UCLA
Computational and Applied Mathematics

Numerical implementation of elastoplasticity theory at finite strains

Koffi Enakoutsa
Yuelian Li

Department of Mathematics
University of California, Los Angeles
Los Angeles, CA, 90095-1555

Contents

1 INTRODUCTION **2**

2 Calculations of $\mathbf{F}^{-1}$ at the times t and $t + \Delta t$ **2**

3 Two-dimensional case **3**

4 Three dimensional case **5**
4.1 Calculation of the rotation from the rotation vector 5
4.2 Calculation of the rate of rotation vector discretized 6
4.3 Calculation of the rate of the rotation vector 7

5 Example: simple shear **8**

1. INTRODUCTION

Writing constitutive equations for elastic-plastic large deformation for metals requires a temporary objective derivative (i.e. independent of the two reference in which it is evaluated); this derivative intervenes on one hand in the hypo-elasticity law, and on the other one, in the case of kinematics hardening, in the evolution equation of the center of the domain of elasticity.

In the formulation adopted in many finite elements codes, the derivative chosen was the most simple one, the Jaumann Derivative, defined by (considering for example the derivative of the Cauchy stress tensor $\mathbf{\Sigma}$):

$$\hat{\mathbf{\Sigma}} = \dot{\mathbf{\Sigma}} + \mathbf{\Sigma}.\mathbf{\Omega} - \mathbf{\Omega}.\mathbf{\Sigma} \tag{1}$$

where $\mathbf{\Omega}$ defines the rate of rotation given by

$$\mathbf{\Omega} = \frac{1}{2}\left(\nabla_{\mathbf{x}}\mathbf{U} - {}^{T}\nabla_{\mathbf{x}}\mathbf{U}\right) \Leftrightarrow \mathbf{\Omega}_{\mathrm{ij}} = \frac{1}{2}\left(\frac{\partial \mathrm{U_i}}{\partial x_{\mathrm{j}}} - \frac{\partial \mathrm{U_j}}{\partial x_{\mathrm{i}}}\right) \tag{2}$$

($\mathbf{x}$, current position vector; $\mathbf{U}$ the speed). The use of this derivative to calculate the behavior in simple shear gives rise to oscillations of the shear stress as function of the strain. Although this prediction only concerns very large deformations and, consequently, no experiment has ever come to demonstrate its unrealistic character, it is considered unsatisfactory, at least for the spirit, by many authors. It therefore seems desirable, to prevent criticism which is always possible, to offer the user of our finite element code the possibility of using another derivative not subject to this drawback.

A possible choice, suggested by Fressengeas and Molinari [1], is to adopt the Green-Naghdi derivative defined by the same formula as in Eq.(1) above, but $\mathbf{\Omega}$ being given here by

$$\mathbf{\Omega} = \dot{\mathbf{R}} \cdot \mathbf{R}^{-1} \tag{3}$$

where $\mathbf{R}$ denotes the polar decomposition of the gradient of deformation $\mathbf{F}$. We recall that this term denotes a multiplicative decomposition of $\mathbf{F}$ of the form

$$\mathbf{F} = \mathbf{R} \cdot \mathbf{S} \tag{4}$$

where $\mathbf{R}$ is a rotation matrix and $\mathbf{S}$ is a symmetric matrix (${}^{t}\mathbf{S} = \mathbf{S}$). Similarly, $\mathbf{F}$ admits the decomposition

$$\mathbf{F} = \tilde{\mathbf{S}} \cdot \mathbf{R} \tag{5}$$

where $\tilde{\mathbf{S}}$ is another symmetric matrix but $\mathbf{R}$ the same rotation matrix. The matrices $\mathbf{R}, \mathbf{S}, \tilde{\mathbf{S}}$ are defined unequivocally if it is specified that they vary continuously and that at the initial time (where $\mathbf{F} = \mathbf{I}$), $\mathbf{R} = \mathbf{S} = \tilde{\mathbf{S}} = \mathbf{I}$.
We describe here the numerical implementation associated with the choice of this derivative and integrated in our finite element code.

