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ROTATION TRANSFORMATIONS FOR TWO-DIMENSIONAL CALCULATIONS

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Abstract—In two-dimensional wave propagation and structural calculations, adjustments are made at each time step to account for the rotation of the material. These adjustments rotate the stress tensor; rotate micro features, such as cracks, with the material; and provide an average rotation angle for the material. Here the nature of the rotation problem and the inaccuracies inherent in the standard Jaumann method for cases of large shear are outlined. A direct method for obtaining the rotation θ of the cell material is described based on the works of Dienes (*Acta Mech.* **32**, 217–232 (1979)) and of Marsden and Hughes (*Mathematical Foundations of Elasticity*, Prentice-Hall, Englewood Cliffs, New Jersey (1983)). Techniques are formulated for rezoning the quantities used in the rotation transformation: one is an exact method based on the invariants of the U matrix; others are approximations based on the components of the U and F matrices. To further explore the nature of the Dienes method, an exact method is developed for the rotation of lines or planes or micro features in the material. The Dienes rotation techniques considered here are necessary under conditions of large shear strain for isotropic and simple anisotropic elastic materials in which all the material is assumed to rotate together. For materials in which yielding occurs, the stresses are correctly provided by the standard Jaumann method, although the rotation angle is not correct for large rotations. For multiple-plane models in which specific planes in the material are followed, neither the Jaumann nor the Dienes rotation treatments are appropriate.

1. INTRODUCTION

Rotation adjustments that are made at each time increment in two-dimensional wave propagation and structural calculations should account for three effects.

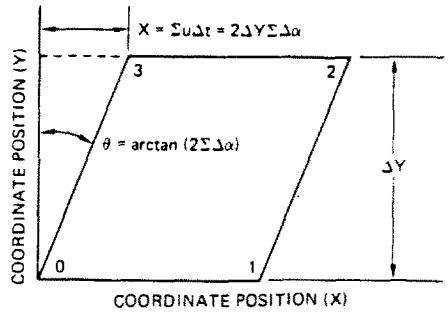
(1) The stress tensor is transformed to account for the material rotation.
(2) Micro features, such as cracks, are rotated with the material.
(3) To aid in understanding the results of calculations, the average rotation of the cell material is computed.

Treatments for these rotation topics are reviewed in the present study. Because the conditions that cause large rotations also require a rezoning treatment in the calculations, means were examined for combining a precise rotation procedure with rezoning. Then a study was made to determine which types of material models and which kinds of problems require rotation adjustments.

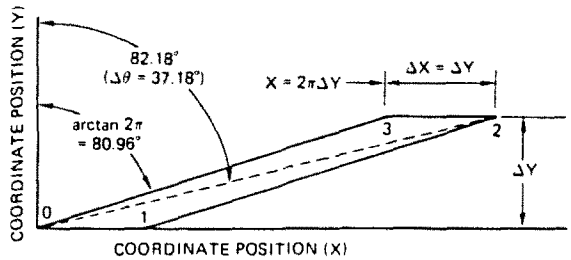
In the last two decades it has been generally recognized that material rotation must be accounted for in stress–strain calculations, or the computed stress tensor will depend on its coordinate system. At present, rotations are commonly accounted for by using the Jaumann rotation rate computed from the coordinate motions of the computational cell

$$\Delta\alpha = (\partial u/\partial y - \partial v/\partial x)\Delta t/2 \tag{1}$$

where $\Delta\alpha$ is the increment of rotation in radians, and u and v are coordinate velocities in the x- and y-directions. In wave propagation codes such as HEMP by Wilkins (1964), these rotation corrections are made by transforming the stress tensor in each cell through the angle $-\Delta\alpha$ so that the tensor remains in the fixed external coordinate system as the material rotates. This Jaumann rotation correction has recently been found to be appropriate only for small shear strains (see, e.g. Dienes (1979)).



(a) Distorted Block After Several Strain Increments



(b) Configuration for $\Sigma\Delta\alpha = \pi$

Fig. 1. Changes in the orientation of lines in a block which has undergone a cumulative deformation, $2\Sigma\Delta\alpha$ of 360°.

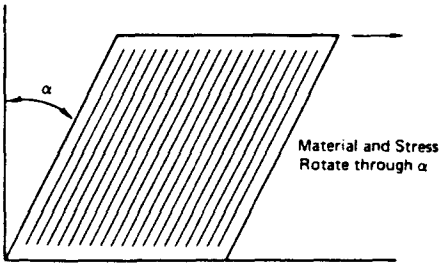
To indicate the nature of the approximation involved in eqn (1), consider a block subjected to simple shear, as shown in Fig. 1(a). The block is sheared by moving points 2 and 3 by $u\Delta t$. From eqn (1), the rotation is

$$\Delta\alpha = \frac{u\Delta t}{2\Delta Y}. \tag{2}$$

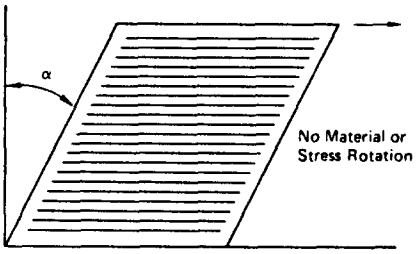
The diagonals of the square rotate by this amount. Yet line 03 rotates by $(u\Delta t)/(\Delta Y) = 2\Delta\alpha$, and line 01 does not rotate. Hence, the combination of shear with rotation appears to produce a complex state in which different elements rotate differently. Thus $\Delta\alpha$ from eqn (2) is only an "average" rotation for the material.

For an example of the difficulty with large rotation problems, consider the case where the incremental motion in Fig. 1(a) gives an angular change of $\Delta\alpha = 1°$. Then continue the motion for 180 increments. Line 03 rotates by about 2° per increment initially. But as it moves from the vertical, the angular change per increment reduces. Line 02 initially rotates by $\Delta\alpha$ per increment; hence, the rotation of this line matches the "average" rotation. But this line also moves away from 45° and so thereafter its rotations are less than $\Delta\alpha$ per increment. The state after 180° of motion is shown in Fig. 1(b). Equations (1) and (2) would give a total angular change of 180°. Yet from Fig. 1(b), it is clear that none of the bounding lines rotated more than 90°, so the average rotation must be less than 45°. (The actual average rotation is about 38°.)

