On VOIGT and KELVIN Matrix Notations of Second-Order Tensors

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The implementation of constitutive models into a computer software necessitates the conversion of abstract tensors into real numbers that can be processed by a computer. This is accomplished (1) by introducing a basis, and (2) by arranging the scalar tensor components into matrices. In literature, such conversion processes are often used ad hoc without any rigorous mathematical derivation or justification. Probably most prominent are the VOIGT and KELVIN matrix notations. These matrix notations use existing symmetries of the tensors and allow to remove any redundant information from the matrix representations. Thus, in this special but very common case, the effective size of the matrices are significantly reduced and with this the computational effort.

In this contribution, the mathematical background for the two mentioned conversion processes is explained. It is shown that VOIGT and KELVIN matrix representations are not restricted to orthonormal bases, and with this not to Cartesian tensors. Moreover, it is demonstrated that the value of a duality pairing is invariant with respect to the conversion process.

1 Mathematical Background of Matrix Representations

Let \( V \) be an \( m \)-dimensional real vector space (without inner product). Then, the dual space of \( V \), denoted by \( V^* \), is the \( m \)-dimensional vector space \( \text{Lin}(V, \mathbb{R}) \), where \( \text{Lin}(V, \mathbb{R}) \) is the vector space of linear mappings from \( V \) onto the field of reals \( \mathbb{R} \). The (co-)vectors \( v^* \) in the dual space \( V^* \) define duality pairings (contractions), denoted by \( (v^*|v)_V = (v|v^*)_V \in \mathbb{R} \), where use is made of the canonical identification \( (V^*)_* \cong V \) (valid for finite-dimensional vector spaces). Let \( V := (v_1, \ldots, v_m) \in \mathbb{R}^m \) be an ordered basis (there are no notions such as orthogonality or normalization available since the vector space \( V \) is not equipped with an inner product structure), then \( V^* := (v^1, \ldots, v^m) \in V^{*m} \) is the dual ordered basis of \( V \) with identical order that is defined by \( (v^i|v)_V := \delta^i_j \), where \( \delta^i_j \) is the KRONECKER delta, which equals 1 if \( i = j \), and equals 0 if \( i \neq j \), with \( i, j \) ranging over the values 1, 2, \ldots, \( m \). The dual ordered basis of \( V^* \) is \( V^* \), i.e., \( (V^*)^* = V \), and \( V^* \) and \( V^* \) are a pair of dual ordered bases. Let \( V \in \mathbb{R}^m \) be an ordered basis, then

\[
v = v^1 v_1 + \cdots + v^m v_m \quad \Rightarrow \quad \begin{bmatrix} v^1 \\ v^2 \\ \vdots \\ v^m \end{bmatrix}^T \in \mathbb{R}^{m \times 1}
\]

is the column matrix representation, and \( [v]_V := [v^1 v^2 \cdots v^m]^T \in \mathbb{R}^{m \times 1} \) is the row matrix representation of the vector \( v \in V \) with respect to the basis \( V \). This establishes a basis-dependent isomorphism, and \( V \cong \mathbb{R}^m \).

Let \( V \subseteq \mathbb{R}^m \) and \( V^* \subseteq \mathbb{R}^{*m} \) be a pair of dual ordered bases, then the matrix representation of a duality pairing of the vectors \( v^* = v^1 v_1 \in \mathbb{R}^m \) and \( v = v^1 v_1 \in \mathbb{R}^m \) reads

\[
\langle v^*|v \rangle_V = v^1 v^1 = [v^1]^T [v^1] = [v^1]^T [v^1] = v^1 v_1 = (v|v^*)_V \in \mathbb{R},
\]

where the EINSTEIN summation convention is used. These concepts can be applied to the nine-dimensional tensor-product space \( V \otimes V \). Let \( V_{\text{Lex}} := (v_1 \otimes v_1, v_1 \otimes v_2, v_1 \otimes v_2, v_2 \otimes v_1, \ldots, v_3 \otimes v_3) \in (V \otimes V)^9 \) be an ordered basis (known as lexicographical order or row-wise stacking), then

\[
\sigma = \sigma^{ij} v_i \otimes v_j \in \mathbb{R}^{9 \times 1} \quad \Rightarrow \quad v_{\text{Lex}}[\sigma] = \begin{bmatrix} \sigma^{11} & \sigma^{12} & \sigma^{13} \\ \sigma^{21} & \sigma^{22} & \sigma^{23} \\ \sigma^{31} & \sigma^{32} & \sigma^{33} \end{bmatrix}^T \in \mathbb{R}^{9 \times 1}.
\]

