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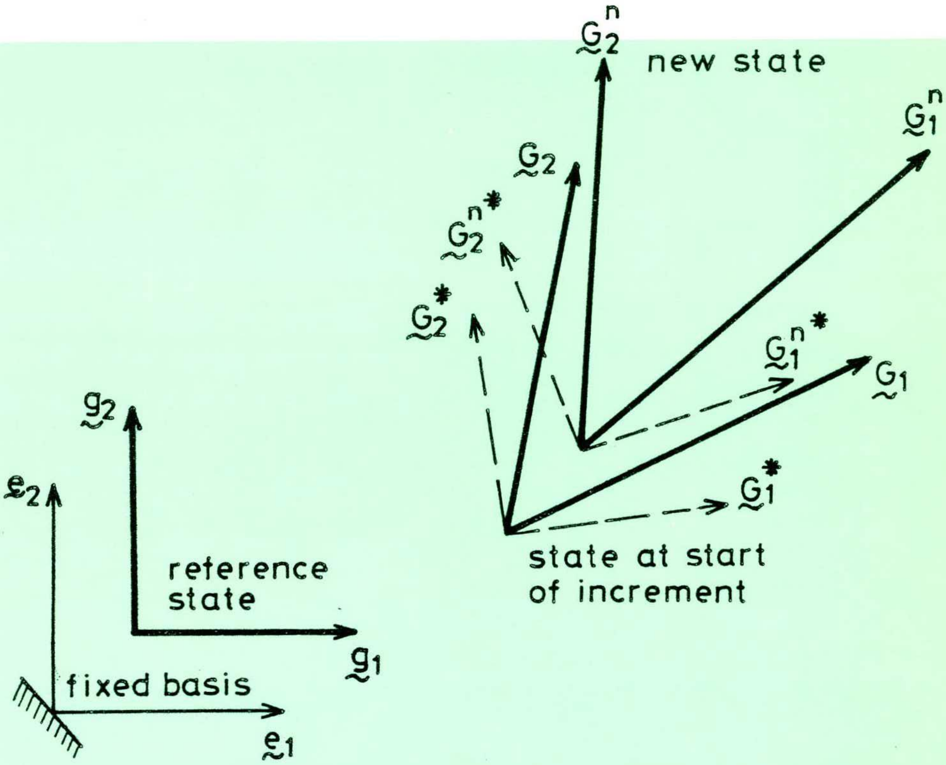

INCREMENTAL CALCULATION OF LARGE DEFORMATION AND MATERIAL ROTATION

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INCREMENTAL CALCULATION OF LARGE DEFORMATION AND MATERIAL ROTATION

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Contents

Summary

The formulation and application of measures for large deformation and material rotation are described. In numerical analysis of the incremental type with large deformation and material rotation these measures are not only needed for a proper interpretation of the deformation but also for the calculation of the objective Jaumann stress increments. When also anisotropic constitutive models are used a proper calculation of the large material rotation can become paramount.
The measures for large deformation and material rotation follow from the common method of polar decomposition of the deformation gradient. For the numerical application of polar decomposition for each increment also the total deformation gradient will have to be calculated. To avoid this in this paper an incremental type of calculation of large deformation and material rotation has been elaborated in which the incremental deformation gradient can be used, which is being calculated anyway. The resulting numerical subroutine has been compared to a numerical subroutine based on polar decomposition considering computational economy and accuracy. It is found that on average the incremental subroutine is slightly more attractive considering computer time while its accumulated errors remain sufficiently small also for large numbers of increments.

Introduction

In the numerical analyses of geotechnical problems the calculation of the deformation and the material rotation is usually needed at least for interpretation of the results. When the magnitudes of the strain and the material rotation are small and when only isotropic constitutive models are being used the strain is usually calculated as the symmetric part of the deformation gradient while for the material rotation the skew part of the deformation gradient is used.
If incremental type of constitutive models are used then this spin of the incremental deformation gradient is used in the relation between the objective Jaumann stress increment and the Cauchy stress increment expressed with respect to the fixed basis of geometrical space.
For geotechnical problems with large deformation and material rotation the aforesaid measures of deformation and material rotation are not suitable anymore. Besides in cases with significant material rotation and anisotropic constitutive models the effects of material anisotropy can only be accounted for properly if the actual material rotation is known.
In such cases more fundamental measures for deformation and rotation are needed as described by the theory of the polar decomposition of the deformation gradient (1, 2, 3). For the direct application of this theory in numerical analysis of the incremental type for each load increment and for each point where stresses, strains and material rotation are needed, first the total deformation gradient would have to be calculated before the actual decomposition could be applied. However usually in such type of analysis for each load increment and at each relevant material point the incremental deformation gradient, approximately proportional to the velocity gradient, is already being calculated. Therefore it could be more economic to apply an incremental type of method for calculating the measures of deformation and material rotation using these incremental deformation gradients. To investigate this possibility in the paper the development of the incremental type of method has been described.

The resulting numerical scheme has been applied to a series of test cases including 360 degrees of material rotation, stretching by a factor of 10 and rotation of the directions of principal strains across 90° degrees with respect to the co-rototional basis of the material. The results have been compared to the results of the alternative common polar decomposition type of approach considering computational economy and accuracy.

Polar decomposition

The measures for large deformation and material rotation can be obtained using polar decomposition (1, 2, 3). To facilitate comparison with the later described incremental method the basis of the relevant part of the polar decomposition method is described first.

The position of the material under consideration is described by the vector $\underset{\sim}{S}$ (see fig. 1). To the material a co-moving curvilinear system of material coordinates Θ^i around this material point is connected. Consequently the co-moving covariant material basevectors $\underset{\sim}{G}_i$ at the current state follow from (4, 5):

$$\underset{\sim}{G}_i = \frac{\partial \underset{\sim}{S}}{\partial \Theta^i} \tag{1}$$

The symbol ~ indicates a vector quantity.

Then a material vector $\underset{\sim}{X}$ to an adjacent material point in an uniformly deformed region at the current state is described by:

$$\underset{\sim}{X} = \Theta^i \underset{\sim}{G}_i \tag{2}$$

At the reference time the position of the material point is given by the vector $\underset{\sim}{s}$. Consequently the covariant material basevectors $\underset{\sim}{g}_i$ at the reference state are described by:

$$\underset{\sim}{g}_i = \frac{\partial \underset{\sim}{s}}{\partial \Theta^i} \tag{3}$$

and a material vector to an adjacent material point at the reference state is described by:

$$\underset{\sim}{x} = \Theta^i \underset{\sim}{g}_i \tag{4}$$

For convenience $\underset{\sim}{g}_i$ will be assumed to consist of cartesian unit vectors coinciding with the fixed cartesian basis $\underset{\sim}{e}_i$.
The transition of the material vector $\underset{\sim}{x}$ at the reference state to the material vector $\underset{\sim}{X}$ at the current state is described by the second order deformation gradient tensor $\underset{\approx}{F}$, namely:

$$\underset{\sim}{X} = \underset{\approx}{F} \bullet \underset{\sim}{x} \tag{5}$$

in which the symbol $\bullet$ indicates the tensor product

and

$$\underset{\approx}{F} = F_{kl} \underset{\sim}{g}_k \underset{\sim}{g}_l \tag{6}$$

is the deformation gradient tensor with components F_{kl} defined on the basevector $\underset{\sim}{g}_k$ of the reference state.

Substitution of eqs. (2), (4) and (6) in eq. (5) gives:

$$\Theta^i \underset{\sim}{G}_i = F_{kl} \underset{\sim}{g}_k \underset{\sim}{g}_l \bullet \Theta^i \underset{\sim}{g}_i$$

or

$$\underset{\sim}{G}_i = F_{ki} \underset{\sim}{g}_k = F_{ik}^T \underset{\sim}{g}_k \tag{7}$$

while:

T indicates a transpose

$$\underset{\sim}{g}_l \bullet \underset{\sim}{g}_i = \delta_{li} \text{ (Kronecker delta)} \tag{8}$$

The deformation gradient can be decomposed into the product of a proper orthogonal transformation tensor $\underset{\approx}{R}$ describing the material rotation and amongst others the symmetric positive definite so called left stretch tensor $\underset{\approx}{V}$ (1, 2, 3), namely:

$$\underset{\approx}{F} = \underset{\approx}{V} \bullet \underset{\approx}{R} \tag{9}$$

while

$$\underset{\approx}{V} = V_{ij}\, \underset{\sim}{g}_i\, \underset{\sim}{g}_j \tag{10}$$

$$\underset{\approx}{R} = R_{kl}\, \underset{\sim}{g}_k\, \underset{\sim}{g}_l \tag{11}$$

and consequently

$$F_{il} = V_{ij}\, R_{jl} \tag{12}$$

The first step of the polar decomposition is the calculation of the so called left Cauchy-Green tensor $\underset{\approx}{C}$:

$$\underset{\approx}{C} = \underset{\approx}{F} \bullet \underset{\approx}{F}^T = F_{ik}\, F_{kj}^{\;T}\, \underset{\sim}{g}_i\, \underset{\sim}{g}_j = V_{ik}\, R_{kl}\, R^T_{lp}\, V_{pj}\, \underset{\sim}{g}_i\, \underset{\sim}{g}_j = V_{ik}\, V_{kj}\, \underset{\sim}{g}_i\, \underset{\sim}{g}_j \tag{13}$$

Next this tensor $\underset{\approx}{C}$ is transformed to its principal axes $\underset{\sim}{H}_i^*$ defined by:

$$\underset{\sim}{H}_i{}^* = \underset{\approx}{Q} \bullet \underset{\sim}{g}_i = Q_{ik}{}^T \underset{\sim}{g}_k \qquad (14)$$

thus:

$$\underset{\sim}{g}_k = Q_{kl} \underset{\sim}{H}_l{}^* \qquad (15)$$

in which Q_{kl} are the components of the rotation tensor.

Substituting eq. (15) in eq. (13) gives the diagonalized version of $\underset{\approx}{C}$:

$$\underset{\approx}{\hat{C}} = Q_{pi}{}^T C_{ij} Q_{jq} \underset{\sim}{H}_p{}^* \underset{\sim}{H}_q{}^* = \hat{C}_{pq} \underset{\sim}{H}_p{}^* \underset{\sim}{H}_q{}^* \qquad (16)$$

From eq. (16) it follows:

$$C_{ij} Q_{jq} = \hat{C}_{qq} Q_{iq} \qquad (17)$$

for each q = 1, 2, 3

in which:

$\hat{C}_{qq}$ are the eigenvalues
Q_{kl} being the components of the rotation tensor, consists of columns of eigenvectors

The numerical calculation of the eigenvalues and eigenvectors (eq. 17) can be performed using a standard subroutine from a library (eg. subroutine FO2ABF of NAG library). From eq. (13) it is learnt that the eigenvalues of eq. (17) are the squares of the eigenvalues of the left stretch tensor $\underset{\approx}{V}$. Conseqently the diagonalized matrix $\hat{V}_{kl}$ can be calculated by substituting the square roots of $\hat{C}_{qq}$, being the principal stretches, on its diagonal.
Finally the components of $\underset{\approx}{V}$ are calculated by applying back-transformation to the fixed basis $\underset{\sim}{g}_i$, thus:

$$V_{kl} = Q_{ki} \hat{V}_{ij} Q_{jl}^{T} \tag{18}$$

When the matrix V_{kl} is known the components of the rotation matrix can be calculated using eq. 12, thus:

$$R_{ij} = F_{ik} V_{kj}^{-1} \tag{19}$$

for which the inverse of V_{kl} has to be calculated too.

