Mathematical Preliminaries

Introductory Course on Multiphysics Modelling

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1 Vectors, tensors, and index notation

1.1 Generalization of the concept of vector

- A **vector** is a quantity that possesses both a **magnitude** and a **direction** and obeys certain laws (of **vector algebra**): the vector addition and the commutative and associative laws, the associative and distributive laws for the multiplication with scalars.
- The vectors are suited to describe physical phenomena, since they are **independent of any system of reference**.

The **concept of a vector** that is independent of any coordinate system **can be generalised** to higher-order quantities, which are called **tensors**. Consequently, vectors and scalars can be treated as lower-rank tensors.

Scalars have a magnitude but no direction. They are tensors of order 0. *Example:* the mass density.

Vectors are characterised by their magnitude and direction. They are tensors of order 1. *Example:* the velocity vector.

Tensors of second order are quantities which multiplied by a vector give as the result another vector. *Example*: the stress tensor.

Higher-order tensors are often encountered in constitutive relations between second-order tensor quantities. *Example:* the fourth-order elasticity tensor.

1.2 Summation convention and index notation

Einstein's summation convention

A summation is carried out over repeated indices in an expression. (The summation sign is skipped.)

Example 1.

$$a_i \, b_i \equiv \sum_{i=1}^3 a_i \, b_i = a_1 \, b_1 + a_2 \, b_2 + a_3 \, b_3$$

$$A_{ii} \equiv \sum_{i=1}^3 A_{ii} = A_{11} + A_{22} + A_{33}$$

$$A_{ij} \, b_j \equiv \sum_{j=1}^3 A_{ij} \, b_j = A_{i1} \, b_1 + A_{i2} \, b_2 + A_{i3} \, b_3 \quad (i = 1, 2, 3) \quad [3 \text{ expressions}]$$

$$T_{ij} \, S_{ij} \equiv \sum_{i=1}^3 \sum_{j=1}^3 T_{ij} \, S_{ij} = T_{11} \, S_{11} + T_{12} \, S_{12} + T_{13} \, S_{13} + T_{21} \, S_{21} + T_{22} \, S_{22} + T_{23} \, S_{23} + T_{31} \, S_{31} + T_{32} \, S_{32} + T_{33} \, S_{33}$$

The principles of index notation:

An index cannot appear more than twice in one term! If necessary, the
normal summation symbol must be used. A repeated index is called a bound or
dummy index.

Example 2.

$$A_{ii}$$
, $C_{ijkl}S_{kl}$, $A_{ij}b_ic_j \leftarrow \text{Correct}$

$$A_{ij}b_jc_j \leftarrow \text{Wrong!}$$

$$\sum_j A_{ij}b_jc_j \leftarrow \text{Correct}$$

A term with more than two-times-repeated index is correct if:

- the summation sign is used, e.g.: $\sum_{i} a_i b_i c_i = a_1 b_1 c_1 + a_2 b_2 c_2 + a_3 b_3 c_3$, or
- the dummy index is underlined, e.g.: $a_i b_i c_i = a_1 b_1 c_1$ or $a_2 b_2 c_2$ or $a_3 b_3 c_3$.
- If the index appears once, it is called a **free index**. The number of free indices determines the order of a tensor.

Example 3.

$$A_{ii}, \quad a_i \, b_i, \quad T_{ij} \, S_{ij} \quad \leftarrow \quad \text{scalars (no free indices)}$$

$$A_{ij} \, b_j \quad \leftarrow \quad \text{a vector (one free index: } i)$$

$$C_{ijkl} \, S_{kl} \quad \leftarrow \quad \text{a second-order tensor (two free indices: } i,j)$$

• The denomination of a dummy index (in a term) is arbitrary since it vanishes after the summation, thus, $a_i b_i \equiv a_j b_j$.