In the foregoing discussion the rotation could be viewed as following crystallographic planes on which the stress acts or as simply following material lines. Thus, it is assumed that the stress tensor follows these planes or lines. Therefore, the stress rotation calculations are made to follow the motion of the planes. However, as pointed out by Drucker (1985), when plastic slip occurs in the material, the crystallographic planes do not follow the macroscopic motion of the material. This ambiguity between the macroscopic motion and the rotation of the planes is illustrated in Fig. 2. The upper part of the figure shows a large shear flow within a crystallographic material with vertical slip lines. Here, for an average differential rotation of $\Delta\alpha$, the lines rotate by $2\Delta\alpha$, and the stress tensor should rotate with these lines. In the lower part of the figure, the slip occurs along the horizontal lines and no rotation occurs in the lines. From the usual macroscopic description of the cell and of the



(a) Simple shear with slip along lines that are initially vertical.



(b) Simple shear with slip along lines that are horizontal.

Fig. 2. Alternate patterns for slip in a crystal with consequent effects on material and stress rotation.

material, one cannot distinguish between these two responses of the material to shear. It would require a detailed theory of plastic flow that includes the rotation of the individual planes in the material (and therefore the development of anisotropy) to distinguish the two behaviors shown in Fig. 2. In the following sections it is assumed that the material remains homogeneous and isotropic throughout the flow, and Drucker's important physical question is temporarily disregarded. His point will be returned to in Section 7.

This paper first presents a review of three recent analyses of the rotation problem. Steps for conducting the analysis are recommended and methods for rezoning the quantities needed in the rotation procedure are discussed. The procedure for the rotation of lines and of the stress tensor are derived separately. Finally, through use of the procedure, the conditions under which the procedure is important are determined.

2. BACKGROUND

Recent work has been done by Dienes (1979), Marsden and Hughes (1983), and Hallquist (1983) in determining the appropriate transformations to undertake to handle the rotation of material undergoing large shear deformations.

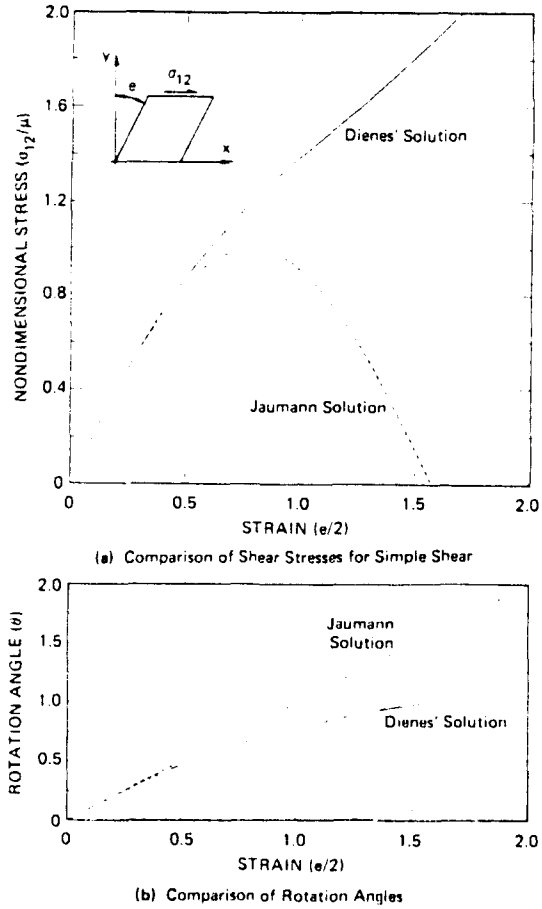
Dienes (1979) has developed a three-dimensional analysis for material rotation, considering the corrections required to transform the stress tensor and determine the correct angle. The analysis was applied to elastic material initially; however, he has noted that the concept is appropriate for any rotation, elastic or plastic. His corrections to the stress tensor take the same form as the Jaumann equations

$$\dot{\sigma} = \dot{\sigma} - \Omega\sigma + \sigma\Omega \tag{3}$$

where $\dot{\sigma}$ is the stress rate tensor corrected for rotation, $\dot{\sigma}$ the stress rate directly from the constitutive equation, and Ω the tensor representing the angular velocity of the material

$$\Omega = \dot{\mathbf{R}}\mathbf{R}^{\mathrm{T}} \tag{4}$$

where $\mathbf{R}$ is the rotation tensor (defined later). Figure 3 (from Dienes' text) shows that σ_{12} grows monotonically with shear strain when Dienes' correction is used, whereas with the traditional Jaumann method the stress oscillates for very large strains.



(a) Comparison of Shear Stresses for Simple Shear

(b) Comparison of Rotation Angles

Fig. 3. Comparison of shear stress and angle of rotation computed by the methods of Dienes and Jaumann in simple shear.

The method outlined by Dienes (1979) is now considered in some detail for determining the rotation of the material of a cell from the locations and velocities of the material. He begins with the deformation and velocity gradient matrices. The problem is solved for the general three-dimensional case, but attention is restricted to a two-dimensional problem. First a description of his solution is presented, then a method based on the development, and finally the numerical procedure he recommends.

Dienes' method begins with the deformation matrix **F** with components

$$F_{ij} = \frac{\partial X_i}{\partial \xi_j} \tag{5}$$

where X_i is the current coordinate and ξ_j the original Eulerian position. Next Dienes derives the material rotation $\boldsymbol{\Omega}$ from the vorticity **W**, left stretch matrix **V**, and the deformation rate matrix **D**. The vorticity and deformation rate matrices are both obtained from the velocity gradient **G**

$$G_{ij} = \frac{\partial u_i}{\partial X_j} \tag{6}$$

where u_i is the velocity in the ith direction. As Dienes also shows, **G** is related to the deformation gradient as follows:

$$\mathbf{G} = \dot{\mathbf{F}}\mathbf{F}^{\mathrm{T}}. \tag{7}$$

The deformation rate matrix **D** is

$$D_{ij} = 1/2(G_{ij} + G_{ji}) \tag{8}$$

and the vorticity **W** is

$$W_{ij} = 1/2(G_{ij} - G_{ji}). \tag{9}$$

The vorticity is the rotation quantity customarily used with the Jaumann rotation computation.