Co-rotational spin

As a consequence of the polar decomposition of the deformation gradient cartesian co-rotational unit basevectors can be defined at the current state by:

$$\underset{\sim}{G}_i^* = \underset{\approx}{R} \bullet \underset{\sim}{g}_i$$

or

$$\underset{\sim}{G}_i^* = R_{kl}\, \underset{\sim}{g}_k\, \underset{\sim}{g}_l \bullet \underset{\sim}{g}_i = R_{ki}\, \underset{\sim}{g}_k = R^T_{\ ik}\, \underset{\sim}{g}_k \tag{20}$$

The transformation between the co-rotational cartesian basevectors G_i^* and the co-moving basevectors $\underset{\sim}{G}_i$ involves only pure deformation, namely:

$$\underset{\sim}{G}_i = \underset{\approx}{V} \bullet \underset{\sim}{G}_i^* \tag{21}$$

The left stretch tensor $\underset{\approx}{V}$ with components V_{kl} defined with respect to the cartesian unit material basevector $\underset{\sim}{g}_i$ at the reference time, can also be expressed with the components V^*_{kl} with respect to the cartesian co-rotational basis $\underset{\sim}{G}_i^*$, namely:

$$\underset{\approx}{V}^* = V^*_{\ kl}\, \underset{\sim}{G}^*_k\, \underset{\sim}{G}^*_l \tag{22}$$

in which the symbol * is added to the tensor $\underset{\approx}{V}^* = \underset{\approx}{V}$ to indicate the basis G^*_k.

The relation between the components of V_{kl} and V^*_{kl} is obtained by substituting in eq. (10) the following relation obtained from eq. (20):

$$\underset{\sim}{g}_i = R_{ik}\, \underset{\sim}{G}^*_k \tag{23}$$

Then the stretch tensor is expressed with respect to the co-rotational basis $\underset{\sim}{G}^*_i$, and

$$\underset{\approx}{V}^* = R^T_{\ ki}\, V_{ij}\, R_{jl}\, \underset{\sim}{G}^*_k\, \underset{\sim}{G}^*_l \tag{24}$$

From eqs. (22) and (24) it follows:

$$V^*_{kl} = R^T_{ki} \, V_{ij} \, R_{jl} \qquad (25)$$

The velocity gradient $\underset{\approx}{L}^*$ with respect to the co-rotational basis $\underset{\sim}{G}^*_i$ can only be dependent on the stretch tensor $\underset{\approx}{V}^*$ and its rate. For small deformations this velocity gradient $\underset{\approx}{L}^*$ has symmetric components so that the material spin with respect to this co-rotational basis is zero. It is shown next that for large deformations this is not the case.
The velocity gradient $\underset{\approx}{L}^*$ is defined by:

$$\dot{\underset{\sim}{X}}^* = \underset{\approx}{L}^* \cdot \underset{\sim}{X}^* \qquad (26)$$

in which:

$$\underset{\sim}{X}^* = \underset{\approx}{V}^* \cdot \underset{\sim}{G}^* \text{ (material vector to an adjacent material point)} \qquad (27)$$

and

$$\dot{\underset{\sim}{X}}^* = \dot{\underset{\approx}{V}}^* \cdot \underset{\sim}{G}^* \qquad (28)$$

while the dot • denotes a time derivative.

Substitution of eqs. (27) and (28) in eq. (26) gives:

$$\dot{\underset{\approx}{V}}^* \cdot \underset{\sim}{G}^* = \underset{\approx}{L}^* \cdot \underset{\approx}{V}^* \cdot \underset{\sim}{G}^*$$

thus

$$\dot{\underset{\approx}{V}}^* = \underset{\approx}{L}^* \cdot \underset{\approx}{V}^* \qquad (29)$$

or:

$$\dot{V}^*_{kq}\, \underset{\sim}{G}^*_k\, \underset{\sim}{G}^*_q = L^*_{kl}\, V^*_{lq}\, \underset{\sim}{G}^*_k\, \underset{\sim}{G}^*_q$$

thus:

$$L^*_{kl} = \dot{V}^*_{kq}\, V^{*-1}_{ql} \tag{30}$$

In eq. (30) both $\dot{V}^*_{kq}$ and V^{*-1}_{ql} are symmetric. However their product L^*_{kl} will in general be non-symmetric. Consequently for large deformations next to the Eulerian strainrate $\underset{\sim}{E}^*$ with respect to the co-rotational cartesian basis $\underset{\sim}{G}_i^*$, thus:

$$\underset{\approx}{E}^* = \frac{(\dot{\underset{\approx}{V}}^* \bullet \underset{\approx}{V}^{*-1} + \underset{\approx}{V}^{*-1} \bullet \dot{\underset{\approx}{V}}^*)}{2} \tag{31}$$

also a spin $\underset{\approx}{\Omega}^*$ occurs namely:

$$\underset{\approx}{\Omega}^* = \frac{(\dot{\underset{\approx}{V}}^* \bullet \underset{\approx}{V}^{*-1} - \underset{\approx}{V}^{*-1} \bullet \dot{\underset{\approx}{V}}^*)}{2} \tag{32}$$

This spin is related to the rotation of the principal strain directions with respect to the co-rotational basis $\underset{\sim}{G}^*_i$. Therefore the spin $\underset{\approx}{\Omega}$ of the mass with respect to the fixed basevectors $\underset{\sim}{e}_i$ will be different from the spin of the co-rotational basis $\underset{\sim}{G}^*_i$ with respect to the fixed basevectors $\underset{\sim}{e}^*_i$. For the latter the rotation of the co-rotational basis $\underset{\sim}{G}^*_i$ and its rate have to be calculated.

Interpretation of left stretch tensor V

The left stretch tensor $\underset{\approx}{V}$ can be related to a Langrangian type of strain tensor, namely:

$$
\begin{aligned}
\underset{\approx}{\eta} &= \frac{1}{2} \left(\underset{\sim}{G}_i \bullet \underset{\sim}{G}_j - \underset{\sim}{g}_i \bullet \underset{\sim}{g}_j \right) \underset{\sim}{g}_i \, \underset{\sim}{g}_j \\
&= \frac{1}{2} \left(F_{ik}^{T} \, F_{jl}^{T} \, \underset{\sim}{g}_k \bullet \underset{\sim}{g}_l - \underset{\sim}{g}_i \bullet \underset{\sim}{g}_j \right) \underset{\sim}{g}_i \, \underset{\sim}{g}_j \\
&= \frac{1}{2} \left(F_{ik}^{T} \, F_{kj} - \delta_{ij} \right) \underset{\sim}{g}_i \, \underset{\sim}{g}_j \\
&= \frac{1}{2} \left(V_{iq} \, V_{qj} - \delta_{ij} \right) \underset{\sim}{g}_i \, \underset{\sim}{g}_j
\end{aligned}
\qquad (33)
$$

Also other interpretations are possible (6).
Besides the left stretch tensor $\underset{\approx}{V}$ can also be interpreted directly in terms of the physical aspects of the deformation. To this end the tensor $\underset{\approx}{V}^*$ is diagonalized by expressing it with respect to basevector $\underset{\sim}{H}_i^*$ orientated along its principal directions:

$$
\underset{\sim}{H}_i^* = \underset{\approx}{Q}^* \bullet \underset{\sim}{G}_i^* = Q^{*T}_{ik} \, \underset{\sim}{G}_k^* \qquad (34)
$$

in which:

$$
\underset{\approx}{Q}^* = Q^*_{kl} \, \underset{\sim}{G}_k^* \, \underset{\sim}{G}_i^* \qquad (35)
$$

is rotation tensor describing the orientation of the principal directions of the deformation with respect to the co-rotational basevectors $\underset{\sim}{G}_i^*$.

Similarly to eqs. (16), (17) and (18) the diagonalized tensor $\hat{\underset{\approx}{V}}$ becomes:

$$\hat{\underset{\approx}{V}} = \hat{V}_{kl} \; \underset{\sim}{H}^*_k \; \underset{\sim}{H}^*_k = Q^{*T}_{ki} \; V^*_{ij} \; Q^*_{jl} \; \underset{\sim}{H}^*_k \; \underset{\sim}{H}^*_l \qquad (36)$$

The principal values of stretches $\hat{V}_1$, $\hat{V}_2$, $\hat{V}_3$ describe the coordinates of the angular point A of a rectangular parallelepiped situated in a cartesian space (see fig. 2). At the start of the deformation the parallelepiped is reduced to a cube with sides of unit length; then the point A has coordinates $\hat{V}_1 = 1$, $\hat{V}_2 = 1$, $\hat{V}_3 = 1$. During consecutive deformation these coordinates change.

Thus in the general case the current state can be described by the material rotation tensor $\underset{\approx}{R}$, describing the material rotation with respect to the fixed basis $\underset{\sim}{e}_i$, the rotation tensor $\underset{\approx}{Q}^*$, describing the rotation between the princial strain directions and the co-rotational basevectors $\underset{\sim}{G}^*_i$, and the 3 principal values of the stretches.

The volumechange is a kind of invariant measure of $\underset{\approx}{V} = \underset{\approx}{V}^*$. It is expressed by:

$$\frac{\Delta Vol}{Vol_o} = I_3 - 1 \qquad (37)$$

For the invariant I_3 the third invariant of the left stretch tensor $\underset{\approx}{V}$ can be used, namely:

$$I_3 = V_{11} V_{22} V_{33} + V_{12} V_{23} V_{31} + V_{21} V_{32} V_{13} +$$

$$- (V_{11} V_{23} V_{32} + V_{22} V_{13} V_{31} + V_{33} V_{12} V_{21}) \qquad (38)$$

The shearing type of deformation can be expressed most easily using the deviatoric tensor component of $\underset{\approx}{V}$, namely

$$\underset{\approx}{V}^d = V^d_{ij}\, \underset{\sim}{g}_i\, \underset{\sim}{g}_j = (V_{ij} - \frac{V_{kl}\,\delta_{kl}}{3}\,\delta_{ij})\, \underset{\sim}{g}_i\, \underset{\sim}{g}_j \qquad (39)$$

The deviatoric component of the vector from the origin of the space of the principal stretches to the corner point A (see fig. 3), defined as length γ, is also an invariant measure. It describes the distortion or shear, namely:

$$\gamma = \sqrt{V^d_{ij}\, V^d_{ij}} =$$

$$= \sqrt{\frac{1}{3}\{(V_{11} - V_{22})^2 + (V_{22} - V_{33})^2 + (V_{33} - V_{11})^2\} + 2\,\{V_{12}{}^2 + V_{23}{}^2 + V_{31}{}^2\}} \qquad (40)$$

The Lode angle Θ^d in the pi-plane of the space of the principal stretches (see fig. 3) is the other invariant measure. It can also be expressed in the components of the tensor $\underset{\approx}{V}^d$, namely

$$\sin 3\Theta^d = -\frac{J_3}{\gamma^3}\, 3\sqrt{6} \qquad (41)$$

in which:

$$J_3 = V^d_{11}\ V^d_{22}\ V^d_{33} + V^d_{12}\ V^d_{23}\ V^d_{31} + V^d_{21}\ V^d_{32}\ V^d_{13} +$$

$$- (V^d_{11}\ V^d_{23}\ V^d_{32} + V^d_{22}\ V^d_{13}\ V^d_{31} + V^d_{33}\ V^d_{12}\ V^d_{21}) \qquad (42)$$

thus:

$\Theta^d = 30°$ for triaxial extension
$\Theta^d = 0°$ for torsion
$\Theta^d = -30°$ for triaxial compression

Interpretation of the rotation tensor

A rotation tensor $\underset{\approx}{R}$ can be expressed in the rotation angles ϕ, Θ, Ψ consecutively applied along its basevectors $\underset{\sim}{g}_1$, $\underset{\sim}{g}_2$ and $\underset{\sim}{g}_3$. In such process an arbitrary vector $\underset{\sim}{b} = b_i \underset{\sim}{g}_i$ will be rotated to $\underset{\sim}{c} = c_i\ \underset{\sim}{g}_i$, namely:

$$\underset{\sim}{c} = \underset{\approx}{R} \bullet \underset{\sim}{b}$$

or:

$$\underset{\sim}{c} = c_k\ \underset{\sim}{g}_k = R^{\phi}_{ki}\ R^{\Theta}{}_{ij}\ R^{\Psi}{}_{jl}\ b_l\ \underset{\sim}{g}_i = R_{kl}\ b_l\ \underset{\sim}{g}_k \tag{43}$$

in which:

$$R^{\phi} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & \sin\phi \\ 0 & -\sin\phi & \cos\phi \end{bmatrix} \tag{44}$$

$$R^{\Theta} = \begin{bmatrix} \cos\Theta & 0 & -\sin\Theta \\ 0 & 1 & 0 \\ \sin\Theta & 0 & \cos\Theta \end{bmatrix} \tag{45}$$

$$R^{\Psi} = \begin{bmatrix} \cos\Psi & \sin\Psi & 0 \\ -\sin\Psi & \cos\Psi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{46}$$

thus:

