Representations of Fourth-Order Cartesian Tensors of Structural Mechanics

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Summary

This paper is concerned with geometrical and algebraic representation of fourth-order Cartesian tensors. As fourth-order tensors are four-dimensional objects, it is difficult to visualize them. A possible way of representation proposed here is based on an orthogonal projection of a four-dimensional cube into a planar octagon. Another way of geometrical visualization is possible by means of a quartic form in the three-dimensional space, though this mapping does not provide a one-to-one correspondence. Different kinds of symmetry and the existence of the inverse are also investigated, and it is established that the stiffness and compliance tensors of general Hooke's law are not inverses of each other. We show that a fourth-order tensor can be represented by a 3×3 matrix whose entries are 3×3 matrices, and also by a 9×9 matrix. The paper summarises some old facts and new results.

Keywords: Fourth-order tensor, geometric representation, algebraic representation, double contraction, single contraction, inverse, symmetry, Hooke tensors.

1. Introduction

Fourth-order tensors were first introduced by Voigt [1], who called them ‘Bitensoren’ along with his term ‘Tensortripel’ for second-order tensors. As tensors have become important in various fields of mathematical and scientific applications in the last few decades including computational mechanics [2], the general and more consistent term of ‘*n*th-order tensor’ has exchanged the old ones. Second-order tensors are in everyday use in the form of common matrices. Third-order tensors are less often used [3], a notable exception is the Levi-Civita tensor. Fourth-order tensors again have an importance in solid mechanics, e.g. in the definition of the stiffness and compliance properties of the general form of Hooke's law.

The two major difficulties regarding the handling of fourth-order tensors are the geometric and algebraic representations. Elements of an *n*th-order object can be placed at the nodes of an *n*-dimensional grid forming an *n*-dimensional cube. The visualization above the third order becomes rather complicated. On the other hand, algebraic descriptions of operations on higher-order tensors involve (multiple) summations making practical calculations difficult to follow. In this paper we discuss and propose representations of fourth-order tensors for better applicability both in geometric and algebraic aspect.

Furthermore, an important field in tensor algebra is related to the definition of the inverse of a tensor. In solid mechanics the relationship between the stiffness and compliance tensors of general Hooke's law bears importance. In numerical computations the said tensors are in most cases represented by 6×6 matrices, the stiffness and compliance matrices of Hooke's law, and operations are performed by using matrix algebra. It makes room for possible confusion of inverse matrices and inverse tensors, e.g. in [4]. We discuss the definition of the identity tensor and the inverse tensor with respect to the symmetry properties of the tensor.

2. Representations

A vector is a series of elements. A second-order tensor, which is represented by a matrix, can be regarded as a series of vectors, or in other words a vector composed of elements being vectors themselves. By generalization a third-order tensor is regarded as a vector composed of elements that are second-order tensors, and a fourth-order tensor as a vector of third-order tensors. If the last index is chosen to refer to the elements of the vector, the notation may go as

$$\mathbf{A}_i, \quad \mathbf{A}_{ij} = (\mathbf{A}_i)_j, \quad \mathbf{A}_{ijk} = (\mathbf{A}_{ij})_k, \quad \mathbf{A}_{ijkl} = (\mathbf{A}_{ijk})_l \tag{1}$$