Example 4.

$$a_i \, b_i = a_1 \, b_1 + a_2 \, b_2 + a_3 \, b_3 = a_j \, b_j$$
 $A_{ii} \equiv A_{jj}, \quad T_{ij} S_{ij} \equiv T_{kl} \, S_{kl}, \quad T_{ij} + C_{ijkl} \, S_{kl} \equiv T_{ij} + C_{ijmn} \, S_{mn}$

1.3 Kronecker delta and permutation symbol

Definition 5 (Kronecker delta).

$$\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$$

- The Kronecker delta can be used to substitute one index by another, for example: $a_i \delta_{ij} = a_1 \delta_{1j} + a_2 \delta_{2j} + a_3 \delta_{3j} = a_j$.
- When Cartesian coordinates are used (with orthonormal base vectors e_1 , e_2 , e_3) the Kronecker delta δ_{ij} is the (matrix) representation of the unity tensor $I = \delta_{ij} e_i \otimes e_j = e_1 \otimes e_1 + e_2 \otimes e_2 + e_3 \otimes e_3$.
- $\mathbf{A} \cdot \mathbf{I} = A_{ij} \delta_{ij} = A_{ii}$ which is the **trace** of the matrix (tensor) \mathbf{A} .

Definition 6 (Permutation symbol).

$$\epsilon_{ijk} = \begin{cases} 1 & \text{for even permutations: } 123, 231, 312 \\ -1 & \text{for odd permutations: } 132, 321, 213 \\ 0 & \text{if an index is repeated} \end{cases}$$

The permutation symbol (or tensor) is widely used in index notation to express the **vector** or **cross product** of two vectors:

$$\mathbf{c} = \mathbf{a} \times \mathbf{b} = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} \rightarrow c_i = \epsilon_{ijk} a_j b_k \rightarrow \begin{cases} c_1 = a_2 b_3 - a_3 b_2 \\ c_2 = a_3 b_1 - a_1 b_3 \\ c_3 = a_1 b_2 - a_2 b_1 \end{cases}$$

1.4 Tensors and their representations

Informal definition of tensor

A **tensor** is a generalized **linear 'quantity'** that can be expressed as a **multi-dimensional array** relative to a choice of basis of the particular space on which it is defined. Thus,

- a tensor is independent of any chosen frame of reference,
- its representation behaves in a specific way under coordinate transformations.

Cartesian system of reference

Let \mathcal{E}^3 be the three-dimensional Euclidean space with a Cartesian coordinate system with three orthonormal base vectors e_1 , e_2 , e_3 , so that

$$e_i \cdot e_j = \delta_{ij}$$
 $(i, j = 1, 2, 3).$

• A **second-order tensor** $T \in \mathcal{E}^3 \otimes \mathcal{E}^3$ is defined by

$$egin{aligned} m{T} := T_{ij} \, m{e}_i \otimes m{e}_j &= T_{11} \, m{e}_1 \otimes m{e}_1 + T_{12} \, m{e}_1 \otimes m{e}_2 + T_{13} \, m{e}_1 \otimes m{e}_3 \\ &+ T_{21} \, m{e}_2 \otimes m{e}_1 + T_{22} \, m{e}_2 \otimes m{e}_2 + T_{23} \, m{e}_2 \otimes m{e}_3 \\ &+ T_{31} \, m{e}_3 \otimes m{e}_1 + T_{32} \, m{e}_3 \otimes m{e}_2 + T_{33} \, m{e}_3 \otimes m{e}_3 \end{aligned}$$

where \otimes denotes the tensorial (or dyadic) product, and T_{ij} is the (matrix) representation of T in the given frame of reference defined by the base vectors e_1 , e_2 , e_3 .

• The second-order tensor $T \in \mathcal{E}^3 \otimes \mathcal{E}^3$ can be viewed as a **linear transformation** from \mathcal{E}^3 onto \mathcal{E}^3 , meaning that it transforms every vector $\mathbf{v} \in \mathcal{E}^3$ into another vector from \mathcal{E}^3 as follows

$$T \cdot v = (T_{ij} e_i \otimes e_j) \cdot (v_k e_k) = T_{ij} v_k (\overbrace{e_j \cdot e_k}^{\delta_{jk}}) e_i$$

$$= T_{ij} v_k \delta_{jk} e_i = T_{ij} v_j e_i = w_i e_i = w \in \mathcal{E}^3 \quad \text{where} \quad w_i = T_{ij} v_j$$

• A **general tensor of order** *n* is defined by

$$T_n := T_{\underbrace{ijk...}_{n \text{ indices}}} \underbrace{e_i \otimes e_j \otimes e_k \otimes ...}_{n \text{ terms}},$$

where $T_{ijk...}$ is its (*n*-dimensional array) representation in the given frame of reference.