$\underset{\approx}{R} = R_{kl}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l$ in which

$$R_{kl} = \left[\begin{array}{c|c|c} \cos\Theta\ \cos\Psi & \cos\Theta\ \sin\Psi & -\sin\Theta \\ -\cos\phi\ \sin\Psi + \sin\phi\ \sin\Theta\ \cos\Psi & \cos\phi\ \cos\Psi + \sin\phi\ \sin\Theta\ \sin\Psi & +\sin\phi\ \cos\Theta \\ \sin\phi\ \sin\Psi + \cos\phi\ \sin\Theta\ \cos\Psi & -\sin\phi\ \cos\Psi + \cos\phi\ \sin\Theta\ \sin\Psi & +\sin\phi\ \mathrm{cis}\Theta \end{array}\right] \tag{47}$$

Incremental method for calculation of large deformation and material rotation

The incremental method for the calculation of the large deformation and material rotation (1, 2, 3) is based on the usage of the velocity gradient $\underset{\approx}{L}$ with respect to the fixed basis $\underset{\sim}{e}_i = \underset{\sim}{g}_i$. This velocity gradient is defined by (see also eqs. (26), (27) and (28)):

$$\underset{\sim}{\dot{X}} = \underset{\approx}{L} \bullet \underset{\sim}{X} \tag{48}$$

$$\underset{\approx}{L} = L_{kl}\, \underset{\sim}{g}_k\, \underset{\sim}{g}_l \tag{49}$$

$\underset{\sim}{X} = \underset{\approx}{F} \bullet \underset{\sim}{x}$ (see eqs. 2 and 5)

and

$$\underset{\sim}{\dot{X}} = \underset{\approx}{\dot{F}} \bullet \underset{\sim}{x} \tag{50}$$

Substituting eqs. (5), (49) and (50) in eq. (48) gives:

$$\underset{\approx}{\dot{F}} \bullet \underset{\sim}{x} = \underset{\approx}{L} \bullet \underset{\approx}{F} \bullet \underset{\sim}{x}$$

thus:

$$\underset{\approx}{\dot{F}} = \underset{\approx}{L} \bullet \underset{\approx}{F}$$

or expressed in the tensor components:

$$\dot{F}_{kl}\, \underset{\sim}{g}_k\, \underset{\sim}{g}_l = L_{kp}\, F_{pl}\, \underset{\sim}{g}_k\, \underset{\sim}{g}_l \tag{51}$$

Using eqs. (12) and (51) the components of the velocity gradient can be related to the components of $\underset{\approx}{V}$ and $\underset{\approx}{R}$ and their rates (1, 2, 3), namely:

$$\dot{F}_{kl}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l = (\dot{V}_{kp}\ R_{pl} + V_{kp}\ \dot{R}_{pl})\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l = L_{kp}\ V_{pq}\ R_{ql}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l$$

thus:

$$L_{kl}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l = (\dot{V}_{kp}\ V^{-1}_{pl} + V_{kp}\ \dot{R}_{pq}\ R^{T}_{qm}\ V^{-1}_{ml})\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l \tag{52}$$

The Eulerian strainrate with respect to the fixed basis becomes:

$$E_{kl}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l = \left(\frac{L_{kl} + L^{T}_{kl}}{2}\right)\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l \tag{53}$$

and the spin becomes:

$$\Omega_{kl}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l = \left(\frac{L_{kl} - L^{T}_{kl}}{2}\right)\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l \tag{54}$$

As was mentioned before (see eq. (32)), the spin of eq. (54) is not equal to the spin $\underset{\approx}{\Omega}^{r}$ of the co-rotational basis $\underset{\sim}{G}^{*}_{i}$ with respect to the fixed basis $\underset{\sim}{g}_k$. The latter is obtained from eq. (52) by putting $\dot{V}_{kp} = 0$ and $V_{kp} = \delta_{kp}$. It is found that:

$$\underset{\approx}{\Omega}^{r} = \Omega^{r}_{kl}\ \ \underset{\sim}{g}_k\ \underset{\sim}{g}_l = \dot{R}_{kp}\ R^{T}_{pl}\ \ \underset{\sim}{g}_k\ \underset{\sim}{g}_l \tag{55}$$

In principle from eq. (52) the rates $\dot{V}_{kp}$ and $\dot{R}_{pq}$ can be calculated if the other quantities V_{kp}, R_{qm} and L_{kl} are known.

Jaumann stress increment

When anisotropic constitutive models with tensors for the description of the material anisotropy are used and when also large deformation and material rotation occur then the spin tensor $\underset{\approx}{\Omega}^r$ of the co-rotational basis $\underset{\sim}{G}_i^*$ with respect to the fixed basis $\underset{\sim}{g}_i$ has to be used in the objective or Jaumann stress rate $\overset{\circ}{\underset{\approx}{\sigma}}$

Then the Jaumann stress rate becomes (1, 2, 3):

$$\overset{\circ}{\sigma}_{kl}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l = (\dot{\sigma}_{kl} + \Omega^{rT}_{kp}\ \sigma_{pl} + \sigma_{kp}\ \Omega^{r}_{pl})\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l \qquad (56)$$

However for the stressincrements as occuring in numerical analysis of the incremental type eq. (56) is not accurate enough because it is expressed in terms of stress rates and not in terms of stress increments. Next a more accurate expression for the stress increments is considered. To this end the following quantities are introduced:

$\underset{\approx}{\sigma} = \sigma_{kl}\ \underset{\sim}{g}_k\ \underset{\sim}{g}_l$ Cauchy stress tensor expressed with respects to the fixed basevectors $\underset{\sim}{g}_i$ at the start of the stress increment (57)

$\underset{\approx}{\sigma}^* = \sigma^*_{kl}\ \underset{\sim}{G}_k^*\ \underset{\sim}{G}_l^*$ Cauchy stress tensor expressed with respect to the co-rotational basevectors $\underset{\sim}{G}_i^*$ at the start of the stress increment (58)

The components of these stress tensors are related by (see also eq. (25)):

$$\sigma_{kl} = R_{kp}\ \sigma^*_{pq}\ R^T_{ql} \qquad (59)$$

Similar quantities are defined at the end of the stress increment using a superindex n.

Then the Cauchy stress at the end of the stress increment becomes:

$$\sigma^{n}_{kl} = R^{n}_{kp} \; \sigma^{*n}_{pq} \; R^{n\,T}_{ql} \tag{60}$$

For convenience the incremental rotation tensor is introduced namely:

$$\underset{\approx}{R}^{r} = R^{r}_{kp} \; \underset{\sim}{g}_{k} \; \underset{\sim}{g}_{p} \tag{61}$$

so that:

$$\underset{\approx}{R}^{n} = \underset{\approx}{R}^{r} \bullet \underset{\approx}{R} = R^{r}_{kp} \; R_{pl} \; \underset{\sim}{g}_{k} \; \underset{\sim}{g}_{l} \tag{62}$$

Using the components of the co-rotational stress increment, namely:

$$\Delta\sigma^{*}_{kl} = \sigma^{*n}_{kl} - \sigma^{*}_{kl} \tag{63}$$

and substituting these in eq. (60) leads to:

$$\begin{aligned} \sigma^{n}_{kl} &= R^{r}_{kp} \; R_{pq} \; \sigma^{*}_{qm} \; R^{T}_{mn} \; R^{r\,T}_{nl} + R^{n}_{kp} \; \Delta\sigma^{*}_{pq} \; R^{n\,T}_{ql} = \\ &= R^{r}_{kp} \; \sigma_{pq} \; R^{r\,T}_{ql} + R^{n}_{kp} \; \Delta\sigma^{*}_{pq} \; R^{n\,T}_{ql} \end{aligned} \tag{64}$$

in which the last term is the objective Jaumann stress increment, to be indicated by:

$$\Delta\overset{\circ}{\sigma}_{kl} = R^{n}_{kp} \; \Delta\sigma^{*}_{pq} \; R^{n\,T}_{ql} = \sigma^{n}_{kl} - R^{r}_{kp} \; \sigma_{pq} \; R^{r\,T}_{ql} \tag{65}$$

From eq. (65) the new Cauchy stress σ^{n}_{kl} can be calculated if the initial stress σ_{pq}, the incremental rotation R_{kp} and the objective Jaumann stress increment $\Delta\overset{\circ}{\sigma}_{kl}$ are known.

Eq. (65) can also be expressed in the form of eq. (56). To this end the spin of the co-rotational basis $\Omega^{r}_{kl}\, \underset{\sim}{g}_k\, \underset{\sim}{g}_l$ (eq. 55) is expressed in terms of the incremental rotation using eq. (62). While using the time increment Δt, it is found that:

$$R^{r}_{kl} = \Omega^{r}_{kl}\ \Delta t + \delta_{kl} \qquad (66)$$

in which δ_{kl} - Kronecker delta.

Substituting eq. (66) in eq. (65) leads to the following expression for the Jaumann stress increment:

$$\Delta\overset{o}{\sigma}_{kl} = \Delta\sigma_{kl} - \Delta t^2\ \Omega^{r}_{kp}\ \sigma_{pq}\ \Omega^{r\,T}_{ql} - \Delta t\ \Omega^{r}_{kp}\ \sigma_{pl} - \Delta t\ \sigma_{kp}\ \Omega^{r\,T}_{pl} \qquad (67)$$

Comparison of eq. (56) with eq. (67) shows that for stress increments also quadratic terms of $\Omega^{r}\Delta t$ occur. Because of its simplicity in numerical analysis (eg. 65) seems more attractive than eq. (67). Therefore in numerical analysis the incremental rotation matrix R^{r}_{kl} will be used and not the spinmatrix Ω^{r}_{kl}.

Application of incremental method in numerical analysis

In the numerical analysis increments occur instead of the timederivatives. The components of the new stretch tensor and the new rotation tensor become respectively:

$$V^{n}_{kl} = V_{kl} + \Delta V_{kl} \tag{68}$$

$$R^{n}_{kl} = R_{kl} + \Delta R_{kl} = R^{r}_{kp} \, R_{pl} \tag{69}$$

Besides instead of the velocity gradient (eq. 51) the incremental deformation gradient defined by $\Delta \underset{\approx}{L} \approx \underset{\approx}{L} \, \Delta t$ occurs, namely (see also eqs. (48), and (50)):

$$\Delta \underset{\sim}{X} = \Delta \underset{\approx}{F} \bullet \underset{\sim}{X} = \Delta \underset{\approx}{L} \bullet \underset{\approx}{F} \bullet \underset{\sim}{x}$$

thus:

$$\Delta F_{kl} \, \underset{\approx}{g}_k \, \underset{\approx}{g}_1 = \Delta L_{kp} \, F_{pl} \, \underset{\approx}{g}_k \, \underset{\approx}{g}_1 \tag{70}$$

while:

$$\Delta F_{kl} = F^{n}_{kl} - F_{kl} = V^{n}_{kp} \, R^{n}_{pl} - V_{kp} \, R_{pl} \tag{71}$$

