Computer methods in applied mechanics and engineering

ELSEVIER

Comput. Methods Appl. Mech. Engrg. 190 (2001) 2753–2770

www.elsevier.com/locate/cma

Some remarks on the compressed matrix representation of symmetric second-order and fourth-order tensors

Peter Helnwein

Institute for Strength of Materials, Vienna University of Technology, Karlsplatz 13, A-1040 Vienna, Austria

Received 1 August 1999; received in revised form 18 April 2000

Dedicated to all students in computational mechanics

Abstract

The mathematical description of physical phenomena requires the use of scalars and tensors of various order. Since many of the second-order and fourth-order tensors used in continuum mechanics possess certain symmetries, a compressed vector or matrix representation, respectively, is frequently used in computational applications such as the FEM and BEM. Use of different storage schemes for different tensors lead to an hypothetical nonuniqueness of such matrix representations. The present paper offers a clarification by investigation of the structure of the underlying six-dimensional vector space. It identifies various types of matrix representations as covariant, contravariant or mixed-variant coordinates in that vector space and thus proves consistency of the matrix representation with classical tensor analysis in $\mathbb{R}^3$. Furthermore, it is shown that an ortho-normal basis for the underlying tensor representation in $\mathbb{R}^3$ does not automatically lead to a normalized space for the compressed matrix representation in $\mathbb{R}^6$. Thus, distinction of covariant and contravariant coordinates is necessary even in that case. Theoretical findings are worked out in detail for symmetric second-order and fourth-order tensors in $\mathbb{R}^3$. Example applications on commonly used fourth-order tensors as well as a comparison of possible computational implementations close the paper.

Keywords: Symmetric tensors; Compressed matrix representation; 6d vector space; Metric; Tensor-to-matrix transition

1. Introduction

The mathematical description of physical phenomena requires the use of scalars and tensors of various order [1–5]. Typical applications of scalars are, e.g., potential functions and temperature, and of vectors (i.e., first-order tensors), displacement or velocity fields or acting forces. Second-order tensors are used as various stress tensors (Cauchy, Kirchhoff, first and second Piola–Kirchhoff, etc.), strain tensors (Cauchy Green–Lagrange, Almansi–Euler, Henkey, etc.) or damage tensors. Typical fourth-order tensors are: the material stiffness tensors, viscoelastic and elastoplastic tangent operators, or structural tensors for anisotropic materials.

All of the above-mentioned tensors obey certain symmetries. Making use of these symmetries, the computational effort for tensor operations can be significantly reduced. Thus, most implementations in computational mechanics, such as the Finite Element Method (FEM) or the Boundary Element Method (BEM) make use of a compressed vector or matrix representation of symmetric second-order and fourth-order tensors (see, e.g., [6–9]). A detailed description of the transition from symmetric tensors into matrix representation is given in [6]. Nevertheless, the explanation given therein is restricted to the matrix representation of a material stiffness tensor relating a strain tensor with a stress tensor. In what follows, this particular case will be identified as *contravariant* representation of a symmetric fourth-order tensor. The mentioned restriction on the tensor-to-matrix transition given in [6] may cause errors when constructing matrix representations of compliance tensors as used in viscoelasticity or some algorithms for elastoplasticity.

0045-7825/01/$ - see front matter
PII: S0045-7825(00)00263-2

Even though the use of matrix representations has a long tradition, the transition from arbitrary fourth-order tensors to 6×6-matrices offers hypothetical non-uniqueness of the matrix representation. A popular example is the matrix representation of the fourth-order deviatoric operator. Applied to the Cauchy stress tensor $\boldsymbol{\sigma}$ it defines the deviatoric stress tensor $\mathbf{s}$ as follows:

$$\mathbf{s} = \mathbb{I}^{\mathrm{dev}} : \boldsymbol{\sigma} \quad \leftrightarrow \quad \begin{Bmatrix} s^{11} \\ s^{22} \\ s^{33} \\ s^{12} \\ s^{23} \\ s^{31} \end{Bmatrix} = \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} \sigma^{11} \\ \sigma^{22} \\ \sigma^{33} \\ \sigma^{12} \\ \sigma^{23} \\ \sigma^{31} \end{Bmatrix}. \tag{1}$$

The right-hand expression of (1) shows the matrix representation of the tensorial expression given on the left-hand side.

Using the deviatoric operator in the elastic constitutive relation between the strain tensor $\boldsymbol{\varepsilon}$ and deviatoric stress tensor $\mathbf{s}$ yields the matrix representation as

$$\mathbf{s} = 2G\mathbb{I}^{\mathrm{dev}} : \boldsymbol{\varepsilon} \quad \leftrightarrow \quad \begin{Bmatrix} s^{11} \\ s^{22} \\ s^{33} \\ s^{12} \\ s^{23} \\ s^{31} \end{Bmatrix} = 2G \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \gamma_{12} \\ \gamma_{23} \\ \gamma_{31} \end{Bmatrix}, \tag{2}$$

where $\gamma_{ij} = 2\varepsilon_{ij}$ are the shear components of the engineering strain. This definition of $\boldsymbol{\varepsilon}$ satisfies the invariance condition $\mathbf{s} : \boldsymbol{\varepsilon} = \{s^{11}\ s^{22}\ s^{33}\ s^{12}\ s^{23}\ s^{31}\}\{\varepsilon_{11}\ \varepsilon_{22}\ \varepsilon_{33}\ \gamma_{12}\ \gamma_{23}\ \gamma_{31}\}^{\mathrm{T}}$.

Comparing the two matrix representations of $\mathbb{I}^{\mathrm{dev}}$ in (1) and (2) demonstrates the source of the hypothetical non-uniqueness of the compressed matrix representation. Two more representations arise in applications using a sequence of fourth-order tensor operators acting one on the other.

The aim of the present paper is to give a clarification on the supposed non-uniqueness on the basis of a six-dimensional vector space and the identification of various types of matrix representations as covariant, contravariant or mixed-variant coordinates in that vector space.

In Section 2, the derivations for the unified explanation of the compressed matrix representation of symmetric second-order and fourth-order tensors will be given.

The theoretical findings given in Section 2 will be discussed in Section 3 by means of the vector representations for stress tensors and strain tensors, respectively, as well as the matrix representations for two commonly used fourth-order tensors. Furthermore, the influence of the type of representation on the computational implementation is discussed by means of a simple numerical example.

2. Matrix representation as first-order and second-order tensors in a six-dimensional vector space

The aim of this chapter is to show that the compressed matrix representation of symmetric second-order and fourth-order tensors in $\mathbb{R}^3$ has tensorial character in $\mathbb{R}^6$. In order to prove this proposition we will develop a basis (it will be identified as a set of symmetric second-order tensors) for the considered vector space in $\mathbb{R}^6$. This enables the definition of a metric and an inner product for this space.

Based on classical tensor analysis we will show that all rules regarding conversion between covariant, contravariant and mixed-variant tensor coordinates appear in the six-dimensional vector space governing the vector (6×1-matrix) representation of symmetric second-order tensors. Using this knowledge, in Section 2.2 we will extend the theory to tensors in $\mathbb{R}^6$ representing symmetric fourth-order tensors in $\mathbb{R}^3$.

A brief summary of the developed framework will be added in Table 1 at the end of this section.

For the derivations given in this section, the following conventions will be used:

- Boldface symbols $\mathbf{T}$, $\mathbf{U}$ and $\mathbf{V}$ denote second-order tensors in $\mathbb{R}^3$ and $\mathbf{A}$ denotes a fourth-order tensor in $\mathbb{R}^3$.
- A bar over a boldface symbol, e.g., $\bar{\mathbf{T}}$ and $\bar{\mathbf{A}}$, generally indicates vector (as 6×1-matrix) and matrix representation, respectively. In order to indicate special representations, i.e. covariant, contravariant or mixed-variant, the notations $\{\bar{T}_a\}, \{\bar{T}^a\}$ or $\{\bar{A}^a_{.b}\}$ will be used instead.
- The indices i, j, k, l, m, n, q, r, s, t indicate summation over 1, 2, 3 while the indices a, b, c, d indicate summation over $1, 2, \ldots, 6$.
- The lowercase boldface symbols $\mathbf{g}_i,\ i = 1, 2, 3$, denote the covariant base vectors in $\mathbb{R}^3$. They are connected to a generally non-normalized skew and arbitrary curved coordinate system. The special case of an ortho-normal basis in $\mathbb{R}^3$ is marked by a hat ($\hat{\mathbf{g}}_i = \hat{\mathbf{g}}^i$ with coordinates $\hat{U}^i = \hat{U}_i$ and $\hat{\mathbf{g}}_i \otimes \hat{\mathbf{g}}_j = \hat{\mathbf{g}}^i \otimes \hat{\mathbf{g}}^j$ with coordinates $\hat{T}^{ij} = \hat{T}_{ij}$).
- The uppercase boldface symbols $\mathbf{G}_a$ and $\mathbf{G}^a$, respectively, denote the covariant and contravariant symmetric tensors used as the basis in the definition of the associated six-dimensional vector space.

2.1. Representation of symmetric second-order tensors as six-dimensional vectors

In this section we will derive the basic relations of a six-dimensional vector space used for the description of the vector (6×1-matrix) representation of symmetric second-order tensors. For this purpose we consider the following equivalent representations of a second-order tensor $\mathbf{T} \in \mathbb{R}^3 \times \mathbb{R}^3$:

$$\mathbf{T} = T^{ij}\mathbf{g}_i \otimes \mathbf{g}_j = T_{ij}\mathbf{g}^i \otimes \mathbf{g}^j. \tag{3}$$

The mixed-variant representations $\mathbf{T} = T^i_{.j}\mathbf{g}_i \otimes \mathbf{g}^j = T_i^{.j}\mathbf{g}^i \otimes \mathbf{g}_j$ are not taken into account in the subsequent development. In this paper we will consider only tensors $\mathbf{T} \in \mathscr{S}$, where

$$\mathscr{S} := \{\mathbf{T} \in \mathbb{R}^3 \times \mathbb{R}^3 \mid \mathbf{T} = \mathbf{T}^t \iff T^{ij} = T^{ji}, T_{ij} = T_{ji}, T^i_{.j} = T_j^{.i}\} \tag{4}$$

is the space of symmetric second-order tensors in $\mathbb{R}^3$.