Example 7. Let $\mathbf{C} \in \mathcal{E}^3 \otimes \mathcal{E}^3 \otimes \mathcal{E}^3 \otimes \mathcal{E}^3$ and $\mathbf{S} \in \mathcal{E}^3 \otimes \mathcal{E}^3$. The fourth-order tensor \mathbf{C} describes a linear transformation in $\mathcal{E}^3 \otimes \mathcal{E}^3$:

$$\begin{aligned} \boldsymbol{C} \bullet \boldsymbol{S} &= \boldsymbol{C} : \boldsymbol{S} = (C_{ijkl} \, \boldsymbol{e}_i \otimes \boldsymbol{e}_j \otimes \boldsymbol{e}_k \otimes \boldsymbol{e}_l) : (S_{mn} \, \boldsymbol{e}_m \otimes \boldsymbol{e}_n) \\ &= C_{ijkl} \, S_{mn} (\boldsymbol{e}_k \cdot \boldsymbol{e}_m) (\boldsymbol{e}_l \cdot \boldsymbol{e}_n) \boldsymbol{e}_i \otimes \boldsymbol{e}_j \\ &= C_{ijkl} \, S_{mn} \, \delta_{km} \, \delta_{ln} \, \boldsymbol{e}_i \otimes \boldsymbol{e}_j = C_{ijkl} \, S_{kl} \, \boldsymbol{e}_i \otimes \boldsymbol{e}_j \\ &= T_{ij} \, \boldsymbol{e}_i \otimes \boldsymbol{e}_j = \boldsymbol{T} \in \mathcal{E}^3 \otimes \mathcal{E}^3 \quad \text{where} \quad T_{ij} = C_{ijkl} \, S_{kl} \end{aligned}$$

1.5 Multiplication of vectors and tensors

Example 8. Let: s be a scalar (a zero-order tensor), v, w be vectors (first-order tensors), R, S, T be second-order tensors, D be a third-order tensor, and C be a fourth-order tensor. The order of tensors is shown explicitly in the expressions below.

Remark: Notice a vital difference between the two dot-operators '•' and '·'. To avoid ambiguity, usually, the operators '·' and '·' are not used, and the dot-operator has the meaning of the (full) dot-product, so that $C_{ijkl}S_{kl} \to C \bullet S$, $T_{ij}S_{ij} \to T \bullet S$, and $T_{ij}S_{jk} \to T \bullet S$.

1.6 Vertical-bar convention and Nabla-operator

Vertical-bar convention

The **vertical-bar** (**or comma**) **convention** is used to facilitate the denomination of partial derivatives with respect to the Cartesian position vectors $\mathbf{x} \sim x_i$, for example,

$$\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{x}} \quad \to \quad \frac{\partial u_i}{\partial x_j} =: u_{i|j}$$

Definition 9 (Nabla-operator).

$$\nabla \equiv (.)_{|i} \, \boldsymbol{e}_{i}$$
 = $(.)_{|1} \, \boldsymbol{e}_{1} + (.)_{|2} \, \boldsymbol{e}_{2} + (.)_{|3} \, \boldsymbol{e}_{3}$

The **gradient**, **divergence**, **curl** (**rotation**), and **Laplacian** operations can be written using the **Nabla-operator**:

$$egin{aligned} & oldsymbol{v} = \operatorname{grad} oldsymbol{s} \equiv \nabla oldsymbol{s} &
ightarrow & v_i = s_{|i|} \ & oldsymbol{T} = \operatorname{grad} oldsymbol{v} \equiv \nabla \otimes oldsymbol{v} &
ightarrow & T_{ij} = v_{i|j} \ & oldsymbol{s} = \operatorname{div} oldsymbol{v} \equiv \nabla \cdot oldsymbol{v} &
ightarrow & s = v_{i|i|} \ & oldsymbol{v} = \operatorname{div} oldsymbol{T} \equiv \nabla \cdot oldsymbol{T} &
ightarrow & v_i = T_{ji|j} \ & oldsymbol{w} = \operatorname{curl} oldsymbol{v} \equiv \nabla \times oldsymbol{v} &
ightarrow & w_i = \epsilon_{ijk} v_{k|j} \ & \operatorname{lapl}(.) \equiv \Delta(.) \equiv \nabla^2(.) &
ightarrow & (.)_{iji} \end{aligned}$$