From eqs. (70) and (71) it follows:

$$\begin{aligned} \Delta L_{kl} &= \Delta F_{kq} \, F^{-1}_{ql} = (V^{n}_{kp} \, R^{n}_{pq} - V_{kp} \, R_{pq}) \, R^{T}_{qs} \, V^{-1}_{sl} \\ &= V^{n}_{kp} \, R^{r}_{pm} \, V^{-1}_{ml} - \delta_{kl} \end{aligned}$$

or:

$$\Delta L_{kl} \, V_{lm} + V_{km} = V^{n}_{kp} \, R^{r}_{pm} \tag{71}$$

From eq. (71) both the incremental rotation and the new stretch tensor can be calculated iteratively. To this end first the difference of the antimetric components of eq. (71) are considered; namely of:

$$\Delta L_{kl}\, V_{lm} + V_{km} - (\Delta L_{kl} V_{lm} + V_{km})^T = V^n_{kp}\ \ R^r_{pm} + (V^n_{kp}\ \ R^r_{pm})^T \tag{72}$$

The antimetric components are expressable as a linear function of the sinus of the rotation angles ϕ, Θ and Ψ of the incremental rotation matrix (see also eq. 47) as will be shown. For convenience first the following quantities are introduced. The components of the present approximation to the new stretch tensor $\underset{\approx}{V}^n$ are described by:

$$V_1 = V\ (1,1);\ V_2 = V(2,2);\ V_3 = V\ (3,3);\ V_4 = V\ (1,2) = V\ (2,1);$$
$$V_5 = V\ (2,3) = V\ (3,2);\ V_6 = (1,3) = V(3,1) \tag{73}$$

The incremental rotation matrix R^r_{kl} is expressed by:

$$R^r_{kl} = \left[\begin{array}{c|c|c} C_1 & \cos\Theta\ \sin\Psi & -\ \sin\Theta \\ -\ \cos\phi\ \sin\Psi + C_2 & C_5 & \cos\Theta\ \sin\phi \\ C_4 + C_3\ \sin\ \Theta & -\cos\Psi\ \sin\phi + C_6 & C_7 \end{array}\right] \tag{74}$$

The functions C_1 up to C_7 can be obtained by comparing eqs. (74) and (47). Substituting eqs. (73) and (74) in eq. (72) the antimetric components become, while using:

$$A_{kl} = \Delta L_{kl}\ V_{lm} + V_{km} \tag{75}$$

$$\begin{bmatrix} \cos\Theta V_2 + \cos\Psi\ V_3 & -V_4 & -\cos\Theta V_6 \\ -\cos\Theta\ V_4 & V_1 + C_3\ V_3 & -\cos\phi\ V_5 \\ -\cos\Psi\ V_6 & -C_3\ V_5 & \cos\Theta\ V_1 + \cos\phi\ V_2 \end{bmatrix} * \begin{Bmatrix} \sin\phi \\ \sin\Theta \\ \sin\Psi \end{Bmatrix} = \begin{Bmatrix} A_{23}-A_{32}-(C_7-C_5)V_5+C_6V_3 \\ -A_{13}+A_{31}-(C_1-C_7)V_6-C_2V_5-C_4V_3 \\ A_{12}-A_{21}-(C_5-C_1)V_4+C_2V_2+C_4V_5-C_6V_6 \end{Bmatrix} \tag{76}$$

For the calculation of the matrix and the vector on the right of eq. (76) the previous estimates of both the angles ϕ, Θ, Ψ and the new stretches V^n_{kl} can be substituted. Then the solution of eq. (76) produces better estimates of the angles to be used in the next iteration. In the first step of this process the angles in the matrix and in the right hand vector are taken as zero and for the estimates of the new stretches the stretches at the start of the increment are used.

In the iteration process the new estimates of the new stretch tensor are calculated using eq. (71); namely:

$$V^n_{kp} = (\Delta L_{kl}\ V_{lm} + V_{km})\ R^{r^T}_{mp} \tag{77}$$

The iteration is terminated when the incremental changes of all angles are sufficiently small, eg. $< 10^{-9}$ radials. Then the components of the new rotation tensor R^n_{kl} are calculated using eq. (69).

This incremental approach has been applied in the numerical subroutine INCR, which has been written in FORTRAN 77 (see Appendix). In the subroutine for the different quantities similar names have been used as in the paper. The different stages of the calculation in the subroutine are clarified by including extra text.

Comparison of numerical performances of both schemes

To be able to decide which of both numerical schemes, the polar decomposition type or the incremental type, would be more attractive for usage in finite element calculations for both schemes the accuracy and the cost in terms of computertime have been determined by using both schemes in a series of test cases. The calculations were performed on a HARRIS H500 computer which has about 11 significant numbers. In each testcase the deformation gradient and the incremental deformation gradient have been defined for a number of increments n by prescribing the material rotation, the principal stretches and the principal strain directions. In the different testseries different combinations have been applied. The different cases A up to T are indicated in table I. As independent variables of the testseries were used the angles ϕ, Θ, Ψ for the material rotation, the principal stretches $\hat{V}_1$ and $\hat{V}_2$, the orientation angles Θ^P and Ψ^P for the description of the principal strains with respect to the co-rotational basis $\underset{\sim}{G}_i^*$, the number of increments n in the testseries and the iteration criterion, describing the maximum allowable incremental change between two consecutive iterations of the angles of the incremental rotation matrix. The resulting maximum errors ΔV and ΔR in the calculated new stretch matrix V_{kl}^n and the new rotation matrix R_{kl}^n have been obtained by comparing all components with the prescribed magnitudes for all steps n. The resulting computertimes are the average durations of the calls of the subroutine per testseries.
The results have been collected in table I. From these results the following observations can be made:

- In series A, B and C rigid material rotations across 360° in n = 360 steps were considered. The rigid material rotations were applied by the angles ϕ, Θ, Ψ respectively. The polar decomposition method showed small errors $\Delta V \approx 10^{-10}$ and $\Delta R \approx 10^{-10}$ while also both accumulated errors of the incremental method were rather small, namely $\Delta V \approx 25 * 10^{-10}$ and $\Delta R \approx 13 * 10^{-10}$. For the incremental method the computertimes were the same for the three cases, namely 4.7 msec. For the polar decomposition method the computertimes were found to be dependent on the angle of the material rotation; for the angles ϕ and Ψ the calculations took about 5.0 msec, but for the angle Θ about 8.5 msec was needed.
  From these results it can be concluded that for rigid material rotation both schemes are rather similar except for the material rotation described by the angle Θ. For such material rotations the polar decomposition method is about 80% more expensive.

- In series D pure stretching with the principal stretch $\hat{V}_1$ from $\hat{V}_1 = 1$ to $\hat{V}_1 = 10$ in n = 360 steps was considered. Again the polar decomposition method showed very small errors. For the incremental method the error $\Delta V \approx 108 * 10^{-10}$, which is still a very small relative error, namely $\frac{\Delta V}{\hat{V}_1} < 10^{-8}$. Relative errors of the order of 10^{-5} or 10^{-6} still seem allowable in practice. For the incremental method the error $\Delta R \approx 10^{-10}$ was also very small. The computer time of the polar decomposition method (5.2 msec) is about 50% higher than the computertime of the incremental method (3.5 msec).
  From these results it can be concluded that for small incremental stretching the polar decomposition method is about 50% more expensive than the incremental method.

- In series E and F a shearing types of deformation were applied by stretching the principal stretch $\hat{V}_1$ from 1 up to 10 while also the principal strain directions were rotated across 90° in n = 360 steps. The principal straindirections were rotated by the angles Θ^P and Ψ^P respectively.

The maximum errors of the polar decomposition method remained very small ($< 5 * 10^{-10}$) while the maximum errors of the incremental method remained limited too ($< 367 * 10^{-10}$). The computer time of the polar decomposition method were found to depend also on the rotation angle of the principal strains; for the rotation angle Θ^P the computer time was higher than for Ψ^P.
From these results it can be concluded that for small incremental shearing without material rotation the polar decomposition method is between 50% and 150% more expensive than the incremental method.

- In series G and H combined material rotations across 360° by angles Θ and Ψ respectively and pure stretching by $\hat{V}_1$ from 1 to 10 were applied in n = 360 increments. The maximum errors of the polar decomposition method were very small again ($< 15 * 10^{-10}$) while the maximum errors of the incremental method were small too ($\Delta V < 579 * 10^{-10}$). For rotation angle Ψ (series H) the computer times for both methods were almost equal (5.9 msec), but for the rotation angle Θ the polar decomposition method was about 50% more expensive than the incremental method.
From these results it can be concluded that for combined material rotation and stretching both methods are equivalent except for the material rotation described by the angle Θ. For such material rotations the polar decomposition method is about 50% more expensive.

- In series I, J, K, L and M combined material rotations across 360° by Θ or Ψ and shearing types of co-rotational deformation, by increasing $\hat{V}_1$ or $\hat{V}_2$ from 1 to 10 and by rotating the principal strain directions with respect to the co-rotational basis across 90° by angles Θ^P or Ψ^P respectively, were applied. Such types of deformation will occur in plane and axi-symmetric deformations. For series I, J, and K this deformation was applied in n = 360 steps, while in series L n = 3600 steps and in series M n = 36000 steps were used. The maximum errors of the polar decomposition method were again very small ($< 10 * 10^{-10}$) while for the incremental method the accumulated maximum errors increased with n.

For n = 360 the maximum errors were small ($\leqslant 563 * 10^{-10}$) but for larger n they became bigger, namely for n = 3600 ($\leqslant 4068 * 10^{-10}$) and for n = 36000 ($\leqslant 43907 * 10^{-10}$). In practice the biggest error ($\approx 5 * 10^{-6}$) is just allowable. For rotation angle Ψ the computer times of both methods were almost equal (5.9 msec), while again for the rotation angle Θ the polar decomposition method was about 50% more expensive than the incremental method.
From these results it can be concluded, that for combined material rotation and shearing, like occur in plane and axisymmetric deformations, both methods are equivalent concerning cost, when the material rotation is described by the angle Ψ. The polar decomposition method is very accurate, but it is about 50% more expensive, when material rotations of the angle Θ occur. In the incremental method the accumulated maximum error remains just small enough ($< 5 * 10^{-6}$) to be allowable in practice, also for a very large number of steps (n = 36000) as could occur in explicit time integration schemes. This accumulated error would decrease with increasing amount of significant numbers of the computer.

- In series N, O, P, Q, R, S and T combined material rotations across 360° of the angle Θ, stretching by increasing $\hat{V}_1$ from 1 to 10 and rotation of principal strain directions by increasing Ψ^P from 0 to 90° were applied. Such types of deformation can only occur in arbitrary 3 dimensional geometries. In series N up to R the number of steps n was increased from n = 36 to n = 36000. In series S and T the iteration criterion was decreased from 10^{-9} as used in the other series to 10^{-8} and 10^{-7}. Again the maximum errors of the polar decomposition method ($< 23 * 10^{-10}$) were very small. For the incremental method accumulated maximum errors increased with the number of steps n from $102 * 10^{-10}$ for n = 36 to $19352 * 10^{-10}$ for n = 36000. Again the latter number is still allowable in practice.
The effect of decreasing the iteration criterion on the maximum error is rather small for the iteration criterion of 10^{-8} but excessive for the iteraton criterion of 10^{-7}. The iteration criterion of 10^{-9} seems to have the right order of magnitude.

For the polar decomposition method the mean computer time per step varied between 9.5 msec and 10.1 msec. For the smallest number of steps ($n = 36$) the polar decomposition method was about 40% cheaper than the incremental method, but for the largest number of steps the polar decomposition method was about 60% more expensive. The number of iterations per step decreased from about 13 for $n = 36$ to about 5 for $n = 360$. As could be expected for the incremental method the computertime per step decreased by about 20% by decreasing the iteration criterion from 10^{-9} to 10^{-7}.
From the results it can be concluded that for general 3 dimensional deformation and small increments of deformation and material rotation the incremental method is somewhat cheaper than the polar decomposition method. In the incremental method the accumulated maximum error remains just acceptable ($< 5 * 10^{-6}$) in practice. For the iteration criterion 10^{-9} is a suitable order of magnitude.