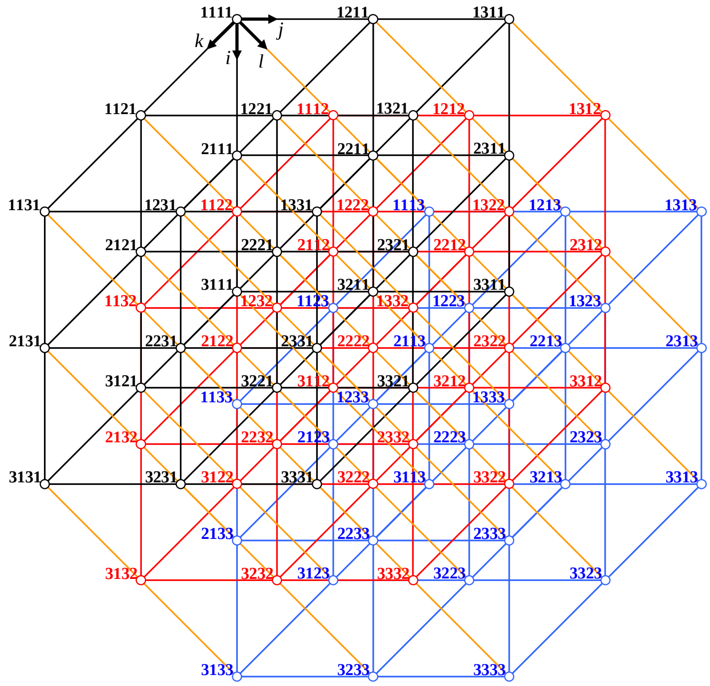

Fig. 1. Representation of a fourth-order tensor in the plane. Only the indices of the 81 elements are shown.

The orthogonal projection of the four-dimensional grid of size 3 into a planar octagon [5] is shown in Fig. 1 where each layer represents a third-order tensor plotted in different colours. Alternatively, in the case of fourth-order tensors, the four-dimensional set can be viewed as 9 two-dimensional layers of size 3×3, and correspondingly the notation goes as

$$\mathbf{A}_{ijkl} = (\mathbf{A}_{ij})_{kl} \tag{2}$$

In this case the layers of the tensor can be arranged in a planar orthogonal grid of size 3×3 as

$$\mathbf{A} = \begin{bmatrix} \begin{bmatrix} 1111 & 1211 & 1311 \\ 2111 & 2211 & 2311 \\ 3111 & 3211 & 3311 \end{bmatrix} & \begin{bmatrix} 1112 & 1212 & 1312 \\ 2112 & 2212 & 2312 \\ 3112 & 3212 & 3312 \end{bmatrix} & \begin{bmatrix} 1113 & 1213 & 1313 \\ 2113 & 2213 & 2313 \\ 3113 & 3213 & 3313 \end{bmatrix} \\ \begin{bmatrix} 1121 & 1221 & 1321 \\ 2121 & 2221 & 2321 \\ 3121 & 3221 & 3321 \end{bmatrix} & \begin{bmatrix} 1122 & 1222 & 1322 \\ 2122 & 2222 & 2322 \\ 3122 & 3222 & 3322 \end{bmatrix} & \begin{bmatrix} 1123 & 1223 & 1323 \\ 2123 & 2223 & 2323 \\ 3123 & 3223 & 3323 \end{bmatrix} \\ \begin{bmatrix} 1131 & 1231 & 1331 \\ 2131 & 2231 & 2331 \\ 3131 & 3231 & 3331 \end{bmatrix} & \begin{bmatrix} 1132 & 1232 & 1332 \\ 2132 & 2232 & 2332 \\ 3132 & 3232 & 3332 \end{bmatrix} & \begin{bmatrix} 1133 & 1233 & 1333 \\ 2133 & 2233 & 2333 \\ 3133 & 3233 & 3333 \end{bmatrix} \end{bmatrix} \tag{3}$$

where only the indices are displayed. Note that (3) is not a 9×9 matrix but an algebraic representation that reflects the structure of the fourth-order tensor. In any layer the last two indices do not vary. A representation can be made by considering layers given by the first two indices instead [2]. In order to create a matrix representation of a tensor that is also applicable to the purposes of algebraic operations, we define a mapping that converts the tensor into a 9×9 matrix as follows. Pairs of indices are mapped to numbers 1 to 9 so that different pairs correspond to different numbers:

$$\Phi:(i,j)\to n,\quad (i,j)=\{(1,1);(1,2);(1,3);(2,1);(2,2);(2,3);(3,1);(3,2);(3,3)\},\quad n=1,\ldots,9 \tag{4}$$

The 9 pairs formed by the first and second indices of the tensor correspond to the rows of the matrix and are listed in an arbitrary order. The pairs of third and fourth indices are listed in the same order referring to the columns of the matrix in a similar way. (One particular mapping sequence was proposed by Nadeau and Ferrari [6].)

