Appendix 1:

Notation

Here we summarize the basic forms of vectors and tensors employed in the text. For more details we refer to literature on vector and tensor algebra, e.g., [BS88, Ber05, BW76, BHW97, Sch97]. Being aware that we lose some of the theories beauty and generality we restrict ourselves in this work to the use of cartesian-coordinate systems with orthonormal base vectors $e_i$. The range of lowercase latin indices is 1, 2, 3. Moreover we adopt Einstein’s summation convention according to which any expression in which an index appears repeatedly is understood to be a sum over the range of this index.

1.1 Scalars

Formally scalars are zeroth-order tensors. Scalars are written here mainly in lowercase greek letters, $\alpha, \beta, \ldots$. Exemtions are made for some physical quantities, e.g., the temperature is denoted by $T$.

1.2 Vectors

First-order tensors are vectors. Vectors are denoted here by boldface lowercase letters, $a, b, \ldots$ and have both direction and length. The corresponding vector spaces are denoted by cursive uppercase letters, i.e., $a \in V, b \in W$. In components a vector is written as

$$a = a_i e_i = a_1 e_1 + a_2 e_2 + a_3 e_3 \equiv [a_1 \ a_2 \ a_3]^T.$$  \hspace{1cm} (1.1)

Vector algebra is well known and may be looked up in many standard mathematical textbooks (e.g. [BHW97, SK91]). We focus here only on the properties of the different products of vectors.
The scalar product (or dot product or inner product) of two vectors \( a \) and \( b \) is denoted by \( a \cdot b \) or equivalently \( \langle a, b \rangle \) and gives a scalar quantity with magnitude \( a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3 \). Properties of the scalar product are (here \( o \) is the zero vector):

\[
\begin{align*}
  a \cdot b &= b \cdot a \quad (1.2) \\
  a \cdot o &= 0 \quad (1.3) \\
  a \cdot a > 0 &\iff a \neq o \quad (1.4) \\
  a \cdot a &= 0 &\iff a = o \quad (1.5) \\
  a \cdot b &= 0 &\iff a \text{ is orthogonal to } b. \quad (1.6)
\end{align*}
\]

The length of a vector is

\[
|a| = (a \cdot a)^{\frac{1}{2}}. \quad (1.7)
\]

A unit vector has length 1, i.e., for the bases vectors of our cartesian coordinates hold

\[
e_i \cdot e_j = \delta_{ij}, \quad (1.8)
\]

where the Kronecker delta \( \delta_{ij} \) equals 1 if \( i = j \) and is zeros otherwise. The length of a vector works as a vector norm. In general, a norm \( ||a|| \) is a non-negative real number with properties

\[
\begin{align*}
  ||a|| &= 0 &\iff a = o \quad (1.9) \\
  ||a|| &< \infty. \quad (1.10)
\end{align*}
\]

The vector product or (cross product) of two vectors \( a \) and \( b \) is written as \( a \times b \) and produces a new vector orthogonal to the plane spanned by \( a \) and \( b \) with components

\[
(a \times b)_i = \epsilon_{ijk} a_j b_k, \quad (1.11)
\]

where \( \epsilon_{ijk} \) is the permutation symbol\(^1\). Another way to compute the cross product easily is given by

\[
a \times b = \det \begin{pmatrix} e_1 & e_2 & e_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{pmatrix}. \quad (1.12)
\]

Note that the magnitude of the resulting vector measures the area spanned by the vectors \( a \) and \( b \), i.e., \( |a \times b| = \text{span}(a, b) \).

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\(^1\) \( \epsilon_{ijk} = 1 \) for \( ijk = 123, 231, 312 \) and \( \epsilon_{ijk} = -1 \) for \( ijk = 132, 213, 321 \) and \( \epsilon_{ijk} = 0 \) for coincident indices.
Properties of cross products are:
\[ a \times b = -b \times a, \]  
\[ a \times b = 0 \iff a \parallel b, \text{ i.e., } a \text{ and } b \text{ are linearly dependent}, \]  
\[ a \cdot (b \times c) = b \cdot (c \times a) = c \cdot (a \times b), \]  
(1.13, 1.14, 1.15)

The last line states a parallelepipedic product (or box product) of the three vectors \( a, b, c \). The expression \( a \cdot (b \times c) \) represents the volume of a parallelepiped spanned by the vectors. The volume is zero if and only if the vectors are linearly dependent. The box product may conveniently be calculated by
\[ (a \times b) \cdot c = \det \begin{pmatrix} a_1 & b_2 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{pmatrix}, \]  
(1.16)

The dyadic product (or tensor product) of two tensors is denoted by \( a \otimes b \). The resulting dyad is a second order tensor with components
\[ (a \otimes b)_{ij} = a_i b_j = \begin{pmatrix} a_1 b_1 & a_1 b_2 & a_1 b_3 \\ a_2 b_1 & a_2 b_2 & a_2 b_3 \\ a_3 b_1 & a_3 b_2 & a_3 b_3 \end{pmatrix}. \]  
(1.17)

For the dyadic product the following relations hold:
\[ (a \otimes b)c = (a(b \cdot c)) = (b \cdot c)a, \]  
\[ (\alpha a + \beta b) \otimes c = \alpha(a \otimes c) + \beta(b \otimes c), \]  
\[ (a \otimes b)(c \otimes d) = (b \cdot c)a \otimes d = a \otimes d(b \cdot c). \]  
(1.18, 1.19, 1.20)

Note that in general,
\[ a \otimes b \neq b \otimes a, \]  
(1.21)
i.e., the dyadic product is not commutative. Also, a dyad can not necessarily be expressed as a single tensor product.
\[ a \otimes b + c \otimes d \neq x \otimes y \text{ for some } x, y. \]  
(1.22)

### 1.3 Second-Order Tensors

Tensors of second order \( A \in (W \otimes V) \) are linear operators that act on a vector \( a \in V \) to generate a vector \( b \in W \). For notation we use boldface latin capitals.
\[ A : V \longrightarrow W \]  
\[ u \mapsto Aa. \]  
(1.23)
Equation (A 1.23 is commonly written as (cf. remarks in Section 1.5)

\[ u = Aa. \]  