Conclusions

The formulation and application of polar decomposition and an incremental method for the calculation of large deformation and material rotation in numerical analyses of the incremental type have been considered. For the application of polar decomposition for each increment also the total deformation gradient will have to be calculated while in the incremental method the incremental deformation gradient can be used, which is being calculated anyway.
Calculations of large deformations and material rotations are not only needed for interpretation of the calculated deformation but also to take proper account of the objective Jaumann stress increment. When anisotropic constitutive models are used the effect of large material rotations can become paramount. It has been shown that for large deformations a spin with respect to the co-rotational basis of the material can occur. Consequently the spin of the co-rotational basis with respect to the fixed basis is not equal to the spin of the mass with respect to this fixed basis. Besides it has been shown that in the expression of the objective Jaumann stress increment this spin of the co-rotational basis not only occurs in a linear way, as in the Jaumann stress rate but in a quadratic way too.
By comparing the performances of the numerical schemes of both methods for several testseries with different kinds of prescribed material rotations and deformations it has been found that for the incremental method the accumulated maximum error remains acceptable in practice ($< 10^{-5}$) also when big numbers of steps (36000) are applied. For numerical analysis with small increments of strain and material rotation on average the incremental method is slightly more attractive concerning computertime.

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Figure captions

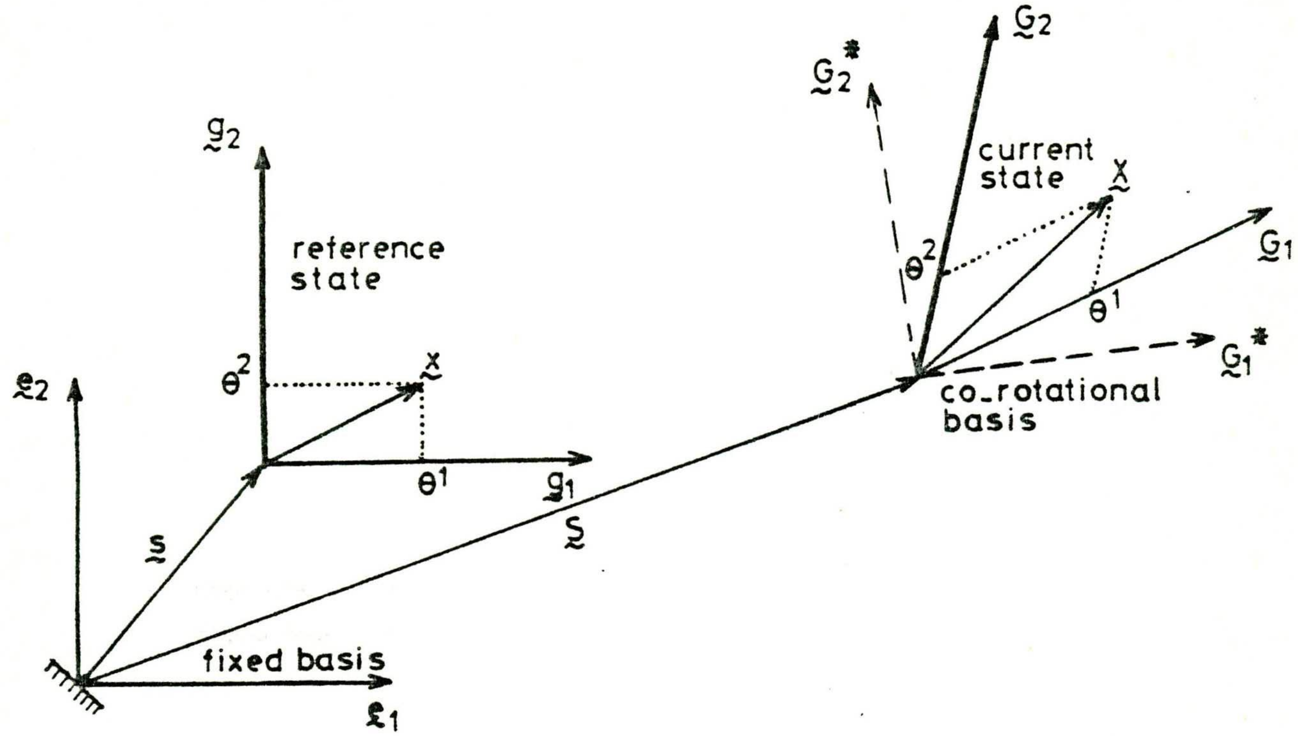
Figure 1. Geometrical space with different basevectors.

Figure 2. Principal stretch space with the parallelepiped described by the principal stretches.

Figure 3. Pi-plane of the principal stretch space with the length γ and the Lode angle Θ^{d} describing the distorsion or shear.

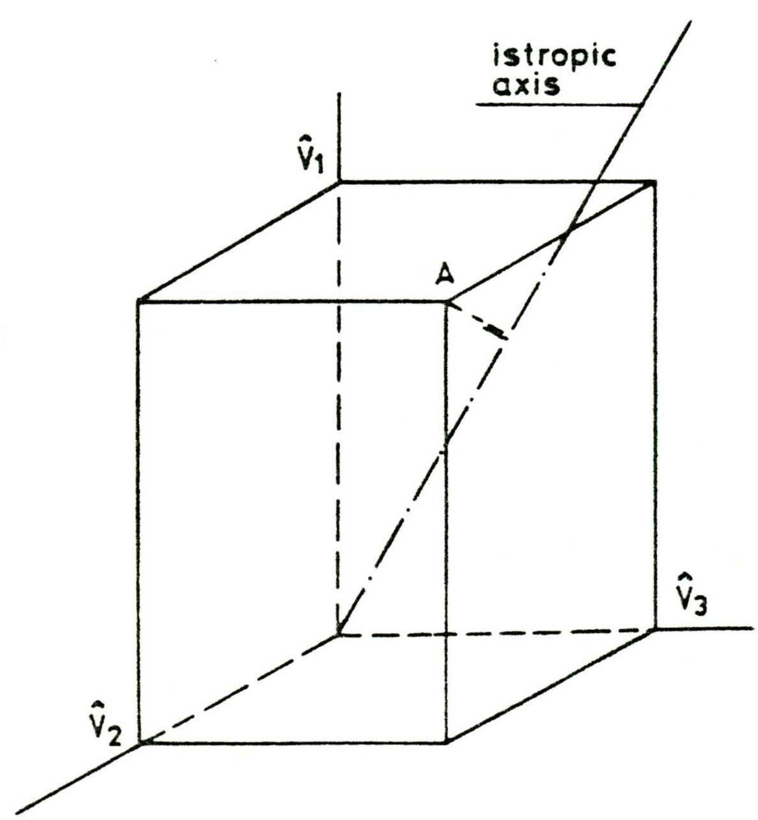
test series	description	prescribed quantities					accuracy				mean computertime per increment $[10^{-3}$ sec.$]$	
		material rotation	magnitude principal stretch	orientation principal stretch	number of increments n	iteration criterion	increm. method		polar decomp.		increm. method	polar decomp.
							$\Delta V^{*}10^{-10}$	$\Delta R^{*}10^{-10}$	$\Delta V^{*}10^{-10}$	$\Delta R^{*}10^{-10}$		
A	rigid rotation	$\phi \rightarrow 360°$	0	0	360	10^{-9}	25	13	1	1	4.7	5.1
B	rigid rotation	$\Theta \rightarrow 360°$	0	0	360	10^{-9}	25	13	1	1	4.7	8.5
C	rigid rotationg	$\upsilon \rightarrow 360°$	0	0	360	10^{-9}	24	13	1	1	4.7	4.9
D	pure stretching	0	$\hat{V}_1 \rightarrow 10$	0	360	10^{-9}	108	1	2	1	3.5	5.2
E	shearing	0	$\hat{V}_1 \rightarrow 10$	$\Theta^P \rightarrow 90°$	360	10^{-9}	367	14	5	3	3.5	9.0
E	shearing	0	$\hat{V}_1 \rightarrow 10$	$\Psi^P \rightarrow 90°$	360	10^{-9}	123	1	4	1	3.5	5.8
G	rotation + stretching	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	0	360	10^{-9}	483	13	14	13	5.8	8.7
H	rotation + stretching	$\Psi \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	0	360	10^{-9}	579	15	4	4	5.8	5.8
I	rotation + shearing	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Theta^P \rightarrow 90°$	360	10^{-9}	526	13	10	10	5.8	8.9
J	rotation + shearing	$\Psi \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi^P \rightarrow 90°$	360	10^{-9}	484	13	5	4	5.8	5.8
K	rotation + shearing	$\Psi \rightarrow 360°$	$\hat{V}_2 \rightarrow 10$	$\Psi^P \rightarrow 90°$	360	10^{-9}	563	13	5	4	5.8	5.8
L	rotation + shearing	$\Psi \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi^P \rightarrow 90°$	3600	10^{-9}	4068	102	5	4	5.8	5.8
M	rotation + shearing	$\Psi \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi^P \rightarrow 90°$	36000	10^{-9}	43907	1279	6	4	5.8	5.8
N	idem	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi^P \rightarrow 90°$	36	10^{-9}	102	16	13	3	16.7	10.1
O	idem	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi^P \rightarrow 90°$	72	10^{-9}	92	30	13	4	12.6	9.9
P	idem	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi^P \rightarrow 90°$	360	10^{-9}	349	13	18	5	8.6	9.7
Q	idem	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi \rightarrow 90°$	3600	10^{-9}	2030	89	20	6	6.9	9.5
R	idem	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi \rightarrow 90°$	36000	10^{-9}	19352	1247	23	6	5.9	9.5
S	idem	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi \rightarrow 90°$	360	10^{-8}	599	106	18	5	8.1	9.7
T	idem	$\Theta \rightarrow 360°$	$\hat{V}_1 \rightarrow 10$	$\Psi \rightarrow 90°$	360	10^{-7}	11279	3407	18	5	7.1	9.7

Table I.



$\underset{\sim}{g}_2$
reference
state
θ^2
$\underset{\sim}{x}$
θ^1
$\underset{\sim}{g}_1$
$\underset{\sim}{e}_2$
$\underset{\sim}{s}$
$\underset{\sim}{S}$
fixed basis
$\underset{\sim}{e}_1$
$\underset{\sim}{G}_2$
$\underset{\sim}{G}_2^*$
current
state
$\underset{\sim}{X}$
θ^2
θ^1
$\underset{\sim}{G}_1$
$\underset{\sim}{G}_1^*$
co-rotational
basis