Operations on fourth-order tensors provide larger variety than those on second-order ones. Addition of tensors is commutative and composed of additions of individual elements. Multiplication operations can be various, e.g. double and quadruple contractions are defined as

$$\mathbf{A}_{ijkl}:\mathbf{B}_{klmn}=\mathbf{C}_{ijmn},\quad c_{ijmn}=\sum_{k=1}^{3}\sum_{l=1}^{3}a_{ijkl}b_{klmn},\quad i,j,m,n=1,2,3 \tag{5}$$

$$\mathbf{A}_{ijkl}::\mathbf{B}_{ijkl}=C,\quad C=\sum_{i=1}^{3}\sum_{j=1}^{3}\sum_{k=1}^{3}\sum_{l=1}^{3}a_{ijkl}b_{ijkl} \tag{6}$$

Quadruple contraction produces a scalar while double contraction yields another fourth-order tensor. However, to calculate the double contraction a double summation of pairs of elements has to be performed. The summation goes by the last two indices of the first tensor, which correspond to the first two indices of the second tensor. Considering a matrix representation that maps the two pairs of indices by the same rule given in Eq.(4), the double contraction of fourth-order tensors can be replaced by single multiplication of matrices, or in other words, single contraction of second-order tensors of dimension 9.

Let us define a second-order tensor of variables as $\mathbf{X}=\mathbf{x}\otimes\mathbf{x}$ where $\mathbf{x}=[x_1,x_2,x_3]$ and $\otimes$ denotes the tensorial product. One can view $\mathbf{X}$ as a 3×3 matrix obtained by the diadic product of vector $\mathbf{x}$ with itself. Now let us create the 'quadratic' form

$$Q=\mathbf{X}:\mathbf{A}:\mathbf{X} \tag{7}$$

of the fourth-order tensor **A**, which is indeed quartic with respect to x_i. It is known that symmetric second-order tensors can be visualized by their quadratic form yielding an ellipsoid in the three-dimensional space. The quartic form (7) of the fourth-order tensor can be applied in a similar manner. Now the equation $Q=1$ displays a fourth-order surface in the Cartesian system (x_1,x_2,x_3), which is not always elliptic. Moreover, its polynomial form contains fifteen terms and thus the mapping of the fourth-order tensor onto the quartic form does not provide a one-to-one correspondence, except for a completely symmetric tensor having 15 different elements. However, it is in direct relationship with the properties of the tensor as shown later in this paper.

3. Group of fourth-order tensors in 3-dimensional space

Let us consider the set G of all fourth-order tensors of dimension 3. They form a group with respect to double contraction if the following requirements are satisfied:

1. (*closure*) $\mathbf{A}:\mathbf{B}\in G$ for all $\mathbf{A},\mathbf{B}\in G$,
2. (*associativity*) $(\mathbf{A}:\mathbf{B}):\mathbf{C}=\mathbf{A}:(\mathbf{B}:\mathbf{C})$ for all $\mathbf{A},\mathbf{B},\mathbf{C}\in G$,
3. (*identity element*) there exist an identity element $\mathbf{I}\in G$ so that $\mathbf{A}:\mathbf{I}=\mathbf{I}:\mathbf{A}=\mathbf{A}$ for all elements $\mathbf{A}\in G$,
4. (*inverse*) for each element $\mathbf{A}\in G$ there exists an inverse element $\mathbf{B}\in G$ so that $\mathbf{A}:\mathbf{B}=\mathbf{B}:\mathbf{A}=\mathbf{I}$.

The requirement of closure is automatically satisfied by definition. Furthermore, it can be shown that the rule of associativity is also satisfied for all fourth-order tensors. However, due to the complexity of symmetry properties, the fourth-order identity tensor is not symmetric thus it is worth considering the identity tensor, its transpose, and its symmetric part as well:

$$\mathbf{I} = \sum_{ijkl} \delta_{ik}\delta_{jl}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \tag{8}$$

$$\mathbf{I}^T = \sum_{ijkl} \delta_{il}\delta_{jk}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l \tag{9}$$

$$\mathbf{I}^S = \frac{1}{2}\left(\mathbf{I} + \mathbf{I}^T\right) \tag{10}$$

where δ and $\mathbf{e}_t$ denote the Kronecker-delta and the unit vector in direction t, respectively. The transpose of a tensor is defined as $\mathbf{B} = \mathbf{A}^T$ if $b_{ijlk} = a_{ijkl}$. The entries of tensors $\mathbf{I}$ and $\mathbf{I}^T$ are only 0 and 1 while $\mathbf{I}^S$ has entries ½ as well.