2. Calculations of $\mathbf{F}^{-1}$ at the times t and t + Δt

The whole problem is to calculate the discretized Green-Naghdi rotation rate $\mathbf{\Omega}\Delta \mathrm{t} \equiv \Delta\mathbf{\Omega} = \Delta\mathbf{R} \cdot \mathbf{R}^{-1}$ (we then deduce for example the discretized Molinari stress rate $\Delta\mathbf{\Sigma} \equiv \Delta\mathbf{\Sigma} + \mathbf{\Sigma}.\Delta\mathbf{\Omega} - \Delta\mathbf{\Omega}\mathbf{\Sigma}.$). This requires calculating the rotations $\mathbf{R}(\mathrm{t}) \equiv \mathbf{R}$ and $\mathbf{R}(\mathrm{t} + \Delta \mathrm{t}) \equiv \mathbf{R}'$ (or $\mathbf{R}$ and $\Delta\mathbf{R} = \mathbf{R}' - \mathbf{R}$), and for this the deformation gradients

$\mathbf{F}(t) \equiv \mathbf{F}$ and $\mathbf{F}(t+\Delta t) \equiv \mathbf{F}'$.
The formula giving $\mathbf{F}'$ is written:

$$\mathbf{F}' = \frac{\partial x'}{\partial \mathbf{X}} = \mathbf{I} + \frac{\partial u'}{\partial \mathbf{X}} \Leftrightarrow F'_{ij} = \delta_{ij} + \frac{\partial u'_i}{\partial X'_j} \tag{6}$$

where $\mathbf{X}$ denotes the position vector at the time 0, x' the position vector at time $t+\Delta t$ and u' the displacement vector at this time $(u' = x' - \mathbf{X})$. However, the use of this formula poses a problem because, when going from the time t to the time $t+\Delta t$, we only have the shape functions relative to the final coordinates x'_i (which prohibits evaluating the derivatives with respect to the initial coordinates X_i). It is therefore more convenient to calculate the inverse of $\mathbf{F}'$ using the formula

$$\mathbf{F}'^{-1} = \frac{\partial \mathbf{X}}{\partial x'} = \mathbf{I} - \frac{\partial u'}{\partial x'} \Leftrightarrow F'^{-1}_{ij} = \delta_{ij} - \frac{\partial u'_i}{\partial X'_J} \tag{7}$$

Of course, it is in fact the discretized version of this equation that we use:

$$F'^{-1}_{ij} = \delta_{ij} - \sum_p \frac{\partial N_p\,(x')}{\partial x'_j} u'_i(p) \tag{8}$$

where the sum is extended to all the nodes of the mesh to which the considered (Gaussian) point belongs, and where $N_p\,(\mathbf{x}')$ and $\mathbf{u}'(p)$ denote respectively the shape function associated with the node p and the displacement (at time $t+\Delta t$) of this node. The inverse of $\mathbf{F}$ can be evaluated as follows:

$$\begin{aligned}&\mathbf{F}^{-1} = \tfrac{\partial \mathbf{X}}{\partial \mathbf{x}} = \tfrac{\partial \mathbf{X}}{\partial \mathbf{x}'} \cdot \tfrac{\partial \mathbf{x}'}{\partial \mathbf{x}} = \mathbf{F}'^{-1} \cdot \left(\mathbf{I} + \tfrac{\partial \Delta \mathbf{u}}{\partial \mathbf{x}}\right) \cong \mathbf{F}'^{-1} \cdot \left(\mathbf{I} + \tfrac{\partial \Delta \mathbf{u}}{\partial \mathbf{x}'}\right)\\ &\Leftrightarrow F^{-1}_{ij} = F'^{-1}_{ik} \cdot \left(\delta_{kj} + \tfrac{\partial \Delta u_k}{\partial x'_j}\right)\end{aligned} \tag{9}$$