fig. 1



istropic
axis
$\hat{V}_1$
A
$\hat{V}_3$
$\hat{V}_2$

fig. 2

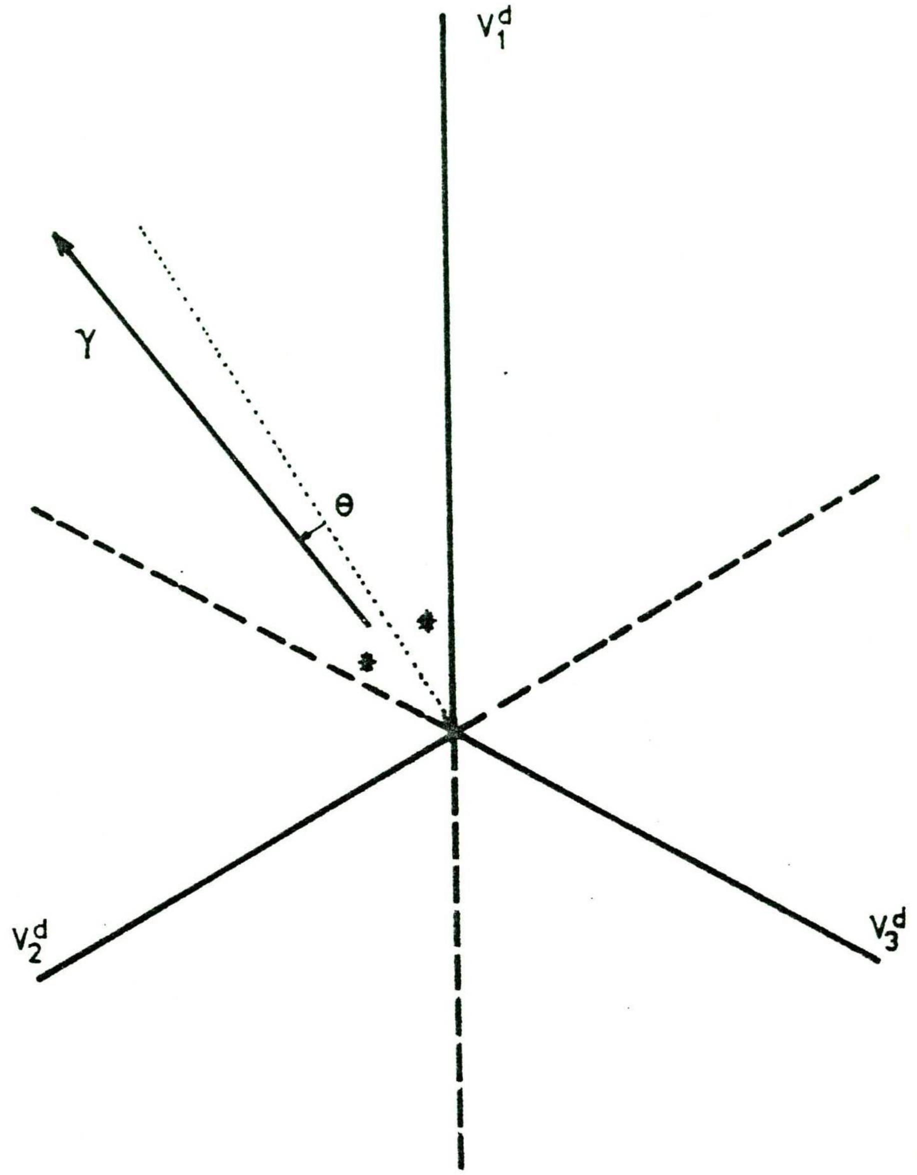


Fig. 3

```
      SUBROUTINE INCR(V,R,L,VN,RN,RS)
C     CALCULATION OF NEW DEFORMATION VN, ROTATION RN AND INCREMENTAL
C     ROTATION RS WHILE OLD DEFORMATION V, ROTATION R AND LOCAL
C     INCREMENTAL DISPLACEMENT GRADIENT L ARE KNOWN.
      COMMON/ GEG/IM(3,3)
      REAL V(6),R(3,3),L(3,3),VN(6),RN(3,3),RR(3,3)
      REAL D,E,P,T,F,PL,TL,FL
      REAL C1,C2,C3,C4,C5,C6,C7,R1,R2,R3
      REAL M11,M21,M31,M12,M22,M32,M13,M23,M33
      REAL S11,S21,S31
      REAL FS,TS,PS,FC,TC,PC
      INTEGER I,J,K
      REAL A(3,3)
C     CALCULATE A=L*V+V
      FOR I=1,3,1
      .  FOR J=1,3,1
      .  .  D=0.0
      .  .  FOR K=1,3,1
      .  .  .  D=D+L(I,K)*V(IM(K,J))
      .  .  ENDFOR
      .  .  A(I,J)=D+V(IM(I,J))
      .  ENDFOR
      ENDFOR
C     FIRST ESTIMATE OF ANGLES F,T,P
      F=0.
      T=0.
      P=0.
C     INITIAL VALUES OF NEW STRETCHTENSOR VN
      FOR I=1,6,1
      .  VN(I)=V(I)
      ENDFOR
C     IMPROVE ANGLES F,T,P UPTO AN ITERATION CRITERION OF
C     DELTA(ANGLE).LT.1.E-9 (WITHIN 20 ITERATIONS)
      FS=0.
      TS=0.
      PS=0.
      FC=1.
      TC=1.
      PC=1.
      C1=1.
      C2=0.
      C3=1.
      C4=0.
      C5=1.
      C6=0.
      C7=1.
```

Subroutine INCR

continued 1

```
LOOP(20)
.  FL=F
.  TL=T
.  PL=P
.  M11=TC*VN(2)+PC*VN(3)
.  M21=-TC*VN(4)
.  M31=-PC*VN(6)
.  M12=-VN(4)
.  M22=VN(1)+C3*VN(3)
.  M32=-C3*VN(5)
.  M13=-TC*VN(6)
.  M23=-FC*VN(5)
.  M33=TC*VN(1)+FC*VN(2)
.  R1=A(2,3)-A(3,2)-(C7-C5)*VN(5)+C6*VN(3)
.  R2=-A(1,3)+A(3,1)-(C1-C7)*VN(6)-C2*VN(5)-C4*VN(3)
.  R3=A(1,2)-A(2,1)-(C5-C1)*VN(4)+C2*VN(2)+C4*VN(5)-C6*VN(6)
.  S11=M22*M33-M32*M23
.  S21=M12*M33-M32*M13
.  S31=M12*M23-M22*M13
.  DET=M11*S11-M21*S21+M31*S31
.  F=(R1*S11-R2*S21+R3*S31)/DET
.  T=((R2-M21*F)*M33-(R3-M31*F)*M23)/S11
.  P=(R3-M31*F-M32*T)/M33
.  D=0.
.  IF (D.LT.DABS(TL-T)) D=DABS(TL-T)
.  IF (D.LT.DABS(PL-P)) D=DABS(PL-P)
.  IF (D.LT.DABS(FL-F)) D=DABS(FL-F)
CALCULATE INCREMENTAL ROTATIONMATRIX RR
.  FS=F
.  TS=T
.  PS=P
.  FC=DSQRT(1.-F**2)
.  TC=DSQRT(1.-T**2)
.  PC=DSQRT(1.-P**2)
.  C1=TC*PC
.  C2=FS*TS*PC
.  C3=FC*PC
.  C4=FS*PS
.  C5=FC*PC+FS*TS*PS
.  C6=FC*TS*PS
.  C7=FC*TC
.  RR(1,1)=C1
.  RR(2,1)=-FC*PS+C2
.  RR(3,1)=C4+C3*TS
.  RR(1,2)=TC*PS
.  RR(2,2)=C5
.  RR(3,2)=-FS*PC+C6
.  RR(1,3)=-TS
.  RR(2,3)=FS*TC
.  RR(3,3)=C7
C      IMPROVE NEW STRETCHTENSOR VN
.  FOR I=1,3,1
.  .  FOR J=1,I,1
.  .  .  E=0.
.  .  .  FOR K=1,3,1
.  .  .  .  E=E+A(I,K)*RR(J,K)
.  .  .  ENDFOR
.  .  .  VN(IM(I,J))=E
.  .  ENDFOR
.  ENDFOR
.  IF (D.LT.1.E-9)
.  .  EXITLOOP
.  ENDIF
ENDLOOP
```

```
C       CALCULATE NEW ROTATION RN
        FOR I=1,3,1
        .  FOR J=1,3,1
        .  .  D=0.0
        .  .  FOR K=1,3,1
        .  .  .  D=D+RR(I,K)*R(K,J)
        .  .  ENDFOR
        .  .  RN(I,J)=D
        .  ENDFOR
        ENDFOR
        RETURN
        END
```

Subroutine INCR

for the incremental calculation of large deformation and material rotation

V-components of left stretchtensor at start of increment	(see eq.10)
R-material rotation matrix at start of increment	(see eq.11)
L-incremental deformation gradient	(see eq.70)
VN-components of left stretchtensor at end of increment	(see eq.68)
RN-material rotation matrix at end of increment	(see eq.69)
RR-incremental rotation matrix	(see eq.69)

```
SUBROUTINE INVV(V,VINV)
CALCULATION OF INVERSE OF V
V=DEFORMATION MATRIX
REAL V(6),VINV(6)
REAL DET
REAL C1,C2,C3,C4,C5,C6
INTEGER I
COVARIANTS, DETERMINANT AND INVERSE OF V
C1=V(2)*V(3)-V(5)**2
C2=V(1)*V(3)-V(6)**2
C3=V(1)*V(2)-V(4)**2
C4=V(5)*V(6)-V(3)*V(4)
C5=V(4)*V(6)-V(1)*V(5)
C6=V(4)*V(5)-V(2)*V(6)
DET=V(1)*C1+V(4)*C4+V(6)*C6
VINV(1)=C1/DET
VINV(2)=C2/DET
VINV(3)=C3/DET
VINV(4)=C4/DET
VINV(5)=C5/DET
VINV(6)=C6/DET
RETURN
END
```

Subroutine INVV

for inversion of a symmetric 3 x 3 matrix

V-components of symmetric 3 x 3 matrix

VINV-components of inverse of V

```
      SUBROUTINE TOROT(V,R,VS)
C     CALCULATION OF CO-ROTATIONAL DEFORMATION
      COMMON/ GEG/IM(3,3)
      REAL V(6),R(3,3),VS(6)
      REAL D
      INTEGER I,J,K
      REAL HH(3,3)
      FOR I=1,3,1
      .  FOR J=1,3,1
      .  .  D=0.
      .  .  FOR K=1,3,1
      .  .  .  D=D+R(I,K)*V(IM(K,J))
      .  .  ENDFOR
      .  .  HH(I,J)=D
      .  ENDFOR
      ENDFOR
      FOR I=1,3,1
      .  FOR J=1,3,1
      .  .  D=0.
      .  .  FOR K=1,3,1
      .  .  .  D=D+HH(I,K)*R(J,K)
      .  .  ENDFOR
      .  .  VS(IM(I,J))=D
      .  ENDFOR
      ENDFOR
      RETURN
      END
```

Subroutine TOROT

for the transformation of a symmetric matrix

from a fixed basis to a co-rotational basis

V- components of symmetric matrix expressed with
   respect to the fixed basis (see eq.25)

R- rotation matrix (see eq.25)

VS-components of the symmetric matrix expressed with

   respect to the co-rotational basis

```
SUBROUTINE FROMROT(VS,R,V)
CALCULATION OF DEFORMATION V WITH RESPECT TO FIXED BASIS
COMMON/ GEG/IM(3,3)
REAL VS(6),R(3,3),V(6)
REAL D
INTEGER I,J,K
REAL HH(3,3)
FOR I=1,3,1
.   FOR J=1,3,1
.   .   D=0.
.   .   FOR K=1,3,1
.   .   .   D=D+R(K,I)*VS(IM(K,J))
.   .   ENDFOR
.   .   HH(I,J)=D
.   ENDFOR
ENDFOR
FOR I=1,3,1
.   FOR J=1,3,1
.   .   D=0.
.   .   FOR K=1,3,1
.   .   .   D=D+HH(I,K)*R(K,J)
.   .   ENDFOR
.   .   V(IM(I,J))=D
.   ENDFOR
ENDFOR
RETURN
END
```

Subroutine FROMROT

for the transformation of a symmetric matrix
from a co-rotational basis to a fixed basis

VS-components of symmetric matrix expressed with respect to the co-rotational basis	(see eq.25)
R -rotation matrix	(see eq.25)
V -components of symmetric matrix expressed with respect to the fixed basis	(see eq.25)

```
      SUBROUTINE POLDEC(F,V,R)
      COMMON /GEG/IM(3,3)
      DIMENSION F(3,3),V(6),R(3,3),
     . CD(3),U(3,3),WORK(10),C(3,3),A(3,3)
C-----------------------------------------------------------------------
C DEZE ROUTINE BEREKENT UIT F DE V EN DE R
C-----------------------------------------------------------------------
      DO 10 M1=1,3
      .  DO 10 M2=1,3
      .  .  D=0.0
      .  .  DO 20 M3=1,3
   20 .  .  .  D=D+F(M1,M3)*F(M2,M3)
   10 .  .  C(M1,M2)=D
      IFAIL=0
      CALL F02ABF(C,3,3,CD,U,3,WORK,IFAIL)
      IF(IFAIL.NE.0) STOP
      DO 30 M1=1,3
   30 .  CD(M1)=DSQRT(CD(M1))
      DO 40 M1=1,3
      .  DO 40 M2=M1,3
      .  .  D=0.0
      .  .  DO 50 M3=1,3
   50 .  .  .  D=D+CD(M3)*U(M1,M3)*U(M2,M3)
   40 .  .  V(IM(M1,M2))=D
      A(1,1)=V(2)*V(3)-V(5)**2
      A(2,2)=V(1)*V(3)-V(6)**2
      A(3,3)=V(1)*V(2)-V(4)**2
      A(1,2)=-(V(4)*V(3)-V(6)*V(5))
      A(2,3)=-(V(1)*V(5)-V(4)*V(6))
      A(1,3)=V(4)*V(5)-V(6)*V(2)
      DET=V(1)*A(1,1)+V(4)*A(1,2)+V(6)*A(1,3)
      A(2,1)=A(1,2)
      A(3,1)=A(1,3)
      A(3,2)=A(2,3)
      DO 60 M1=1,3
      .  DO 60 M2=1,3
      .  .  D=0.0
      .  .  DO 70 M3=1,3
   70 .  .  .  D=D+A(M1,M3)*F(M3,M2)
   60 .  .  R(M1,M2)=D/DET
      RETURN
      END
```