Our analysis has shown that the transpose tensor and the symmetric part may satisfy the third requirement for certain types of fourth-order tensors. Furthermore, special tensors can be found that satisfy the equations in the fourth requirement with $\mathbf{I}$ and $\mathbf{I}^T$ but are not unique solutions and hence cannot be regarded as inverse tensors. We have divided the set of fourth-order tensors into subsets with respect to symmetry in order to assess the requirements individually. These subsets are referred to as ‘types’ in the following. We consider symmetry by the equality of certain elements, and a list of types shown in Table 1 has been created.

Table 1. Symmetry types of fourth-order tensors displaying indices referring to identical elements, the maximum number of different elements (N_{max}), and the notation.

Symmetry properties	$N_{\max}$	Notation
all permutations of *ijkl*	15	15
$a_{ijkl} = a_{klij} = a_{jikl} = a_{ijlk}$	21	21
$a_{ijkl} = a_{jikl} = a_{ijlk} = a_{jilk}$	36	36
$a_{ijkl} = a_{jilk}$	45	45a
$a_{ijkl} = a_{klij}$	45	45b
$a_{ijkl} = a_{jikl}$	54	54a
$a_{ijkl} = a_{ijlk}$	54	54b
none	81	81

Though some of the types are not subsets of other ones, one can generally say that the maximum number of different elements is less for higher types of symmetry and such tensors satisfy criteria of some of the lower types as well. Surprisingly, the identity tensor $\mathbf{I}$ and its transpose $\mathbf{I}^T$ satisfy only criteria 45a and 45b while the symmetric part $\mathbf{I}^S$ satisfies all except 15. The properties are summarized in Table 2.

Table 2. Fulfilment of symmetry definitions (symbol ×) with respect to different types of tensors (columns) and type criteria (rows). Note that some tensor types comply with several type criteria.

Type	$\mathbf{A}^{15}$	$\mathbf{A}^{21}$	$\mathbf{A}^{36}$	$\mathbf{A}^{45a}$	$\mathbf{A}^{45b}$	$\mathbf{A}^{54a}$	$\mathbf{A}^{54b}$	$\mathbf{I}$	$\mathbf{I}^T$	$\mathbf{I}^S$
15	×									
21	×	×								×
36	×	×	×							×
45a	×	×	×	×				×	×	×
45b	×	×	×		×			×	×	×
54a	×	×	×			×				×
54b	×	×	×				×			×
81	×	×	×	×	×	×	×	×	×	×

Though the associativity criterion is satisfied for all fourth-order tensors, the double contraction does not always yield output of the same symmetry type. Symmetry is preserved in the case of types 36, 45a, 54a, 54b, and 81, but is reduced in the case of types 15, 21, and 45b, i.e. the requirement of closure is satisfied only in the former case.

Double contraction of fourth-order tensors with the identity tensor, its transpose, and its symmetric part yields various results depending on the symmetry type. In the case of higher symmetry types (15, 21, 36) the third criterion of group definition is satisfied for the identity tensor as well as for its transpose and symmetric part. On the other hand, in the case of types 54a and 54b double contraction with $\mathbf{I}^S$ violates the criterion since the two contractions give different results, while in the case of types 45a, 45b, and 81 double contraction fails with both $\mathbf{I}^T$ and $\mathbf{I}^S$. The results are summarized in Table 3.

Table 3. Fulfilment of the criterion of identity element (symbol ×) with respect to symmetry types of tensors coupled with the identity tensor, its transpose and its symmetric part.