The left stretch matrix **V** is named for its position in the defining relation

$$\mathbf{F} = \mathbf{VR} \tag{10}$$

where **R** is the rotation tensor. To compute **V**, he forms the product **B**

$$\mathbf{B} = \mathbf{FF}^{\mathrm{T}} \tag{11}$$

from which he derives **V** by the method of Bellman (1960)

$$\mathbf{V} = \mathbf{B}^{1/2}. \tag{12}$$

The rotation tensor **R** is obtained by inverting eqn (10)

$$\mathbf{R} = \mathbf{V}^{-1}\mathbf{F} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}. \tag{13}$$

With this definition of the rotation tensor, the rotation is positive counterclockwise. From the **D** and **V** matrices he defines two more matrices

$$\mathbf{Z} = \mathbf{DV} - \mathbf{VD} \tag{14}$$

and

$$\mathbf{S} = [\mathbf{I}\,\mathrm{tr}(\mathbf{V}) - \mathbf{V}]^{-1}. \tag{15}$$

His angular velocity of the material axes, ω ($=\Omega_{21}$) is then given by

$$\omega = W_{21} + S_{33}Z_{21}. \tag{16}$$

Thus the SZ term acts as a correction to the rotation W which is customarily used in the Jaumann rate equations.

In his paper Dienes gave the following steps for computing the rotation in a computer code, but did not recommend this procedure.

(1) Compute the current $\mathbf{F}^n$ and $\mathbf{G}^{n+1/2}$ from the nodal positions and velocities. Evaluate $\mathbf{D}^{n+1/2}$ and $\mathbf{W}^{n+1/2}$ from $\mathbf{G}^{n+1/2}$. Here n refers to the beginning of the time step, so quantities labeled $n+1/2$ are defined at the middle of the time step.

(2) Compute $\mathbf{V}^n$ from the square root of $\mathbf{FF}^{\mathrm{T}}$ (eqns (11) and (12)).

(3) Compute $\mathbf{R}^n$ and θ^n from eqn (13).

(4) Compute $\mathbf{S}^{n+1/2}$ and $\mathbf{Z}^{n+1/2}$ from $\mathbf{V}^n$ and $\mathbf{D}^{n+1/2}$ (eqns (14) and (15)).

(5) Compute $\omega^{n+1/2}$ from eqn (16).

This procedure requires computation of the **F** matrix (hence, storage of the original Eulerian coordinate ξ). The time consuming steps are the computation of the square root of $\mathbf{F}\mathbf{F}^{\mathrm{T}}$ and the matrix inversion for determining **S**. The procedure is very accurate.

Dienes recommended a second procedure with the following steps.

(1) Compute $\mathbf{G}^{n+1/2}$ and then $\mathbf{W}^{n+1/2}$ from $\mathbf{G}^{n+1/2}$ (eqns (6) and (9)).
(2) Compute $\mathbf{Z}^{n+1/2}$ from $\mathbf{V}^n$ and $\mathbf{D}^{n+1/2}$ (eqn (14)).
(3) Calculate $\mathbf{S}^n$ from $\mathbf{V}^n$ (eqn (15)).
(4) Obtain $\dot{\mathbf{V}}^{n+1/2}$ from $\mathbf{G}^{n+1/2}\mathbf{V}^n - \mathbf{V}^n(\mathbf{W}^{n+1/2} + \mathbf{S}^n\mathbf{Z}^{n+1/2})$ (Dienes' eqn (7.5)).
(5) Update $\mathbf{V}^{n+1}$ from $\mathbf{V}^n$ and $\dot{\mathbf{V}}^{n+1/2}$.
(6) Compute the angular velocity ω from eqn (16).

This method requires storage of **V**, but not of the original Eulerian coordinates. The lengthy calculation is the matrix inversion in step 3. This second method is also very accurate. Note that in both of these approaches Dienes gets the rotation quantity $\omega = \dot{\theta}$ explicitly, and in the first method, θ and **R** are also obtained.

Marsden and Hughes (1983) have suggested a simplified way to obtain the stretch matrix from the **B** matrix. Instead of computing **V**, they obtain the right stretch matrix **U**. This matrix is defined by

$$\mathbf{F} = \mathbf{R}\mathbf{U}. \tag{17}$$

They begin the computation by forming the product matrix **C**

$$\mathbf{C} = \mathbf{F}^{\mathrm{T}}\mathbf{F}. \tag{18}$$

Then **U** is given by

$$\mathbf{U} = \frac{\mathbf{C} + \sqrt{(\det \mathbf{C})}}{\sqrt{(\operatorname{tr}\mathbf{C} + 2\sqrt{(\det \mathbf{C})})}}. \tag{19}$$

Thus their method has the following steps.

(1) Compute $\dot{\mathbf{F}}^n$ from $\mathbf{G}^{n+1/2}$ and $\mathbf{F}^n$ from eqn (7), and evaluate $\mathbf{F}^{n+1} = \mathbf{F}^n + \dot{\mathbf{F}}^n\Delta t$.
(2) Compute $\mathbf{U}^{n+1}$ from $\mathbf{F}^{n+1}$ as in eqn (19).
(3) Compute $\mathbf{R}^{n+1} = \mathbf{F}^{n+1}(\mathbf{U}^{n+1})^{-1}$.

Marsden and Hughes do not explicitly compute θ or ω because they are not needed for the rotation of the stress tensor.

Hallquist (1983) uses the method of Marsden and Hughes (1983) in his NIKE2D code. In this finite element code he computes the $\mathbf{R}^n$, $\mathbf{R}^{n+1/2}$, and $\mathbf{R}^{n+1}$ rotation tensors. With $\mathbf{R}^n$ he rotates the initial stress tensor $\boldsymbol{\sigma}^n$ from the external coordinate system to the material orientation. The strain increment $\Delta\boldsymbol{\varepsilon}^{n+1/2}$ is rotated to the material orientation with $\mathbf{R}^{n+1/2}$. Then $\boldsymbol{\sigma}^{n+1}$ is computed by the material model, and the stress tensor is transformed back to the external coordinate system. **R** is not stored between cycles, so the three-step procedure above is performed three times at each cell and each cycle.