where $\mathbf{x}$ denotes the position vector at the time t and $\Delta\mathbf{u}$ the increment of displacement between the times t and $t+\Delta t(\Delta\mathbf{u} = \mathbf{u}' - \mathbf{u}$, $\mathbf{u} \equiv$ move at the time t). The error made by replacing $\partial\Delta\mathbf{u}/\partial\mathbf{x}$ by $\partial\Delta\mathbf{u}/\partial\mathbf{x}'$ is negligible because of the second order in Δt whereas the algorithm used is of the first order. The derivatives $\partial\Delta\mathbf{u}_k/\partial\mathbf{x}'_j$ are of course still evaluated here using the gradients of the shape functions (relative to the coordinates $\mathbf{x}'_i$).

3. Two-dimensional case

We must now calculate $\mathbf{R}$ and $\mathbf{R}'$, or $\mathbf{R}$ and $\Delta\mathbf{R}$, and the discretized rotation rate $\Delta\boldsymbol{\Omega}$. We are going to distinguish here the two-dimensional and three-dimensional cases, because we will not proceed in the same way in the two cases (direct calculation of $\mathbf{R}$ and $\mathbf{R}$ without storage in the two-dimensional case, calculation of $\mathbf{R}$ and $\Delta\mathbf{R}$ with storage of $\mathbf{R}$ in the three-dimensional case). Let us consider first the two-dimensional case. Since we do not know $\mathbf{F}$ and $\mathbf{F}'$ directly but their inverses, it is convenient to consider the polar decompositions of these inverses:

$$\mathbf{F}^{-1} = \mathcal{R} \cdot \mathcal{S} = \tilde{\mathcal{S}} \cdot \mathcal{R},\ \mathbf{F}'^{-1} = \mathcal{R}' \cdot \mathcal{S}' = \tilde{\mathcal{S}}' \cdot \mathcal{R}' \tag{10}$$

where $\mathcal{R}$ and $\mathcal{R}'$ are the rotation matrices, $\mathcal{S}, \tilde{\mathcal{S}}, \mathcal{S}', \tilde{\mathcal{S}}'$ symmetric matrices . The quantities $\mathcal{R}$ and $\mathcal{R}'$ are none other than the inverses of $\mathbf{R}$ and $\mathbf{R}'$: indeed, for$\mathbf{F}$ for example, we have:

$$\mathbf{F}^{-1} = \tilde{S} \cdot \mathcal{R} \Rightarrow \mathbf{F} = R^{-1} \cdot \tilde{\mathcal{S}}^{-1}; \tag{11}$$

the comparison with Eq.(5) and the uniqueness of $\mathcal{R}$ and $\mathcal{S}$ show that $\mathcal{R}^{-1} = \mathbf{R}$. If we know how to calculate $\mathcal{R}$ and $\mathcal{R}'$, we can easily deduce the discretized rotation rate:

$$\mathbf{\Delta\Omega} = \mathbf{\Delta R} \cdot \mathbf{R^{-1}} \cong \mathbf{\Delta R} \cdot \mathbf{R'^{-1}} = (\mathbf{R'} - \mathbf{R}) \cdot \mathbf{R'^{-1}} = \mathbf{1} - \mathbf{R} \cdot \mathbf{R'^{-1}} = \mathbf{1} - \mathcal{R}^{\mathbf{-1}} \cdot \mathcal{R}'. \tag{12}$$

The problem is therefore reduced to the calculation of the rotations $\mathcal{R}$ and $\mathcal{R}'$ or to that, equivalent, of the matrices $\mathcal{S}$ and $\mathcal{S}'$, of the polar decompositions of $\mathbf{F}^{-1}$ and $\mathbf{F}'^{-1}$. Consider for example that of $\mathbf{F}^{-1}$. Let us introduce the matrix of dilatations (symmetric and known)

$$C = {}^{T}\mathbf{F}^{-1} \cdot \mathbf{F}^{-1}. \tag{13}$$

Thus, we have

$$C = {}^{T}(\mathcal{R}.\mathcal{S}).\mathcal{R}.\mathcal{S} = {}^{T}\mathcal{S}.{}^{T}\mathcal{R}.\mathcal{R}.\mathcal{S} = \mathcal{S}^2. \tag{14}$$

