ijk\ell}\,e_{k\ell}$):

$$\boxed{E^{ijk\ell} = \mu\left(g^{ik}\,g^{j\ell} + g^{i\ell}\,g^{jk}\right) + \lambda\,g^{ij}\,g^{k\ell}}$$

4.4. Hooke's law for isotropic materials: compliance $C_{ijk\ell}$

The tensor-inverse of $E^{ijk\ell}$ is called **compliance** $\underline{\underline{C}}$:

$$\tau^{ij} = E^{ijk\ell}\, e_{kl} \qquad\qquad e_{ij} = C_{ijk\ell}\, \tau^{k\ell}.$$

Let us inverse the Hooke's law (ie. express $\underline{e}$ as a function of $\underline{\tau}$):

$$\underline{\tau} = 2\,\mu\,\underline{e} + \lambda\,\mathrm{tr}(\underline{e})\,\underline{\underline{Id}}$$

Take a trace:

$$\mathrm{tr}(\underline{\tau}) = 2\,\mu\,\mathrm{tr}(\underline{e}) + 3\,\lambda\,\mathrm{tr}(\underline{e}) = (2\,\mu + 3\,\lambda)\;\mathrm{tr}(\underline{e})$$

Plug back $\mathrm{tr}(\underline{e})$ into the Hooke's law above to get

$$\underline{\tau} = 2\,\mu\underline{e} + \frac{\lambda}{2\,\mu + 3\,\lambda}\,\mathrm{tr}(\underline{\tau})\,\underline{\underline{Id}}$$

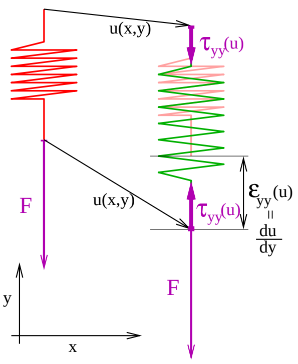
Hence,

$$\underline{e} = \frac{1}{2\mu}\left(\underline{\tau} - \frac{\lambda\,\mathrm{tr}(\underline{\tau})}{2\mu+3\lambda}\,\underline{\underline{Id}}\right) \quad \text{or} \quad e_{ij} = \underbrace{\frac{1}{2\mu}\left(g_{ik}\,g_{j\ell} - \frac{\lambda}{2\mu+3\lambda}\,g_{k\ell}\,g_{ij}\right)}_{C_{ijk\ell}}\,\tau^{k\ell}$$

4.5. Hooke's law: Young's modulus E, Poisson's ratio ν

Material constants in Hooke's law **by analogy with linear springs:**

In 1D, spring stiffness $\quad E = \dfrac{\text{force } F}{\text{relative elongation } \varepsilon}$



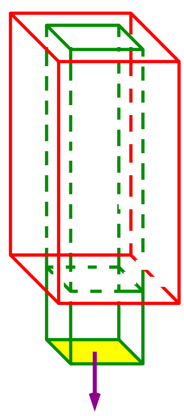
Compare with a special case in 3D:

Mono-axial loading

Suppose $\tau^{ij} = 0$ for all i, j, except $\tau^{11} \neq 0$.
Compliance-form of a 3D Hooke's law gives:

$$e_{11} = \frac{1}{2\mu}\left(1 - \frac{\lambda}{2\mu + 3\lambda}\right)\tau_{11} = \frac{\mu + \lambda}{\mu\,(2\mu + 3\lambda)}\,\tau_{11}$$

$$e_{22} = e_{33} = -\frac{\lambda}{2\mu\,(2\mu + 3\lambda)}\,\tau_{11}$$



4.5. Hooke's law: Young's modulus E, Poisson's ratio ν

Young's modulus defined as apparent "1D spring stiffness" in the case of mono-axial loading, ie:

$$E = \frac{\tau^{11}}{e_{11}} = \frac{\mu + \lambda}{\mu\,(2\mu + 3\lambda)}$$

with τ^{11} and e_{11} from the mono-axial loading in cartesian coordinates.

