# Numerical trial of a statistical method to find the preferred frames of reference of elastic tensors

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## ABSTRACT

A simple method to obtain the preferred frame of reference of an elastic tensor using statistical techniques (Easley and Brown, 1992) was implemented successfully in a computer program. The program was tested on cubic elastic tensors. A numerical trial is shown.

## INTRODUCTION

In general an elastic tensor contains 81 non-zero components, 21 of which can be considered to be independent. If the tensor has some symmetries, aside from those intrinsic to elastic tensors, then these 21 components are in general dependent quantities. Direct inspection of the components of a tensor in general does not make the interdependence clear. In the preferred frame of reference, where the coodinate planes are coincident with the planes of symmetry of the tensor, the dependence becomes far more obvious. It is of interest, therefore, to find the preferred frame of reference. Direct methods to obtain the preferred frame have been devised. The most notable of these 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 (1993). 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 many of the crystal classes. Thus the diagonalization of this matrix will yield eigen vectors which should represent the unit vectors of the preferred frame of reference.

These are both viable methods with some points that can be expanded upon. These points are discussed in more detail in (Easley and Brown, 1992). The method used here (Easley and Brown, 1992) is statistical in nature and addresses some of the weaknesses of the analytical methods; however, being a statistical method it has its own shortcomings. The flowchart in figure 1 indicates the statistical method implemented, for greater detail refer to the paper (Easley and Brown, 1992).The example is for the cubic case, but the method is easily adapted to the other crystal classes.

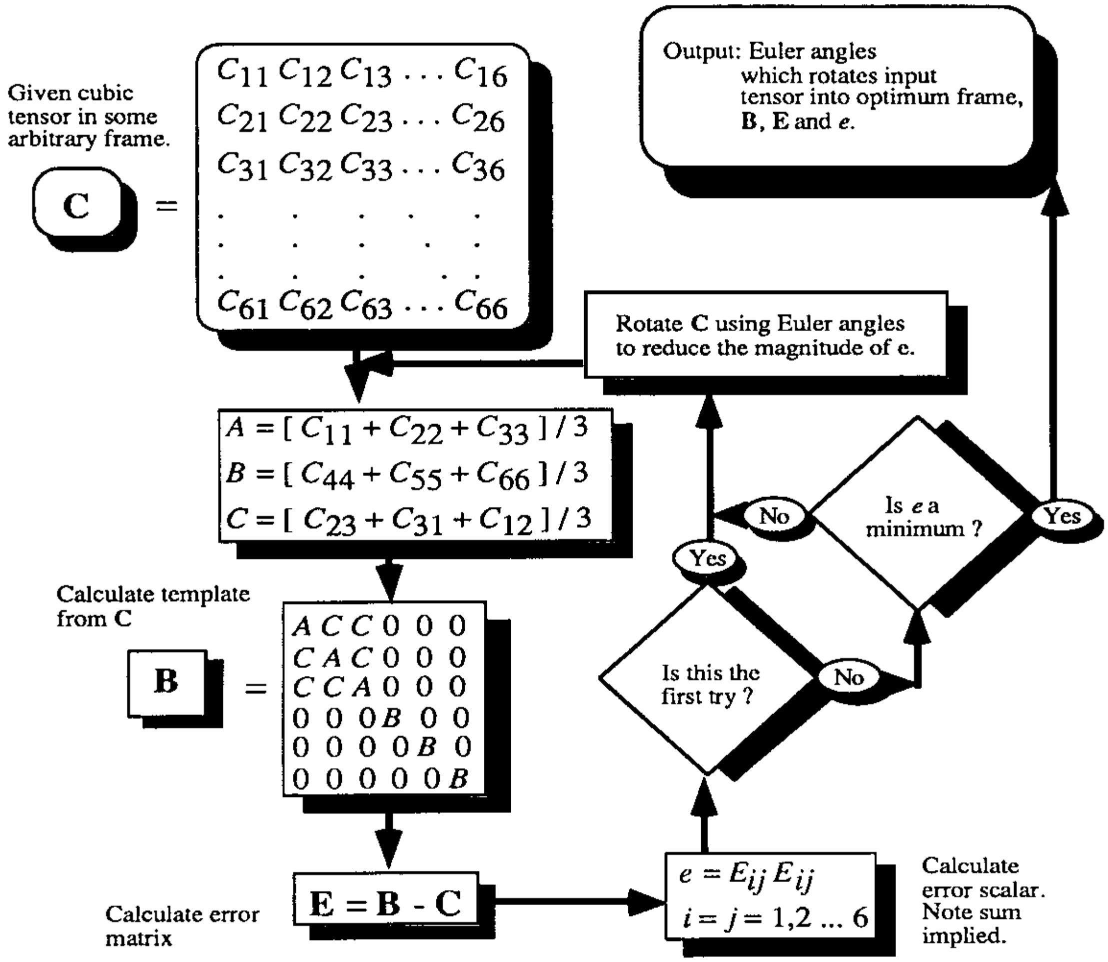


FIG. 1: Flowchart indicating the method used to rotate elastic tensors in arbitrary frames of reference to their preferred frames of reference (Cubic example).