Thus $\mathcal{S}$ appears as the square root of C. This square root is uniquely defined given the requirements that it is symmetric, a continuous function of time (like C) and identical to the identity at the initial time. Let assume that :

$$C = \begin{bmatrix} a & b \\ b & c \end{bmatrix}; \mathcal{S} = \begin{bmatrix} \alpha & \beta \\ \beta & \gamma \end{bmatrix} \tag{15}$$

The matrix equation $C = \mathcal{S}^2$ is then written:

$$\begin{cases} \alpha^2 + \beta^2 & = \mathrm{a} \\ \beta(\alpha + \gamma) & = b \\ \beta^2 + \gamma^2 & = \mathrm{c} \end{cases} . \tag{16}$$

In addition, the matrix equation $C = (det(\mathcal{S}))^2$ is then written as:

$$\Delta \equiv \mathrm{ac} - \mathrm{b}^2 = (\alpha\gamma - \beta)^2 \Rightarrow \alpha\gamma - \beta^2 = \sqrt{\Delta}, \tag{17}$$

the choice of the sign in front of the radical results from the continuity and that initially, $\Delta = 1, \alpha = \gamma = 1, \beta = 0$. Adding this result to Eq.$(16)_1$ on one hand, Eq.$(16)_3$ on the other hand, we obtain:

$$\begin{cases} \alpha(\alpha + \gamma) = a + \sqrt{\Delta} \\ \gamma(\alpha + \gamma) = c + \sqrt{\Delta} \end{cases} \tag{18}$$

the addition of these equations gives $(\alpha + \gamma)^2 = a + c + 2\sqrt{\Delta}$, i.e. $\alpha + \gamma = \sqrt{\mathrm{a} + \mathrm{c} + 2\sqrt{\Delta}}$ given that initially, $\mathrm{a} = \mathrm{c} = 1, \Delta = 1, \alpha = \gamma = 1$. Transferring this result to Eq.(18) and Eq.$(16)_2$, we finally obtain:

$$\begin{cases} \alpha = \frac{a+\sqrt{\Delta}}{\sqrt{a+c+2\sqrt{\Delta}}} \\ \beta = \frac{b}{\sqrt{a+c+2\sqrt{\Delta}}} \\ \gamma = \frac{c+\sqrt{\Delta}}{\sqrt{a+c+2\sqrt{\Delta}}} \end{cases} \tag{19}$$

These equations allow the calculation of $\mathcal{S}$ as a function of C. The expression of $\mathcal{R}$ follows immediately thanks to the formula $\mathcal{R} = \mathbf{F}^{-1} \cdot \mathcal{S}^{-1}$.

4. Three dimensional case

We have seen, in the two-dimensional case, that the calculation of $\mathcal{R}$ or $\mathcal{S}$ is equivalent to that of the square root of C, itself fundamentally equivalent to the diagonalization of this matrix. In the two-dimensional case, this results in painless extractions of square roots. In the three-dimensional case, it is a question of solving an equation of the 3rd degree, which is more unpleasant and costly in computing time. We therefore use another, faster method, consisting of an incremental calculation of $\mathbf{R}$ (and $\mathbf{R}'$) and requiring storage, Gauss point by Gauss point , of $\mathbf{R}$. This method would indeed also lead to faster calculations in the two-dimensional case, but its use is not possible in this case because of the need to store $\mathbf{R}$.