	15	21	36	45a	45b	54a	54b	81
$\mathbf{I}$	×	×	×	×	×	×	×	×
$\mathbf{I}^T$	×	×	×			×	×	
$\mathbf{I}^S$	×	×	×					

The definition of the inverse element in the fourth criterion means that all 81 elements of the inverse tensor **B** have to be chosen so that the two equations (one for the right inverse and one for the left inverse) are satisfied. According to the operation of double contraction defined by Eq.(5) two inhomogeneous systems of linear equations are formulated, both comprised of 81 equations with 81 variables. The systems of equations yield unique solutions if the ranks of the coefficient matrix and of the extended matrix are both 81. The inverse tensor exists if the left inverse and the right inverse obtained from the two systems of equations are identical according to the fourth requirement of the group definition.

We have examined all symmetry types with respect to the existence of the inverse tensor **B** such that $\mathbf{A}:\mathbf{B}=\mathbf{B}:\mathbf{A}=\mathbf{I}$ according to the fourth requirement. We found that only tensors of types 45a, 45b, and 81 comply with this requirement. Moreover, tensors of type 45a satisfy the equations also if the identity tensor is replaced by its transpose or its symmetric part, and the symmetry properties are preserved as well while in this case tensors of types 45b and 81 yield different solutions for the left inverse and the right inverse.

For all other types both the coefficient matrix and the extended matrix have rank deficiency, thus a unique inverse is not possible to obtain. In the case of types 54a and 54b the system of equation yields no solution for either the left inverse or the right inverse or both.

Even though unique solution is not possible, the higher symmetry types (15, 21, 36) can yield solutions if the symmetric part $\mathbf{I}^S$ of the identity tensor is used. Now the ranks of the coefficient matrix and the extended matrix are equally 54, i.e. an infinite set of solutions of 27 parameters is obtained. They can be taken arbitrarily, however, a suitable choice of parameters yield a solution of high symmetry. They are of types 21, 21, and 36 for tensor types 15, 21, and 36, respectively. These special left and right tensors are identical in all three cases. The results are summarized in Table 4.

Table 4. Fulfilment of the criterion of inverse element (symbol ×) with respect to symmetry types of tensors coupled with the identity tensor, its transpose and its symmetric part; symbols ! denote non-unique solutions of equations.

	15	21	36	45a	45b	54a	54b	81
$\mathbf{I}$				×	×			×
$\mathbf{I}^T$				×				
$\mathbf{I}^S$	!	!	!	×				

To conclude, the set of all fourth-order tensors do not form a group with double contraction because the third and the fourth requirements are not satisfied for all tensors. Associativity is satisfied for all types but closure only for certain ones. The types show large variety with respect to the criteria regarding the identity element and the inverse element. The result are shown in Table 5. One can conclude that the requirements of group definition can be satisfied only in the case of types 45a and 81 for the identity tensor $\mathbf{I}$. On the other hand, it is interesting to observe that in the case of higher symmetry types the equations with the symmetric part of the identity tensor in the fourth criterion lead neither to contradiction nor to unique solutions, hence inverse tensor does not exist. In this case all tensors involved exhibit rank deficiency in their matrix representations defined by Eq.(4).

Table 5. Fulfilment of group definition (symbol ×) with respect to symmetry types; symbols ! denote non-unique solution of equations; in the last two rows the relevant tensors are displayed.

	15	21	36	45a	45b	54a	54b	81
1			×	×		×	×	×
2	×	×	×	×	×	×	×	×
3	$\mathbf{I}\ \mathbf{I}^T\ \mathbf{I}^S$	$\mathbf{I}\ \mathbf{I}^T\ \mathbf{I}^S$	$\mathbf{I}\ \mathbf{I}^T\ \mathbf{I}^S$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}\ \mathbf{I}^T$	$\mathbf{I}\ \mathbf{I}^T$	$\mathbf{I}$
4	!	!	!	$\mathbf{I}\ \mathbf{I}^T\ \mathbf{I}^S$	$\mathbf{I}$			$\mathbf{I}$

4. Hooke tensors

The stiffness and compliance tensors of general Hooke’s law are fourth-order tensors, which are usually given in a form of a 6×6 reduced matrix. The relationship between the stress and strain tensors defines the mapping between the fourth-order tensors and the reduced matrices [7]. The stiffness and compliance tensors comply with symmetry type 21. The most important consequence is that the two tensors are not inverses of each other. (Note that the reduced matrices are indeed in inverse relationship according to matrix inverse definition.)

