Elastic tensors and their preferred frames of reference

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ABSTRACT

Even though tensors have an existence independent of what frame we choose to represent them in, it is inevitable that we need to utilize the numbers representing the tensor in a certain frame of reference. The elastic tensor is no exception; if we choose the wrong frame of reference the tensor components will in general be all non-zero, which is cumbersome to work with, even though correct. If we choose the preferred frame we gain two things: minimization of dependent non-zero elements and information as to the symmetry orientation represented by the elastic tensor. We propose to approach the problem in a statistical manner.

INTRODUCTION

We will use the definition that a tensor **T** of order m is a multilinear functional on an n dimensional vector space V_n equipped with an inner product $(\cdot,\cdot)$. These are all abstract quantities. The properties of **T** are determined by choosing an arbitrary set of m vectors from V_n such as $\{\mathbf{v}_1,\mathbf{v}_2,\cdots,\mathbf{v}_m\}$, and examining the scalar defined by $\mathbf{T}(\mathbf{v}_1,\mathbf{v}_2,\cdots,\mathbf{v}_m)$ and doing this for all sets of vectors $\{\mathbf{v}_1,\mathbf{v}_2,\cdots,\mathbf{v}_m\}$. In general we choose an orthonormal basis in V_n say $\{\mathbf{x}_1,\mathbf{x}_2,\cdots,\mathbf{x}_n\}$, then represent the vectors above as $\mathbf{v}_i = (\mathbf{v}_i,\mathbf{x}_j)\,\mathbf{x}_j$ for $i = 1,\ldots,m$, summation on repeated indices being in effect. With this in mind we can write:

$$\mathbf{T}(\mathbf{v}_1\,\mathbf{v}_2,\cdots,\mathbf{v}_m) = (\mathbf{v}_1,\mathbf{x}_{j_1})(\mathbf{v}_2,\mathbf{x}_{j_2})\cdots(\mathbf{v}_m,\mathbf{x}_{j_m})\;\mathbf{T}(\mathbf{x}_{j_1},\mathbf{x}_{j_2},\cdots,\mathbf{x}_{j_m}), \qquad (1)$$

where we have relied heavily on the multilinearity of **T**. To cast equation (1) in a more familiar form we can define the following scalars:

$$\begin{aligned} T_{j_1j_2\cdots j_m} &= \mathbf{T}(\mathbf{x}_{j_1},\mathbf{x}_{j_2},\cdots,\mathbf{x}_{j_m}) \,, \qquad (2)\\ v_1^{j_1} &= (\mathbf{v}_1,\mathbf{x}_{j_1}) \,,\\ v_2^{j_2} &= (\mathbf{v}_2,\mathbf{x}_{j_2}) \,,\\ &\vdots\\ v_m^{j_m} &= (\mathbf{v}_m,\mathbf{x}_{j_m}) \,. \end{aligned}$$

The first scalar in equation (2) is just the commonly used tensor component and the rest are the components of the vectors. All of these scalars are defined only with respect to the basis we chose. Thus equation (1) can be rewritten with the aid of definition (2) as:

$$\mathbf{T}(\mathbf{v}_1\,\mathbf{v}_2,\cdots,\mathbf{v}_m) = v_1^{j_1}v_2^{j_2}\cdots v_m^{j_m}\,T_{j_1j_2\cdots j_m}. \qquad (3)$$

Now consider the case when we have a different orthonormal basis $\{\tilde{\mathbf{x}}_1, \tilde{\mathbf{x}}_2, \cdots, \tilde{\mathbf{x}}_n\}$. Then definition (2) and equation (3) give us:

$$\mathbf{T}(\tilde{\mathbf{x}}_{i_1}, \tilde{\mathbf{x}}_{i_2}, \cdots, \tilde{\mathbf{x}}_{i_m}) = \tilde{\mathrm{T}}_{i_1 i_2 \cdots i_m} = \tilde{\mathrm{x}}_{i_1}^{j_1} \tilde{\mathrm{x}}_{i_2}^{j_2} \cdots \tilde{\mathrm{x}}_{i_m}^{j_m} \, \mathrm{T}_{j_1 j_2 \cdots j_m}, \qquad (4)$$