(1.24)

Any second order tensor may be expressed as a dyad, e.g.,

\[ A = A_{ij}e_i \otimes e_j. \]  

(1.25)

The nine components of (the matrix of) tensor \( A \) are

\[ (A)_{ij} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}. \]  

(1.26)

Sum, difference, multiplication with a scalar and further operations of second order tensors are defined analogously to vector and matrix algebra. For example, the transpose of tensor \( A \) in equation (A 1.25), \( A^\top \), is given by

\[ A^\top = A_{ij}e_j \otimes e_i \equiv (A)_{ji} = \begin{pmatrix} A_{11} & A_{21} & A_{31} \\ A_{12} & A_{22} & A_{32} \\ A_{13} & A_{23} & A_{33} \end{pmatrix}. \]  

(1.27)

The magnitude of Tensor \( A \) is defined as the Frobenius norm of its matrix representation, i.e.,

\[ |A| := \|(A)_{ij}\|_F = (A_{ij}A_{ij})^{1/2}. \]  

(1.28)

The second order unit (or identity) tensor is defined by \( I \), the corresponding zero tensor is \( O \). Additional properties of second order tensors are summarized in Section 2.1.

The double scalar product (contractive product) is denoted by \( A : B \) or equivalently \( \langle A, B \rangle \) and yields a scalar. In components the scalar product evaluates to

\[ (A : B)_{ij} = A_{ij}B_{ij}. \]  

(1.29)

Note that for the double scalar product holds

\[ A : B = B : A \equiv \langle A, B \rangle = \langle B, A \rangle, \]  

(1.30)

and, moreover,

\[ A : (B : C) = (B^\top A) : C = (AC^\top) : B \]  

(1.31)

\[ A : (a \otimes b) = a \cdot Ab \]  

(1.32)

\[ (a \otimes b)(c \otimes d) = (a \cdot b)(c \cdot d). \]  

(1.33)
A special case of the last equation is
\[(e_i \otimes e_j)(e_k \otimes e_l) = (e_i \cdot e_j)(e_k \cdot e_l) = \delta_{ij}\delta_{kl}.\] (1.34)

The tensor product (or dot product) of two second order tensors is written as by \(AB\) (here as commonly written without a dot). The result is again a second order tensor with components
\[(AB)_{ij} = A_{ik}B_{kj}.\] (1.35)

The matrix product is not commutative, i.e., in general
\[AB \neq BA.\] (1.36)

Moreover holds
\[(AB)^\top = B^\top A^\top.\] (1.37)

The dyadic product of two second order tensor consequently generates a fourth order tensor. The definition and properties of the dyadic product follow analogously to equation (1.18-1.22). Computed in components we write
\[(A \otimes B)_{ijkl} = C_{ijkl} = A_{ij}B_{kl},\] (1.38)
resulting in \(3^4 = 81\) entries for the result \(C_{ijkl}\).

## 1.4 Higher-Order Tensors

Generally, a third order tensor, \(<3>D\), has 27 components \(D_{ijk}\) and a fourth order tensor, \(<4>C\), has 81 components \(C_{ijkl}\). This sequence can be continued but tensors of order higher than four are not subject of this work.

For further use we define here the corresponding unit and zero tensor of order four, \(<4>I\) and \(<4>O\), respectively. Finally we note that a fourth order tensor may be expressed with the help of the three Cartesian basis vectors as
\[<4>C = C_{ijkl}e_i \otimes e_j \otimes e_k \otimes e_l.\] (1.39)
1.5 Remark

Throughout this work equations are formulated in tensor notation, in matrix notation and sometimes indicial notation. For readability we use the same notation for matrices as for tensors but we will not use connective symbols. Moreover, for finite element implementation tensors are often converted into matrices and vectors by using the Voigt-matrix notation, cf. e.g. [R.83, ZT03]. To illustrate the notations we formulate here an energy-like scalar expression in the different ways.

\[
\tensor{x} \cdot \tensor{A} \equiv \transpose{\tensor{x}} \tensor{A} \equiv x_{ij} A_{ijkl} x_{kl}. \tag{1.40}
\]
2 Appendix 2:
Some Rules of Tensor Algebra and Calculus

In this chapter some fundamental rules of tensor manipulations in the 3D-Euclidian space are summarized for reference. All statements are given without proof. For more details consult the textbooks [Ber05, Gek06, Wri01] among others.

2.1 Decompositions, invariants and eigenvalues of tensors

Here we summarize operations on tensors of second order $A \in \mathbb{R}^3 \times \mathbb{R}^3$ applied within this work. If necessary, the extension to tensors of higher order is straightforward.

**Determinate, inverse, orthogonality, symmetry and antisymmetry**

The *determinate* of a tensor is given by the determinate of its matrix representation in equation (A 1.26), $\det A = \det(A)_{ij}$, with properties

\begin{align*}
\det A^\top &= \det A \tag{2.1} \\
\det(\alpha A) &= \alpha^3 \det A \tag{2.2} \\
\det(AB) &= \det A \det B. \tag{2.3}
\end{align*}

Presuming a non-singular tensor, i.e., $\det A \neq 0$, than exists an unique *inverse* $A^{-1}$ of tensor $A$ satisfying the relation

$$A^{-1}A = AA^{-1} = I. \tag{2.4}$$
Some fundamental rules for the inverse of a tensor are

\[ (A^{-1})^{-1} = A \]  \hspace{1cm} (2.5)

\[ (\alpha A)^{-1} = \frac{1}{\alpha} A^{-1} \]  \hspace{1cm} (2.6)

\[ (AB)^{-1} = B^{-1} A^{-1} \]  \hspace{1cm} (2.7)

\[ A^{-2} = A^{-1} A^{-1} \]  \hspace{1cm} (2.8)

\[ \det A^{-1} = \frac{1}{\det A} \]  \hspace{1cm} (2.9)

Moreover we defined an abbreviation,

\[ A^{-\top} := (A^{-1})^\top = (A^\top)^{-1}. \]  \hspace{1cm} (2.10)

For the Inverse of a second-order tensor holds the Sherman-Morrison-Formula.

\[ (A + a \otimes b)^{-1} = A^{-1} - \frac{A^{-1} a \otimes b A^{-1}}{I + b A^{-1} a}. \]  \hspace{1cm} (2.11)

A second order tensor \( R \) is said to be orthogonal if

\[ RR^\top = R^\top R = I. \]  \hspace{1cm} (2.12)

This implies, \( R^{-1} = R^\top \) and, additionally, \( (\det R)^2 = 1 \).