4.1. Calculation of the rotation from the rotation vector

In fact, the storage of the rotation matrix itself is less economical (9 quantities to store) and redundant, the coefficients being related due to the relationship ${}^T\mathbf{R}.\mathbf{R} = \mathbf{R}.{}^T\mathbf{R} = \mathbf{I}$. The most economical way to proceed[1] consists in storing the 3 components of the rotation vector $\mathbf{V}$ defined by:

$$\mathbf{V} = \theta\mathbf{v} \tag{20}$$

where θ denotes the angle of rotation and $\mathbf{v}$ the unit vector parallel with the axis of rotation. θ is a priori defined modulo 2π, but it is obvious that we can change the sign of θ and $\mathbf{v}$ without modifying $\mathbf{R}$; there is therefore uniqueness of θ and $\mathbf{v}$ only if it is specified that θ is in the interval $[0,\pi]$.

The first problem that arises is therefore to reconstruct the rotation matrix $\mathbf{R}$ from the rotation vector $\mathbf{V}$. For this, let us calculate the image, by the rotation $\mathbf{R}$, of any vector $\mathbf{W}$. The projection of $\mathbf{W}$ on the axis of rotation is $(\mathbf{v}.\mathbf{W})\mathbf{v} = \frac{1}{\theta^2}(\mathbf{V}.\mathbf{W})\mathbf{V}$; this projection is rotation invariant. The projection of $\mathbf{W}$ on the plane perpendicular to the axis of rotation is $\mathbf{W}' = \mathbf{W} - \frac{1}{\theta^2}(\mathbf{V}.\mathbf{W})\mathbf{V}$; after rotation, this projection becomes:

$$\cos\theta\mathbf{W}' + \sin\theta\mathbf{v}\wedge\mathbf{W}' = \cos\theta\left[\mathbf{W} - \frac{1}{\theta^2}(\mathbf{V}.\mathbf{W})\mathbf{V}\right] + \frac{\sin\theta}{\theta}\mathbf{V}\wedge\left[\mathbf{W} - \frac{1}{\theta^2}(\mathbf{V}.\mathbf{W})\mathbf{V}\right] = \cos\theta\left[\mathbf{W} - \frac{1}{\theta^2}(\mathbf{V}.\mathbf{W})\mathbf{V}\right] + \frac{\sin\theta}{\theta}\mathbf{V}\wedge\mathbf{W}. \tag{21}$$

In total, $\mathbf{W}$ thus becomes, after rotation,

$$\mathbf{R}.\mathbf{W} = \frac{1-\cos\theta}{\theta^2}(\mathbf{V}.\mathbf{W})\mathbf{V} + \cos\theta\mathbf{W} + \frac{\sin\theta}{\theta}\mathbf{V}\wedge\mathbf{W}. \tag{22}$$

The components of $\mathbf{R}$ are therefore given, given that $(\mathbf{V}\wedge\mathbf{W})_{\mathrm{i}} = \varepsilon_{\mathrm{ikj}}\cdot\mathrm{V_k W_j}$ where ε denotes the permutation tensor (completely anti-symmetric), by the formula:

$$\mathrm{R_{ij}} = \frac{1-\cos\theta}{\theta^2}\mathrm{V_i V_j} + \cos\theta\delta_{\mathrm{ij}} + \frac{\sin\theta}{\theta}\varepsilon_{\mathrm{ikj}}\mathrm{V_k}, \theta \equiv \|\mathbf{V}\| \tag{23}$$

[1] A classic method is to store the quaternion associated with the rotation; but this quaternion has 4 components instead of 3.

4.2. Calculation of the rate of rotation vector discretized

We now come to the central problem, which is to calculate, from the knowledge of $\mathbf{R}, \mathbf{F}^{-1}, \mathbf{F}'^{-1}$, the discretized rotation rate $\Delta\mathbf{\Omega} = \mathbf{\Delta R}.\mathbf{R^{-1}}$, or rather the associated discretized rotation rate vector $\Delta\omega$, defined by:

$$\forall \mathbf{W} : \Delta\Omega.\mathbf{W} = \Delta\omega \wedge \mathbf{W}. \tag{24}$$