Subroutine POLDEC

for polar decomposition of a deformation gradient

F-matrix of deformation gradient	(see eqs.(5) and (12))
V-components of left stretchtensor	(see eqs.(10)and (12))
R-rotation matrix	(see eqs.(11)and (12))

Sunroutine FO2ABF is part of the NAG library

```
SUBROUTINE DRAAI(FI,THET,PSI,R)
CALCULATION OF ROTATIONMATRIX R AS A FUNCTION OF FI,THET,PSI
REAL FI,THET,PSI
REAL R(3,3)
REAL FS,TS,PS,FC,TC,PC
FS=DSIN(FI)
TS=DSIN(THET)
PS=DSIN(PSI)
FC=DCOS(FI)
TC=DCOS(THET)
PC=DCOS(PSI)
R(1,1)=TC*PC
R(2,1)=-FC*PS+FS*TS*PC
R(3,1)=FS*PS+FC*TS*PC
R(1,2)=TC*PS
R(2,2)=FC*PC+FS*TS*PS
R(3,2)=-FS*PC+FC*TS*PS
R(1,3)=-TS
R(2,3)=FS*TC
R(3,3)=FC*TC
RETURN
END
```

Subroutine DRAAI

for the calculation of the rotation matrix

on the basis of given rotation angtes

FI -rotation angle (see eq.47)

THET-rotation angle (see eq.47)

PSI -rotation angle (see eq.47)

R -rotation matrix (see eq.47)

```
C
      SUBROUTINE HOEK(R,TH,FI,PSI)
      DIMENSION R(3,3),F(4)
      DATA PI /3.141593/
C -------------------------------------------------------------------------
C    BEPAALT DE HOEKEN VAN ORTHONORMAAL ASSENSTELSEL R(RECHTSDRAAIEND)
C -------------------------------------------------------------------------
C..... HOEK TH
      TH=DASIN(-R(1,3)/1.000001)
C..... HOEK FI
      E1=R(2,3)/DCOS(TH)
      E2=R(3,3)/DCOS(TH)
      E1=E1/1.000001
      E2=E2/1.000001
      F(1)=DASIN(E1)
      F(2)=-PI-F(1)
      IF (F(1).GT.0.0) F(2)=PI-F(1)
      F(3)=DACOS(E2)
      F(4)=-F(3)
      IF(DABS(F(1)-F(3)).LT.1.E-03) FI=F(1)
      IF(DABS(F(1)-F(4)).LT.1.E-03) FI=F(1)
      IF(DABS(F(2)-F(3)).LT.1.E-03) FI=F(2)
      IF(DABS(F(2)-F(4)).LT.1.E-03) FI=F(2)
C..... HOEK PSI
      E1=R(1,2)/DCOS(TH)
      E2=R(1,1)/DCOS(TH)
      E1=E1/1.000001
      E2=E2/1.000001
      F(1)=DASIN(E1)
      F(2)=-PI-F(1)
      IF (F(1).GT.0.0) F(2)=PI-F(1)
      F(3)=DACOS(E2)
      F(4)=-F(3)
      IF(DABS(F(1)-F(3)).LT.1.E-03) PSI=F(1)
      IF(DABS(F(1)-F(4)).LT.1.E-03) PSI=F(1)
      IF(DABS(F(2)-F(3)).LT.1.E-03) PSI=F(2)
      IF(DABS(F(2)-F(4)).LT.1.E-03) PSI=F(2)
C..... OMZETTING VAN RADIALEN NAAR GRADEN
      TH=180.0*TH/PI
      FI=180.0*FI/PI
      PSI=180.0*PSI/PI
      RETURN
      END
```

Subroutine HOEK

for calculation of rotation angles of a rotation matrix

R	-rotation matrix	(see eq.47)
TH	-rotation angle	(see eq.47)
FI	-rotation angle	(see eq.47)
PSI	-rotation angle	(see eq.47)

```
      SUBROUTINE INVAR(V,DEO,GI,TH)
      DIMENSION V(6),VN(6)
      DATA PI /3.141593/
C-----------------------------------------------------------------------
C BEPAALT DE INVARIANTEN VAN DE SYMMETRISCHE TENSOR V
C-----------------------------------------------------------------------
      C11=V(2)*V(3)-V(5)**2
      C12=-V(4)*V(3)+V(5)*V(6)
      C13=V(4)*V(5)-V(2)*V(6)
      DELTA=V(1)*C11+V(4)*C12+V(6)*C13
      DEO=DELTA-1.0
      CC=(V(1)+V(2)+V(3))/3.0
      DO 10 M1=1,3
      VN(M1)=V(M1)-CC
   10 CONTINUE
      DO 20 M1=4,6
      VN(M1)=V(M1)
   20 CONTINUE
      D=0.0
      DO 30 M1=1,3
      M2=M1+3
   30 D=D+VN(M1)**2+2.0*(VN(M2)**2)
      GI=DSQRT(D)
      C11=VN(2)*VN(3)-VN(5)**2
      C12=-VN(4)*VN(3)+VN(5)*VN(6)
      C13=VN(4)*VN(5)-VN(2)*VN(6)
      X3=VN(1)*C11+VN(4)*C12+VN(6)*C13
      X1=0.0
      IF(DABS(GI).GT.1.0E-10) X1=-(X3*3.0*DSQRT(6.0))/(GI**3)
      X1=X1/1.00001
      TH=DASIN(X1)/3.0
      TH=180.0*TH/PI
      RETURN
      END
```

Subroutine INVAR

for calculation of invariant measures of large deformation

V	- components of left stretchtensor	(see eq.10)
DEO	- relative volume change	(see eq.37)
GI	- measure of distorsion or shear	(see eq.40)
TH	- angle in pi-plane of principal stretchspace	(see eq.41)

```
C       IN FILE ROTDEF
C       DETERMINATION OF V AND R USING INCREMENTAL METHOD AND
C       POLAR DECOMPOSITION.
C
        REAL PI,FI,T,P,TIME,TIMINC,TIMPOL,FF,TT,PP
        REAL ERV,ERR,ERVP,ERRP
        INTEGER I,J,K,JJ,NN,JJERV,JJERR,JJERVP,JJERRP
        COMMON /GEG/ IM(3,3)
        REAL VICO(6),VIC(6),VIO(6),VI1(6),V1C(6),V10(6),V11(6)
        REAL V2C(6),V20(6),V21(6),SG1(6),DSG1(6),SG2(6),DSG2(6)
        REAL RIO(3,3),RI1(3,3),R10(3,3),R11(3,3),R20(3,3),R21(3,3)
        REAL RR11(3,3),RR21(3,3),RH(3,3),SGH(6)
        REAL FI1(3,3),L(3,3),HH(3,3),VINV(6)
        DATA IM/1,4,6,4,2,5,6,5,3/
C
C       INITIATION
        ERV=0.
        ERR=0.
        ERVP=0.
        ERRP=0.
        PI=4.*DATAN(1.)
        NN=360
        FOR I=1,3,1
        .  FOR J=1,3,1
        .  .  RIO(I,J)=0.0
        .  .  R10(I,J)=0.0
        .  .  R20(I,J)=0.0
        .  ENDFOR
        .  VIO(I)=1.0
        .  VIO(I+3)=0.0
        .  V10(I)=1.0
        .  V10(I+3)=0.0
        .  V20(I)=1.0
        .  V20(I+3)=0.0
        .  RIO(I,I)=1.0
        .  R10(I,I)=1.0
        .  R20(I,I)=1.0
        .  SG1(I)=1.
        .  SG1(I+3)=0.
        .  SG2(I)=1.
        .  SG2(I+3)=0.
        ENDFOR
        SG1(1)=2.
        SG2(1)=2.
        FI=0.0
        T=0.0
        P=0.0
        FF=0.
        TT=0.
        PP=0.
        TIMINC=0.
        TIMPOL=0.
C
```

```
CALCULATION OF INCREMENTS
FOR JJ=1,NN,1
DESCRIBE VI1 AND RI1
.   P=2.*PI*FLOAT(JJ)/FLOAT(NN)
.   CALL DRAAI(FI,T,P,RI1)
.   PP=2.*PI*FLOAT(JJ)/FLOAT(NN)/4.
.   CALL DRAAI(FF,TT,PP,RH)
.   FOR I=1,3,1
.   .   VICO(I)=1.0
.   .   VICO(I+3)=0.0
.   ENDFOR
.   VICO(1)=1.+9.*FLOAT(JJ)/FLOAT(NN)
.   CALL FROMROT(VICO,RH,VIC)
.   CALL FROMROT(VIC,RI1,VI1)
DESCRIBE FI1
.   FOR I=1,3,1
.   .   FOR J=1,3,1
.   .   .   D=0.0
.   .   .   FOR K=1,3,1
.   .   .   .   D=D+VI1(IM(I,K))*RI1(K,J)
.   .   .   ENDFOR
.   .   .   FI1(I,J)=D
.   .   ENDFOR
.   ENDFOR
DESCRIBE L:  LOCAL INCREMENTAL DISPLACEMENT INCREMENT
.   CALL INVV(VI0,VINV)
.   FOR I=1,3,1
.   .   FOR J=1,3,1
.   .   .   D=0.
.   .   .   FOR K=1,3,1
.   .   .   .   D=D+(RI1(I,K)-RI0(I,K))*RI0(J,K)
.   .   .   ENDFOR
.   .   .   L(I,J)=D
.   .   ENDFOR
.   ENDFOR
.   FOR I=1,3,1
.   .   FOR J=1,3,1
.   .   .   D=0.
.   .   .   FOR K=1,3,1
.   .   .   .   D=D+VI1(IM(I,K))*L(K,J)
.   .   .   ENDFOR
.   .   .   HH(I,J)=D
.   .   ENDFOR
.   ENDFOR
.   FOR I=1,3,1
.   .   FOR J=1,3,1
.   .   .   D=0.0
.   .   .   FOR K=1,3,1
.   .   .   .   D=D+(VI1(IM(I,K))-VI0(IM(I,K))+HH(I,K))*VINV(IM(K,J))
.   .   .   ENDFOR
.   .   .   L(I,J)=D
.   .   ENDFOR
.   ENDFOR
```