If \( \det(R) = 1 \) tensor \( R \) prescribes a rotation \( (R \in SO3) \), if \( \det(R) = -1 \) then tensor \( R \) prescribes a reflection. Hence, a linear transformation with an orthogonal tensor satisfies the condition

\[ Ru \cdot Rv = u \cdot R^\top Rv = u \cdot v \]  \hspace{1cm} (2.13)

for all vectors \( u \) and \( v \). This states the well known property of two vectors that their length as well as the angle between them is preserved during rotation.

Any tensor \( A \) can uniquely be decomposed into a symmetric and an antisymmetric tensor.

\[ A = \text{sym}(A) + \text{skew}(A) \]  \hspace{1cm} (2.14)

where we define

\[ \text{sym}(A) = \frac{1}{2} (A + A^\top), \]  \hspace{1cm} (2.15)

\[ \text{skew}(A) = \frac{1}{2} (A - A^\top). \]  \hspace{1cm} (2.16)
Then for any second order tensor $A$ and $B$ holds

\[
\text{sym}(A) : B = \text{sym}(A) : B^\top = \text{sym}(A) : \text{sym}(B), \tag{2.17}
\]

\[
\text{skew}(A) : B = -\text{skew}(A) : B^\top = \text{skew}(A) : \text{skew}(B), \tag{2.18}
\]

\[
\text{sym} (\text{skew}(A)) = \text{skew} (\text{sym}(A)) = 0. \tag{2.19}
\]

Finally let’s state that a second order tensor is said to be \textbf{positive definite} if for all $x \neq o$

\[
x \cdot Ax > 0. \tag{2.20}
\]

Positive definite tensors are symmetric and have, as a consequence of $\det A > 0$, only positive entries on the main diagonal. The tensor is \textbf{positive semi-definite} if

\[
x \cdot Ax \geq 0, \tag{2.21}
\]

and negative (semi)-definite otherwise.

\section*{Trace and deviator of a second-order tensor}

Every second-order tensor $A$ can be decomposed into a spherical tensor $\alpha I$ and a deviatoric tensor $\text{dev } A$.

\[
A = \alpha I + \text{dev } A. \tag{2.22}
\]

The spherical tensor is related to the trace of tensor $A$ which is a scalar denoted by $\text{tr } A$. The trace is given by

\[
\text{tr } A = A_{11} + A_{22} + A_{33} = A_{ii}. \tag{2.23}
\]

Then the decomposition reads

\[
A = \frac{1}{3} \text{tr } A \ I + \text{dev } A. \tag{2.24}
\]

The trace has the properties

\[
\text{tr } A = \text{tr } A^\top, \tag{2.25}
\]

\[
\text{tr } (A + B) = \text{tr } A + \text{tr } B, \tag{2.26}
\]

\[
\text{tr } (\alpha AB) = \alpha \text{tr } (AB) = \alpha \text{tr } (BA), \tag{2.27}
\]

\[
\text{tr } (A^\top B) = \text{tr } (AB^\top) = \text{tr } (B^\top A) = \text{tr } (BA^\top). \tag{2.28}
\]

The trace of a tensor may equivalently be computed by the double scalar product

\[
\text{tr } A = A : I = I : A. \tag{2.29}
\]
In other words, the deviatoric part of tensor \( A \) is defined from equation 2.24 by

\[
\text{dev} \, A = A - \frac{1}{3} \text{tr} A \, I,
\]

or, in components,

\[
\text{dev} \, A_{ij} = A_{ij} - \frac{1}{3} A_{ij} \delta_{ij}.
\]

**Invariants, eigenvalues and spectral decomposition**

Let a general Tensor \( A \) have \( n \) eigenvalues \( \{ \lambda_\alpha, \ \alpha = 1, \ldots n \}. \) Correspondingly there are \( n \) right eigenvectors \( \{ u_\alpha, \ \alpha = 1, \ldots n \}, \) and \( n \) left eigenvectors \( \{ v_\alpha, \ \alpha = 1, \ldots n \}. \) Thus,

\[
Au_\alpha = \lambda_\alpha u_\alpha, \quad \alpha = 1, \ldots, n, \quad (2.32)
\]

\[
v_\alpha A = A^T v_\alpha = \lambda_\alpha v_\alpha, \quad \alpha = 1, \ldots, n. \quad (2.33)
\]

The set of homogeneous algebraic equations to determine the eigenvalues \( \lambda_\alpha \) and the right eigenvectors \( u_\alpha \) is the well known **characteristic equation**

\[
(A - \lambda_\alpha I) u_\alpha = 0, \quad (2.34)
\]

which may be stated analogously for (2.33). Then the **spectral representation** of \( A \) reads

\[
A = \sum_{\alpha=1}^{n} \lambda_\alpha u_\alpha \otimes v_\alpha. \quad (2.35)
\]

The components \( A_{ij} \) of tensor \( A \) relative to a basis of **principal directions** form a diagonal matrix where the eigenvalues of \( A \) are the diagonal elements

\[
(A)_{ij} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}. \quad (2.36)
\]

The **characteristic polynomial**, also known as the Cayley-Hamilton polynomial, for a second-order tensor, is the equation resulting from the eigenvalue problem (2.34), i.e.,

\[
\det (A - \lambda_\alpha I) = 0, \quad \text{giving}
\]

\[
\lambda_\alpha^3 - I_1 A \lambda_\alpha^2 - I_2 A \lambda_\alpha - I_3 A = 0. \quad (2.37)
\]
2.1 Decompositions, invariants and eigenvalues of tensors