Some vector calculus identities:

•
$$\nabla \times (\nabla s) = \mathbf{0}$$
 (curl grad = $\mathbf{0}$)

Proof.

$$\nabla \times (\nabla s) = \epsilon_{ijk} (s_{|k})_{|j} = \epsilon_{ijk} s_{|kj} = \begin{cases} \text{for } i = 1: \ s_{|23} - s_{|32} = 0 \\ \text{for } i = 2: \ s_{|31} - s_{|13} = 0 \end{cases}$$

$$\text{for } i = 3: \ s_{|12} - s_{|21} = 0$$

• $(\nabla \cdot (\nabla \times \boldsymbol{v}) = 0)$ (div curl = 0)

Proof.

$$\nabla \cdot (\nabla \times \boldsymbol{v}) = \left(\epsilon_{ijk} \, v_{k|j} \right)_{|i} = \epsilon_{ijk} \, v_{k|ji} = \left(v_{3|21} - v_{3|12} \right) + \left(v_{1|32} - v_{1|23} \right) + \left(v_{2|13} - v_{2|31} \right) = 0$$

• $\nabla \times (\nabla \times \boldsymbol{v}) = \nabla(\nabla \cdot \boldsymbol{v}) - \nabla^2 \boldsymbol{v}$ (curl curl = grad div - lapl)

Proof.

$$\begin{array}{rcl} \nabla\times(\nabla\times\boldsymbol{v}) & \to & \epsilon_{mni}\big(\epsilon_{ijk}\,v_{k|j}\big)_{|n} = \epsilon_{mni}\epsilon_{ijk}\,v_{k|jn} \\ \text{for } m=1: & \epsilon_{1ni}\epsilon_{ijk}\,v_{k|jn} = \epsilon_{123}\big(\epsilon_{312}\,v_{2|12} + \epsilon_{321}\,v_{1|22}\big) + \epsilon_{132}\big(\epsilon_{213}\,v_{3|13} + \epsilon_{231}\,v_{1|33}\big) \\ & = \big(v_{2|2} + v_{3|3}\big)_{|1} - \big(v_{1|22} + v_{1|33}\big) \\ & = \big(v_{1|1} + v_{2|2} + v_{3|3}\big)_{|1} - \big(v_{1|11} + v_{1|22} + v_{1|33}\big) \\ & = \big(v_{i|i}\big)_{|1} - v_{1|ii} = \big(\nabla\cdot\boldsymbol{v}\big)_{|1} - \nabla^2v_{1} \\ \text{for } m=2: & \epsilon_{2ni}\epsilon_{ijk}\,v_{k|jn} = \big(v_{i|i}\big)_{|2} - v_{2|ii} = \big(\nabla\cdot\boldsymbol{v}\big)_{|2} - \nabla^2v_{2} \\ \text{for } m=3: & \epsilon_{3ni}\epsilon_{ijk}\,v_{k|jn} = \big(v_{i|i}\big)_{|3} - v_{3|ii} = \big(\nabla\cdot\boldsymbol{v}\big)_{|3} - \nabla^2v_{3} \end{array}$$

2 Integral theorems

2.1 General idea

Integral theorems of vector calculus,

- the **classical** (Kelvin-)**Stokes' theorem** (the curl theorem),
- Green's theorem,
- Gauss theorem (the Gauss-Ostrogradsky divergence theorem),

are special cases of the **general Stokes' theorem**, which generalizes the **fundamental theorem of calculus**.

Fundamental theorem of calculus relates scalar integral to boundary points:

$$\int_{a}^{b} f'(x) dx = f(b) - f(a)$$

Stokes's (curl) theorem relates surface integrals to line integrals. *Applications:* e.g. conservative forces.