Let us introduce the six-tuple $\bar{\mathbf{T}} = \{\bar{T}^a\} = \{\bar{T}^1\ \bar{T}^2\ \bar{T}^3\ \bar{T}^4\ \bar{T}^5\ \bar{T}^6\}^t$. We will refer to the components $\bar{T}^a$ as coordinates of the vector space defined by

$$\mathscr{S}^* := \{\bar{\mathbf{T}} \in \mathbb{R}^6 \mid \bar{T}^a\mathbf{G}_a = \mathbf{T} \in \mathscr{S}\}. \tag{5}$$

The tensors $\mathbf{G}_a \in \mathscr{S}$ form the covariant basis of the vector space $\mathscr{S}^*$. In what follows they will be referred to as *base tensors*. Definition (5) describes the mapping from a first-order tensor in $\mathbb{R}^6$ (i.e., from a vector in $\mathbb{R}^6$) onto a second-order tensor in $\mathscr{S} \subset \mathbb{R}^3 \times \mathbb{R}^3$.

Then we define the inner product $\langle\bar{\mathbf{U}}, \bar{\mathbf{V}}\rangle$ with $\bar{\mathbf{U}}$ and $\bar{\mathbf{V}} \in \mathscr{S}^*$ as

$$\langle\bar{\mathbf{U}}, \bar{\mathbf{V}}\rangle := \mathbf{U} : \mathbf{V} = \bar{U}^a\bar{V}^b\mathbf{G}_a : \mathbf{G}_b = \bar{U}^a\bar{V}^bG_{ab}, \tag{6}$$

where

$$G_{ab} := \langle\mathbf{G}_a, \mathbf{G}_b\rangle = \mathbf{G}_a : \mathbf{G}_b = \mathbf{G}_b : \mathbf{G}_a = \langle\mathbf{G}_b, \mathbf{G}_a\rangle = G_{ba} \tag{7}$$

are the covariant coordinates of the metric tensor in $\mathscr{S}^*$. Note that the summation convention in $\mathscr{S}^*$ forces the sum $\sum_{a=1}^{6}$.

As can be seen from (6) and (7), the inner product defined by (6) satisfies

$$\langle\bar{\mathbf{U}}, \bar{\mathbf{V}}\rangle = \langle\bar{\mathbf{V}}, \bar{\mathbf{U}}\rangle \quad \text{and} \quad \langle\bar{\mathbf{U}}, \bar{\mathbf{U}}\rangle > 0 \quad \forall\, \bar{\mathbf{U}} \neq \bar{\mathbf{0}}. \tag{8}$$

In order to obtain a simpler expression for the inner product defined by (6) we introduce a contravariant set of base-tensors in $\mathscr{S}^*$ by the condition

$$\langle\mathbf{G}_a, \mathbf{G}^b\rangle = \langle\mathbf{G}^b, \mathbf{G}_a\rangle = \delta_a^b, \tag{9}$$

where δ_a^b are the coordinates of the Kronecker tensor in $\mathbb{R}^6$. According to (6), any tensor $\mathbf{U} \in \mathscr{S}$ can be described by means of $\bar{\mathbf{U}} \in \mathscr{S}^*$ as

$$\mathbf{U} = \{\mathbf{G}_1\ \mathbf{G}_2\ \mathbf{G}_3\ \mathbf{G}_4\ \mathbf{G}_5\ \mathbf{G}_6\}\{\bar{U}^a\}. \tag{10}$$

Hence, the contravariant base tensors $\mathbf{G}^a$ can be expressed as

$$\mathbf{G}^a := G^{ba}\mathbf{G}_b. \tag{11}$$

Building the inner product of (11) with $\mathbf{G}_c$ yields under consideration of (9) and (7)

$$\langle \mathbf{G}_c, \mathbf{G}^a \rangle = G^{ba}\langle \mathbf{G}_c, \mathbf{G}_b \rangle \ \Rightarrow\ \delta_c^a = G_{cb}G^{ba}. \tag{12}$$

From (12) we obtain the coefficients G^{ba} as

$$\{G^{ba}\} = \{G_{ab}\}^{-1} \tag{13}$$

and by means of (11) the contravariant base tensors $\mathbf{G}^a$. Eq. (13) is a well-known definition of the contravariant coordinates of the metric tensor in $\mathbb{R}^6$. Thus, the coefficients $G^{ab} = \langle \mathbf{G}^a, \mathbf{G}^b \rangle$ are identified as those coordinates.

Using the contravariant base tensors $\mathbf{G}^a$, the coordinates $\bar{T}^a$ are obtained from definition (5) and under consideration of (9) as

$$\boxed{\mathbf{T} : \mathbf{G}^b = \bar{T}^a \langle \mathbf{G}_a, \mathbf{G}^b \rangle = \bar{T}^b}. \tag{14}$$

Eq. (14) defines the map $\mathscr{S} \to \mathscr{S}^*$.

Building the inner product of the invariance condition

$$\mathbf{T} = \bar{T}^a\mathbf{G}_a = \bar{T}_a\mathbf{G}^a \tag{15}$$

with $\mathbf{G}_b$ and $\mathbf{G}^b$, respectively, yields under consideration of (9) and (11) the transformation for the coordinates in $\mathscr{S}^*$ as

$$\boxed{\bar{T}_b = G_{ab}\bar{T}^a = G_{ba}\bar{T}^a} \quad \text{and} \quad \boxed{\bar{T}^b = G^{ab}\bar{T}_a = G^{ba}\bar{T}_a}. \tag{16}$$

Using matrix notation, the transformations from contravariant to covariant coordinates and vice versa are obtained as

$$\{\bar{T}_b\} = \{G_{ba}\}\{\bar{T}^a\} \quad \text{and} \quad \{\bar{T}^b\} = \{G^{ba}\}\{\bar{T}_a\}. \tag{17}$$

Based on the covariant and contravariant coordinates as defined by (16) the definition of the inner product as given by (6) can be simplified as follows:

$$\langle \bar{\mathbf{U}}, \bar{\mathbf{V}} \rangle := \bar{U}^a\bar{V}_a = \bar{U}_a\bar{V}^a \quad \forall\ \bar{\mathbf{U}}, \bar{\mathbf{V}} \in \mathscr{S}^*. \tag{18}$$

Using vector notation (6×1-matrix), definition (18) can be expressed as

$$\langle \bar{\mathbf{U}}, \bar{\mathbf{V}} \rangle := \{\bar{U}^a\}^t\{\bar{V}_b\} = \{\bar{U}_a\}^t\{\bar{V}^b\}. \tag{19}$$

The inner product as given by (18) and (19) is equivalent to the *scalar invariant* $\operatorname{tr}\mathbf{UV} = \mathbf{U} : \mathbf{V}$ of the related tensors $\mathbf{U}$ and $\mathbf{V} \in \mathscr{S}$.

Remark 2.1. Note that the matrix operations $\{\bar{U}_a\}^t\{\bar{V}_b\}$ and $\{\bar{U}^a\}^t\{\bar{V}^b\}$ have no tensorial equivalent and thus are *not invariant* under changes of the coordinate frame.

2.1.1. Base tensors and metric of the most common matrix representations

The most common compressed representations of symmetric tensors in continuum mechanics are the direct use of coordinates for stresses and the use of engineering strains (which use $\gamma_{ij} = 2\varepsilon_{ij}$ for the shear components) as the components in a vector (6×1-matrix) representation. Using the interpretation as a six-dimensional vector space as outlined above, it will be shown that both representations are equivalent but represent covariant and contravariant coordinates in $\mathscr{S}^*$.

In order to obtain such a representation we have to define the covariant base tensors as follows

$$\begin{aligned}
\mathbf{G}_1 &= \mathbf{g}_1 \otimes \mathbf{g}_1, \quad \mathbf{G}_4 = \mathbf{g}_1 \otimes \mathbf{g}_2 + \mathbf{g}_2 \otimes \mathbf{g}_1,\\
\mathbf{G}_2 &= \mathbf{g}_2 \otimes \mathbf{g}_2, \quad \mathbf{G}_5 = \mathbf{g}_2 \otimes \mathbf{g}_3 + \mathbf{g}_3 \otimes \mathbf{g}_2,\\
\mathbf{G}_3 &= \mathbf{g}_3 \otimes \mathbf{g}_3, \quad \mathbf{G}_6 = \mathbf{g}_3 \otimes \mathbf{g}_1 + \mathbf{g}_1 \otimes \mathbf{g}_3.
\end{aligned} \tag{20}$$

Consideration of the covariant coordinates $g_{ij} = g_{ji}$ of the *metric tensor* in $\mathbb{R}^3$ yields the related metric tensor – given in matrix notation – as

$$\{G_{ab}\} = \begin{bmatrix}
g_{11}g_{11} & g_{12}g_{12} & g_{31}g_{31} & 2g_{11}g_{12} & 2g_{12}g_{31} & 2g_{31}g_{11}\\
 & g_{22}g_{22} & g_{23}g_{23} & 2g_{12}g_{22} & 2g_{22}g_{23} & 2g_{23}g_{12}\\
 & & g_{33}g_{33} & 2g_{31}g_{23} & 2g_{23}g_{33} & 2g_{33}g_{31}\\
 & \text{symm.} & & 2(g_{11}g_{22}+g_{12}g_{12}) & 2(g_{12}g_{23}+g_{31}g_{22}) & 2(g_{31}g_{12}+g_{23}g_{11})\\
 & & & & 2(g_{22}g_{33}+g_{23}g_{23}) & 2(g_{23}g_{31}+g_{12}g_{33})\\
 & & & & & 2(g_{33}g_{11}+g_{31}g_{31})
\end{bmatrix}. \tag{21}$$

Remark 2.2. For the special case of an ortho-normal basis $\{\hat{\mathbf{g}}_1, \hat{\mathbf{g}}_2, \hat{\mathbf{g}}_3\}$ in $\mathbb{R}^3$, the metric tensor (21) of the six-dimensional vector space $\mathscr{S}^*$ simplifies to

$$\{G_{ab}\} = \begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0\\
0 & 1 & 0 & 0 & 0 & 0\\
0 & 0 & 1 & 0 & 0 & 0\\
0 & 0 & 0 & 2 & 0 & 0\\
0 & 0 & 0 & 0 & 2 & 0\\
0 & 0 & 0 & 0 & 0 & 2
\end{bmatrix}. \tag{22}$$

As can be seen from the coordinates of the metric tensor (22), even in this particular case, $\mathscr{S}^*$ is an orthogonal but in general not normalized vector space. Thus leading to $\bar{U}_a \neq \bar{U}^a$ even if $U_{ij} = U^{ij}$.