From the foregoing it appears that there are procedures available to transform the stress tensor and to follow the rotation of the cell material. However, it is not clear how these methods can be used under conditions in which rezoning is also being used. The rotation procedures with rezoning are examined in a later section.

3. AVERAGE CELL ROTATION IN TWO-DIMENSIONAL CALCULATIONS

In this section a practical means for performing the rotation calculation is developed. Later, in Section 7, conditions for which this procedure is appropriate are considered. The following requirements will be considered for judging the system to be practical:

(a) only the current nodal positions and velocities are required, but not a history of these quantities;

(b) the system should minimize the computational time and the additional storage;

(c) the system must permit standard rezoning procedures to occur, that is, rezoning should not disturb the rotation calculation, and the new variables required (if any) must be rezonable.

The method proposed here begins with the computation of the matrices $\mathbf{G}^{n+1/2}$, $\dot{\mathbf{F}}^{n+1/2}$, and $\mathbf{F}^{n+1}$. Then θ is computed from the polar decomposition theorem. From θ and the stored value of θ_0 the increment $\Delta\theta$ is computed. The rezoning aspect of this calculation is treated in the next section. Here the definition of the deformation matrix $\mathbf{F}$, the computation of θ, and tests of the procedure are examined.

3.1. *Deformation matrix calculation*

The deformation matrix defined in eqn (5) must be determined in a way that is natural for the finite-difference codes. To begin, the current coordinates X_i are written as functions of the initial coordinates (ξ and η) and time

$$X_i = f_i(\xi, \eta, t) \tag{20}$$

and this function is computed by fitting it to the nodes around a cell at some time. A single function $\mathbf{F}$ is required that represents the cell material, yet the function must be fitted to the K nodes around the cell. For this fitting purpose one could define the function X_{ik}, the X_i value at the kth node, by the series

$$X_{ik} = A_{i0} + A_{i1}\xi + A_{i2}\eta + A_{i3}\xi\eta + A_{i4}\xi^2 + A_{i5}\eta^2 + \cdots \tag{21}$$

where A_{im} are constants obtained by the fitting process. By differentiating eqn (21) for X_i with respect to ξ or η, the deformation gradient F_{ij} is obtained according to eqn (5). For a four-node cell, these components of $\mathbf{F}$ are

$$\begin{aligned}
F_{11} &= \frac{\partial x}{\partial \xi} = \frac{x_{13}\eta_{24} - x_{24}\eta_{13}}{A_0 + A_1} \\
F_{12} &= \frac{\partial x}{\partial \eta} = \frac{x_{24}\xi_{13} - x_{13}\xi_{24}}{A_0 + A_1} \\
F_{21} &= \frac{\partial y}{\partial \xi} = \frac{y_{13}\eta_{24} - y_{24}\eta_{13}}{A_0 + A_1} \\
F_{22} &= \frac{\partial y}{\partial \eta} = \frac{y_{24}\xi_{13} - y_{13}\xi_{24}}{A_0 + A_1}
\end{aligned} \tag{22}$$

where $x_{mn} = x_m - x_n$, $\xi_{mn} = \xi_m - \xi_n$, and m and n refer to node numbers. The A_0 and A_1 factors are the areas of the cell at the beginning and end of the increment. Clearly, in this method the original coordinates ξ_m and η_m must be retained for all cells. Yet these original coordinates are not rezonable quantities, so this method of computing F cannot be used with rezoning.

An alternate method for determining $\mathbf{F}$ is to start with an initial value, and update it at each time step in the calculation using $\dot{\mathbf{F}}$ computed from eqn (7)

$$\dot{\mathbf{F}}^{n+1/2} \approx \mathbf{G}^{n+1/2}(\mathbf{F}^{-1})^n \tag{23}$$

where n indicates that these matrices are from the nth time step. The $\dot{\mathbf{F}}$ factor is not exactly centered in this calculation. The $\mathbf{F}$ at the next time step is calculated using $\dot{\mathbf{F}}$

$$\mathbf{F}^{n+1} = \mathbf{F}^n + \dot{\mathbf{F}}^{n+1/2}\Delta t. \tag{24}$$

This second method, using $\dot{\mathbf{F}}$, seems the most direct, but requires storage of $\mathbf{F}$ from the previous cycle. This method of computing $\mathbf{F}$ is chosen for the procedure.

3.2. *Computation of the rotation angle* θ

For computing the rotation angle θ the left and right stretch matrices $\mathbf{V}$ and $\mathbf{U}$, and the rotation tensor $\mathbf{R}$ are considered. Because of the symmetry of $\mathbf{V}$ and $\mathbf{U}$, and because $\mathbf{R}$ represents a counterclockwise rotation of θ, one can recognize that one can write these matrices in the following way:

$$\mathbf{V} = \begin{bmatrix} V_{11} & V_{12} \\ V_{12} & V_{22} \end{bmatrix}, \quad \mathbf{U} = \begin{bmatrix} U_{11} & U_{12} \\ U_{12} & U_{22} \end{bmatrix} \text{ and } \mathbf{R} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}. \tag{25}$$

Equations (10) and (17) can be written out term by term and solved for the unknown components $\mathbf{V}$, $\mathbf{U}$, and $\mathbf{R}$

$$\begin{aligned} F_{11} &= V_{11}\cos\theta + V_{12}\sin\theta = U_{11}\cos\theta - U_{12}\sin\theta \\ F_{12} &= -V_{11}\sin\theta + V_{12}\cos\theta = U_{12}\cos\theta - U_{22}\sin\theta \\ F_{21} &= V_{12}\cos\theta + V_{22}\sin\theta = U_{11}\sin\theta + U_{12}\cos\theta \\ F_{22} &= -V_{12}\sin\theta + V_{22}\cos\theta = U_{12}\sin\theta + U_{22}\cos\theta. \end{aligned} \tag{26}$$

The solution of either set of four simultaneous equations leads to

$$\tan\theta = \frac{F_{21} - F_{12}}{F_{11} + F_{22}}. \tag{27}$$

The angle θ can be obtained with the arctangent function or, for small angles, with the series expansion for arctan θ.