The scalar coefficients of the characteristic polynomial are the principal invariants of tensor $\mathbf{A}$. The explicit expressions for the three principal invariants of a second-order tensor are

\[
I_1^A = \text{tr} \mathbf{A} \quad (2.38)
\]

\[
I_2^A = \frac{1}{2} ((\text{tr} \mathbf{A})^2 - \text{tr} (\mathbf{A}^2)) = \text{tr} \mathbf{A}^{-1} \det \mathbf{A} = \text{tr} (\text{cof} \mathbf{A}) \quad (2.39)
\]

\[
I_3^A = \det \mathbf{A} \quad (2.40)
\]

Equivalently, we can claim that for every second-order tensor the principal invariants fulfil the Cayley-Hamilton equation:

\[
\mathbf{A}^3 - I_1^A \mathbf{A}^2 - I_2^A \mathbf{A} - I_3^A \mathbf{I} = 0, \quad (2.41)
\]

or, explicitly,

\[
\mathbf{A}^3 - \text{tr} \mathbf{A} \mathbf{A}^2 - \text{tr} (\text{cof} \mathbf{A}) \mathbf{A} - \det \mathbf{A} \mathbf{I} = 0. \quad (2.42)
\]

The principle invariants of tensor $\mathbf{A}$ expressed with the eigenvalues are given with

\[
I_1^A = \lambda_1 + \lambda_2 + \lambda_3 \quad (2.43)
\]

\[
I_2^A = \lambda_1 \lambda_2 + \lambda_1 \lambda_3 + \lambda_2 \lambda_3 \quad (2.44)
\]

\[
I_3^A = \lambda_1 \lambda_2 \lambda_3. \quad (2.45)
\]

The principal invariant do — by definition — not depend on the coordinate system. Note that the definition of an invariant is not unique, e.g., a multiplication of an invariant with any scalar factor yields another invariant value. Widely used are also the so-called basic invariants, the invariants of a tensor $\mathbf{A}$ defined as the traces of powers of $\mathbf{A}$,

\[
\hat{I}_A = \text{tr} \mathbf{A} = \mathbf{I} : \mathbf{A} \quad (2.46)
\]

\[
\hat{II}_A = \text{tr} (\mathbf{A}^2) = \mathbf{I} : \mathbf{A}^2 \quad (2.47)
\]

\[
\hat{III}_A = \text{tr} (\mathbf{A}^3) = \mathbf{I} : \mathbf{A}^3. \quad (2.48)
\]

Because of their practical importance we re-formulate the second invariant (2.39) here in terms of the tensor components

\[
I_2^A = \alpha (A_{ii} A_{jj} - A_{ji} A_{ij}) \quad (2.49)
\]

where we denote by $\alpha$ a factor which is $\frac{1}{2}$ in equation (2.39) but may also be determined by the physical nature of the referring tensor.
Finally, we state that for the invariants of the deviatoric part of tensor $A$ the following relations hold:

\[ J_1^A \equiv I_1^{\text{dev}A} = 0 \]  
\[ J_2^A \equiv I_2^{\text{dev}A} = -\frac{1}{2} \text{tr}(\text{dev} A)^2 \]  
\[ J_3^A \equiv I_3^{\text{dev}A} = \det(\text{dev} A) = \frac{1}{3} \text{tr}(\text{dev} A)^3, \]

or, applying equation (2.38–2.40),

\[ J_2^A = I_2^A - \frac{1}{3} (I_1^A)^2 \]  
\[ J_3^A = I_3^A - \frac{1}{3} I_1^A I_2^A + \frac{2}{27} (I_1^A)^3. \]

### Derivatives of a second order tensor

The derivatives of the principal invariants of a second order tensor with respect to the tensor itself are given here for reference:

\[ \frac{\partial I_1^A}{\partial A} = I \quad \text{or} \quad \frac{\partial I_1^A}{\partial A_{ij}} = \delta_{ij} \]  
\[ \frac{\partial I_1^A}{\partial A} = I \quad \text{or} \quad \frac{\partial I_1^A}{\partial A_{ij}} = \delta_{ij} \]  
\[ \frac{\partial I_1^A}{\partial A} = I \quad \text{or} \quad \frac{\partial I_1^A}{\partial A_{ij}} = \delta_{ij} \]

### Some rules of transformation for the deformation gradient

The deformation gradient works between current and reference placement, is a two point tensor and thus denoted with a small and a capital index as in \( \dot{\mathbf{F}} \). Within a cartesian coordinate system the deformation gradient $F = \partial \mathbf{x} / \partial \mathbf{X}$ and its inverse relation $F^{-T} = \partial \mathbf{X} / \partial \mathbf{x}$ can also be written as:

\[ F = F_{iJ} = \frac{\partial x_i}{\partial X_J} e_J \otimes e_i \quad F^T = F_{ji} = \frac{\partial x_i}{\partial X_J} e_i \otimes e_J \]  
\[ F^{-1} = F^{-1}_{iJ} = \frac{\partial X_J}{\partial x_i} e_J \otimes e_i \quad F^{-T} = F^{-1}_{ji} = \frac{\partial X_J}{\partial x_i} e_i \otimes e_J \]
2.2 Gauss’s integral theorem and divergence theorem

Some useful differential relations for the deformation gradient are summarized here:

\[
\frac{\partial F}{\partial F} = \mathbf{I} \quad \text{or} \quad \frac{\partial F_{ij}}{\partial F_{kL}} = \delta_{ik} \delta_{jL} \tag{2.59}
\]

\[
\frac{\partial F^{-T}}{\partial F} = -F^{-T}F^{-T} \quad \text{or} \quad \frac{\partial F^{-1}}{\partial F_{kL}} = -F^{-1}_{jk} F^{-1}_{Li} \tag{2.60}
\]

\[
\frac{\partial \det(F)}{\partial F} = \det(F)F^{-T} \quad \text{or} \quad \frac{\partial \mathcal{J}}{\partial F_{ij}} = \mathcal{J} F^{-1}_{ji} \tag{2.61}
\]

\[
\frac{\partial \text{tr}(F^T \cdot F)}{\partial F} = 2F \quad \text{or} \quad \frac{\partial (F_{mN} F_{mN})}{\partial F_{ij}} = 2F_{ij} \tag{2.62}
\]

Equation (2.59), (2.60) and (2.62) follow by direct calculation following the rules summarized in the appendix 1. The proof of (2.61) is lengthy but can be found in [TN65].