To some terms in $(\Delta \mathrm{t})^2$, $\Delta\omega = \dot{\mathbf{R}} \cdot \mathbf{R^{-1}}$ is anti-symmetric; to any such matrix $\mathbf{A}$ is associated a vector a such that $\forall \mathbf{W}, \mathbf{A}.\mathbf{W} = \mathbf{a} \wedge \mathbf{W}.$

From $\mathbf{R}, \mathbf{F}^{-1}, \mathbf{F}'^{-1}$, we easily form the matrices

$$\begin{cases} \Delta\mathbf{M} = \mathbf{R}.\left(\mathbf{F}^{-1} - \mathbf{F}'^{-1}\right) \\ \tilde{\mathbf{S}}^{-1} = \mathbf{R}.\mathbf{F}^{-1} \end{cases} \tag{25}$$

($\tilde{\mathbf{S}}^{-1}$ is none other than the inverse of the matrix $\tilde{\mathbf{S}}$ of the polar decomposition Eq.(5)'). Let $\Delta\tilde{\mathbf{S}} = \tilde{\mathbf{S}}' - \tilde{\mathbf{S}}$, where $\tilde{\mathbf{S}}'^{-1}$ denotes the symmetric matrix of the polar decomposition Eq.(5)) at the time $\mathrm{t} + \Delta\mathrm{t}$.
We have

$$\tilde{\mathbf{S}}'^{-1} = (\tilde{\mathbf{S}} + \Delta\tilde{\mathbf{S}})^{-1} = \left[\tilde{\mathbf{S}}.\left(\mathbf{I} + \tilde{\mathbf{S}}^{-1}.\Delta\tilde{\mathbf{S}}\right)\right]^{-1} \cong \left(\mathbf{I} - \tilde{\mathbf{S}}^{-1}.\Delta\tilde{\mathbf{S}}\right).\tilde{\mathbf{S}}^{-1}. \tag{26}$$

Therefore:

$$\begin{aligned} \Delta\mathbf{M} &= \mathbf{R}.\left(\mathbf{F}^{-1} - \mathbf{F}'^{-1}\right) = \mathbf{R}.\left[{}^{T}\mathbf{R}.\tilde{\mathbf{S}}^{-1} - \left({}^{T}\mathbf{R} + {}^{T}\Delta\mathbf{R}\right).\left(\tilde{\mathbf{S}}^{-1} - \tilde{\mathbf{S}}^{-1}.\Delta\tilde{\mathbf{S}}.\tilde{\mathbf{S}}^{-1}\right)\right] \\ &\cong \mathbf{R}.\left({}^{T}\mathbf{R}.\tilde{\mathbf{S}}^{-1}.\Delta\tilde{\mathbf{S}}.\tilde{\mathbf{S}}^{-1} - {}^{T}\Delta\mathbf{R}.\tilde{\mathbf{S}}^{-1}\right) \\ &= \tilde{\mathbf{S}}^{-1}.\Delta\tilde{\mathbf{S}}.\tilde{\mathbf{S}}^{-1} - \mathbf{R}.{}^{T}\Delta\mathbf{R}.\tilde{\mathbf{S}}^{-1} \\ &= \tilde{\mathbf{S}}^{-1}.\Delta\tilde{\mathbf{S}}.\tilde{\mathbf{S}}^{-1} + \Delta\mathbf{\Omega}.\tilde{\mathbf{S}}^{\mathbf{-1}}. \end{aligned} \tag{27}$$

As a consequence

$$\Delta\mathbf{M} - {}^{T}\Delta\mathbf{M} = \Delta\mathbf{\Omega}.\mathbf{S}^{-1} + \tilde{\mathbf{S}}^{-1}.\Delta\mathbf{\Omega}. \tag{28}$$