To find the rotation rate ω, the current orientation θ of the material is first computed from tan θ (eqn (27)). Then

$$\omega \approx \frac{\theta - \theta_0}{\Delta t} \tag{28}$$

where θ_0 is the orientation at the previous cycle.

3.3. *Computation of* $\mathbf{V}$, $\mathbf{U}$, *and* $\mathbf{R}$

For the rezoning procedures considered later it may be necessary to obtain the $\mathbf{V}$ and $\mathbf{U}$ matrices, and the $\mathbf{R}$ tensor. If these are of interest, one can proceed as follows. The sine and cosine factors in $\mathbf{R}$ can be computed from components of the deformation matrix, using eqns (26)

$$\sin\theta = \frac{F_{21} - F_{12}}{\sqrt{((F_{21} - F_{12})^2 + (F_{11} + F_{22})^2)}}. \tag{29a}$$

$$\cos\theta = \frac{F_{11} + F_{22}}{\sqrt{((F_{21} - F_{12})^2 + (F_{11} + F_{22})^2)}}. \tag{29b}$$

With the sine and cosine available, one can simply solve for the $\mathbf{V}$ components from eqns (26)

$$
\begin{aligned}
V_{11} &= F_{11}\cos\theta - F_{12}\sin\theta \\
V_{12} &= F_{11}\sin\theta + F_{12}\cos\theta \\
&= F_{21}\cos\theta - F_{22}\sin\theta \\
V_{22} &= F_{21}\sin\theta + F_{22}\cos\theta.
\end{aligned} \tag{30}
$$

The U components are

$$
\begin{aligned}
U_{11} &= F_{11}\cos\theta + F_{21}\sin\theta \\
U_{12} &= -F_{11}\sin\theta + F_{21}\cos\theta \\
&= F_{12}\cos\theta + F_{22}\sin\theta \\
U_{22} &= -F_{12}\sin\theta + F_{22}\cos\theta.
\end{aligned} \tag{31}
$$

An alternate procedure to the above would involve using Hughes' method of finding **U** by taking the square root of $\mathbf{F}^{\mathrm{T}}\mathbf{F}$: the results are identical.

3.4. *Summary of the method*

In summary, the strategy suggested for two-dimensional problems differs slightly from those of Dienes and Hughes. One is interested mainly in obtaining the rotation angle θ and the increment $\Delta\theta$. In this method it is necessary to store the full **F** matrix and the rotation θ. During each time step one makes the following computations.

(1) Compute **G** (eqn (6)), and evaluate **D** (eqn (8)) and **W** (eqn (9)) from it.

(2) Using **G** and the stored **F**, compute $\dot{\mathbf{F}}$ (eqn (23)), and evaluate the current **F** matrix (eqn (24)).

(3) Compute $\tan\theta$ (eqn (27)) and evaluate θ. Adjust θ as needed to account for the ambiguity of the arctangent.

(4) Compute the increment of rotation from $\Delta\theta = \theta - \theta_0$.

(5) Perform the stress rotation calculations using $\Delta\theta$ in the same way that one generally used W_{12}.

The stress rotation calculations have the form

$$
\begin{aligned}
\sigma_{xx} &= \sigma_{xx0} - 2\sigma_{xy0}\Delta\theta \\
\sigma_{yy} &= \sigma_{yy0} + 2\sigma_{xy0}\Delta\theta \\
\sigma_{zz} &= \sigma_{zz0} \\
\sigma_{xy} &= \sigma_{xy0} + (\sigma_{xx0} - \sigma_{yy0})\Delta\theta.
\end{aligned} \tag{32}
$$

This new procedure requires five storage locations per cell (four Fs and θ) in addition to those for the usual Jaumann computations. The computation time for the procedure is mainly taken by the additional square root (eqn (29)) and the arctangent.

3.5. *Tests of the rotation procedure*

A number of tests were made on the foregoing rotation procedure to evaluate its accuracy and speed, and especially to determine whether it works correctly for very large angles. The following problems were run.

(1) Apply a uniform tension to a body and then gradually rotate the body, computing the current stress tensor at each step. This is a rigid body rotation so the angle and stress tensor should be obtainable even using the Jaumann method with $\omega = W_{21}$.

(2) Extend a block gradually while rotating it. This problem includes some rigid body rotation, yet is a more complex test. The results should match those of test 1 at the end point.

(3) Shear a block in simple shear and follow the computed orientation θ and the stress tensor.

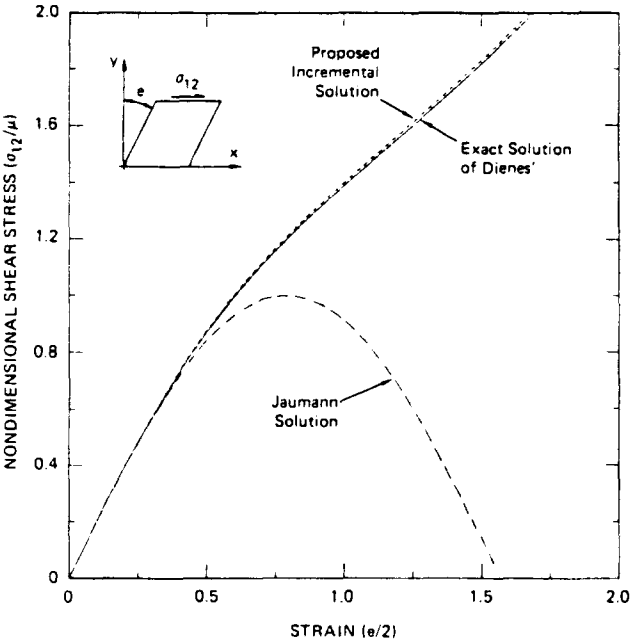


Fig. 4. Comparison of shear stress computed incrementally by the proposed method with the exact solution.