2.2 Gauss’s integral theorem and divergence theorem

Because of its importance in continuum mechanics we state here a general form of Gauss’s integral theorem and a the special case known as divergence theorem. For proofs and more details consult the mathematical textbooks as, e.g., [Gek06, Hac92].

A general version of Gauss’s integral theorem reads

\[
\int_{\Omega \setminus \Lambda} \text{grad} \circ \mathbf{A}(\mathbf{x}) dV = \int_{\partial \Omega} \mathbf{n} \circ \mathbf{A}(\mathbf{x}) dS + \int_{\Lambda} \mathbf{n} \circ [\mathbf{A}(\mathbf{x})] dS. \tag{2.63}
\]

Equation (2.63) includes the classical theorems of Gauss and Stokes as special cases. In this version the tensorial fields \( \mathbf{A}(\mathbf{x}) \) defined in the region \( \Omega \) may be discontinuous at a surface of discontinuity \( \Lambda \). The function

\[
[a] = a^+ - a^-
\]

is the difference of the values of the field quantity \( a \) on both sides of the surface of discontinuity. The index “ + ” refers to the side with positive outward-pointing unit normal \( \mathbf{n} \) and the index “ - ” refers to the opposite side, i.e., the side where the positive surface normal \( \mathbf{n} \) points to. The symbol \( \circ \) in equation (2.63) summarizes three different possible operations, namely: multiplication with a scalar field, scalar product with a vectorial or tensorial field, or vector (wedge) product with a vector field.
Let now $\Omega$ be a bounded open subset of $\mathbb{R}^n$ with smooth (or piecewise smooth) boundary $\partial \Omega$. Let $a = [a_1 \ldots a_n]$ be a smooth vector (or tensorial) field defined in $\mathbb{R}^n$, or at least in $\Omega \cup \partial \Omega$. Again $n$ be the unit outward-pointing normal of $\partial \Omega$. Then follows

$$\int_{\Omega} \text{div} \ a \ dV_0 = \int_{\partial \Omega} n a \ dS,$$

(2.65)

where as above $dV$ is the element of volume in $\mathbb{R}^n$ and $dS$ is the element of surface area on $\partial \Omega$. Equation (2.65) is cited in the text as divergence theorem.

## 2.3 Reynolds’ transport theorem

To conclude this summary we present a fundamental theorem to evaluate a time derivative in some changing volume. The rate of any scalar or tensorial function $\Psi(x, t)$ in a time depending volume $V(t)$ is

$$\frac{d}{dt} \int_{V(t)} \Psi(x, t) \ dV = \frac{d}{dt} \int_{V_0} \Psi(\varphi(X, t), t) \ J(X, t) \ dV$$

(2.66)

Evaluating the right hand side of 2.66$^1$, transferring it to the current placement and applying the divergence theorem gives Reynolds’ transport theorem

$$\frac{d}{dt} \int_{V(t)} \Psi \ dV = \int_{V(t)} \frac{\partial \Psi}{\partial t} \ dV + \int_{\partial V(t)} \Psi \cdot v \cdot n \ dS,$$

(2.67)

where we dropped the arguments for readability. The first term in (2.67) denotes the local time rate of the spacial field $\Psi(x, t)$, the second term characterizes the outward normal flux, i.e., the rate of transport of $\Psi \cdot v$ across a fixed boundary $\partial V$ of region $V(t)$. Assuming $\Psi(x, t)$ to be sufficiently smooth, the local form of (2.67) is the material time derivative,

$$\frac{d}{dt} = \frac{\partial \Psi}{\partial t} + \text{grad} \ \Psi \cdot v.$$

(2.68)

$^1$Note that $J V_0 = \frac{d}{dt} V(t)$ and $\frac{\partial}{\partial t} = \text{div} v(x, t)$. 

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Here we summarize some linear spaces and norms naturally to use in finite element approximations. The definitions are given for scalar functions. The analogous definition for vector valued functions are obtained by applying the definition to each one of the components. For more detailed expressions we refer to the mathematical literature, e.g., [BS94, CL91, GR80, GRT88]. Throughout this section let \( \Omega \in \mathbb{R}^d \) be a bounded open set.

Let \( u : \mathbb{R}^d \rightarrow \mathbb{R} \) and let \( \alpha \) be a multi-index\(^1\). Then we write the partial derivatives of a function by

\[
D^\alpha u = \frac{\partial^{|\alpha|} u}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}.
\]

**Definition:** Frobenius-norm. Let \( u \in \mathbb{R}^\alpha \) and let \( \alpha \) be a multi-index. Then we define the norm

\[
\|u\|_F = \sqrt{u_{\alpha_1}^2 + \cdots + u_{\alpha_d}^2}.
\]

(4.2)

If \( u \in \mathbb{R}^n \) is a vector definition (4.2) coincides with the definition of the Euclidian norm.

The Lebesque-space \( \mathbb{L}^p(\Omega) \), \( p \geq 1 \), is the linear space of functions \( u : \Omega \rightarrow \mathbb{R} \) which are Lebesque-measurable, i.e., the ess \( \sup_{\Omega} u < \infty \).

**Definition:** \( \mathbb{L}^p \)-norm. Let \( u \in \mathbb{L}^p(\Omega) \), \( p \geq 1 \). Then we define the norm

\[
\|u\|_p = \left( \int_\Omega |u|^{1/p} \, dx \right)^{1/p}.
\]

(4.3)

According to custom we refer to functions \( \mathbb{L}^2(\Omega) \) as functions which are square integrable over \( \Omega \). All piecewise continuous functions \( u \) belong to \( \mathbb{L}^2(\Omega) \).

