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 and the summation symbol is skipped.

Example 0.

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

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

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

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

The principles of index notation:

■ An index cannot appear more than twice in one term! If necessary, the standard summation symbol (\sum) must be used. A repeated index is called a **bound** or **dummy index**.

Example 0.

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

$$A_{ij} b_j c_j \leftarrow \text{Wrong!}$$

$$\sum_j A_{ij} b_j c_j \leftarrow \text{Correct}$$

A term with an index repeated more than two times 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 an index appears once, it is called a **free index**. The number of free indices determines the order of a tensor.

Example 0.

$$A_{ii}\,,\quad a_i\,b_i\,,\quad T_{ij}\,S_{ij} \quad \leftarrow \quad \text{scalars (no free indices)} \ A_{ij}\,b_j \quad \leftarrow \quad \text{a vector (one free index: } i) \ C_{ijkl}\,S_{kl} \quad \leftarrow \quad \text{a second-order tensor (two free indices: } i,j)$$

■ The denomination of dummy index (in a term) is arbitrary, since it vanishes after summation, namely: $a_i b_i \equiv a_j b_j \equiv a_k b_k$, etc.

Example 0.

$$a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3 = a_j b_j$$

$$A_{ii} \equiv A_{jj} , \quad T_{ij} S_{ij} \equiv T_{kl} S_{kl} , \quad T_{ij} + C_{ijkl} S_{kl} \equiv T_{ij} + C_{ijmn} S_{mn}$$

1.3 Kronecker delta and permutation symbol

Definition 0 (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: $a_i \, \delta_{ij} = a_1 \, \delta_{1j} + a_2 \, \delta_{2j} + a_3 \, \delta_{3j} = a_j$, i.e., here $i \to j$.
- 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 $I = e_1 \otimes e_1 + e_2 \otimes e_2 + e_3 \otimes e_3 = \delta_{ij} e_i \otimes e_j$.
- $A \bullet I = A_{ij} \delta_{ij} = A_{ii}$ which is the **trace** of the matrix (tensor) A.

Definition 0 (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:

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

Tensors and their representations 1.4

Informal definition of tensor

A tensor is a generalized linear 'quantity' that can be expressed as a multidimensional array relative to a choice of basis of the particular space on which it is defined. Therefore:

- 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

$$T := T_{ij} \mathbf{e}_i \otimes \mathbf{e}_j = T_{11} \mathbf{e}_1 \otimes \mathbf{e}_1 + T_{12} \mathbf{e}_1 \otimes \mathbf{e}_2 + T_{13} \mathbf{e}_1 \otimes \mathbf{e}_3$$
$$+ T_{21} \mathbf{e}_2 \otimes \mathbf{e}_1 + T_{22} \mathbf{e}_2 \otimes \mathbf{e}_2 + T_{23} \mathbf{e}_2 \otimes \mathbf{e}_3$$
$$+ T_{31} \mathbf{e}_3 \otimes \mathbf{e}_1 + T_{32} \mathbf{e}_3 \otimes \mathbf{e}_2 + T_{33} \mathbf{e}_3 \otimes \mathbf{e}_3$$

where \otimes denotes the tensorial (or dyadic) product, and T_{ij} is the (matrix) repre**sentation** 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 tensor of order n is defined by

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

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

Example 0. Let $C \in \mathcal{E}^3 \otimes \mathcal{E}^3 \otimes \mathcal{E}^3 \otimes \mathcal{E}^3$ and $S \in \mathcal{E}^3 \otimes \mathcal{E}^3$. The fourth-order tensor C describes a linear transformation in $\mathcal{E}^3 \otimes \mathcal{E}^3$:

$$C \bullet S = C : S = (C_{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l) : (S_{mn} e_m \otimes e_n)$$

$$= C_{ijkl} S_{mn} (e_k \cdot e_m) (e_l \cdot e_n) e_i \otimes e_j$$

$$= C_{ijkl} S_{mn} \delta_{km} \delta_{ln} e_i \otimes e_j = C_{ijkl} S_{kl} e_i \otimes e_j$$

$$= T_{ij} e_i \otimes e_j = T \in \mathcal{E}^3 \otimes \mathcal{E}^3 \quad \text{where} \quad T_{ij} = C_{ijkl} S_{kl}$$