(4) Shear a block during rotation and follow the orientation and stress tensor.

These tests were all performed using the foregoing procedure. In each case 400 steps were used and the stresses and orientation θ were examined at several intermediate steps as well as at the end. The rotation was through an angle of 360°. In all cases the value of θ obtained was within 0.1% of the exact value. The error was found to be directly related to the imposed angular increment. The stress computation obtained in simple shear is shown in Fig. 4, and compared with the exact solution of Dienes.

4. REZONING OF THE ROTATION QUANTITIES

During a large distortion computation it is usually necessary to rezone the cells, that is, to construct a new mesh with less distortion in the individual cells. After the new mesh is constructed, the properties in the old cells are assigned to the new cells. Generally, each new cell will contain some material from two or more of the old cells. The properties (energy, pressure, stress tensor, yield strength, plastic strain, etc.) of the mixed materials in the new cell are computed by weighting each property according to the mass contributed by the old cell. For example, property P is computed from

$$P_{\text{new}} = \frac{\sum_{k=1}^{K} m_k P_k}{\sum_{k=1}^{K} m_k} \tag{33}$$

where m_k is the mass contributed by the kth old cell to the new cell. This mass-weighting method is essentially an averaging technique, and thus it causes some smearing of the properties during rezoning.

To fit into the rezoning procedure, it is essential that the variables used in the rotation calculation be rezonable in a manner like that in eqn (33). The matrices **F** and **V** (or **U**), and the scalar θ have been selected as candidates for rezoning. The angle θ is scalar and represents a physical quantity which can be appropriately averaged in combining properties from two groups; hence the angle is rezonable.

The stretch matrices each represent the state of distortion in the cell material. Following Dienes (1979), they can be diagonalized as follows:

$$\mathbf{U} = \mathbf{T}\Lambda\mathbf{T}^{-1} \tag{34}$$

where Λ is diagonal, and $\mathbf{T}$ represents an orthogonal transformation. Hence the fundamental information contained in $\mathbf{V}$ or $\mathbf{U}$ is Λ_{11}, Λ_{22}, and the transformation angle α associated with $\mathbf{T}$, where

$$\mathbf{T} = \begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix}. \tag{35}$$

These three quantities (Λ_{11}, Λ_{22}, and α) meet the criteria for averageable quantities, and therefore are rezonable. An alternate set of independent quantities are the trace and determinant of $\mathbf{U}$, and the angle α. Here the determinant of $\mathbf{U}$ has the physical meaning of the exponential of the areal strain, and hence, it is a quantity that one may especially want to preserve during rezoning. The five quantities are all readily computed from the $\mathbf{U}$ matrix

$$\text{trace}\,\mathbf{U} = \text{tr}\,\mathbf{U} = U_{11} + U_{22} \tag{36}$$

$$\text{determinant}\,\mathbf{U} = \det\mathbf{U} = U_{11}U_{22} - U_{12}^2 \tag{37}$$

$$\Lambda_{11}, \Lambda_{22} = \frac{\text{tr}\,\mathbf{U}}{2} \pm \sqrt{\left(\frac{1}{4}(\text{tr}\,\mathbf{U})^2 - \det\mathbf{U}\right)} \tag{38}$$

$$\alpha = \frac{1}{2}\arctan\frac{2U_{12}}{U_{11} - U_{22}}. \tag{39}$$

Similar rezoning results are obtained by using the set Λ_{11}, Λ_{22}, and α or the set tr $\mathbf{U}$, det $\mathbf{U}$, and α. Following the rezoning of these invariants, the new $\mathbf{U}$ matrix is constructed by computing $\mathbf{U} = \mathbf{T}\Lambda\mathbf{T}^{-1}$ with the new Λ and $\mathbf{T}$ (from α) tensors.

The foregoing is clearly a lengthy procedure so it is worthwhile to form an approximate method. For a first approximation, one may choose to rezone the U_{ij} components, yet preserve the areal strain (det $\mathbf{U}$). To start the calculation $\mathbf{U}$ is computed from $\mathbf{F}$ using either eqn (19) or (31). Then the areal strain factor $A = \det\mathbf{U}$ is computed and a $\mathbf{u}$ matrix with reduced components is generated

$$u_{ij} = U_{ij}/\sqrt{A}. \tag{40}$$

These reduced $\mathbf{u}$ matrices are then used in the rezoning process to form a reduced matrix for the new cell

$$u_{ij_z} = \frac{\sum m_k U_{ijk}/\sqrt{A_k}}{\sum m_k}. \tag{41}$$

Next the determinant $A_z = \det u_{ij_z}$ is computed and the areal strain factor from the old cells is rezoned

$$\bar{A} = \frac{\sum m_k A_k}{\sum m_k}. \tag{42}$$

Finally the $\mathbf{U}$ matrix for the new cell is formed

$$U_{ij} = u_{ijs}\sqrt{(\bar{A}/A_s)}. \tag{43}$$

In this way the new **U** has a mass-weighted areal strain. This rezoning method was tested for cases in which there were large rotations combined with either extension or shear. For 180° differences between rotations of the old cells, the **U** matrix components for the new cell were all within 1% of the exact value for the extension case and within 10% of the exact value for the shearing case. For the usual strain and rotation levels, this procedure should be satisfactory.

A simpler and faster rezoning approximation can be made by rezoning the **F** components directly. The determinant of **F** also equals the exponential of the areal strain, so one can preserve the areal strain using a procedure like that above. As with the **U** matrix, one starts by calculating the reduced components of **F** for the new cell

$$F_{ijs} = \frac{\sum m_k F_{ijk}/\sqrt{A_k}}{\sum m_k}. \tag{44}$$

The areal strain factor for the reduced F matrix is computed: $A_s = \det F_{ijs}$. Then the components of the F matrix for the new cell

$$\bar{F}_{ij} = F_{ijs}\sqrt{(\bar{A}/A_s)}. \tag{45}$$

Rezoning tests with the **F** components showed that nonsense was obtained when old cells with rotations that differed by 180° were used. Errors of approximately 10% in the **F** components were obtained when the rotations of the old cells were within 45°, for either extension or shearing. Hence, the use of **F** in rezoning could only be considered satisfactory for fairly small angular differences between old cells.