Let \( V_{\text{Vec}} := (v_1 \otimes v_1, v_2 \otimes v_1, v_3 \otimes v_1, v_1 \otimes v_2, v_2 \otimes v_1, \ldots, v_3 \otimes v_3) \in (V \otimes V)^9 \) be a second alternative ordered basis (known as vectorization or column-wise stacking), then

\[
\sigma = \sigma^{ij} v_i \otimes v_j \in \mathbb{R}^{9 \times 1} \quad \Rightarrow \quad v_{\text{Vec}}[\sigma] = \begin{bmatrix} \sigma^{11} & \sigma^{21} & \sigma^{31} \\ \sigma^{12} & \sigma^{22} & \sigma^{32} \\ \sigma^{13} & \sigma^{23} & \sigma^{33} \end{bmatrix}^T \in \mathbb{R}^{9 \times 1}.
\]

Based on this, the duality pairing (double contraction) of the vector \( \sigma \in \text{Sym}(V^* \otimes V^*) \) (a contravariant or stress-like quantity) and the vector \( \varepsilon \in \text{Sym}(V^* \otimes V^*) \) (a covariant or strain-like quantity) reads

\[
\langle \sigma|\varepsilon \rangle_{V^* \otimes V^*} = \varepsilon^{ij} \sigma_{ij} = (\sigma|v_{\text{Vec}}(\varepsilon))_{V^*} = \varepsilon[\sigma]_{V_{\text{Vec}}}(\varepsilon)_{V_{\text{Vec}}} + \varepsilon^{ij} \sigma_{ij} = \varepsilon[\sigma]_{V_{\text{Vec}}}(\varepsilon)_{V_{\text{Vec}}}.
\]

It is seen that the value of a duality pairing is independent of the matrix representations used to calculate it (the matrix representation of the duality pairing is well-defined). However, nine multiplications are necessary to calculate the double contraction in general.

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2 Matrix Representations of Symmetric Second-Order Tensors

Let \{v_1, v_2, v_3\} be a basis for the vector space \(V\) (not necessarily an orthonormal basis since \(V\) is not equipped with an inner product structure). Due to the three-dimensional continuum physics’ context, the dimension of the vector space \(V\) is chosen to be three. For incorporation of the symmetry, the basis representation of a tensor, \(\sigma = \sigma_{ij} v_i \otimes v_j \in V \otimes V\) (not necessarily symmetric), is written as

\[
\sigma = \sigma^{11} D_{11} + \sigma^{22} D_{22} + \sigma^{33} D_{33} + \sigma^{(23)} S_{23} + \sigma^{(31)} S_{31} + \sigma^{(12)} S_{12} + \sigma^{[12]} A_{12} + \sigma^{[13]} A_{13} + \sigma^{[21]} A_{21},
\]

where \(\sigma^{(ij)} := \frac{1}{2}(\sigma_{ij} + \sigma_{ji})\) and \(\sigma^{[ij]} := \frac{1}{2}(\sigma_{ij} - \sigma_{ji})\) are the symmetrized \((\sigma^{(ij)} = \sigma^{(ji)})\) and skew-symmetrized \((\sigma^{[ij]} = -\sigma^{[ji]}))\) scalar coefficients of \(\sigma\), respectively, and

\[
D_{11} \equiv v_1 \otimes v_1, \quad D_{22} \equiv v_2 \otimes v_2, \quad D_{33} \equiv v_3 \otimes v_3,
\]

\[
S_{23} \equiv v_2 \otimes v_3 + v_3 \otimes v_2 = S_{32}, \quad S_{31} \equiv v_3 \otimes v_1 + v_1 \otimes v_3 = S_{13}, \quad S_{12} \equiv v_1 \otimes v_2 + v_2 \otimes v_1 = S_{21},
\]

\[
A_{12} \equiv v_1 \otimes v_2 - v_2 \otimes v_1 = -A_{21}, \quad A_{13} \equiv v_1 \otimes v_3 - v_3 \otimes v_1 = -A_{31}, \quad A_{21} \equiv v_2 \otimes v_1 - v_1 \otimes v_2 = -A_{12}.
\]

If \(\sigma\) is symmetric \((\sigma^{ij} = \sigma^{ji})\), the last three components are all zero. If \(\sigma\) is skew-symmetric \((\sigma^{ij} = -\sigma^{ji})\), the first six components are all zero. Even if \(\sigma\) is symmetric or skew-symmetric, the tensor has still nine components, of which some are linearly independent or zero.