Green's theorem is a two-dimensional special case of Stokes' theorem.

Gauss (divergence) theorem relates volume integrals to surface integrals. *Applications:* analysis of flux, pressure.

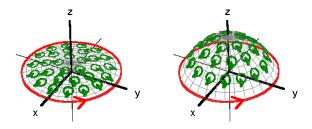
2.2 Stokes' theorem

Theorem 10 (Stokes' curl theorem). Let C be a simple closed curve spanned by a surface S with unit normal n. Then, for a continuously differentiable vector field f:



$$\int_{S} (\nabla \times \boldsymbol{f}) \cdot \underline{\boldsymbol{n}} \, dS = \int_{C} \boldsymbol{f} \cdot d\boldsymbol{r}$$

- *Formal requirements:* the surface S must be open, orientable and piecewise smooth with correspondingly orientated, simple, piecewise smooth boundary (curve) C.
- Stokes' theorem implies that **the flux** of $\nabla \times f$ **through a surface** S depends only on the boundary C of S and is therefore **independent of the surface's shape**.



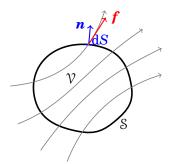
• **Green's theorem in the plane** may be viewed as a special case of Stokes' theorem (with f = [u(x, y), v(x, y), 0]):

$$\int_{S} \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) dx dy = \int_{C} u dx + v dy$$

2.3 Gauss-Ostrogradsky theorem

Theorem 11 (Gauss divergence theorem). Let the region V be bounded by a simple surface S with unit outward normal n. Then, for a continuously differentiable vector field f:

$$\int_{\mathcal{V}} \nabla \cdot \boldsymbol{f} \, dV = \int_{\mathcal{S}} \boldsymbol{f} \cdot \underline{\boldsymbol{n}} \, dS; \quad in \ particular \quad \int_{\mathcal{V}} \nabla f \, dV = \int_{\mathcal{S}} f \, \boldsymbol{n} \, dS.$$



- The divergence theorem is a result that relates the flow (that is, flux) of a vector field through a surface to the behavior of the vector field inside the surface.
- Intuitively, it states that the sum of all sources minus the sum of all sinks gives the net flow out of a region.

3 Time-harmonic approach

Dynamic problems. In dynamic problems, the field variables depend upon position x and time t, for example, u = u(x, t).

Separation of variables. In many cases, the governing PDEs can be solved by expressing u as a product of functions that each depend only on one of the independent variables: $u(\mathbf{x},t) = \hat{u}(\mathbf{x})\check{u}(t)$.

Steady state. A system is in steady state if its recently observed behaviour will continue into the future. An opposite situation is called the transient state which is often a start-up in many steady state systems. An important case of steady state is the time-harmonic behaviour.

Time-harmonic solution. If the time-dependent function $\check{u}(t)$ is a time-harmonic function (with the frequency f), the solution can be written as

$$u(\boldsymbol{x},t) = \hat{u}(\boldsymbol{x})\cos(\omega t + \alpha(\boldsymbol{x}))$$

where $\omega = 2\pi f$ is called the **circular** (or **angular**) **frequency**, $\alpha(x)$ is the **phase-angle shift**, and $\hat{u}(x)$ can be interpreted as a **spatial amplitude**.

Complex notation of time-harmonic problems

A convenient way to handle time-harmonic problems is in **complex notation** with the real-part as a physically meaningful solution:

$$u(\boldsymbol{x},t) = \hat{u}(\boldsymbol{x})\cos\left(\omega t + \alpha(\boldsymbol{x})\right) = \hat{u}\Re\left\{\underbrace{\cos(\omega t + \alpha) + \mathrm{i}\sin(\omega t + \alpha)}_{\tilde{u}}\right\}$$
$$= \hat{u}\Re\left\{\exp[(\mathrm{i}(\omega t + \alpha)]\right\} = \Re\left\{\underbrace{\hat{u}\exp(\mathrm{i}\alpha)}_{\tilde{u}}\exp(\mathrm{i}\omega t)\right\} = \Re\left\{\underbrace{\tilde{u}\exp(\mathrm{i}\omega t)}_{\tilde{u}}\right\}$$

where the so-called **complex amplitude** (or **phasor**) is introduced:

$$\tilde{u} = \tilde{u}(\mathbf{x}) = \hat{u}(\mathbf{x}) \exp(i\alpha(\mathbf{x})) = \hat{u}(\mathbf{x})(\cos\alpha(\mathbf{x}) + i\sin\alpha(\mathbf{x}))$$