## NUMERICAL TRIAL

The numerical trial begins with a specific cubic elastic tensor in one of its preferred frames and represented in the standard 6x6 matrix notation as:

$$\mathbf{C} = \begin{bmatrix} 3.1500 & 1.8500 & 1.8500 & 0.0000 & 0.0000 & 0.0000 \\ 1.8500 & 3.1500 & 1.8500 & 0.0000 & 0.0000 & 0.0000 \\ 1.8500 & 1.8500 & 3.1500 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 2.5000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 2.5000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 2.5000 \end{bmatrix}. \qquad (1)$$

The frame of reference is then rotated by the Euler angles $\theta = 35^\circ$, $\varphi = 16^\circ$, and $\psi = 52^\circ$. This results in a matrix representation of **C** very different from equation (1), as shown below:

$$\mathbf{C}' = \begin{bmatrix} 3.5169 & 1.8237 & 1.5094 & 0.0003 & 0.7344 & -0.1172 \\ 1.8237 & 3.3647 & 1.6616 & 0.5416 & -0.0610 & 0.2429 \\ 1.5094 & 1.6616 & 3.6789 & -0.5419 & -0.6734 & -0.1257 \\ 0.0003 & 0.5416 & -0.5419 & 2.3116 & -0.1257 & -0.0610 \\ 0.7344 & -0.0610 & -0.6734 & -0.1257 & 2.1594 & 0.0003 \\ -0.1172 & 0.2429 & -0.1257 & -0.0610 & 0.0003 & 2.4737 \end{bmatrix}. \tag{2}$$

The prime symbol in equation (2) indicates that a rotation of the frame of reference has occurrred, but we must keep in mind that we are still dealing with the same tensor. As can be seen by the representation of tensor **C** in equation (2), it would be difficult to determine what symmetries, if any, may exist for this tensor. Following the recipe of flowchart 1 we calculate the template associated with $\mathbf{C}'$ as given by equation (2). This results in:

$$\mathbf{B}_1 = \begin{bmatrix} 3.5202 & 1.6649 & 1.6649 & 0.0000 & 0.0000 & 0.0000 \\ 1.6649 & 3.5202 & 1.6649 & 0.0000 & 0.0000 & 0.0000 \\ 1.6649 & 1.6649 & 3.5202 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 2.3149 & 0.0000 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 2.3149 & 0.0000 \\ 0.0000 & 0.0000 & 0.0000 & 0.0000 & 0.0000 & 2.3149 \end{bmatrix}, \tag{3}$$

where the subscript 1 indicates the template associated with the first iteration and no rotations have been applied to equation (2). By direct comparison with equation (1) we can see that there is a large difference. The error scalar associated with this template is $e = 3.580657$, which is rather large. We now attempt to find rotations which will minimize the error scalar. At each stage of minimization a new rotated realization of the elastic tensor $\mathbf{C}'$ is calculated, as well as its associated template. This procedure is repeated until our optimization criterion is met. For this case, 14 iterations were necessary to satisfy the optimization criterion. At this point the Euler angles were found to be $\theta = -52.000027$, $\varphi = -16.000008$, and $\psi = 55.000027$. When these Euler angles are used to rotate equation (2), the following results:

$$\mathbf{C}' = \begin{bmatrix} 3.1500 & 1.8500 & 1.8500 & -0.0000 & -0.0000 & 0.0000 \\ 1.8500 & 3.1500 & 1.8500 & 0.0000 & -0.0000 & -0.0000 \\ 1.8500 & 1.8500 & 3.1500 & -0.0000 & 0.0000 & 0.0000 \\ -0.0000 & 0.0000 & -0.0000 & 2.5000 & 0.0000 & 0.0000 \\ -0.0000 & -0.0000 & 0.0000 & 0.0000 & 2.5000 & -0.0000 \\ 0.0000 & -0.0000 & 0.0000 & 0.0000 & -0.0000 & 2.5000 \end{bmatrix}. \tag{4}$$

By directly comparing $\mathbf{C}'$ of equation (4) to **C** of equation (1) we find that they are identical. The error scalar is zero up to the fourth decimal place. We have come full circle and found a set of Euler angles which will give a reference frame in which our elastic tensor will have a representation in its standard form.

## CONCLUSION

A simple method to find the preferred frame of reference of an elastic tensor was shown to work with cubic tensors. A particular numerical trial was shown.

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## REFERENCES

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