Substitution of (21) into (13), of the result and (20) into (11), and consideration of the transformation rule $\mathbf{g}^i = g^{ij}\mathbf{g}_j$ with $\{g^{ij}\} = \{g_{ij}\}^{-1}$ yields the contravariant base tensors as

$$\begin{aligned}
\mathbf{G}^1 &= \mathbf{g}^1 \otimes \mathbf{g}^1, \quad \mathbf{G}^4 = \frac{1}{2}(\mathbf{g}^1 \otimes \mathbf{g}^2 + \mathbf{g}^2 \otimes \mathbf{g}^1),\\
\mathbf{G}^2 &= \mathbf{g}^2 \otimes \mathbf{g}^2, \quad \mathbf{G}^5 = \frac{1}{2}(\mathbf{g}^2 \otimes \mathbf{g}^3 + \mathbf{g}^3 \otimes \mathbf{g}^2),\\
\mathbf{G}^3 &= \mathbf{g}^3 \otimes \mathbf{g}^3, \quad \mathbf{G}^6 = \frac{1}{2}(\mathbf{g}^3 \otimes \mathbf{g}^1 + \mathbf{g}^1 \otimes \mathbf{g}^3).
\end{aligned} \tag{23}$$

Condition (9) can easily be verified for $\mathbf{G}_a$ and $\mathbf{G}^b$ according to (20) and (23), respectively. The coordinates $\bar{T}^a$ are derived from (3) and (14) by means of (23) as

$$\begin{aligned}
&\bar{T}^1 = T^{11}, \quad \bar{T}^2 = T^{22}, \quad \bar{T}^3 = T^{33}, \quad \bar{T}^4 = \frac{1}{2}(T^{12} + T^{21}) = T^{12}, \quad \bar{T}^5 = \frac{1}{2}(T^{23} + T^{32}) = T^{23},\\
&\bar{T}^6 = \frac{1}{2}(T^{31} + T^{13}) = T^{31},
\end{aligned} \tag{24a}$$

or in vector (6×1-matrix) notation as

$$\boxed{\{\bar{T}^a\} = \{T^{11}\ T^{22}\ T^{33}\ T^{12}\ T^{23}\ T^{31}\}^t}. \tag{24b}$$

Substitution of (24a) and (21) into (17) and consideration of the transformation rule $T_{ij} = g_{ik} g_{jl} T^{kl}$ yields the covariant coordinates in $\mathscr{S}^*$ as

$$\begin{aligned}&\bar{T}_1 = T_{11}, \quad \bar{T}_2 = T_{22}, \quad \bar{T}_3 = T_{33},\\ &\bar{T}_4 = T_{12} + T_{21} = 2T_{12}, \quad \bar{T}_5 = T_{23} + T_{32} = 2T_{23}, \quad \bar{T}_6 = T_{31} + T_{13} = 2T_{31},\end{aligned} \tag{25a}$$

or in vector (6×1-matrix) notation as

$$\{\bar{T}_a\} = \{T_{11}\ T_{22}\ T_{33}\ 2T_{12}\ 2T_{23}\ 2T_{31}\}^t. \tag{25b}$$

According to the representation theory of vector and tensor functions, any vector possesses exactly one scalar invariant I. By means of the equivalence

$$I = \bar{T}^a \bar{T}_a \equiv T^{ij} T_{ij} \ \leftrightarrow \ I = \{\bar{T}^a\}^t \{\bar{T}_a\} \equiv \mathbf{T} : \mathbf{T}, \tag{26}$$

this invariant is identified as the second invariant $S_2 = \operatorname{tr} \mathbf{T}^2 = \mathbf{T} : \mathbf{T}$ of the second-order tensor $\mathbf{T} \in \mathscr{S}$. Thus, even if the vector (6×1-matrix) representation enables the full and unique reconstruction of $\mathbf{T}$, it reduces the number of invariants from three to one. Hence, the matrix representation $\bar{\mathbf{T}} \in \mathscr{S}^*$ does not recover the whole integrity basis of $\mathbf{T} \in \mathscr{S}$. This shortcoming has been pointed out in the literature for second-order tensors as well as for fourth-order tensors [4].

Remark 2.3. The derivations given in (5)–(25b) have shown that in consequence of the mapping $\mathscr{S} \to \mathscr{S}^*$ even an ortho-normal basis in $\mathbb{R}^3$ may yield a non-normalized basis in the six-dimensional representation, i.e., in $\mathscr{S}^*$. Thus, one needs to take care to distinguish between covariant and contravariant coordinates in $\mathscr{S}^*$ even in the special case when there is no difference between them in the underlying space $\mathscr{S}$.

2.1.2. Normalized tensorial basis in $\mathscr{S}^*$

An ortho-normal basis $\hat{\mathbf{G}}_a = \hat{\mathbf{G}}^a$ in $\mathscr{S}^*$ can be obtained from an ortho-normal basis $\{\hat{\mathbf{g}}_1, \hat{\mathbf{g}}_2, \hat{\mathbf{g}}_3\}$ in $\mathbb{R}^3$ and normalization of the tensorial basis given in (20). This leads to a diagonal shape of the metric tensor. The normalization is achieved by

$$\hat{\mathbf{G}}_a = \frac{1}{\sqrt{G_{aa}}} \mathbf{G}_a \quad \text{and} \quad \hat{\mathbf{G}}^a = \frac{1}{\sqrt{G^{aa}}} \mathbf{G}^a = \sqrt{G^{aa}} \mathbf{G}_a = \hat{\mathbf{G}}_a \qquad \text{(no sum)} \tag{27}$$

where $\mathbf{G}_a$ is defined by (20) but based on an ortho-normal basis $\{\hat{\mathbf{g}}_1, \hat{\mathbf{g}}_2, \hat{\mathbf{g}}_3\}$ instead of a general basis $\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\}$. Using the related coordinates of the metric tensor as given in (22) yields the ortho-normal basis in $\mathscr{S}^*$ as

$$\begin{aligned}&\hat{\mathbf{G}}_1 = \hat{\mathbf{G}}^1 = \hat{\mathbf{g}}_1 \otimes \hat{\mathbf{g}}_1, \quad \hat{\mathbf{G}}_4 = \hat{\mathbf{G}}^4 = \frac{1}{\sqrt{2}}(\hat{\mathbf{g}}_1 \otimes \hat{\mathbf{g}}_2 + \hat{\mathbf{g}}_2 \otimes \hat{\mathbf{g}}_1),\\ &\hat{\mathbf{G}}_2 = \hat{\mathbf{G}}^2 = \hat{\mathbf{g}}_2 \otimes \hat{\mathbf{g}}_2, \quad \hat{\mathbf{G}}_5 = \hat{\mathbf{G}}^5 = \frac{1}{\sqrt{2}}(\hat{\mathbf{g}}_2 \otimes \hat{\mathbf{g}}_3 + \hat{\mathbf{g}}_3 \otimes \hat{\mathbf{g}}_2),\\ &\hat{\mathbf{G}}_3 = \hat{\mathbf{G}}^3 = \hat{\mathbf{g}}_3 \otimes \hat{\mathbf{g}}_3, \quad \hat{\mathbf{G}}_6 = \hat{\mathbf{G}}^6 = \frac{1}{\sqrt{2}}(\hat{\mathbf{g}}_3 \otimes \hat{\mathbf{g}}_1 + \hat{\mathbf{g}}_1 \otimes \hat{\mathbf{g}}_3).\end{aligned} \tag{28}$$

The related coordinates are obtained as $\hat{T}^a = \sqrt{G_{aa}} \bar{T}^a$ and $\hat{T}^a = \sqrt{G^{aa}} \bar{T}^a = (1/\sqrt{G_{aa}}) \bar{T}_a$. Using (24a) and (22) as well as (25a) and (22) yields

$$\begin{aligned}&\hat{T}_1 = \hat{T}^1 = \hat{T}_{11}, \quad \hat{T}_4 = \hat{T}^4 = \frac{1}{\sqrt{2}}(\hat{T}_{12} + \hat{T}_{21}) = \sqrt{2}\hat{T}_{12},\\ &\hat{T}_2 = \hat{T}^2 = \hat{T}_{22}, \quad \hat{T}_5 = \hat{T}^5 = \frac{1}{\sqrt{2}}(\hat{T}_{23} + \hat{T}_{32}) = \sqrt{2}\hat{T}_{23},\\ &\hat{T}_3 = \hat{T}^3 = \hat{T}_{33}, \quad \hat{T}_6 = \hat{T}^6 = \frac{1}{\sqrt{2}}(\hat{T}_{31} + \hat{T}_{13}) = \sqrt{2}\hat{T}_{31},\end{aligned} \tag{29}$$

or in vector (6×1 matrix) notation

$$\boxed{\{\hat{T}^a\} = \{\hat{T}_a\} = \{\hat{T}_{11}\ \hat{T}_{22}\ \hat{T}_{33}\ \sqrt{2}\hat{T}_{12}\ \sqrt{2}\hat{T}_{23}\ \sqrt{2}\hat{T}_{31}\}^t}. \tag{30}$$

Thus, in the ortho-normal representation of $\mathscr{S}^*$ no distinction between covariant and contravariant representation is required.

2.2. Representation of symmetric fourth-order tensors as six-dimensional square matrices

Now consider a fourth-order tensor $\mathbf{A} \in \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3$ and the following equivalent representations:

$$\mathbf{A} = A^{ijkl}\mathbf{g}_i \otimes \mathbf{g}_j \otimes \mathbf{g}_k \otimes \mathbf{g}_l = A_{ijkl}\mathbf{g}^i \otimes \mathbf{g}^j \otimes \mathbf{g}^k \otimes \mathbf{g}^l = A^{ij}_{..kl}\mathbf{g}_i \otimes \mathbf{g}_j \otimes \mathbf{g}^k \otimes \mathbf{g}^l = A_{ij}^{..kl}\mathbf{g}^i \otimes \mathbf{g}^j \otimes \mathbf{g}_k \otimes \mathbf{g}_l. \tag{31}$$

In most applications in continuum mechanics using fourth-order tensors, $\mathbf{A}$ is in

$$\mathscr{T} := \{\mathbf{A} \in \mathscr{S} \times \mathscr{S} \subset \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \mid A_{ijkl} = A_{jikl} = A_{jilk} = A_{ijlk}\}, \tag{32}$$

i.e., the space of fourth-order tensors in $\mathbb{R}^3$ with symmetries with respect to the first two and the last two indices of their covariant as well as their contravariant coordinates. Note that the mixed-variant coordinates satisfy $A^{i.kl}_{.j} = A^{ikl}_{j}$ but $A^{i.kl}_{.j} \neq A^{j.kl}_{.i}$.