Multiplication of vectors and tensors

Example 0. Let: s be a scalar (a zero-order tensor), v, w be vectors (first-order tensor) sors), R, S, T be second-order tensors, D be a third-order tensor, and C be a fourthorder tensor. The order of tensors is shown explicitly in the expressions below.

$$s = \mathbf{v} \bullet \mathbf{w} = \mathbf{v} \mathbf{w} = \mathbf{v} \cdot \mathbf{w} \rightarrow v_i w_i = s$$

$$\mathbf{v} = \mathbf{T} \mathbf{w} = \mathbf{T} \cdot \mathbf{v} \rightarrow T_{ij} w_j = v_i$$

$$\mathbf{R} = \mathbf{T} \mathbf{S} = \mathbf{T} \cdot \mathbf{S} \rightarrow T_{ij} S_{jk} = R_{ik}$$

$$s = \mathbf{T} \bullet \mathbf{S} = \mathbf{T} \cdot \mathbf{S} \rightarrow T_{ij} S_{ij} = s$$

$$\mathbf{T} = \mathbf{C} \bullet \mathbf{S} = \mathbf{C} \cdot \mathbf{S} \rightarrow C_{ijkl} S_{kl} = T_{ij}$$

$$\mathbf{T} = \mathbf{v} \mathbf{D} = \mathbf{v} \cdot \mathbf{D} \rightarrow v_k D_{kij} = T_{ij}$$

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 $T_{ij} S_{jk} \to C \bullet S$ TS.

Vertical-bar convention and Nabla operator 1.6

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 $x \sim x_i$, for example,

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

Definition 0 (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**:

$$\mathbf{v} = \operatorname{grad} s \equiv \nabla s \quad \rightarrow \quad v_i = s_{|i}$$

$$\mathbf{T} = \operatorname{grad} \mathbf{v} \equiv \nabla \otimes \mathbf{v} \quad \rightarrow \quad T_{ij} = v_{i|j}$$

$$s = \operatorname{div} \mathbf{v} \equiv \nabla \cdot \mathbf{v} \quad \rightarrow \quad s = v_{i|i}$$

$$\mathbf{v} = \operatorname{div} \mathbf{T} \equiv \nabla \cdot \mathbf{T} \quad \rightarrow \quad v_i = T_{ji|j}$$

$$\mathbf{w} = \operatorname{curl} \mathbf{v} \equiv \nabla \times \mathbf{v} \quad \rightarrow \quad w_i = \epsilon_{ijk} v_{k|j}$$

$$\operatorname{lapl}(.) \equiv \Delta(.) \equiv \nabla^2(.) \quad \rightarrow \quad (.)_{|ii}$$

Some vector calculus identities:

Proof:

$$\nabla \times (\nabla s) = \epsilon_{ijk} \big(s_{|k} \big)_{|j} = \epsilon_{ijk} \, s_{|kj} = \begin{cases} \text{for } i = 1 \text{: } s_{|23} - s_{|32} = 0 \\ \text{for } i = 2 \text{: } s_{|31} - s_{|13} = 0 \\ \text{for } i = 3 \text{: } s_{|12} - s_{|21} = 0 \end{cases}$$

QED

Proof:

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

 $\nabla \cdot (\nabla s) = \nabla^2 s$ (div grad = lapl)

Proof:

$$\nabla \cdot (\nabla s) = (s_{|i})_{|i} = s_{|ii} = s_{|11} + s_{|22} + s_{|33} \equiv \nabla^2 s$$

QED

Proof:

QED

Integral theorems

2.1 General idea

Integral theorems of vector calculus, namely:

- 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:

$$\int_{a}^{b} f'(x) \, \mathrm{d}x = f(b) - f(a)$$

Stokes's (curl) theorem relates surface integrals to line integrals. Applications: for example, conservative forces.