Example 12. Consider a **linear dynamic system** characterized by the matrices of stiffness K, damping C, and mass M:

$$Kq(t) + C\dot{q}(t) + M\ddot{q}(t) = Q(t)$$

where Q(t) is the dynamic excitation (a time-varying force) and q(t) is the system's response (displacement).

• Let the driving force Q(t) be harmonic with the angular frequency ω and the (real) amplitude \hat{Q} :

$$Q(t) = \hat{Q}\cos(\omega t) = \hat{Q}\Re\{\cos(\omega t) + i\sin(\omega t)\} = \Re\{\hat{Q}\exp(i\omega t)\}$$

• Since the system is linear the response q(t) will also be harmonic with the same angular frequency but (in general) shifted by the phase angle α :

$$\begin{split} q(t) &= \hat{q} \cos(\omega t + \alpha) = \hat{q} \,\Re \big\{ \cos(\omega t + \alpha) + \mathrm{i} \sin(\omega t + \alpha) \big\} \\ &= \hat{q} \,\Re \big\{ \exp[\mathrm{i}(\omega t + \alpha)] \big\} = \Re \big\{ \underbrace{\hat{q} \,\exp(\mathrm{i}\,\alpha)}_{\tilde{q}} \exp(\mathrm{i}\,\omega t) \big\} = \Re \big\{ \underbrace{\tilde{q} \,\exp(\mathrm{i}\,\omega t)}_{\tilde{q}} \big\} \end{split}$$

Here, \hat{q} and \tilde{q} are the real and complex amplitudes, respectively. The real amplitude \hat{q} and the phase angle α are unknowns; thus, unknown is the complex amplitude $\tilde{q} = \hat{q} (\cos \alpha + i \sin \alpha)$.

• Now, one can substitute into the system's equation

$$Q(t) \leftarrow \hat{Q} \exp(i\omega t),$$

$$q(t) \leftarrow \tilde{q} \exp(i\omega t), \quad \text{so that} \quad \dot{q}(t) = \tilde{q} i\omega \exp(i\omega t), \quad \ddot{q}(t) = -\tilde{q} \omega^2 \exp(i\omega t)$$

to easily obtain the following algebraic equation for the unknown complex amplitude \tilde{q} :

$$[K + i\omega C - \omega^2 M]\tilde{q} = \hat{Q}$$

• For the Rayleigh damping model, where $C = \beta_K K + \beta_M M$ (β_K and β_M are real constants), this equation can be presented as follows:

$$\left[ilde{K} - \omega^2 ilde{M}
ight] ilde{q} = \hat{Q} \,, \quad ext{where} \quad ilde{K} = K ig(1 + \mathrm{i}\,\omega\,eta_K ig) \,, \quad ilde{M} = M ig(1 + rac{eta_M}{\mathrm{i}\,\omega} ig)$$

are complex matrices.

• Having computed the complex amplitude \tilde{q} for the given frequency ω , one can finally find the time-harmonic response as the real-part of the complex solution:

$$q(t) = \Re \big\{ \tilde{q} \, \exp(\mathrm{i} \, \omega \, t) \big\} = \hat{q} \, \cos(\omega \, t + \alpha), \quad \text{where} \quad \begin{cases} \hat{q} = |\tilde{q}| \\ \alpha = \arg(\tilde{q}) \end{cases}$$

Here, $|\tilde{q}| = \sqrt{\Re{\{\tilde{q}\}^2 + \Im{\{\tilde{q}\}^2}}}$ is the absolute value or modulus of the complex number \tilde{q} , and $\arg(\tilde{q}) = \arctan\left(\frac{\Im{\{\tilde{q}\}}}{\Re{\{\tilde{q}\}}}\right)$ is called the argument or angle of \tilde{q} .