where

$$\tilde{\mathrm{x}}_i^j = (\tilde{\mathbf{x}}_i, \mathbf{x}_j),$$

are just the direction cosines relating one frame to the other. Equation (4) shows that the components of a tensor can be quite different from one frame to the other, and also provides a means of going from one to the other. The elastic tensor is no different. Its components are directly related in the same fashion to the frame of reference we choose to express it in. Many people have devised means to take an arbitrary representation of the elastic tensor and determine the symmetry properties of the underlying tensor. Most notable is the work of Backus (1970) who decomposed the representation of the elastic tensor to a series of vector bouquets and showed that, by direct observation of the symmetry of these bouquets, one can determine the symmetry of the underlying tensor. A second method is described by Baerheim (1992). He notes that the symmetric mapping of the asymmetric part of the representation of the elastic tensor is diagonal in the preferred frame of reference for all crystal classes except triclinic, monoclinic and trigonal cases. Thus the diagonalization of this matrix will yield eigen-vectors which should represent the preferred coordinate system.

These are both good methods with some points which can be built upon. The method of Backus requires visual inspection, which can probably be automated, and there is no work which shows how stable the technique is to small perturbations. The method of Baerheim is direct but is not universally applicable, and I have not seen the effects of small perturbations to this method. Thus I propose to study a statistical method which should be universal and not sensitive to small perturbations.

STATISTICAL DETERMINATION OF THE PREFERRED FRAME OF REFERENCE FOR ELASTIC TENSORS

I will use the standard two-index notation for all the development. but all bold face capital letters will represent the tensor which underlies the matrix representation. A reference for the two index notation can be found in Baerheim's (1992) paper. I will be developing the idea for the cubic symmetry class. The cubic elastic tensor represented in the preferred frame of reference has the following form in two index notation:

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix} . \qquad (5)$$

This show the cubic tensor has only three independent elements. Now consider the tensor is some arbitrary frame of reference. In general its representation will no longer be appear as simple in appearance as equation (5) but will have many non zero entries as:

$$\mathbf{A} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} & A_{15} & A_{16} \\ A_{12} & A_{22} & A_{23} & A_{24} & A_{25} & A_{26} \\ A_{13} & A_{23} & A_{33} & A_{34} & A_{35} & A_{36} \\ A_{14} & A_{24} & A_{34} & A_{44} & A_{45} & A_{46} \\ A_{15} & A_{25} & A_{35} & A_{45} & A_{55} & A_{56} \\ A_{16} & A_{26} & A_{36} & A_{46} & A_{56} & A_{66} \end{bmatrix} . \qquad (6)$$

In order to find the frame which causes equation (6) to become closest to equation (7), I propose to form the new matrix below:

$$\mathbf{B} = \begin{bmatrix} B_{11} & B_{12} & B_{12} & 0 & 0 & 0 \\ B_{12} & B_{11} & B_{12} & 0 & 0 & 0 \\ B_{12} & B_{12} & B_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & B_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & B_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & B_{44} \end{bmatrix} , \qquad (7)$$

where

$$B_{11} = \frac{1}{3}(A_{11} + A_{22} + A_{33}) ,$$

$$B_{44} = \frac{1}{3}(A_{44} + A_{55} + A_{66}) ,$$

and

$$B_{12} = \frac{1}{3}(A_{12} + A_{13} + A_{23}) .$$

We now form the difference $\mathbf{E} = R(\mathbf{B} - \mathbf{A})$, which I will call the error tensor. The symbol $R(\cdot)$ represents the rotation from one frame of reference to another as given by equation (4); this is where the distinction becomes important that the rotation is actually performed on the tensor and not its matrix representation. The rotation can be represented by Euler angles or some other set of three appropriate variables. Let the matrix representation of E have the elements E_{ij}. We now form the scalar:

$$\varepsilon = \sum_{i=1}^{6} \sum_{j=1}^{6} w_{ij} E_{ij}^2 , \qquad (8)$$

which shall be called the error term. At this point we are free to use a number of optimization techniques such as GLI to minimize equation (8). Weights w_{ij} have been introduced to add additional control. The template matrix **B** can be customized for all symmetry systems in the same manner as above, and so is not restricted to cubic symmetry. When equation (8) is minimized, the resulting **B** will be our closest representation of **A** within the confines of this fixed symmetry system. We can also examine the error matrix **E** to see how the error is distributed and the magnitude of the individual terms. The Euler angles will define the new coordinate system, which provides information as to the underlying symmetry of the tensor **A**. The use of methods like GLI should also stabilize the method to small perturbations.

CONCLUSION

A new method to obtain the preferred reference frame of an arbitrary elastic tensor is proposed. Compared to earlier methods, it has the advantage that: small perturbations will not strongly influence the estimated representation, errors are clearly seen and easily adaptable to all symmetry classes.

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