Let \(V_\sigma := (D_{11}, D_{22}, D_{33}, S_{23}, S_{31}, S_{12}) \in (V \otimes V)^6\) and \(V_\varepsilon := (V_\sigma)^* \in (V^* \otimes V^*)^6\) be a pair of dual ordered bases for the six-dimensional subspaces of symmetric tensors in \(\text{Sym}(V \otimes V)\) and \(\text{Sym}(V^* \otimes V^*)\), respectively, then

\[
\sigma = \sigma^{ij} v_i \otimes v_j \in \text{Sym}(V \otimes V) \quad \Leftrightarrow \quad [\sigma]_{V_\sigma} = [\sigma^{11} \sigma^{22} \sigma^{33} \sigma^{(23)} \sigma^{(31)} \sigma^{(12)}] \in M_{1\times 6}^6
\]

\[
\varepsilon = \varepsilon^{ij} v^i \otimes v^j \in \text{Sym}(V^* \otimes V^*) \quad \Leftrightarrow \quad [\varepsilon]_{V_\varepsilon} = [\varepsilon^{11} \varepsilon^{22} \varepsilon^{33} \varepsilon^{(23)} \varepsilon^{(31)} \varepsilon^{(12)}]^T \in M_{6\times 1}^6
\]

are the VOIGT matrix representations of contravariant (stress-like) and covariant (strain-like) quantities, respectively. The VOIGT matrix representation (used, e.g., in crystal physics [1–3], and in the finite element method) treats contravariant and covariant scalar tensor components differently.

Let \(M_\sigma := (D_{11}, D_{22}, D_{33}, 2^{-\frac{1}{2}} S_{23}, 2^{-\frac{1}{2}} S_{31}, 2^{-\frac{1}{2}} S_{12}) \in (V \otimes V)^6\) and \(M_\varepsilon := (M_\sigma)^* \in (V^* \otimes V^*)^6\) be an alternative pair of dual ordered bases, then

\[
\sigma = \sigma^{ij} v_i \otimes v_j \in \text{Sym}(V \otimes V) \quad \Leftrightarrow \quad [\sigma]_{M_\sigma} = [\sigma^{11} \sigma^{22} \sigma^{33} \sqrt{2} \sigma^{(23)} \sqrt{2} \sigma^{(31)} \sqrt{2} \sigma^{(12)}] \in M_{1\times 6}^6
\]

\[
\varepsilon = \varepsilon^{ij} v^i \otimes v^j \in \text{Sym}(V^* \otimes V^*) \quad \Leftrightarrow \quad [\varepsilon]_{M_\varepsilon} = [\varepsilon^{11} \varepsilon^{22} \varepsilon^{33} \sqrt{2} \varepsilon^{(23)} \sqrt{2} \varepsilon^{(31)} \sqrt{2} \varepsilon^{(12)}]^T \in M_{6\times 1}^6
\]

are the KELVIN matrix representations (also known as MANDEL matrix representations) of contravariant (stress-like) and covariant (strain-like) quantities, respectively. The KELVIN matrix representation (used, e.g., in anisotropic elasticity [4–7]) treats contravariant and covariant scalar tensor components identically (an observation that was already made by Bechtherew [8] in the 1920s).

Based on these reduced matrix representations, the duality pairing becomes

\[
\langle [\sigma]_{V_\sigma} \rangle_{V^* \otimes V} = \sigma^{ij} \varepsilon_{ij} = [\sigma]_{V_\sigma} V_\varepsilon [\varepsilon] = [\sigma]_{M_\sigma} M_\varepsilon [\varepsilon] = \varepsilon^{ij} \sigma_{ij} = [\varepsilon]_{V_\varepsilon} V_\sigma [\sigma] = [\varepsilon]_{M_\varepsilon} M_\sigma [\sigma] = (\langle \varepsilon \rangle)_{V^* \otimes V}.
\]

As is the general case, the value of duality pairing is independent of the matrix representations used to calculate it. However, only six multiplications are necessary to calculate the double contraction (twice the strain-energy density in linear elasticity).

3 Conclusions

Since the underlying vector space \(V\) is not equipped with an inner product, it becomes obvious that VOIGT and KELVIN matrix representations are not restricted to orthonormal bases and with this not to Cartesian tensors. The value of a duality pairing is invariant with respect to the conversion process. The factor two in VOIGT matrix representation shows up due to the pair of dual ordered bases used, \(V_\sigma\) and \(V_\varepsilon\), and not due to any (ortho”) normalization. The KELVIN matrix representation allows an identical treatment of purely contravariant or purely covariant scalar tensor components and appears therefore more natural.

References

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