Based on these initial observations a two-branch plan for rezoning was developed, depending on the range in the rotation angles in the old cells contributing to the new cell.

(1) Cells with angular differences less than 20°: mass weight the components of the **F** matrix.

(2) Cells with large angular differences: derive the **U** matrix and θ for each contributing cell. Mass weight **U** and θ. Then recover **F** for the new cell.

5. EFFECT OF YIELDING ON ROTATION

For material that may yield and remain isotropic, the same rotation procedures can be used as for the elastic material. However, the continued straining tends to eliminate the errors in the stress transformation, so the stresses are accurate whether or not they are correctly transformed. The results of an ideal plastic calculation of simple shear with a yield strength of 20% of the shear modulus gave the results shown in Fig. 5. The very large yield value was used to emphasize the importance of errors in the rotation transformation. The exact and Jaumann solutions for stress in the presence of yielding are essentially indistinguishable. However, the angle calculation for the yielded case by the Jaumann method still has the inaccuracy illustrated in Fig. 3(b). Hence, if the rotation angle is not needed, the Jaumann solution is very satisfactory for yielding in isotropic material.

6. DEVELOPMENT OF THE ANALYSIS FOR ROTATION OF LINES

The rotation analysis is developed first for the motion of a line in a linear velocity field. This result is applied to the rotation of material features such as microcracks. Then the line analysis is applied to determine the average rotation of a block undergoing large shear deformation.

A line segment L in a linear velocity field will be stretched (or shortened) and rotated. Consider here only the rotation aspect. The rotation rate $\mathrm{d}\theta/\mathrm{d}t$ is given by the dot product

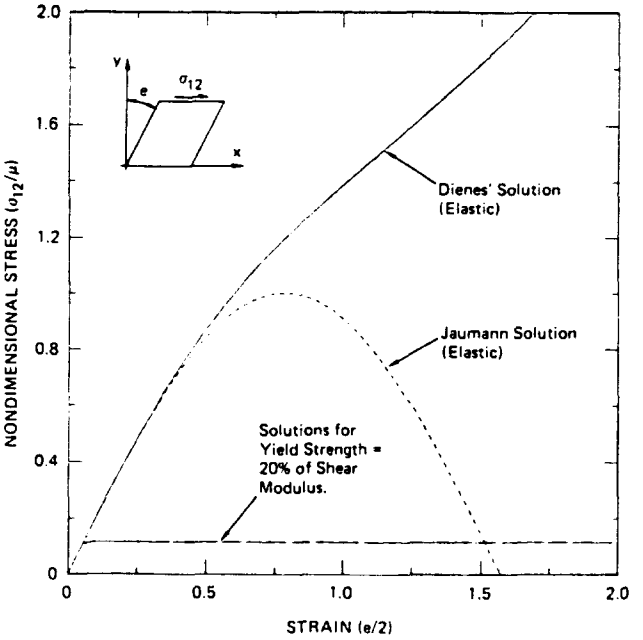


Fig. 5. Comparison of shear stresses from Dienes' and Jaumann's solutions for elastic and plastic cases.

$$\frac{d\theta}{dt} = -\frac{1}{|L|}\frac{d\vec{\delta}\cdot\vec{n}}{dt} \tag{46}$$

where $\vec{n}$ is the unit normal to line L, $\vec{\delta}$ is the displacement of one end of the line with respect to the other, and L is the line length. The linear velocity field is written in terms of velocities u and v in the x- and y-directions. Then $d\vec{\delta}/dt$ can be written in terms of the x- and y-coordinates and the Δx and Δy lengths of the line

$$\frac{1}{|L|}\frac{d\vec{\delta}}{dt} = \vec{i}\frac{(\partial u/\partial x)\Delta x + (\partial u/\partial y)\Delta y}{|L|} + \vec{j}\frac{(\partial v/\partial x)\Delta x + (\partial v/\partial y)\Delta y}{|L|}$$

$$= \vec{i}\left(\frac{\partial u}{\partial x}\cos\theta + \frac{\partial u}{\partial y}\sin\theta\right) + \vec{j}\left(\frac{\partial v}{\partial x}\cos\theta + \frac{\partial v}{\partial y}\sin\theta\right). \tag{47}$$

The angle θ is the angle of the line with respect to the x-coordinate, measured positively counterclockwise. Similarly the normal vector $\vec{n}$ is

$$\vec{n} = \vec{i}\sin\theta - \vec{j}\cos\theta. \tag{48}$$

When the expressions for $d\vec{\delta}/dt$ and $\vec{n}$ are placed in eqn (46), the increment of rotation is obtained

$$\frac{d\theta}{dt} = -\frac{\partial u}{\partial x}\sin\theta\cos\theta - \frac{\partial u}{\partial y}\sin^2\theta + \frac{\partial v}{\partial x}\cos^2\theta + \frac{\partial v}{\partial y}\sin\theta\cos\theta. \tag{49}$$

Equation (49) is used to obtain the rotation for lines or other line-like features in two-dimensional calculations.

Now consider the rotation of several lines in a block of material as a means of obtaining the average rotation of the material. Assume that the block has a large number of lines drawn on it. Then the block is sheared and the motion of the lines is followed. If a simple shear $\omega = dx/dt = \partial u/\partial y$ is applied, then the rotation rate $d\theta/dt$ of a line originally at an angle θ_0 from the X-axis is