Poisson's ratio measures transversal vs. axial elongation

$$\nu = -\frac{e_{22}}{e_{11}} = \frac{\lambda}{2\,(\mu + \lambda)}$$

Relative volume change:

$$\frac{dV - dV_0}{dV_0} = e_{11} + e_{22} + e_{33} = (1 - 2\,\nu)\; e_{11}$$

ie. $\nu = 0.5$ for incompressible materials

4.6. Hooke's law for isotropic materials: summary

Isotropic material characterized by two constants:

- shear modulus μ and bulk modulus K,

$$\mu = \frac{E}{2\,(1+\nu)} \qquad K = \frac{1}{3}\,(2\mu + 3\lambda) = \frac{1}{3}\,\frac{E}{1-2\nu}$$

- Lamé's coefficients μ and λ,

$$\mu = \frac{E}{2\,(1+\nu)} \qquad \lambda = \frac{E\,\nu}{(1+\nu)(1-2\nu)} = K - \frac{2\,\mu}{3}$$

- Young's modulus E and Poisson's ratio ν,

$$E = \frac{\mu\,(2\mu + 3\lambda)}{\mu + \lambda} \qquad \nu = \frac{\lambda}{2(\mu + \lambda)}$$

4.6. Hooke's law for isotropic materials: summary

Corresponding form of Hooke's law:

- using shear modulus μ and bulk modulus K, in deviator form:

$$\tilde{\tau}^i_j = 2\,\mu\,\tilde{e}^i_j \qquad , \qquad s = 3\,K\,e$$

- using Lamé's coefficients μ and λ:

$$\tau^{ij} = \mu\left(g^{ik}\,g^{j\ell} + g^{i\ell}\,g^{jk}\right)\,e_{k\ell} + \lambda\,g^{ij}\,g^{k\ell}\,e_{k\ell}$$

Or in global form

$$\underline{\underline{\tau}} = 2\,\mu\underline{\underline{e}} + \frac{\lambda}{2\,\mu + 3\,\lambda}\,\mathrm{tr}(\underline{\underline{\tau}})\,\underline{\underline{Id}}$$

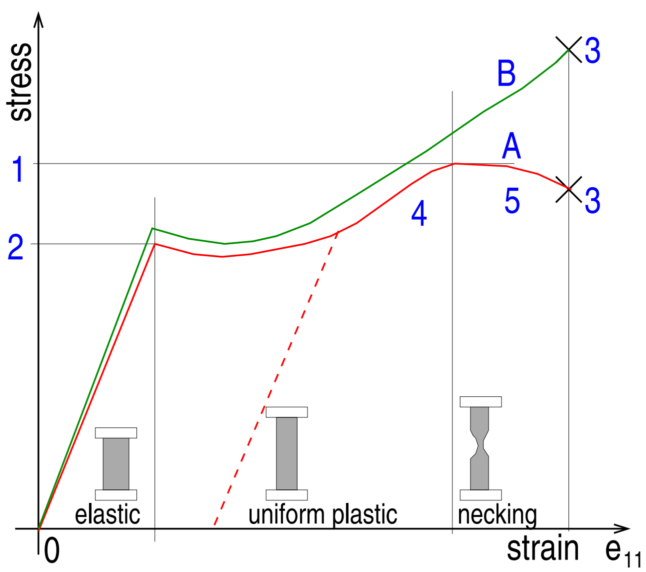
- using Young's modulus E and Poisson's ratio ν:

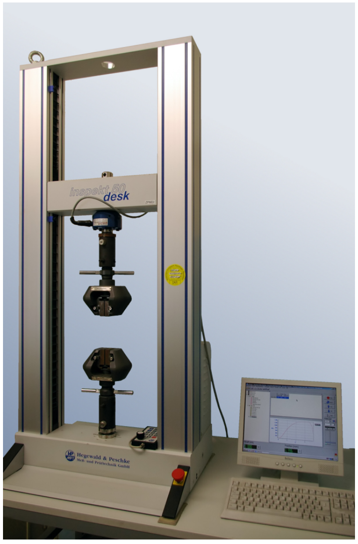
$$\tau^{ij} = \frac{E}{2(1+\nu)}\left(\frac{2\nu}{1-2\nu}\,g^{ij}\,g^{k\ell} + g^{ik}\,g^{j\ell} + g^{i\ell}\,g^{jk}\right)\,e_{k\ell}$$

- large deformations: Saint Venant-Kirchhoff material

$$\Psi(\underline{\underline{\varepsilon}}) = \mu\,\mathrm{tr}(\underline{\underline{\varepsilon}}^2) + \frac{\lambda}{2}\left[\mathrm{tr}(\underline{\underline{\varepsilon}})\right]^2 \qquad , \qquad T^{ij} = \frac{\partial\Psi}{\partial\varepsilon_{ij}}$$

4.7. Hooke's law: measuring stress-strain curve for steel





1 Ultimate Strength
2 Yield Strength (elastic limit)
3 Rupture
4 Strain hardening region
5 Necking region
A 1st Piola-Kirchhoff stress $\sigma = \dfrac{F}{A_0}$
B Euler stress $\tau = \dfrac{F}{A}$