Now introduce a 6×6 matrix representation of the form

$$\bar{\mathbf{A}} = \{\bar{A}^{ab}\} = \begin{bmatrix} \bar{A}^{11} & \bar{A}^{12} & \bar{A}^{13} & \bar{A}^{14} & \bar{A}^{15} & \bar{A}^{16} \\ \bar{A}^{21} & \bar{A}^{22} & \bar{A}^{23} & \bar{A}^{24} & \bar{A}^{25} & \bar{A}^{26} \\ \bar{A}^{31} & \bar{A}^{32} & \bar{A}^{33} & \bar{A}^{34} & \bar{A}^{35} & \bar{A}^{36} \\ \bar{A}^{41} & \bar{A}^{42} & \bar{A}^{43} & \bar{A}^{44} & \bar{A}^{45} & \bar{A}^{46} \\ \bar{A}^{51} & \bar{A}^{52} & \bar{A}^{53} & \bar{A}^{54} & \bar{A}^{55} & \bar{A}^{56} \\ \bar{A}^{61} & \bar{A}^{62} & \bar{A}^{63} & \bar{A}^{64} & \bar{A}^{65} & \bar{A}^{66} \end{bmatrix} \tag{33}$$

and view the matrix elements as coordinates of the second-order vector (tensor) space $\mathscr{T}^*$ defined as

$$\mathscr{T}^* := [\bar{\mathbf{A}} \in \mathbb{R}^6 \times \mathbb{R}^6 | \bar{A}^{ab}\mathbf{G}_a \otimes \mathbf{G}_b = \mathbf{A} \in \mathscr{T}]. \tag{34}$$

The tensors $\mathbf{G}_a \in \mathscr{S}$ are the base tensors of the vector space $\mathscr{S}^*$. Definition (34) describes the mapping from a second-order tensor in $\mathbb{R}^6$ onto a fourth-order tensor in $\mathscr{T}$.

The coordinates $\bar{A}^{ab}$ can be obtained from definition (34) and under consideration of (9) as

$$\boxed{\mathbf{G}^a : \mathbf{A} : \mathbf{G}^b = \bar{A}^{cd}\langle \mathbf{G}^a, \mathbf{G}_c\rangle\langle \mathbf{G}_d, \mathbf{G}^b\rangle = \bar{A}^{ab}}. \tag{35}$$

Eq. (35) defines the map $\mathscr{T} \to \mathscr{T}^*$.

Using definition (23) for the base tensors $\mathbf{G}^a$ and the transition formula (35) for the map $\mathscr{T} \to \mathscr{T}^*$ leads to the coordinates

$$\bar{A}^{ab} = \frac{1}{4}(A^{ijkl} + A^{jikl} + A^{ijlk} + A^{jilk}) = A^{ijkl}, \tag{36}$$

where $a = 1,2,3,4,5,6$ maps to $ij(kl) = 11,22,33,12,23,31$, respectively. The 6×6 matrix representation based on the contravariant coordinates of $\mathbf{A} \in \mathscr{T}$ given in (36) thus is obtained as

$$\{\bar{A}^{ab}\} = \begin{bmatrix} A^{1111} & A^{1122} & A^{1133} & A^{1112} & A^{1123} & A^{1131} \\ A^{2211} & A^{2222} & A^{2233} & A^{2212} & A^{2223} & A^{2231} \\ A^{3311} & A^{3322} & A^{3333} & A^{3312} & A^{3323} & A^{3331} \\ A^{1211} & A^{1222} & A^{1233} & A^{1212} & A^{1223} & A^{1231} \\ A^{2311} & A^{2322} & A^{2333} & A^{2312} & A^{2323} & A^{2331} \\ A^{3111} & A^{3122} & A^{3133} & A^{3112} & A^{3123} & A^{3131} \end{bmatrix}. \tag{37}$$

In cases where $\mathbf{A} \in \mathscr{T}$ exhibits the extended symmetry

$$A^{ijkl} = A^{klij}, \tag{38}$$

the matrix representation given in (37) exhibits the symmetry $\bar{A}^{ab} = \bar{A}^{ba}$, i.e., $\{A^{ab}\} = \{A^{ab}\}^t$.

Based on the invariance condition

$$\mathbf{A} = \bar{A}^{ab}\mathbf{G}_a \otimes \mathbf{G}_b = \bar{A}^{a}_{.b}\mathbf{G}_a \otimes \mathbf{G}^b = \bar{A}^{.b}_{a}\mathbf{G}^a \otimes \mathbf{G}_b = \bar{A}_{ab}\mathbf{G}^a \otimes \mathbf{G}^b \tag{39}$$

the inner products $\mathbf{G}^a : \mathbf{A} : \mathbf{G}_b, \mathbf{G}_a : \mathbf{A} : \mathbf{G}^b$, and $\mathbf{G}_a : \mathbf{A} : \mathbf{G}_b$, yield the transformation rules for the mixed-variant and covariant coordinates, respectively, as

$$\boxed{\bar{A}^{a}_{.b} = G_{bc}\bar{A}^{ac}, \quad \bar{A}^{.b}_{a} = G_{ac}\bar{A}^{cb}, \quad \bar{A}_{ab} = G_{ac}G_{bd}\bar{A}^{cd}}. \tag{40}$$

These are the standard transformations of second-order tensors in $\mathbb{R}^6$.

Using (21) and the transformation rules

$$A^{ij}_{..kl} = g_{kt}g_{lq}A^{ijtq}, \quad A^{..kl}_{ij} = g_{ir}g_{js}A^{rskl}, \quad A_{ijkl} = g_{ir}g_{is}g_{kt}g_{lq}A^{rstq}, \tag{41}$$

leads to the matrix representations

$$\{\bar{A}^{a}_{.b}\} = \begin{bmatrix} A^{11}_{..11} & A^{11}_{..22} & A^{11}_{..33} & 2A^{11}_{..12} & 2A^{11}_{..23} & 2A^{11}_{..31} \\ A^{22}_{..11} & A^{22}_{..22} & A^{22}_{..33} & 2A^{22}_{..12} & 2A^{22}_{..23} & 2A^{22}_{..31} \\ A^{33}_{..11} & A^{33}_{..22} & A^{33}_{..33} & 2A^{33}_{..12} & 2A^{33}_{..23} & 2A^{33}_{..31} \\ A^{12}_{..11} & A^{12}_{..22} & A^{12}_{..33} & 2A^{12}_{..12} & 2A^{12}_{..23} & 2A^{12}_{..31} \\ A^{23}_{..11} & A^{23}_{..22} & A^{23}_{..33} & 2A^{23}_{..12} & 2A^{23}_{..23} & 2A^{23}_{..31} \\ A^{31}_{..11} & A^{31}_{..22} & A^{31}_{..33} & 2A^{31}_{..12} & 2A^{31}_{..23} & 2A^{31}_{..31} \end{bmatrix}, \tag{42a}$$

$$\{\bar{A}^{.b}_{a}\} = \begin{bmatrix} A^{..11}_{11} & A^{..22}_{11} & A^{..33}_{11} & A^{..12}_{11} & A^{..23}_{11} & A^{..31}_{11} \\ A^{..11}_{22} & A^{..22}_{22} & A^{..33}_{22} & A^{..12}_{22} & A^{..23}_{22} & A^{..31}_{22} \\ A^{..11}_{33} & A^{..22}_{33} & A^{..33}_{33} & A^{..12}_{33} & A^{..23}_{33} & A^{..31}_{33} \\ 2A^{..11}_{12} & 2A^{..22}_{12} & 2A^{..33}_{12} & 2A^{..12}_{12} & 2A^{..23}_{12} & 2A^{..31}_{12} \\ 2A^{..11}_{23} & 2A^{..22}_{23} & 2A^{..33}_{23} & 2A^{..12}_{23} & 2A^{..23}_{23} & 2A^{..31}_{23} \\ 2A^{..11}_{31} & 2A^{..22}_{31} & 2A^{..33}_{31} & 2A^{..12}_{31} & 2A^{..23}_{31} & 2A^{..31}_{31} \end{bmatrix}, \tag{42b}$$

and

$$\{\bar{A}_{ab}\} = \begin{bmatrix} A_{1111} & A_{1122} & A_{1133} & 2A_{1112} & 2A_{1123} & 2A_{1131} \\ A_{2211} & A_{2222} & A_{2233} & 2A_{2212} & 2A_{2223} & 2A_{2231} \\ A_{3311} & A_{3322} & A_{3333} & 2A_{3312} & 2A_{3323} & 2A_{3331} \\ 2A_{1211} & 2A_{1222} & 2A_{1233} & 4A_{1212} & 4A_{1223} & 4A_{1231} \\ 2A_{2311} & 2A_{2322} & 2A_{2333} & 4A_{2312} & 4A_{2323} & 4A_{2331} \\ 2A_{3111} & 2A_{3122} & 2A_{3133} & 4A_{3112} & 4A_{3123} & 4A_{3131} \end{bmatrix}. \tag{42c}$$

The matrix representations based on mixed-variant and covariant coordinates as given in (42a), (42b), and (42c), respectively, can be obtained directly from the contravariant representation (37) by means of the transformations given in (40) as follows:

$$\{\bar{A}^{A}_{.b}\} = \{\bar{A}^{ac}\}\{G_{cb}\}, \quad \{\bar{A}^{.b}_{a}\} = \{G_{ac}\}\{\bar{A}^{cb}\}, \quad \{\bar{A}_{ab}\} = \{G_{ac}\}\{\bar{A}^{cd}\}\{G_{db}\}. \tag{43}$$

Table 1
Summary of the framework for the tensor-to-matrix transition developed in Section 2. No restrictions to the coordinate system in $\mathbb{R}^3$ apply

Covariant base vectors and metric in $\mathbb{R}^3$:

$$\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\} \Rightarrow g_{ij} := \mathbf{g}_i \cdot \mathbf{g}_j \tag{I}$$

Contravariant base vectors and metric in $\mathbb{R}^3$*defined by* $\mathbf{g}_i \cdot \mathbf{g}^j = \delta_i^j$:

$$\{\mathbf{g}^1, \mathbf{g}^2, \mathbf{g}^3\} \Rightarrow \{g^{ij}\} := \{\mathbf{g}^i \cdot \mathbf{g}^j\} = \{g_{ij}\}^{-1} \tag{II}$$