Let $\Delta\mathbf{m}$ be the (known) vector associated with the anti-symmetric matrix $\Delta\mathbf{M} - {}^{T}\Delta\mathbf{M}.$ We then have $\Delta\mathrm{M_{ij}} - \Delta\mathrm{M_{ji}} = \varepsilon_{\mathrm{ikj}}\Delta\mathrm{m_k}$, and likewise $\Delta\Omega_{\mathrm{ij}} = \varepsilon_{\mathrm{ikj}}\Delta\omega_{\mathrm{k}}$. The previous equation is therefore written as:

$$\varepsilon_{\mathrm{ikj}}\Delta\mathrm{m_k} = \Delta\Omega_{\mathrm{ik}}.\tilde{S}^{-1}_{\mathrm{kj}} + \tilde{\mathrm{S}}^{-1}_{\mathrm{ik}}\Delta\Omega_{\mathrm{kj}} = \varepsilon_{\mathrm{ilk}}\Delta\omega_1\tilde{S}^{-1}_{\mathrm{kj}} + \tilde{\mathrm{S}}^{-1}_{\mathrm{ik}}\varepsilon_{\mathrm{klj}}.\Delta\omega_{\mathrm{l}}. \tag{29}$$

Multiplying on the right and on the left by $\varepsilon_{\mathrm{ijp}}$ we obtain

$$\begin{aligned} \varepsilon_{\mathrm{ikj}}\varepsilon_{\mathrm{ijp}}\Delta\mathrm{m_k} &= -\varepsilon_{\mathrm{ijk}}\varepsilon_{\mathrm{ijp}}\Delta\mathrm{m_k} = -2\delta_{\mathrm{kp}}\Delta\mathrm{m_k} = -2\Delta\mathrm{m_p} \\ &= \varepsilon_{\mathrm{ilk}}\varepsilon_{\mathrm{ijp}}\Delta\omega_1\tilde{\mathrm{S}}^{-1}_{\mathrm{kj}} + \varepsilon_{\mathrm{klj}}\varepsilon_{\mathrm{ijp}}\tilde{\mathrm{S}}^{-1}_{\mathrm{ik}}\Delta\omega_1 \\ &= \left(\delta_{\mathrm{lj}}.\delta_{\mathrm{kp}} - \delta_{\mathrm{lp}}.\delta_{\mathrm{kj}}\right)\tilde{\mathrm{S}}^{-1}_{\mathrm{kj}}\Delta\omega_1 + \left(\delta_{\mathrm{kp}}.\delta_{\mathrm{li}} - \delta_{\mathrm{ki}}\cdot\delta_{\mathrm{lp}}\right)\tilde{\mathrm{S}}^{-1}_{\mathrm{ik}}\Delta\omega_1 \\ &= \tilde{\mathrm{S}}^{-1}_{\mathrm{pj}}\Delta\omega_{\mathrm{j}} - \tilde{\mathrm{S}}^{-1}_{\mathrm{jj}}\Delta\omega_{\mathrm{p}} + \tilde{\mathrm{S}}^{-1}_{\mathrm{ip}}\Delta\omega_{\mathrm{i}} - \tilde{\mathrm{S}}^{-1}_{\mathrm{ii}}\Delta\omega_{\mathrm{p}} \\ &= 2\tilde{\mathrm{S}}^{-1}_{\mathrm{pj}}\Delta\omega_{\mathrm{j}} - 2\tilde{S}^{-1}_{\mathrm{jj}}\Delta\omega_{\mathrm{p}} \\ &\Rightarrow \Delta\mathrm{m_p} = \left[\left(\mathrm{tr}\tilde{\mathbf{S}}^{-1}\right)\delta_{\mathrm{pj}} - \tilde{\mathrm{S}}^{-1}_{\mathrm{pi}}\right]\Delta\omega_{\mathrm{j}}, \end{aligned} \tag{30}$$

This can be written as:

$$\Delta\mathbf{m} = \left[\left(\mathrm{tr}\tilde{\mathbf{S}}^{-1}\right)\mathbf{I} - \tilde{\mathbf{S}}^{-1}\right].\Delta\omega. \tag{31}$$