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

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

Stokes' theorem

Theorem 1 (Stokes' curl theorem). Let \mathcal{C} be a simple closed curve spanned by a surface S with unit normal n. Then, for a continuously differentiable vector field f:



$$\int_{\mathbb{S}} (\nabla \times \boldsymbol{f}) \cdot \underbrace{\boldsymbol{n} \, \mathrm{d} \boldsymbol{S}}_{\mathbf{d} \boldsymbol{S}} = \int_{\mathbb{C}} \boldsymbol{f} \cdot \mathrm{d} \boldsymbol{r}$$

- Formal requirements: the surface S must be open, orientable and piecewise smooth with a correspondingly orientated, simple, piecewise and smooth boundary curve C.
- Stokes' theorem implies that **the flux** of $\nabla \times f$ **through a surface** \mathcal{S} depends only on the boundary \mathcal{C} of \mathcal{S} and is therefore **independent of the surface's shape** (see Figure 1).

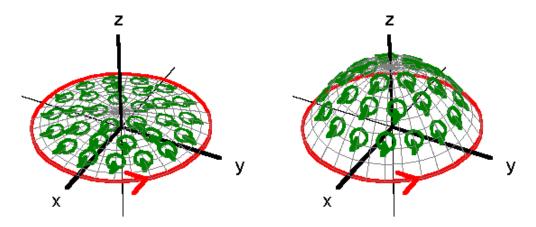


FIGURE 1

■ 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 2 (Gauss divergence theorem). Let the region \mathcal{V} be bounded by a simple surface \mathcal{S} with unit outward normal n (see Figure 2). Then, for a continuously differentiable vector field f:

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

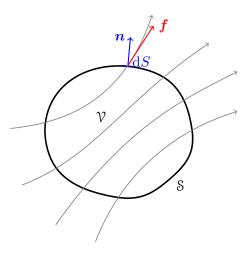


FIGURE 2

- 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

3.1 Types of dynamic problems

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 **angular** (or **circular**) **frequency**, $\alpha(\boldsymbol{x})$ is the **phase-angle shift**, and $\hat{u}(\boldsymbol{x})$ can be interpreted as a **spatial amplitude**.Here: ω – the angular frequency, $\alpha(\boldsymbol{x})$ – the phase-angle shift, $\hat{u}(\boldsymbol{x})$ – the spatial amplitude.

3.2 Complex-valued notation

A complex-valued notation for time-harmonic problems

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

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

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

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

3.3 A practical example

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

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

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-valued) amplitude \hat{Q} :

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

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

$$q(t) = \hat{q} \cos(\omega t + \alpha) = \hat{q} \operatorname{Re} \left\{ \cos(\omega t + \alpha) + i \sin(\omega t + \alpha) \right\}$$
$$= \hat{q} \operatorname{Re} \left\{ \exp[i(\omega t + \alpha)] \right\} = \operatorname{Re} \left\{ \underbrace{\hat{q} \exp(i \omega)}_{\tilde{q}} \exp(i \omega t) \right\}$$
$$= \operatorname{Re} \left\{ \tilde{q} \exp(i \omega t) \right\}$$

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

$$\begin{split} Q(t) \; \leftarrow \; \hat{Q} \, \exp(\mathrm{i} \, \omega \, t) \,, \\ q(t) \; \leftarrow \; \tilde{q} \, \exp(\mathrm{i} \, \omega \, t) \,, \quad \text{so that} \quad \dot{q}(t) = \tilde{q} \, \mathrm{i} \, \omega \, \exp(\mathrm{i} \, \omega \, t) \,, \quad \ddot{q}(t) = -\tilde{q} \, \omega^2 \, \exp(\mathrm{i} \, \omega \, t) \end{split}$$

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

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

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

$$\left[\tilde{K} - \omega^2 \, \tilde{M}\right] \tilde{q} = \hat{Q} \,, \quad \text{where} \quad \tilde{K} = K \big(1 + \mathrm{i} \, \omega \, \beta_K \big) \,, \quad \tilde{M} = M \bigg(1 + \frac{\beta_M}{\mathrm{i} \, \omega} \bigg)$$

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:

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

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