Covariant base tensors in $\mathscr{S}^* \subset \mathbb{R}^6$:

$$\begin{aligned} \mathbf{G}_1 &= \mathbf{g}_1 \otimes \mathbf{g}_1, & \mathbf{G}_4 &= \mathbf{g}_1 \otimes \mathbf{g}_2 + \mathbf{g}_2 \otimes \mathbf{g}_1, \\ \mathbf{G}_2 &= \mathbf{g}_2 \otimes \mathbf{g}_2, & \mathbf{G}_5 &= \mathbf{g}_2 \otimes \mathbf{g}_3 + \mathbf{g}_3 \otimes \mathbf{g}_2, \\ \mathbf{G}_3 &= \mathbf{g}_3 \otimes \mathbf{g}_3, & \mathbf{G}_6 &= \mathbf{g}_3 \otimes \mathbf{g}_1 + \mathbf{g}_1 \otimes \mathbf{g}_3. \end{aligned} \tag{III}$$

Contravariant base tensors in $\mathscr{S}^* \subset \mathbb{R}^6$ *defined by* $\langle \mathbf{G}_a, \mathbf{G}^b \rangle = \delta_a^b$:

$$\begin{aligned} \mathbf{G}^1 &= \mathbf{g}^1 \otimes \mathbf{g}^1, & \mathbf{G}^4 &= \tfrac{1}{2}(\mathbf{g}^1 \otimes \mathbf{g}^2 + \mathbf{g}^2 \otimes \mathbf{g}^1), \\ \mathbf{G}^2 &= \mathbf{g}^2 \otimes \mathbf{g}^2, & \mathbf{G}^5 &= \tfrac{1}{2}(\mathbf{g}^2 \otimes \mathbf{g}^3 + \mathbf{g}^3 \otimes \mathbf{g}^2), \\ \mathbf{G}^3 &= \mathbf{g}^3 \otimes \mathbf{g}^3, & \mathbf{G}^6 &= \tfrac{1}{2}(\mathbf{g}^3 \otimes \mathbf{g}^1 + \mathbf{g}^1 \otimes \mathbf{g}^3). \end{aligned} \tag{IV}$$

Metric of $\mathscr{S}^* \subset \mathbb{R}^6$:

$$G_{ab} = \langle \mathbf{G}_a, \mathbf{G}_b \rangle = \mathbf{G}_a : \mathbf{G}_b, \quad G^{ab} = \langle \mathbf{G}^a, \mathbf{G}^b \rangle = \mathbf{G}^a : \mathbf{G}^b, \quad \{G^{ab}\} = \{G_{ab}\}^{-1} \tag{V}$$

Transition from $\mathscr{S} \subset \mathbb{R}^3 \times \mathbb{R}^3 \to \mathscr{S}^* \subset \mathbb{R}^6$:

$$\bar{T}^a = \mathbf{T} : \mathbf{G}^a, \quad \bar{T}_a = \mathbf{T} : \mathbf{G}_a = G_{ab} \bar{T}^b \tag{VI}$$

$$\{\bar{T}^a\} = \{T^{11}\ T^{22}\ T^{33}\ T^{12}\ T^{23}\ T^{31}\}^t, \quad \{\bar{T}^a\} = \{T_{11}\ T_{22}\ T_{33}\ 2T_{12}\ 2T_{23}\ 2T_{31}\}^t \tag{VII}$$

Transition from $\mathscr{T} \subset \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathscr{T}^* \subset \mathbb{R}^6 \times \mathbb{R}^6$:

$$\bar{A}^{ab} = \mathbf{G}^a : \mathbf{A} : \mathbf{G}^b = \frac{1}{4}\left(A^{ijkl} + A^{jikl} + A^{ijlk} + A^{jilk}\right) \tag{VIII}$$

$$\bar{A}_a^{\cdot b} = \mathbf{G}_a : \mathbf{A} : \mathbf{G}^b = G_{ac} \bar{A}^{cb} \tag{IX}$$

$$\bar{A}^a_{\cdot b} = \mathbf{G}^a : \mathbf{A} : \mathbf{G}_b = G_{bc} \bar{A}^{ac} \tag{X}$$

$$\bar{A}_{ab} = \mathbf{G}_a : \mathbf{A} : \mathbf{G}_b = G_{ac} G_{bd} \bar{A}^{cd} \tag{XI}$$

For the matrix representation of (VII)–(XI) see (37) and (42a)–(42c). For the matrix notation of the conversion from contravariant to covariant and mixed-variant coordinates see (43).

2.2.1. Normalized tensorial basis in $\mathscr{T}^*$

In Section 2.1.2 an ortho-normal basis $\hat{\mathbf{G}}_a = \hat{\mathbf{G}}^a$ has been derived and given in (28). Substitution of (28) into (35) yields the matrix representation for a normalized vector space $\mathscr{T}^*$ as

$$\{\hat{A}_{ab}\} = \begin{bmatrix} \hat{A}_{1111} & \hat{A}_{1122} & \hat{A}_{1133} & \sqrt{2}\hat{A}_{1112} & \sqrt{2}\hat{A}_{1123} & \sqrt{2}\hat{A}_{1131} \\ \hat{A}_{2211} & \hat{A}_{2222} & \hat{A}_{2233} & \sqrt{2}\hat{A}_{2212} & \sqrt{2}\hat{A}_{2223} & \sqrt{2}\hat{A}_{2231} \\ \hat{A}_{3311} & \hat{A}_{3322} & \hat{A}_{3333} & \sqrt{2}\hat{A}_{3312} & \sqrt{2}\hat{A}_{3323} & \sqrt{2}\hat{A}_{3331} \\ \sqrt{2}\hat{A}_{1211} & \sqrt{2}\hat{A}_{1222} & \sqrt{2}\hat{A}_{1233} & 2\hat{A}_{1212} & 2\hat{A}_{1223} & 2\hat{A}_{1231} \\ \sqrt{2}\hat{A}_{2311} & \sqrt{2}\hat{A}_{2322} & \sqrt{2}\hat{A}_{2333} & 2\hat{A}_{2312} & 2\hat{A}_{2323} & 2\hat{A}_{2331} \\ \sqrt{2}\hat{A}_{3111} & \sqrt{2}\hat{A}_{3122} & \sqrt{2}\hat{A}_{3133} & 2\hat{A}_{3112} & 2\hat{A}_{3123} & 2\hat{A}_{3131} \end{bmatrix}, \tag{44}$$

satisfying the identity

$$\{\hat{A}_{ab}\} = \{\hat{A}^{ab}\} = \{\hat{A}^a_{\cdot b}\} = \{\hat{A}_a^{\cdot b}\}. \tag{45}$$

Thus, in the ortho-normal representation of $\mathscr{T}^*$ no distinction between covariant and contravariant representations is necessary.

3. Example applications

Within this section we will study the application of the proposed framework to the finite element implementation of tensorial equations. First we will review the common vector representation and identify it with the covariant and contravariant coordinates in $\mathscr{S}^*$.

In the subsequent Sections 3.2 and 3.3 we will investigate the effect on the fourth-order identity tensor and on the linear elastic material stiffness tensor. The first tensor appears as part of many operators such as, e.g., the deviatoric operator used in the problem given in Section 1. The material stiffness tensor and, in particular, its inverse are representative for many fourth-order tensors appearing in continuum and algorithmic tangent operators for nonlinear elasticity, viscoelasticity or elastoplasticity.

Applications for mixed-variant representation may occur in nonlinear creep laws for isotropic and anisotropic material where a series of fourth-order tensor operators act on a stress tensor or strain tensor. Avoiding the overhead due to a discussion of such a material law a simple numerical example application will be discussed in Section 3.4. Nevertheless, this example will demonstrate all steps of the tensor-to-matrix transition as required in most numerical implementations of tensorial equations.

3.1. Vector representation for stress tensors and strain tensors

The intention of this short section is to review the vector representations for stress tensors and strain tensors as used in standard finite element books using the presented mathematical framework. Consider any symmetric stress tensor $\boldsymbol{\sigma}$ with contravariant coordinates σ^{ij}. The commonly used vector representation proposed in, e.g., [6–8] is

$$\{\boldsymbol{\sigma}\} = \{\sigma^{11}\ \sigma^{22}\ \sigma^{33}\ \sigma^{12}\ \sigma^{23}\ \sigma^{31}\}^t. \tag{46}$$

Comparing (46) with (24b) identifies the standard vector representation of stress tensors as the *contravariant* coordinates of $\bar{\boldsymbol{\sigma}}$ in $\mathscr{S}^*$.

Now consider any symmetric strain tensor $\boldsymbol{\varepsilon}$ with covariant coordinates ε_{ij}. The vector representation given in, e.g., [6–8] is

$$\{\boldsymbol{\varepsilon}\} = \{\varepsilon_{11}\ \varepsilon_{22}\ \varepsilon_{33}\ 2\varepsilon_{12}\ 2\varepsilon_{23}\ 2\varepsilon_{31}\}^t. \tag{47}$$

The term $2\varepsilon_{ij}, i \neq j$ is often referred to as the engineering strain γ_{ij}. Comparing (47) with (25b) identifies the standard vector representation of strain tensors as the *covariant* coordinates of $\bar{\boldsymbol{\varepsilon}}$ in $\mathscr{S}^*$.

Remark 3.1. The representations given in (46) and (47) are valid for arbitrary coordinate systems. The special case of ortho-normal coordinates then implies $\sigma^{ij} = \sigma_i^{\cdot j} = \sigma^i_{\cdot j} = \sigma_{ij}$ and $\varepsilon^{ij} = \varepsilon_i^{\cdot j} = \varepsilon^i_{\cdot j} = \varepsilon_{ij}$, which is not required for the proposed general framework.