Programme ROTDEF

continued 2

```
C      OUTPUT OF THE PRESCRIBED DEFORMATION AND ROTATION
       .  IF (JJ.EQ.1.OR.JJ.EQ.NN)
       .  .  WRITE(6,) VI0
       .  .  WRITE(6,) RI0
       .  .  WRITE(6,) VI1
       .  .  WRITE(6,) RI1
       .  .  WRITE(6,) FI1
       .  .  WRITE(6,) L
       .  .  WRITE(6,) VIC
       .  .  WRITE(6,1)
       .  ENDIF
C      END OF DESCRIPTION OF VI1,RI1,FI1,L
C
C      START INCREMENTAL CALCULATION
       .  CALL SETTIM
       .  CALL INCR(V10,R10,L,V11,R11,RR11)
       .  CALL GETTIM(TIME)
       .  TIMINC=TIMINC+TIME
       .  CALL TOROT(V11,R11,V1C)
       .  FOR I=1,6,1
       .  .  IF (ERV.LT.DABS(V11(I)-VI1(I)))
       .  .  .  JJERV=JJ
       .  .  .  ERV=DABS(V11(I)-VI1(I))
       .  .  ENDIF
       .  ENDFOR
       .  FOR I=1,3,1
       .  .  FOR J=1,3,1
       .  .  .  IF (ERR.LT.DABS(R11(I,J)-RI1(I,J)))
       .  .  .  .  JJERR=JJ
       .  .  .  .  ERR=DABS(R11(I,J)-RI1(I,J))
       .  .  .  ENDIF
       .  .  ENDFOR
       .  ENDFOR
C      CALCULATE STRESSINCREMENT FOR CONSTANT CO-ROTATIONAL STRESS.
       .  CALL FROMROT(SG1,RR11,SGH)
       .  FOR I=1,6,1
       .  .  DSG1(I)=SGH(I)-SG1(I)
       .  .  SG1(I)=SGH(I)
       .  ENDFOR
       .  IF (JJ.EQ.1.OR.JJ.EQ.NN)
       .  .  WRITE(6,) V10
       .  .  WRITE(6,) R10
       .  .  WRITE(6,) V11
       .  .  WRITE(6,) R11
       .  .  WRITE(6,) RR11
       .  .  WRITE(6,) SG1
       .  .  WRITE(6,) DSG1
       .  .  WRITE(6,) V1C
       .  .  WRITE(6,) JJERV,ERV,JJERR,ERR
       .  .  TIMINC=TIMINC/FLOAT(JJ)
       .  .  WRITE(6,) TIMINC
       .  .  WRITE(6,450) TIME
  450  .  .  FORMAT('0 DE INCREMENTELE BEREKENING DUURT',F15.9,/)
       .  .  WRITE(6,1)
       .  ENDIF
```

Programme ROTDEF

continued 3

```
START POLAR DECOMPOSITION
.  CALL SETTIM
.  CALL POLDEC(FI1,V21,R21)
.  FOR I=1,3,1
.  .  FOR J=1,3,1
.  .  .  D=0.
.  .  .  FOR K=1,3,1
.  .  .  .  D=D+R21(I,K)*R20(J,K)
.  .  .  ENDFOR
.  .  .  RR21(I,J)=D
.  .  ENDFOR
.  ENDFOR
.  CALL GETTIM(TIME)
.  TIMPOL=TIMPOL+TIME
.  FOR I=1,6,1
.  .  IF (ERVP.LT.DABS(V21(I)-VI1(I)))
.  .  .  JJERVP=JJ
.  .  .  ERVP=DABS(V21(I)-VI1(I))
.  .  ENDIF
.  ENDFOR
.  FOR I=1,3,1
.  .  FOR J=1,3,1
.  .  .  IF (ERRP.LT.DABS(R21(I,J)-RI1(I,J)))
.  .  .  .  JJERRP=JJ
.  .  .  .  ERRP=DABS(R21(I,J)-RI1(I,J))
.  .  .  ENDIF
.  .  ENDFOR
.  ENDFOR
CALCULATE STRESSINCREMENT FOR CONSTANT CO-ROTATIONAL STRESS.
.  CALL FROMROT(SG2,RR21,SGH)
.  FOR I=1,6,1
.  .  DSG2(I)=SGH(I)-SG2(I)
.  .  SG2(I)=SGH(I)
.  ENDFOR
.  IF (JJ.EQ.1.OR.JJ.EQ.NN)
.  .  CALL TOROT(V21,R21,V2C)
.  .  WRITE(6,) V21
.  .  WRITE(6,) R21
.  .  WRITE(6,) RR21
.  .  WRITE(6,) SG2
.  .  WRITE(6,) DSG2
.  .  WRITE(6,) V2C
.  .  WRITE(6,) JJERVP,ERVP,JJERRP,ERRP
.  .  TIMPOL=TIMPOL/FLOAT(JJ)
.  .  WRITE(6,) TIMPOL
.  .  WRITE(6,460) TIME
460 .  .  FORMAT('0 DE POLAIRE DECOMPOSITIE DUURT',F15.9,/)
.  .  WRITE(6,3)
.  ENDIF
```

```
C
C     UPDATING
      .  FOR I=1,3,1
      .  .  FOR J=1,3,1
      .  .  .  RI0(I,J)=RI1(I,J)
      .  .  .  R10(I,J)=R11(I,J)
      .  .  .  R20(I,J)=R21(I,J)
      .  .  ENDFOR
      .  .  VI0(I)=VI1(I)
      .  .  VI0(I+3)=VI1(I+3)
      .  .  V10(I)=V11(I)
      .  .  V10(I+3)=V11(I+3)
      .  .  V20(I)=V21(I)
      .  .  V20(I+3)=V21(I+3)
      .  ENDFOR
C
      ENDFOR
      STOP
C     PASS OVER 1 LINE
1     FORMAT( )
C     PASS OVER 2 LINES
2     FORMAT(/)
C     PASS OVER 3 LINES
3     FORMAT(//)
C     GO TO NEW PAGE
4     FORMAT('1')
C     EXPECT 3*27 SYMBOLS TO BE READ
5     FORMAT(27A3)
C     EXPECT 3*27 SYMBOLS TO BE PRINTED
6     FORMAT(' ',27A3)
      END
```

Programme ROTDEF

for the comparison of the accuracy and the computertime of the subroutines INCR and POLDEC

```
 1.000000000          1.000000000          1.000000000          0.000000000        VI0
 0.000000000          0.000000000
 1.000000000          0.000000000          0.000000000          0.000000000        RI0
 1.000000000          0.000000000          0.000000000          0.000000000
 1.000000000
 1.024988103          1.000011897        0.9999999999       5.4524234190E-04       VI1
 0.000000000          0.000000000
0.9998476951      -1.7452406437E-02        0.000000000       1.7452406437E-02       RI1
0.9998476951          0.000000000          0.000000000          0.000000000
1.0000000000
 1.024822476      -1.6907454772E-02        0.000000000       1.8433668259E-02       FI1
0.9998691063          0.000000000          0.000000000          0.000000000
0.9999999999
2.4822476219E-02  -1.6907454772E-02        0.000000000       1.8433668259E-02       L
-1.3089372579E-04     0.000000000          0.000000000          0.000000000
-7.2759576141E-11
 1.024999524          1.000000476        1.0000000000       1.0908169369E-04       VIC
 0.000000000          0.000000000

 1.000000000          1.000000000          1.000000000          0.000000000        V10
 0.000000000          0.000000000
 1.000000000          0.000000000          0.000000000          0.000000000        R10
 1.000000000          0.000000000          0.000000000          0.000000000
 1.000000000
 1.024988103          1.000011897        0.9999999999       5.4524234201E-04       V11
 0.000000000          0.000000000
0.9998476952      -1.7452406437E-02        0.000000000       1.7452406437E-02       R11
0.9998476952          0.000000000          0.000000000          0.000000000
 1.000000000
 0.000000000          0.000000000          0.000000000          0.000000000        RR11
 0.000000000          0.000000000          0.000000000          0.000000000
 0.000000000
 0.000000000          0.000000000          0.000000000          0.000000000        SG1
 0.000000000          0.000000000
-2.000000000         -1.000000000         -1.000000000          0.000000000        DSG1
 0.000000000          0.000000000
 1.024999524          1.000000476        0.9999999999       1.0908169395E-04       V1C
 0.000000000          0.000000000
       1    2.9103830457E-11          1    1.4551915228E-11                         JJERV,ERV,JJERR,ERR
 5.9000000000E-03                                                                  TIMINC

DE INCREMENTELE BEREKENING DUURT     0.005900000

 1.024988103          1.000011897        0.9999999999       5.4524234179E-04       V21
 0.000000000          0.000000000
0.9998476952      -1.7452406437E-02        0.000000000       1.7452406437E-02       R21
0.9998476952          0.000000000          0.000000000          0.000000000
 1.000000000
0.9998476952      -1.7452406437E-02        0.000000000       1.7452406437E-02       RR21
0.9998476952          0.000000000          0.000000000          0.000000000
 1.000000000
 1.999695413          1.000304586          1.000000000       1.7449748351E-02       SG2
 0.000000000          0.000000000
-3.0458651600E-04   3.0458647234E-04       0.000000000       1.7449748351E-02       DSG2
 0.000000000          0.000000000
 1.024999524          1.000000476        0.9999999999       1.0908169327E-04       V2C
 0.000000000          0.000000000
       1    2.1827872843E-11          1    1.4551915228E-11                         JJERVP,ERVP,JJERRP,ERRP
 5.7999999990E-03                                                                  TIMPOL

DE POLAIRE DECOMPOSITIE DUURT    0.005800000
```

Example of output of programme ROTDEF

for the first increment

```
1.004271106          9.970728894          0.9999999999         0.1957420025          VI0
0.000000000          0.000000000
0.9998476951         1.7452406585E-02     0.000000000          -1.7452406585E-02     RI0
0.9998476951         0.000000000          0.000000000          0.000000000
1.0000000000
0.9999999999         9.999999999          0.9999999999         1.8515056939E-09      VI1
0.000000000          0.000000000
1.0000000000         1.6000666492E-10     0.000000000          -1.6000666492E-10     RI1
1.0000000000         0.000000000          0.000000000          0.000000000
1.0000000000
0.9999999999         3.4515723429E-09     0.000000000          1.6914990290E-09      FI1
9.999999999          0.000000000          0.000000000          0.000000000
0.9999999999
-9.2289379875E-04    -0.3706520314        0.000000000          -1.7863182030E-02     L
1.0059467983E-02     0.000000000          0.000000000          0.000000000
0.000000000
1.0000000000         10.000000000         1.0000000000         4.1144570978E-10      VIC
0.000000000          0.000000000

1.004271101          9.970728846          0.9999999999         0.1957420033          V10
0.000000000          0.000000000
0.9998476939         1.7452407283E-02     0.000000000          -1.7452407250E-02     R10
0.9998476939         0.000000000          0.000000000          0.000000000
1.000000000
0.9999999958         9.999999951          0.9999999999         3.5024640965E-09      V11
0.000000000          0.000000000
0.9999999987         8.6129148258E-10     0.000000000          -8.2786755229E-10     R11
0.9999999987         0.000000000          0.000000000          0.000000000
1.000000000
0.000000000          0.000000000          0.000000000          0.000000000           RR11
0.000000000          0.000000000          0.000000000          0.000000000
0.000000000
0.000000000          0.000000000          0.000000000          0.000000000           SG1
0.000000000          0.000000000
0.000000000          0.000000000          0.000000000          0.000000000           DSG1
0.000000000          0.000000000
0.9999999932         9.999999926          0.9999999999         -3.9149199062E-09     V1C
0.000000000          0.000000000
   360    4.8370566219E-08        350    1.3096723706E-09                          JJERV,ERV,JJERR,ERR
5.8152777765E-03                                                                   TIMINC

DE INCREMENTELE BEREKENING DUURT      0.005800000

0.9999999999         9.999999999          0.9999999999         1.8515056938E-09      V21
0.000000000          0.000000000
1.000000000          1.6000666493E-10     0.000000000          -1.6000666488E-10     R21
1.000000000          0.000000000          0.000000000          0.000000000
1.000000000
0.9998476951         -1.7452406423E-02    0.000000000          1.7452406426E-02      RR21
0.9998476952         0.000000000          0.000000000          0.000000000
1.000000000
2.000000068          1.000000014          1.000000049          -1.7065644897E-08     SG2
0.000000000          0.000000000
3.0458703986E-04     -3.0458711262E-04    1.4551915228E-11     1.7449749275E-02      DSG2
0.000000000          0.000000000
0.9999999999         9.999999999          0.9999999999         4.1144571008E-10      V2C
0.000000000          0.000000000
   310    4.9476511777E-10        291    3.7471181713E-10                          JJERVP,ERVP,JJERRP,ERRP
5.7811111089E-03                                                                   TIMPOL

DE POLAIRE DECOMPOSITIE DUURT     0.005700000
```

Example of output of programme ROTDEF

for the last increment