\(^1\)A multi-index \( \alpha \) of dimension \( d \) is an array \( \{\alpha_1, \ldots, \alpha_d\} \) of nonnegative integers, \( \alpha \in \mathbb{N}^d \). The degree \( |\alpha| \) of the multi-index is the sum \( \alpha_1 + \cdots + \alpha_d \). For example: a quadratic polynomial in two dimensions has \( |\alpha| = 6 \) independent coefficients with indices \( \alpha = \{00\}, \{10\}, \{01\}, \{20\}, \{11\}, \{02\} \).
The **Sobolev-space** $W^{m,p}(\Omega)$ is the linear space of functions $u : \Omega \to \mathbb{R}$ such that $D^\alpha u \in L^p(\Omega)$ in the distributional sense. In other words, these are functions in $L^p(\Omega)$ whose distributional derivatives up to order $m$ are themselves in $L^p(\Omega)$.

**Definition: Sobolev Seminorm.** Let $u : \Omega \to \mathbb{R}$ be $m$-times continuously differentiable in $\Omega$, $m \geq 0$. Then we define the seminorm

$$|u|_{m,p} = \left( \sum_{|\alpha| = m} \int_\Omega |D^\alpha u|^p \, dx \right)^{1/p}. \quad \text{(4.4)}$$

**Definition: Sobolev norm.** Let $u : \Omega \to \mathbb{R}$ be $m$-times continuously differentiable in $\Omega$, $m \geq 0$. Then we define the norm

$$\|u\|_{m,p} = \left( \sum_{k=0}^m \int_\Omega |u|_{k,p} \, dx \right)^{1/p}. \quad \text{(4.5)}$$

The Sobolev space $W^{m,p}(\Omega)$ is a complete normed space, or Banach space, under the norm (4.5).

The **Hilbert space** $H^m(\Omega)$, $m \geq 0$ is the Sobolev-space $W^{m,2}(\Omega)$. The particular space $H^0(\Omega)$ coincides with the Lebesgue space $L^2(\Omega)$.

For instance, all piecewise continuous functions $u$ with piecewise continuous first derivatives belong to $H^1(\Omega)$.

**Definition: Hilbert norm.** Let $u : \Omega \to \mathbb{R}$ be $m$-times continuously differentiable in $\Omega$, $m \geq 0$. Then we define the norm

$$\|u\|_m = \left( \sum_{k=0}^m |u|^2_k \right)^{1/2}. \quad \text{(4.6)}$$

The Hilbert space $H^m(\Omega)$ the space of functions over $\Omega$ which can be obtained as limits of smooth functions under the norm $\| \cdot \|_m$. These limits may be thought of as functions which are square integrable over $\Omega$ and whose distributional derivatives of order up to $m$ are themselves square integrable. In addition, the Hilbert spaces $H^m(\Omega)$ are spaces with the inner product

$$(u,v)_m = \sum_{|\alpha| = m} \int_\Omega D^\alpha u \cdot D^\alpha v \, dx. \quad \text{(4.7)}$$
5 Appendix 4:

Evaluation of the exponential and logarithmic mapping and their derivatives

Here algorithms for the computation of the exponential and logarithmic mapping and their first and second linearizations according to Radovitzky and Ortiz [RO99] are given.

Let $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times n}$ be square matrices, not necessarily symmetric. The exponential of $A$ is defined as

$$\exp(A) = \sum_{k=0}^{\infty} \frac{1}{k!} A^k$$

(5.1)

provided that the series converges. The logarithm of $B$ is defined as

$$\log(B) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} (B - I)^k$$

(5.2)

provided that the series converges.

5.1 Spectral representation

Let $A$ have eigenvalues $\{\lambda_\alpha, \alpha = 1, \ldots, n\}$, right eigenvectors $\{u_\alpha, \alpha = 1, \ldots, n\}$, and left eigenvectors $\{v_\alpha, \alpha = 1, \ldots, n\}$. Thus,

$$A u_\alpha = \lambda_\alpha u_\alpha, \quad \alpha = 1, \ldots, n,$$

(5.3)

$$A^T v_\alpha = \lambda_\alpha v_\alpha, \quad \alpha = 1, \ldots, n,$$

(5.4)
and

\[ A = \sum_{\alpha=1}^{n} \lambda_{\alpha} u_{\alpha} \otimes v_{\alpha} \]  

(5.5)

The exponential of $A$ then admits the spectral representation

\[ \exp(A) = \sum_{\alpha=1}^{n} e^{\lambda_{\alpha}} u_{\alpha} \otimes v_{\alpha} \]  

(5.6)

We wish to linearize the exponential mapping twice. To this end, we begin by recalling that the solution to the problem

\[ \dot{x}(t) = Ax(t) + f(t), \quad t \geq 0 \]  

(5.7)

\[ x(0) = x_0 \]  

(5.8)

in $\mathbb{R}^n$ is

\[ x(t) = \exp(tA)x_0 + \int_{0}^{t} \exp((t-\tau)A)f(\tau) \, d\tau, \quad t \geq 0 \]  

(5.9)

It therefore follows that $\exp(A)_{ij}$ is the $i$th component of the solution of the initial-value problem (5.7 - 5.8) at $t = 1$ with $f(t) = 0$ and $x_0 = e_j \equiv j$th standard basis vector in $\mathbb{R}^n$.