Linearly elastic materials are classified with respect to the symmetry of their atomic (crystal) structure. The symmetry systems are: triclinic, monoclinic, orthorhombic, trigonal, hexagonal, tetragonal, cubic, and isotropic; each class is characterized by planes and rotational axes of symmetry, see e.g. [1]. The symmetry properties of the crystal structure is reflected in the symmetry properties and in the number of different elements of the tensor.

Let us consider the quartic form defined in Eq.(7) for the crystal groups above. Our calculations show that the surface in the Cartesian system (x_1, x_2, x_3) exhibits the same symmetry properties as the crystal system. For example, the trigonal system has a threefold axis of rotation (and in certain cases also another three twofold axes of rotation in a perpendicular direction to the threefold axis) just as well as its surface representation has. Such material is the corundum (Al_2O_3) where the elements of the 6×6 reduced stiffness matrix are c_{11}=497,5 GPa, c_{12}=162,7 GPa, c_{13}=115,5 GPa, c_{14}=22,5 GPa, c_{33}=503,3 GPa, c_{44}=147,4 GPa, see [8]. The quartic surface shown in Fig. 2 is

$$497{,}5x_1^3 + 497{,}5x_2^4 + 501x_3^4 - 90x_2^3x_3 + 995x_1^2x_2^2 + 820{,}6x_1^2x_3^2 + 820{,}6x_2^2x_3^2 + 270x_1^2x_2x_3 = 1 \quad (11)$$

5. Conclusions

We have shown that a fourth-order tensor can be visualized as an orthogonal projection of the four-dimensional cube and can be represented as a matrix whose elements are matrices. It is also possible to create a mapping that converts the double contraction of fourth-order tensors of dimension 3 into a single contraction of second-order tensors of dimension 9 reducing computational difficulties. Different types of fourth-order tensors can be defined with respect to symmetry properties. We have found that the set of all tensors coupled with double contraction does not form a group but the subset of general non-symmetrical tensors and the subset of a special symmetry type do. Tensors of the symmetry type which represents the Hooke tensors of solid mechanics do not form a group and have no inverse tensor either. It means that the stiffness and compliance tensors are not inverses of each other in spite of the fact that the stiffness and compliance tensors applied in succession transform the strain tensor into the stress tensor and back again. The special behaviour is also exhibited in the rank deficiency of the matrix representation of the tensors.

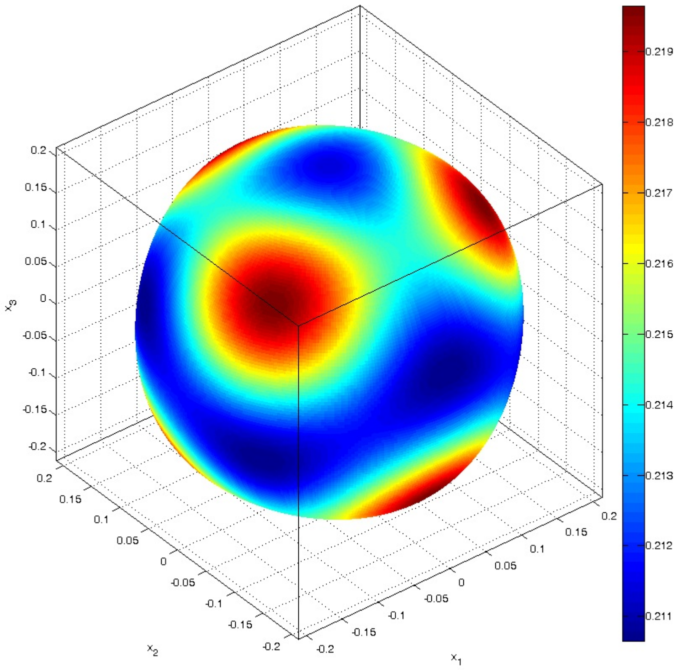

Fig. 2. Representation of the trigonal stiffness tensor of corundum (Al_2O_3) in the Cartesian system (x_1,x_2,x_3) by its quartic surface. Colours indicate distance from the origin.

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