5. Linear thermo-elasticity: Duhamel-Neumann's law

Consider also temperature: Taylor expansion of strain energy:

$$\begin{aligned}\Psi(e,T) &= \Psi_0(T) + E^{ij}(T)\, e_{ij} + \frac{1}{2} E^{ijk\ell}(T)\, e_{ij}\, e_{k\ell} + \dots \\ &= \Psi_0(T) + \left[E^{ij}(T_0) + \frac{\partial E^{ij}}{\partial T}(T-T_0) + \dots\right] e_{ij} \\ &\quad + \frac{1}{2}\left[E^{ijk\ell}(T_0) + \frac{\partial E^{ijk\ell}}{\partial T}(T-T_0) + \dots\right] e_{ij}\, e_{k\ell} + \dots\end{aligned}$$

Suppose $|T - T_0| << T_0$ and small deformations and neglect all (mixed) 3rd order terms and higher.

Duhamel-Neumann's law: from $\tau^{ij} = \frac{\partial \Psi}{\partial e_{ij}}$ we obtain:

$$\boxed{\tau^{ij} = E^{ij}_{T_0} + E^{ijk\ell}\, e_{k\ell} - \beta^{ij}\,(T - T_0)}$$

with $\beta^{ij} = -\frac{\partial E^{ij}}{\partial T}$. For isotropic materials $\beta^{ij} = \beta\, g^{ij}$.
Usually, we take T_0 with no pre-strain, $E^{ij}_{T_0} = 0$.

5. Linear thermo-elasticity: Duhamel-Neumann's law

From the Hooke's law, we can write:

$$\tau^i_j = 2\,\mu\, e^i_j + \lambda\, \delta^i_j\, e^\ell_\ell - \beta^i_j\,(T - T0)$$

Let us derive the compliance-form $\underline{\underline{e}} = e(\underline{\underline{\tau}}, T)$:
Index-contraction of the above gives

$$\tau^i_i = (2\mu{+}3\lambda)\, e^\ell_\ell - \beta^k_k\,(T{-}T_0) \quad \text{ie.} \quad e^\ell_\ell = \frac{1}{2\mu + 3\lambda}\left[\tau^i_i + \beta^k_k\,(T - T_0)\right]$$

Substitute it back to the Duhamel-Neumann's law to obtain

$$e^i_j = \frac{1}{2\mu}\left[\delta^i_k\,\delta^\ell_j - \frac{\lambda}{2\mu{+}3\lambda}\delta^i_j\,\delta^\ell_k\right]\tau^k_\ell \underbrace{-\frac{1}{2\mu}\left(\frac{\lambda}{2\mu{+}3\lambda}\,\delta^i_j\,\beta^m_m - \beta^i_j\right)}_{\alpha^i_j\text{...thermal dilatation coeff}}(T{-}T_0)$$

6. Constitutive law for heat flux $\mathbf{q}$: Fourier's law

Suppose simple thermo-mechanical continuum, small deformations:

$$\mathbf{q} = \mathbf{q}(T, \underline{\nabla} T, \underline{\underline{e}})$$

Use first-order Taylor expansion around a deformation-free configuration at T_0 to approximate:

$$q^i = k_0^i + k_1^i\,(T - T_0) + k_2^{ij}\,\nabla_j T + k_3^{ijk}\,e_{jk}$$

with some coefficients k_0^i, k_1^i and k_3^{ijk}.
This law must not contradict the 2nd law of thermodynamics in particular there must be (cf. Section 2 and 3 above):

$$\frac{q^i}{T}\nabla_i T = \frac{1}{T}\left(k_0^i + k_1^i\,(T - T_0) + k_2^{ij}\,\nabla_j T + k_3^{ijk}\,e_{jk}\right)\,\nabla_i T \leq 0$$

for any state of the continuum, ie. $\forall\ T > 0$ and $\forall\ \underline{\underline{e}}$. This is satisfied only if

$$k_0^i = k_1^i \equiv 0 \qquad , \qquad k_3^{ijk} \equiv 0 \qquad \text{and } -[k_2^{ij}] \text{ is sym.positive definite}$$

6. Constitutive law for heat flux $\mathbf{q}$: Fourier's law

Hence, we have derived the **Fourier's law** for heat flux:

$$\boxed{q^i = -k^{ij}\,\nabla_j T \qquad , \qquad \mathbf{q} = \underline{\underline{k}} \cdot \nabla T}$$

with **the heat conductivity tensor** $\underline{\underline{k}}$, $k^{ij} = -k_2^{ij}$, $[k^{ij}]$ is a symmetric positive definite matrix.

For isotropic materials: $\underline{\underline{k}} = k\,\underline{\underline{Id}}$.