Imagine now perturbing the matrix $A$ to $A + \delta A$ in (5.7 - 5.8), resulting in a perturbed solution $x(t) + \delta x(t)$. To first order, $\delta x(t)$ is the solution of the problem

\[ \dot{\delta x}(t) = A\delta x(t) + \delta Ax(t), \quad t \geq 0 \]  

(5.10)

\[ \delta x(0) = 0 \]  

(5.11)

Using (5.9), the solution of this problem is found to be

\[ \delta x(t) = \int_{0}^{t} \exp((t-\tau)A)\delta A \exp(\tau A) \, d\tau \]  

(5.12)

But we also have

\[ x(t) + \delta x(t) = \exp(t(A + \delta A))x_0 \sim [\exp(tA) + D\exp(tA)\delta A]x_0 + \text{hot} \]  

(5.13)

Comparing (5.12) and (5.13) yields

\[ D\exp(A)\delta A = \int_{0}^{1} \exp((1-\tau)A)\delta A \exp(\tau A) \, d\tau \]  

(5.14)
or, in components

\[
D\exp(A)_{ijkl} = \int_0^1 \exp((1 - \tau)A)_{ik} \exp(\tau A)_{lj} \, d\tau \tag{5.15}
\]

In order to evaluate this integral we may make use of representation (5.5) to write (5.15) in the form

\[
D\exp(A)_{ijkl} = \sum_{\alpha=1}^n e^{\lambda_\alpha} \sum_{\beta=1}^n \left[ \int_0^1 e^{\tau(\lambda_\beta - \lambda_\alpha)} \, d\tau \right] u_{\alpha i} v_{\alpha k} u_{\beta l} v_{\beta j} \tag{5.16}
\]

which evaluates to

\[
D\exp(A)_{ijkl} = \sum_{\alpha=1}^n \sum_{\beta=1}^n f(\lambda_\alpha, \lambda_\beta) u_{\alpha i} v_{\alpha k} u_{\beta l} v_{\beta j} \tag{5.17}
\]

or, in invariant notation

\[
D\exp(A) = \sum_{\alpha=1}^n \sum_{\beta=1}^n f(\lambda_\alpha, \lambda_\beta) u_\alpha \otimes v_\beta \otimes u_\alpha \otimes v_\beta \tag{5.18}
\]

In these expressions we have written

\[
f(\lambda_\alpha, \lambda_\beta) = \frac{e^{\lambda_\beta} - e^{\lambda_\alpha}}{\lambda_\beta - \lambda_\alpha} \quad \text{if} \quad \lambda_\beta \neq \lambda_\alpha \tag{5.19}
\]

\[
f(\lambda_\alpha, \lambda_\alpha) = e^{\lambda_\alpha} \quad \text{otherwise} \tag{5.20}
\]

Note that the above expressions are valid even when eigenvalues are repeated.

In order to determine the second derivative of the exponential mapping we may differentiate (5.15) to obtain

\[
D^2\exp(A)_{ijklmn} = \int_0^1 (1 - \tau)D\exp((1 - \tau)A)_{ikmn} \exp(\tau A)_{lj} \, d\tau \\
+ \int_0^1 \tau \exp((1 - \tau)A)_{ik} D\exp(\tau A)_{ljmn} \, d\tau \tag{5.21}
\]

Inserting (5.5) and (5.17) into this expression gives

\[
D^2\exp(A)_{ijklmn} = \\
\sum_{\alpha=1}^n \sum_{\beta=1}^n \sum_{\gamma=1}^n \left[ \int_0^1 (1 - \tau) f((1 - \tau)\lambda_\alpha, (1 - \tau)\lambda_\beta) e^{\tau \lambda_\gamma} \, d\tau \right] u_{\alpha i} v_{\alpha m} u_{\beta n} v_{\beta j} u_{\gamma l} v_{\gamma k} \\
+ \sum_{\alpha=1}^n \sum_{\beta=1}^n \sum_{\gamma=1}^n \left[ \int_0^1 \tau f(\tau \lambda_\alpha, \tau \lambda_\beta) e^{(1 - \tau)\lambda_\gamma} \, d\tau \right] u_{\alpha i} v_{\alpha m} u_{\beta n} v_{\beta j} u_{\gamma l} v_{\gamma k} \tag{5.22}
\]
5.1 Spectral representation

Defining
\[
g(\lambda_\alpha, \lambda_\beta, \lambda_\gamma) = \int_0^1 \tau f(\tau \lambda_\alpha, \tau \lambda_\beta) e^{(1-\tau)\lambda_\gamma} \, d\tau
\]  \hspace{1cm} (5.23)

(5.22) simplifies to
\[
D^2 \exp(A)_{ijklmn} = 
\sum_{\alpha=1}^n \sum_{\beta=1}^n \sum_{\gamma=1}^n g(\lambda_\alpha, \lambda_\beta, \lambda_\gamma) v_{am} u_{bn} [u_{ai} v_{\beta j} u_{\gamma k} v_{\gamma l} + u_{ai} v_{\beta k} u_{\gamma l} v_{\gamma j}]
\]  \hspace{1cm} (5.24)

which is the sought expression.

The derivatives of the logarithmic mapping can be obtained directly from the previous expressions by recognizing that \( \log = \exp^{-1} \) and using the properties of inverse functions. This leads to
\[
D \log(B)_{ijkl} = D \exp(A)^{-1}_{ijkl}
\]  \hspace{1cm} (5.25)

\[
D^2 \log(B)_{ijklmn} = -D \exp(A)^{-1}_{ijpq} D \exp(A)^{-1}_{rskl} D \exp(A)^{-1}_{tumn} D^2 \exp(A)_{pqrstn}
\]  \hspace{1cm} (5.26)

where \( A = \exp(B) \). The first of these expressions evaluates to
\[
D \log(B)_{ijkl} = \sum_{\alpha=1}^n \sum_{\beta=1}^n f(\mu_\alpha, \mu_\beta) u_{ai} v_{\alpha k} u_{\beta l} v_{\beta j}
\]  \hspace{1cm} (5.27)

where \( \{\mu_\alpha, \alpha = 1, \ldots n\} \) are the eigenvalues of \( B \), \( \{u_\alpha, \alpha = 1, \ldots n\} \) are its right eigenvectors, and \( \{v_\alpha, \alpha = 1, \ldots n\} \) its left eigenvectors. In invariant notation
\[
D \log(B) = \sum_{\alpha=1}^n \sum_{\beta=1}^n f(\mu_\alpha, \mu_\beta) u_\alpha \otimes v_\beta \otimes v_\alpha \otimes u_\beta
\]  \hspace{1cm} (5.28)

where we write
\[
f(\mu_\alpha, \mu_\beta) = \begin{cases} 
\frac{\log \mu_\beta - \log \mu_\alpha}{\mu_\beta - \mu_\alpha} & \text{if } \mu_\beta \neq \mu_\alpha \\
1/\mu_\alpha & \text{otherwise}
\end{cases}
\]  \hspace{1cm} (5.29)