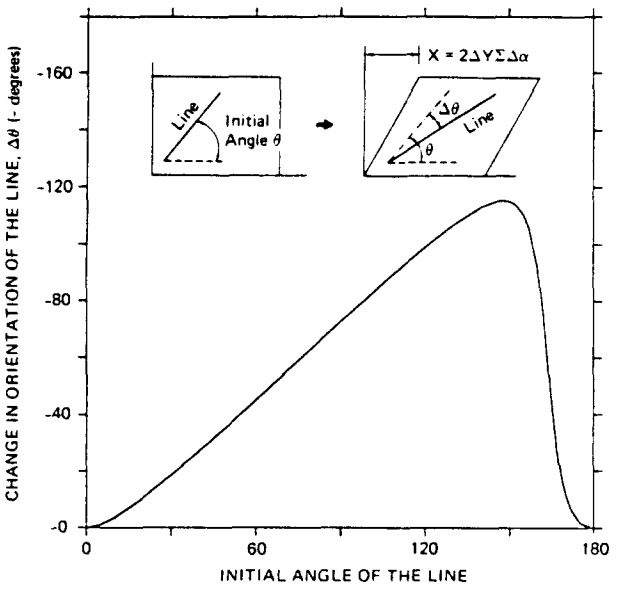


Fig. 6. Distortion of a block in simple shear.

$$\frac{d\theta}{dt} = -\omega \sin^2\theta = -\frac{d\alpha}{dt}\sin^2\theta. \tag{50}$$

For a constant ω, this equation can be integrated over time to obtain

$$\cot\theta = \cot\theta_0 + \Delta\alpha \tag{51}$$

or

$$\Delta\theta = \theta - \theta_0 = \operatorname{arccot}(\cot\theta_0 + \Delta\alpha) - \theta_0. \tag{52}$$

Now the average rotation for a cell can be found by finding the average $\Delta\theta$ for a large number of planes. A set of 18 planes uniformly distributed from $\theta_0 = 0^\circ$ to 170° was studied. Simple shear strain like that in Fig. 1 was imposed in 1° increments for 180 steps. As shown in Fig. 6, the rotations of the planes varied from 0° to 115°.

Next imagine that a number of lines during the shearing calculation had been tracked, and the accuracy that could be achieved with this method was determined. First the use of an orthogonal pair of lines is considered. The average rotations of pairs which were initially orthogonal ranged from 36° to 80°, compared with the exact value of $57.52^\circ = \arctan \pi/2$. The accuracy of the average rotation gradually improved as sets of 4 lines and 8 lines were considered. The average rotation for all 18 planes was 57.64°. This variation in the range of average rotation angles is illustrated in Fig. 7. Hence, the correct rotation of the material can be found by following the rotation of lines, but this procedure does not provide high accuracy unless a large number of lines are used.

7. APPLICATIONS TO CONSTITUTIVE RELATIONS

The foregoing rotation calculations are intended for use with constitutive relations so that the stresses computed are objective, that is, independent of the motion of the coordinate system. The type of constitutive relation determines the information required from the rotation procedure. Three types of relations are identified below.

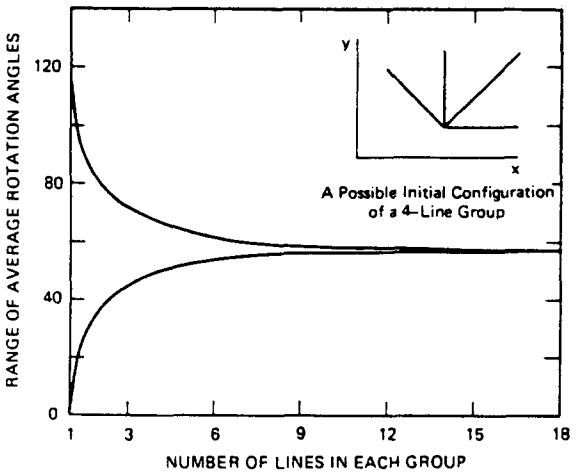


Fig. 7. Variation in range of average rotation angle with number of lines in the group.

(1) Isotropic elastic material. For isotropic material, the calculation can be conducted either by rotating the stresses to the material coordinates using the **R** tensor, or the stresses can be incremented using $\Delta\theta$ as in eqns (32). The results in Fig. 3 show the inaccuracies involved in the stresses and the rotation angle by neglecting a precise rotation procedure.

(2) Isotropic plastic material. As noted in Section 5, for material that may yield, the same rotation procedures can be used as for the elastic material. The results of an ideal plastic calculation of simple shear showed that the exact and Jaumann solutions for stress are essentially indistinguishable. However, the angle calculation for the yielded case by the Jaumann method still has the inaccuracy illustrated in Fig. 3(b).

(3) Anisotropic material. For calculations with anisotropic material it is necessary to know the orientation of the material coordinates. In such a material it is often assumed that the material planes all rotate together, maintaining their fixed angular relationship (under conditions of large distortion, this fixity of angles is certainly not achieved according to the results in Fig. 6). The rotation tensor **R** or the angles θ and $\Delta\theta$ are required for the calculation.

(4) Multiple-plane models. Models such as BFRACT (Seaman *et al.* (1985)) and SHEAR (Seaman and Dein (1983)) contain a series of internal planes that follow the material motion. The rotation of these planes is computed correctly from the velocity gradient matrix **G** according to the equations in Section 6. These models account for the relative motion of several planes, and the gradual development of anisotropy. Hence, these constitutive relations do not require any additional rotation treatment.

8. SUMMARY

The rotation problem in two-dimensional calculations has been treated to determine methods appropriate to finite-difference wave propagation calculations involving rezoning. First, the nature of the rotation problem and the inaccuracies inherent in the standard Jaumann method for cases of large shear strain were outlined. A direct method for obtaining the rotation θ of the cell material was outlined based on the works of Dienes (1979) and Marsden and Hughes (1983). The deformation matrix **F** is stored for each cell. The current angle θ is obtained from

$$\tan\theta = \frac{F_{21} - F_{12}}{F_{11} + F_{22}}. \tag{27}$$

Three methods were explored for rezoning the quantities used in the calculation. A theoretically exact rezoning method based on the invariants of the **U** matrix, and approximations based on the **U** and **F** components are outlined. To explore further the

nature of Dienes' method, an exact method was developed for the rotation of lines or planes in the material.

The rotation technique of Dienes is necessary under conditions of large shear strain for isotropic and simple anisotropic elastic materials in which all the material is assumed to rotate together. For materials in which yielding occurs the stresses are correctly provided by the standard Jaumann method, although the rotation angle is not correct for large distortions. For multiple plane material models in which specific planes in the material are followed, neither the Dienes nor the Jaumann rotation treatment is appropriate.

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