3.2. The fourth-order identity tensor

The fourth-order identity tensor $\mathbb{I}$ is defined by the condition (see, e.g. [4])

$$\mathbb{I} : \mathbf{U} = \mathbf{U}, \tag{48}$$

where $\mathbf{U} \in \mathbb{R}^3 \times \mathbb{R}^3$ is an arbitrary second-order tensor. Restricting $\mathbf{U}$ to $\mathscr{S}$, i.e., to symmetric second-order tensors, this condition is usually rewritten as

$$\mathbb{I} : \mathbf{U} = \frac{1}{2}(\mathbf{U} + \mathbf{U}^t). \tag{49}$$

Using (49) leads to a fourth-order tensor $\mathbb{I} \in \mathscr{T}$ while (48) in general does not. [1] From condition (49) we obtain the coordinates of $\mathbb{I}$ as

$$\{\mathbb{I}\}^{ij}_{..kl} = \frac{1}{2}(\delta^i_k\delta^j_l + \delta^i_l\delta^j_k) \iff \{\mathbb{I}\}_{ijkl} = \frac{1}{2}(g_{ik}g_{jl} + g_{il}g_{jk}). \tag{50}$$

3.2.1. Ortho-normal coordinates in $\mathbb{R}^3$

Consider ortho-normal coordinates in $\mathbb{R}^3$ and the definition of the base tensors as given in (20). This yields the coordinates of the metric tensor in $\mathscr{S}^*$ as given by (22). The matrix representations of $\mathbb{I}$ are found by means of (37) and (43) as

$$\{\bar{\mathbb{I}}^{ab}\} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} \end{bmatrix}, \quad \{\bar{\mathbb{I}}_{ab}\} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{bmatrix}, \tag{51a}$$

and

$$\{\bar{\mathbb{I}}_a^{.b}\} = \{\bar{\mathbb{I}}^a_{.b}\} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}. \tag{51b}$$

For better understanding of the above representations consider the trivial operation

$$\mathbb{I} : \mathbb{I} = \mathbb{I}. \tag{52}$$

Rewriting it using coordinate (index) notation yields

$$\mathbb{I}_{ijmn}\mathbb{I}^{mnkl} = \mathbb{I}_{ij}^{..kl} \mapsto \{\bar{\mathbb{I}}_{ac}\}\{\bar{\mathbb{I}}^{cb}\} = \{\bar{\mathbb{I}}_a^{.b}\} \tag{53a}$$

or

$$\mathbb{I}^{ijmn}\mathbb{I}_{mnkl} = \mathbb{I}^{ij}_{..kl} \mapsto \{\bar{\mathbb{I}}^{ac}\}\{\bar{\mathbb{I}}_{cb}\} = \{\bar{\mathbb{I}}^a_{.b}\} \tag{53b}$$

or

$$\mathbb{I}^{ij}_{..mn}\mathbb{I}^{mnkl} = \mathbb{I}^{ijkl} \mapsto \{\bar{\mathbb{I}}^a_{.c}\}\{\bar{\mathbb{I}}^{cb}\} = \{\bar{\mathbb{I}}^{ab}\} \tag{53c}$$

or

$$\mathbb{I}^{ij}_{..mn}\mathbb{I}^{mn}_{..kl} = \mathbb{I}^{ij}_{..kl} \mapsto \{\bar{\mathbb{I}}^a_{.c}\}\{\bar{\mathbb{I}}^c_{.b}\} = \{\bar{\mathbb{I}}^a_{.b}\}. \tag{53d}$$

The correctness of (53a), (53b), (53c), and (53d) can be easily verified by means of (51a) and (51b).

Remark 3.2. Note that the matrix representations (53a), (53b), (53c), and (53d) of the trivial identity (52) are different although the coordinates $\mathbb{I}_{ijkl} = \mathbb{I}^{ijkl} = \mathbb{I}_{ij}^{..kl} = \mathbb{I}^{ij}_{..kl}$ are identical because of the ortho-normal basis in $\mathbb{R}^3$. Hence, covariant and contravariant coordinates need to be distinguished in the matrix representation.

[1] Condition (48) leads to the coordinates $\{\mathbb{I}\}^{ij}_{..kl} = \delta^i_k\delta^j_l$.

3.3. Isotropic elasticity: material stiffness tensor

The material stiffness tensor for linear elastic material is just one example of a tangent operator appearing in mechanics. Nevertheless, this tensor and, in particular, its inverse are sufficient to demonstrate the consequences of the framework developed in Section 2. The discussion given in this section should enable the reader to answer most questions observed in the tensor-to-matrix transition of tangent operators in linear viscoelasticity and elastoplasticity.

The material stiffness tensor $\mathbb{C}$ for isotropic linear elasticity is defined as (see, e.g. [9])

$$\mathbb{C} = K\mathbf{1}\otimes\mathbf{1} + 2G\left(\mathbb{I} - \frac{1}{3}\mathbf{1}\otimes\mathbf{1}\right), \tag{54}$$

where K is the bulk modulus, G the shear modulus and $\mathbf{1}$ is the second-order identity tensor with coordinates $\{\mathbf{1}\}_i^j = \delta_i^j$ ($\{\mathbf{1}\}_{ij} = g_{ij}$). The inverse of $\mathbb{C}$ is obtained as

$$\mathbb{C}^{-1} = \frac{1}{9K}\mathbf{1}\otimes\mathbf{1} + \frac{1}{2G}\left(\mathbb{I} - \frac{1}{3}\mathbf{1}\otimes\mathbf{1}\right). \tag{55}$$

Eq. (55) can be verified by means of

$$\mathbb{C} : \mathbb{C}^{-1} = \mathbb{I}. \tag{56}$$

3.3.1. Ortho-normal coordinates in $\mathbb{R}^3$

In most applications in continuum mechanics the base tensors given in (20) are used. Furthermore, the symmetric stress tensors (Cauchy stress, Kirchhoff stress and second Piola–Kirchhoff stress) are restricted to the contravariant representation and the strain tensors (Cauchy strain, Almansi strain, Greens strain, Henkey strain) are restricted to the covariant representation. Such a choice enables simple physical interpretation of the coordinates $\bar{\sigma}^a$ and $\bar{\varepsilon}_b$ of the matrix representation.

As in Section 3.2.1, consider ortho-normal coordinates in $\mathbb{R}^3$ and the definition of the base tensors as given in (20). This yields the coordinates of the metric tensor in $\mathscr{S}^*$ as given by (22).

The matrix representation of the fourth-order tensor $\mathbf{1}\otimes\mathbf{1}$ is identical for covariant, contravariant and both mixed-variant representations given in (37), (42a), (42b), and (42c), respectively. It is obtained as

$$\{\overline{\mathbf{1}\otimes\mathbf{1}}_{ab}\} = \{\overline{\mathbf{1}\otimes\mathbf{1}}^{ab}\} = \{\overline{\mathbf{1}\otimes\mathbf{1}}_a^{.b}\} = \{\overline{\mathbf{1}\otimes\mathbf{1}}^a_{.b}\} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{57}$$

The contravariant description of $\mathbb{C}$ follows from (54) under consideration of the left-hand equation in (51a) and (57) as

$$\{\bar{\mathbb{C}}^{ab}\} = \begin{bmatrix} \lambda+2G & \lambda & \lambda & 0 & 0 & 0 \\ & \lambda+2G & \lambda & 0 & 0 & 0 \\ & & \lambda+2G & 0 & 0 & 0 \\ & & & G & 0 & 0 \\ & \text{symm.} & & & G & 0 \\ & & & & & G \end{bmatrix}, \tag{58}$$

with $\lambda = K - \frac{2}{3}G$. The contravariant representation of the inverse tensor given in (55) then follows as

$$\{\bar{\mathbb{C}}^{(-1)ab}\} = \begin{bmatrix} \bar{\lambda} + \frac{1}{2G} & \bar{\lambda} & \bar{\lambda} & 0 & 0 & 0 \\ & \bar{\lambda} + \frac{1}{2G} & \bar{\lambda} & 0 & 0 & 0 \\ & & \bar{\lambda} + \frac{1}{2G} & 0 & 0 & 0 \\ & & & \frac{1}{4G} & 0 & 0 \\ & \text{symm.} & & & \frac{1}{4G} & 0 \\ & & & & & \frac{1}{4G} \end{bmatrix}, \tag{59}$$

with $\bar{\lambda} = 1/9K - 1/6G$. It can be proven easily that the contravariant representation (59) is *not* the inverse of the 6×6-matrix representation of $\mathbb{C}$ given by (58). Rewriting (56) as $\{\bar{\mathbb{C}}^{ac}\}\{\bar{\mathbb{C}}^{(-1)}_{cb}\} = \{\bar{\mathbb{I}}^{a}_{.b}\}$ yields the consistent representation of the inverse as the covariant representation of $\mathbb{C}^{-1}$ as

$$\{\bar{\mathbb{C}}^{(-1)}_{ab}\} = \begin{bmatrix} \bar{\lambda} + \frac{1}{2G} & \bar{\lambda} & \bar{\lambda} & 0 & 0 & 0 \\ & \bar{\lambda} + \frac{1}{2G} & \bar{\lambda} & 0 & 0 & 0 \\ & & \bar{\lambda} + \frac{1}{2G} & 0 & 0 & 0 \\ & & & \frac{1}{G} & 0 & 0 \\ & \text{symm.} & & & \frac{1}{G} & 0 \\ & & & & & \frac{1}{G} \end{bmatrix}. \tag{60}$$

The inverse to the contravariant representation (59) of $\mathbb{C}^{-1}$ can be found by rewriting (56) as $\{\bar{\mathbb{C}}_{ac}\}\{\bar{\mathbb{C}}^{(-1)cb}\} = \{\bar{\mathbb{I}}_{a}^{.b}\}$. Thus, it is the covariant representation of $\mathbb{C}$ as

$$\{\bar{\mathbb{C}}_{ab}\} = \begin{bmatrix} \lambda + 2G & \lambda & \lambda & 0 & 0 & 0 \\ & \lambda + 2G & \lambda & 0 & 0 & 0 \\ & & \lambda + 2G & 0 & 0 & 0 \\ & & & 4G & 0 & 0 \\ & \text{symm.} & & & 4G & 0 \\ & & & & & 4G \end{bmatrix}. \tag{61}$$

Furthermore, a mixed-variant representation based on $\{\bar{\mathbb{C}}_{a}^{.c}\}\{\bar{\mathbb{C}}^{(-1).b}_{\quad c}\} = \{\bar{\mathbb{I}}_{a}^{.b}\}$ is possible. An example of the mixed-variant approach will be given in Section 3.4.

Remark 3.3. Note that even if the fourth-order tensor $\mathbb{C} \in \mathscr{T}$ satisfies the symmetry condition (38), its mixed-variant representation does not need to be symmetric. Nevertheless, for the proposed isotropic tensor we obtain a symmetric mixed-variant representation.