(5.30)

Note that the above expressions are valid even when eigenvalues are repeated.
5.2 Taylor series expansion

For small $A$ it may be cheaper to evaluate the exponential mapping and its derivatives directly from its series expansion (5.1). Likewise, for $B$ close to the identity it may be cost-effective to use (5.2) directly. To this end, it proves convenient to express (5.1) in the form

$$
\exp(A) = \sum_{k=0}^{\infty} \exp^{(k)}(A) \tag{5.31}
$$

where the terms $\exp^{(k)}(A)$ in the expansion follow from the recurrence relation

$$
\exp^{(0)}(A) = I \tag{5.32}
$$

$$
\exp^{(k+1)}(A) = \frac{1}{k+1} \exp^{(k)}(A)A, \quad k = 0, \ldots \tag{5.33}
$$

Here $I$ is the identity matrix. It follows from this representation that

$$
D\exp(A) = \sum_{k=1}^{\infty} D\exp^{(k)}(A) \tag{5.34}
$$

where

$$
D\exp^{(1)}(A) = DA \tag{5.35}
$$

$$
D\exp^{(k+1)}(A) =
\frac{1}{k+1} [D\exp^{(k)}(A)A + \exp^{(k)}(A)DA], \quad k = 1, \ldots \tag{5.36}
$$

In components

$$
D\exp^{(1)}(A)_{ijkl} = \delta_{ik}\delta_{jl} \tag{5.37}
$$

$$
D\exp^{(k+1)}(A)_{ijkl} =
\frac{1}{k+1} [D\exp^{(k)}(A)_{ijkl}A_{pj} + \exp^{(k)}(A)_{ik}\delta_{jl}], \quad k = 1, \ldots \tag{5.38}
$$

Likewise

$$
D^2\exp(A) = \sum_{k=2}^{\infty} D^2\exp^{(k)}(A) \tag{5.39}
$$

where

$$
D^2\exp^{(2)}(A) = \frac{1}{2} D^2A^2 \tag{5.40}
$$

$$
D^2\exp^{(k+1)}(A) =
\frac{1}{k+1} \{D^2\exp^{(k)}(A)A + 2\text{sym}[D\exp^{(k)}(A)DA]\}, \quad k = 2, \ldots \tag{5.41}
$$
In components

\[ D^2 \exp^{(2)}(A)_{ijklmn} = \frac{1}{2} (\delta_{ik} \delta_{lm} \delta_{jn} + \delta_{im} \delta_{kn} \delta_{jl}) \]  
(5.42)

\[ D^2 \exp^{(k+1)}(A)_{ijklmn} = \frac{1}{k+1} [D^2 \exp^{(k)}(A)_{ipklmn} A_{pj} + D\exp^{(k)}(A)_{imkn} \delta_{jn} + D\exp^{(k)}(A)_{ikmn} \delta_{jl}], \quad k = 2, \ldots \]  
(5.43)

The logarithmic mapping can be given a similar treatment. Begin by expressing (5.2) in the form

\[ \log(B) = \sum_{k=1}^{\infty} \log^{(k)}(B) \]  
(5.44)

where the terms \( \log^{(k)}(B) \) in the expansion follow from the recurrence relation

\[ \log^{(1)}(B) = B - I \]  
(5.45)

\[ \log^{(k+1)}(B) = -\frac{k}{k+1} \log^{(k)}(B)(B - I), \quad k = 1, \ldots \]  
(5.46)

It follows from this representation that

\[ D\log(B) = \sum_{k=1}^{\infty} D\log^{(k)}(B) \]  
(5.47)

where

\[ D\log^{(1)}(B) = DB \]  
(5.48)

\[ D\log^{(k+1)}(B) = \]  
\[ -\frac{k}{k+1} [D\log^{(k)}(B)(B - I) + \log^{(k)}(B)DB], \quad k = 1, \ldots \]  
(5.49)

In components

\[ D\log^{(1)}(B)_{ijkl} = \delta_{ik} \delta_{jl} \]  
(5.50)

\[ D\log^{(k+1)}(B)_{ijkl} = \]  
\[ -\frac{k}{k+1} [D\log^{(k)}(B)_{ipkl}(B_{pj} - \delta_{pj}) + \log^{(k)}(B)_{ik\delta_{jl}}], \quad k = 1, \ldots \]  
(5.51)

Likewise

\[ D^2\log(B) = \sum_{k=2}^{\infty} D^2\log^{(k)}(B) \]  
(5.52)

where

\[ D^2\log^{(2)}(B) = \frac{1}{2} D^2B^2 \]  
(5.53)

\[ D^2\log^{(k+1)}(B) = \]  
\[ -\frac{k}{k+1} [D^2\log^{(k)}(B)(A - I) + 2\text{sym}[D\log^{(k)}(B)DB]], \quad k = 2, \ldots \]  
(5.54)
5.2 Taylor series expansion

In components

\[ D^{2}\log^{(2)}(B)_{ijklmn} = \frac{1}{2}(\delta_{ik}\delta_{lm}\delta_{jn} + \delta_{im}\delta_{kn}\delta_{jl}) \]  

\[ D^{2}\log^{(k+1)}(B)_{ijklmn} = -\frac{k}{k+1}[D^{2}\log^{(k)}(B)_{ipklmn}(A_{pj} - \delta_{pj}) + D\log^{(k)}(B)_{inkl}\delta_{jn} + D\log^{(k)}(B)_{ikmn}\delta_{jl}], \quad k = 2, \ldots \]
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