3.3.2. Ortho-normal coordinates in $\mathscr{S}^*$

Using an ortho-normal basis in $\mathscr{S}^*$ as given be (28) leads to the matrix representation given by (44). Hence, the material stiffness tensor $\mathbb{C}$ is of the form

$$\{\hat{\mathbb{C}}_{ab}\} = \{\hat{\mathbb{C}}^{ab}\} = \{\hat{\mathbb{C}}^{a}_{.b}\} = \{\hat{\mathbb{C}}_{a}^{.b}\} = \begin{bmatrix} \lambda + 2G & \lambda & \lambda & 0 & 0 & 0 \\ & \lambda + 2G & \lambda & 0 & 0 & 0 \\ & & \lambda + 2G & 0 & 0 & 0 \\ & & & 2G & 0 & 0 \\ & \text{symm.} & & & 2G & 0 \\ & & & & & 2G \end{bmatrix}, \tag{62}$$

and the inverse tensor $\mathbb{C}^{-1}$ is obtained as

$$\{\hat{\mathbb{C}}^{(-1)}_{ab}\} = \{\hat{\mathbb{C}}^{(-1)ab}\} = \{\hat{\mathbb{C}}^{(-1)a}_{\quad .b}\} = \{\hat{\mathbb{C}}^{(-1).b}_{\quad a}\} = \begin{bmatrix} \bar{\lambda} + \frac{1}{2G} & \bar{\lambda} & \bar{\lambda} & 0 & 0 & 0 \\ & \bar{\lambda} + \frac{1}{2G} & \lambda & 0 & 0 & 0 \\ & & \bar{\lambda} + \frac{1}{2G} & 0 & 0 & 0 \\ & & & \frac{1}{2G} & 0 & 0 \\ & \text{symm.} & & & \frac{1}{2G} & 0 \\ & & & & & \frac{1}{2G} \end{bmatrix}. \tag{63}$$

Such a representation avoids the treatment of covariant and contravariant representations. The reason why it it not standard in commercial as well as scientific FEM-codes is the lack of a direct physical interpretation for the coordinates $\hat{T}^a = \hat{T}_a$ as given by (29).

3.4. Derivatives of second-order tensor functions

Fourth-order tensors occur in tangent operators of nonlinear second-order tensor functions. In mechanics such tensor functions represent, e.g., the mathematical formulation of material laws. For some of these tangent operators the tensor-to-matrix transition requires the use of a mixed-variant matrix representation. Since the discussion of material laws exceeds the aim of this paper a numerical example has been chosen such that the application of mixed-variant matrix representations can be demonstrated without being forced to discuss any material law. Nevertheless, this example carefully points out why a mixed-variant matrix representation makes sense. The observations apply to any advanced material model without restrictions.

3.4.1. Iterative solution of a nonlinear tensorial equation

A common tensor function in finite deformation continuum mechanics is the exponential function $\exp[\mathbf{X}]\colon \mathscr{S} \to \mathscr{S}$. It is defined as

$$\mathbf{Y} = \exp[\mathbf{X}] := \mathbf{1} + \sum_{n=1}^{\infty} \frac{1}{n!}\mathbf{X}^n, \tag{64}$$

where $\mathbf{X} \in \mathscr{S}$ and $\mathbf{Y} \in \mathscr{S}$ are symmetric second-order tensors and $\mathbf{X}^n, n > 1$, is defined by $\mathbf{X}^n := \mathbf{X} \cdot \mathbf{X}^{n-1}$ with $\mathbf{X}^1 = \mathbf{X}$.

Now consider the problem formulated as follows: *Solve the nonlinear equation*

$$\boxed{\mathbf{R}(\mathbf{X}) := \mathbf{Y} - \exp[\mathbf{X}] = \mathbf{0}} \tag{65}$$

for $\mathbf{X} \in \mathscr{S}$ *for a given tensor* $\mathbf{Y} \in \mathscr{S}$.

Note that the considered problem possesses a closed form solution

$$\mathbf{X} = \ln[\mathbf{Y}] = \sum_{\alpha=1}^{3} \ln(\mu_\alpha)\overset{\alpha}{\mathbf{m}}, \tag{66}$$

where μ_1, μ_2 and μ_3 are the real eigenvalues of $\mathbf{Y}$ and $\{\overset{\alpha}{\mathbf{m}}\}$ the related eigenvector bases. An algorithm for the direct computation of the eigenvector bases is given in Appendix A. Because of the logarithm in (66), a solution exists only for three positive eigenvalues of $\mathbf{Y}$. This solution is used for verification only.

The derivative of the exponential function frequently appears as part of a tangent operator in more realistic applications where closed form solutions cannot be obtained. Thus, for demonstration purposes, let us solve (65) by means of a full Newton–Raphson iteration in $\mathscr{S}^*$. The related iterative procedure in $\mathscr{S}$ is

Table 2
Algorithm for the iterative solution of the non-linear tensorial Eq. (65)

Initiate $k = 0$ (k is the iteration counter) and $\mathbf{X}^{(0)} = \mathbf{1}+$ small perturbation

$$\mathbf{R}^{(k)} = \mathbf{Y} - \exp[\mathbf{X}^{(k)}] \tag{I}$$

If $\mathbf{R}^{(k)} : \mathbf{R}^{(k)} \leqslant$ tolerance, $\mathbf{X}^{(k)}$ is the solution of (I) at the chosen tolerance.
Otherwise proceed with

$$\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}] : \Delta\mathbf{X} = \mathbf{R}^{(k)} \Rightarrow \Delta\mathbf{X} = (\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}])^{-1} : \mathbf{R}^{(k)} \tag{II}$$

$$\mathbf{X}^{(k+1)} = \mathbf{X}^{(k)} + \Delta\mathbf{X} \tag{III}$$

Set $k = k + 1$ and proceed with (I).

Table 3
Matrix representation of the iterative procedure using a mixed-variant representation of $\partial_{\mathbf{X}} \exp[\mathbf{X}]$

Initiate $k=0$ and $\{\bar{X}_a^{(0)}\} = \bar{\mathbf{1}}$ + small perturbation $= \{1.00\ 1.01\ 0.99\ 0\ 0\ 0\}^t$

$$\{\bar{R}_a^{(k)}\} = \{\bar{Y}_a\} - \{\exp[\mathbf{X}^{(k)}]_a\} \tag{I}$$

If $(\mathbf{R}^{(k)}, \mathbf{R}^{(k)}) = \{\bar{R}_a^{(k)}\}^t\{\bar{R}^{(k)a}\} \leqslant$ tolerance, $\{\bar{X}_a^{(k)}\}$ is the solution of (I).
Otherwise proceed with

$$\{\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]_a^{\ b}\}\{\Delta\bar{X}_b\} = \{\bar{R}_a^{(k)}\} \Rightarrow \{\Delta\bar{X}_b\} = \{\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]^{(-1).a}_{\ \ \ \ \ \ \ b}\}\{\bar{R}_a^{(k)}\} \tag{II}$$

$$\{\bar{X}_b^{(k+1)}\} = \{\bar{X}_b^{(k)}\} + \{\Delta\bar{X}_b\} \tag{III}$$

Set $k = k+1$ and proceed with (I).

shown in Table 2. The tangent operator $\partial_{\mathbf{X}} \exp[\mathbf{X}]$ is given in Appendix A. It is a fourth-order tensor possessing all symmetries listed in the definition of $\mathscr{T}$ given in (32).

The transition of the sequence (I)–(III) in Table 2 to its matrix representation can be done by means of the covariant, the contravariant or both mixed-variant formulations for $\partial_{\mathbf{X}} \exp\ [\mathbf{X}]$.

Let us consider the covariant represtation for $\mathbf{X}$ and $\mathbf{Y}$ as given by (25b). Then the mixed-variant approach as given in Table 3 seems to be the natural matrix representation of the previous iteration algorithm.

Remark 3.4. The fourth-order tensor $\partial_{\mathbf{X}} \exp\ [\mathbf{X}^{(k)}]$ as defined in Table 6 is in $\mathscr{T}$, i.e., it is symmetric, while the mixed-variant matrix representation given by (42a) is not symmetric. Thus the formulation given in Table 3 requires the inversion of a non-symmetric 6×6-matrix.

In order to avoid the inversion of a non-symmetric matrix, the algorithm given Table 2 may be reformulated by means of the covariant matrix representation of $\partial_{\mathbf{X}} \exp\ [\mathbf{X}]$ as shown in Table 4. This preserves the symmetry of the fourth-order tensor even in the 6×6 matrix representation but requires changes in the update of $\{\bar{X}_b\}$.

3.4.2. Numerical example

In order to verify the matrix representations proposed in Tables 3 and 4 a numerical test will be performed in this section. In order to demonstrate the effect of an incorrect tensor-to-matrix transition two examples both with inconsistent matrix representation are added and compared with the two proper versions.

Solve Eq. (65) for $\mathbf{X}$ with

$$\mathbf{Y} = \begin{bmatrix} 7 & 2 & 4 \\ 2 & 5 & 1 \\ 4 & 1 & 6 \end{bmatrix} \mapsto \{\bar{Y}_a\} = \{7\ 5\ 6\ 4\ 2\ 8\}^t. \tag{67}$$

Table 4
Matrix representation of the iterative procedure using the covariant representation of $\partial_{\mathbf{X}} \exp[\mathbf{X}]$

Initiate $k=0$ and $\{\bar{X}_a^{(0)}\} = \bar{\mathbf{1}}+$ small perturbation $= \{1.00\ 1.01\ 0.99\ 0\ 0\ 0\}^t$

$$\{\bar{R}_a^{(k)}\} = \{\bar{Y}_a\} - \{\exp[\mathbf{X}^{(k)}]_a\} \tag{I}$$

If $(\mathbf{R}^{(k)}, \mathbf{R}^{(k)}) = \{\bar{R}_a^{(k)}\}^t\{\bar{R}^{(k)a}\} \leqslant$ tolerance, $\{\bar{X}_a^{(k)}\}$ is the solution of (I).
Otherwise proceed with

$$\{\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]_{ab}\}\{\Delta\bar{X}^b\} = \{\bar{R}_a^{(k)}\} \Rightarrow \{\Delta\bar{X}^b\} = \{\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]^{(-1)ba}\}\{\bar{R}_a^{(k)}\} \tag{II}$$

$$\{\bar{X}_b^{(k+1)}\} = \{\bar{X}_b^{(k)}\} + \{G_{ba}\}\{\Delta\bar{X}^a\} \tag{III}$$

Set $k = k+1$ and proceed with (I).

Table 5
Residual norm $\langle \bar{\mathbf{R}}^{(k)}, \bar{\mathbf{R}}^{(k)} \rangle / \langle \bar{\mathbf{R}}^{(0)}, \bar{\mathbf{R}}^{(0)} \rangle$ obtained by means of the representations according to **a**: Table 3, **b**: Table 4, **c**: symmetrized approach given by (69) and **d**: with covariant representation but update of $\{\bar{X}_a\}$ according to Table 3

k	**a**	**b**	**c**	**d**
0	$0.10000 \times 10^{+1}$	$0.10000 \times 10^{+1}$	$0.10000 \times 10^{+1}$	$0.10000 \times 10^{+1}$
1	$0.36210 \times 10^{+2}$	$0.36210 \times 10^{+2}$	$0.36210 \times 10^{+2}$	$0.22839 \times 10^{+1}$
2	$0.36757 \times 10^{+1}$	$0.36757 \times 10^{+1}$	$0.21558 \times 10^{+8}$	$0.16113 \times 10^{+0}$
3	$0.22245 \times 10^{+0}$	$0.22245 \times 10^{+0}$	$0.51979 \times 10^{+7}$	0.82743×10^{-2}
4	0.32714×10^{-2}	0.32714×10^{-2}	$0.65574 \times 10^{+6}$	0.11551×10^{-2}
5	0.13870×10^{-5}	0.13870×10^{-5}	$0.87480 \times 10^{+5}$	0.27938×10^{-3}
6	0.27840×10^{-12}	0.27840×10^{-12}	$0.11768 \times 10^{+5}$	0.69325×10^{-4}
7	0.11214×10^{-25}	0.11214×10^{-25}	$0.15658 \times 10^{+4}$	0.17266×10^{-4}
8			$\vdots$	0.43084×10^{-5}
9			divergent	0.10761×10^{-5}
10				0.26890×10^{-6}
11				0.67208×10^{-7}
12				0.16800×10^{-7}
13				0.41998×10^{-8}
14				0.10499×10^{-8}
15				0.26247×10^{-9}

Eq. (66) as well as both iterative procedures given in Tables 3 and 4 yield the result

$$\{\bar{X}_a\} = \begin{bmatrix} 1.667887 \\ 1.539923 \\ 1.537122 \\ 0.675707 \\ 0.147045 \\ 1.427738 \end{bmatrix} \quad \mapsto \quad \mathbf{X} = \begin{bmatrix} 1.667887 & 0.337854 & 0.713869 \\ 0.337854 & 1.539923 & 0.073522 \\ 0.713869 & 0.073522 & 1.537122 \end{bmatrix}. \tag{68}$$

Table 5 shows the relative residual norm $\langle \bar{\mathbf{R}}^{(k)}, \bar{\mathbf{R}}^{(k)} \rangle / \langle \bar{\mathbf{R}}^{(0)}, \bar{\mathbf{R}}^{(0)} \rangle$ for each iteration step of the algorithm given in Table 3 (column **a**) and Table 4 (column **b**). Furthermore, it presents the relative residual norm obtained from the algorithm given in Table 3 but using the symmetrized mixed-variant matrix representation

$$\frac{1}{2}(\{\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]_{a}^{\cdot b}\} + \partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]_{a}^{\cdot b}\}^{t}) \tag{69}$$

instead of $\{\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]_{a}^{\cdot b}\}$ (column **c**) and the use of the covariant representation of $\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]$ with the update for $\mathbf{X}$ as given in Table 3 (column **d** of Table 5).

The results demonstrate that both representations given in Tables 3 and 4, respectively, are equivalent and obtain the solution at a quadratic rate of asymptotic convergence. Using the symmetrized mixed-variant matrix representation (69) causes divergence of the iterative procedure. Using the (symmetric) covariant representation $\{\partial_{\mathbf{X}} \exp[\mathbf{X}^{(k)}]_{ab}\}$ within the sequence given in Table 3, i.e. an inconsistent representation of the algorithm given in Table 2, causes loss of the quadratic rate of asymptotic convergence.

4. Conclusions

The discussion of the proposed six-dimensional vector space and its metric enabled a simple explanation of various types of vector and matrix representations of symmetric second-order and fourth-order tensors, respectively, as covariant, contravariant or mixed-variant coordinates in this space. We have proven that all of the mentioned representations enable the full and unique reconstruction of the symmetric tensors in $\mathbb{R}^3$.

We further demonstrated that even though the tensors in $\mathscr{S}$ and $\mathscr{S}^*$ as well as in $\mathscr{T}$ and $\mathscr{T}^*$ are uniquely connected, the integrity basis for tensors in $\mathscr{S}^*$ and $\mathscr{T}^*$ reproduces only a subset of the integrity basis found for tensors in $\mathscr{S}$ and $\mathscr{T}$, respectively.

Special effort has been made with the discussion of ortho-normal coordinates in $\mathbb{R}^3$. Such coordinate systems are used in many applications of the FEM or BEM. In an ortho-normal coordinate system the covariant and contravariant coordinates are identical in $\mathbb{R}^3$. Investigating the metric of the related six-dimensional representation pointed out that, even in that particular case, the matrix representation is related to a generally *not normalized* vector space. Thus, we could show the need for covariant, contravariant and mixed-variant coordinates for all matrix representations of tensorial equations. A set of example applications on commonly used second-order and fourth-order tensors demonstrated the application of the proposed framework.

It has been shown that the presented clarification of the mathematical structure of the compressed matrix representation yields a simple framework for the transition of symmetric second-order and fourth-order tensors to the corresponding vector (6×1 matrix) and 6×6 matrix representations. A compact summary of the transition formulas has been given in the paper. These formulas are not restricted to any special coordinate system but include all types of non-normalized, skew and curvilinear coordinate systems.

Table 6
Eigenvector basis of a tensor $\mathbf{X}$ and derivative of the second-order tensor function exp $[\mathbf{X}]$ with respect to $\mathbf{X}$ derived from the formulas given by Miehe [10]

Invariants:

$$I_1 = \operatorname{tr}\mathbf{X}, \quad I_2 = \frac{1}{2}[(\operatorname{tr}\mathbf{X})^2 - \operatorname{tr}\mathbf{X}^2], \quad I_3 = \det\mathbf{X} \in \mathbb{R} \tag{I}$$

Principal values: these are obtained as roots of the characteristic polynomial

$$-\lambda^3 + I_1\lambda^2 - I_2\lambda + I_3 = 0 \quad \Rightarrow \quad \{\lambda_1, \lambda_2, \lambda_3\} \tag{II}$$

For what follows, we define $\lambda_4 \equiv \lambda_1$ and $\lambda_5 \equiv \lambda_2$.
Eigenvector bases:

$$D_\alpha = (\lambda_\alpha - \lambda_{\alpha+1})(\lambda_\alpha - \lambda_{\alpha+2}) \tag{III}$$

$$\overset{\alpha}{\mathbf{m}} = \overset{\alpha\,t}{\mathbf{m}} = \frac{1}{D_\alpha}[\mathbf{X} - (I_1 - \lambda_\alpha)\mathbf{1} + I_3\lambda_\alpha^{-1}\mathbf{X}^{-1}] \in \mathscr{S} \tag{IV}$$

Computation of exp $[\mathbf{X}]$:

$$\exp[\mathbf{X}] = \sum_{\alpha=1}^{3} \exp[\lambda_\alpha]\overset{\alpha}{\mathbf{m}} \quad \in \mathscr{S} \tag{V}$$

Derivative of exp [X] *with respect to* $\mathbf{X}$

$$\partial_{\mathbf{X}} \exp[\mathbf{X}] = a\mathbb{I} - b\mathbb{I}_{\mathbf{X}^{-1}} + \sum_{\alpha=1}^{3} d_\alpha \overset{\alpha}{\mathbf{m}} \otimes \overset{\alpha}{\mathbf{m}} \in \mathscr{T} \tag{VI}$$

with

$$a = \sum_{\beta=1}^{3} \frac{\lambda_\beta}{D_\beta}\exp(\lambda_\beta) \tag{VII}$$

$$b = I_3 \sum_{\beta=1}^{3} \frac{1}{D_\beta}\exp(\lambda_\beta) \tag{VIII}$$

$$d_\alpha = \exp(\lambda_\alpha) + \sum_{\beta=1}^{3} \frac{\lambda_\beta}{D_\beta}\exp(\lambda_\beta)[I_3\lambda_\beta^{-1} - \lambda_\alpha^2]\lambda_\alpha^{-2} \tag{IX}$$

and the fourth-order tensor $\mathbb{I}_{\mathbf{X}^{-1}}$ defined as

$$\{\mathbb{I}_{\mathbf{X}^{-1}}\}_{ijkl} = \frac{1}{2}\left(X_{ik}^{(-1)}X_{jl}^{(-1)} + X_{jk}^{(-1)}X_{il}^{(-1)}\right) \tag{X}$$

Acknowledgements

The author receives financial support from the APART-program of the Austrian Academy of Sciences, which is gratefully acknowledged. Furthermore, he wishes to thank Ch. Hellmich, P. Pivonka, U. Hirschböck and A. Hanhijärvi for discussions initiating the present paper, and J. Betten, B. Pichler, Ch. Schranz and L. Mackenzie for helpful comments.

Appendix A. Computation of $\exp[\mathbf{X}]$ and $\partial_{\mathbf{X}}\exp[\mathbf{X}]$

An arbitrary tensor $\mathbf{X} \in \mathscr{S}$ can be expressed by means of its eigenvalues λ_1, λ_2 and λ_3 and the eigenvector basis $\{\overset{1}{\mathbf{m}}, \overset{2}{\mathbf{m}}, \overset{3}{\mathbf{m}}\}$ as $\mathbf{X} = \sum_{\alpha=1}^{3} \lambda_\alpha \overset{\alpha}{\mathbf{m}}$. The eigenvalues are obtained as the roots of the third-order characteristic polynomial by means of a direct formula given by Malvern [2]. The definition of the eigenvector basis $\{\overset{\alpha}{\mathbf{m}}\}, \alpha = 1, 2, 3$ and an alternative formula for the efficient computation of $\exp[\mathbf{X}]$ has been explained by Miehe [10]. The derivative $\partial_{\mathbf{X}} \exp[\mathbf{X}]$ used in Section 3.4 is defined by means of the directional derivative as follows:

$$D_{\boldsymbol{\eta}} \exp[\mathbf{X}] := \left.\frac{\mathrm{d}}{\mathrm{d}\epsilon}\right|_{\epsilon=0} \exp[\mathbf{X} + \epsilon\boldsymbol{\eta}] = \partial_{\mathbf{X}} \exp[\mathbf{X}] : \boldsymbol{\eta} \quad \forall\, \boldsymbol{\eta} \in \mathscr{S}. \tag{A.1}$$

For a detailed explanation and derivation see [10] and references therein. A summary of required formulas is given in Table 6.

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