Thus we can obtain the discretized rotation rate vector $\Delta\omega$ from $\Delta\mathbf{m}$ (i.e. $\Delta\mathbb{M}$) by simply inverting a matrix 3×3 (which is much less expensive in calculation time than a diagonalization):

$$\Delta\omega = \left[\left(\mathrm{tr}\tilde{\mathbf{S}}^{-1}\right)\mathbf{I} - \tilde{\mathbf{S}}^{-1}\right].\Delta\mathbf{m}. \tag{32}$$

We then easily deduce the discretized rotation rate $\Delta\Omega$ by the formula $\Delta\mathbf{\Omega}_{\mathrm{ij}} = \varepsilon_{\mathrm{ikj}}\Delta\omega_{\mathrm{k}}$.

4.3. Calculation of the rate of the rotation vector

Finally, the vector $\Delta\omega$ being known, it is necessary to calculate and store the rotation $\mathbf{R}+\Delta\mathbf{R}$ at the time t, or more precisely the vector of rotation $\mathbf{V}+\Delta\mathbf{V}$ at this time t.
An additional advantage here is storing $\mathbf{V}+\Delta\mathbf{V}$ rather than $\mathbf{R}+\Delta\mathbf{R}$. In the second case, since the step Δt is not, numerically, infinitely small, the calculation of $\Delta\mathbf{R}$ inevitably leads to a matrix $\mathbf{R}+\Delta\mathbf{R}$ which is no longer strictly orthogonal. In the first, on the contrary, regardless of the vector $\mathbf{V}+\Delta\mathbf{V}$ calculated, the use, at the next time step, of the formula Eq.(18)with this rotation vector leads to a strictly orthogonal matrix.

To calculate $\Delta\mathbf{V}$, let us rewrite Eq.(17) with the unit vector $\mathbf{W}$ instead of the vector $\mathbf{V}=\theta\mathbf{v}$, and differentiate it with respect to time, $\mathbf{W}$ being assumed fixed:

$$\begin{aligned}
&\mathbf{R}.\mathbf{W} = (1-\cos\theta)(\mathrm{v}.\mathbf{W})\mathrm{v} + (\cos\theta\mathbf{W} + \sin\theta\mathrm{v}\wedge\mathbf{W})\\
&\quad\Rightarrow \Delta\mathbf{R}.\ \mathbf{W} = \Delta\theta.\ \sin\theta(\mathrm{v}\cdot\mathbf{W})\mathrm{v} + (1-\cos\theta)(\Delta\mathrm{v}.\ \mathbf{W})\mathrm{v} + (1-\cos\theta)(\mathrm{v}.\ \mathbf{W})\Delta\mathrm{v}\\
&\quad - \Delta\theta\cdot\sin\theta\mathbf{W} + \Delta\theta\cdot\cos\theta\mathrm{v}\wedge\mathbf{W} + \sin\theta\Delta\mathrm{v}\wedge\mathbf{W}.
\end{aligned}$$

Let us apply this relation to the vector $\mathbf{W}=\mathbf{v}$ as $\Delta\mathrm{v}.\mathrm{v}=0$ (v being unitary at any time), we obtain:

$$\begin{aligned}
\Delta\mathbf{R}\cdot\mathrm{v} &= \Delta\theta\cdot\sin\theta\mathrm{v} + (1-\cos\theta)\Delta\mathrm{v}\cdot\Delta\theta\cdot\sin\theta\mathrm{v} + \sin\theta(\Delta\mathrm{v})\wedge\mathrm{v}\\
&= (1-\cos\theta)\Delta\mathrm{v} + \sin\theta(\Delta\mathrm{v})\wedge\mathrm{v}.
\end{aligned}$$

Now, for any vector $\mathbf{W}$, we have $\Delta\mathbf{R}\cdot\mathbf{R}^{-1}.\ \mathbf{W} = \Delta\Omega.\mathbf{W} = \Delta\omega\wedge\mathbf{W}$. For $\mathbf{W}=\mathbf{v}$, we have $\mathbf{R}^{-1}.\mathrm{v}=\mathrm{v}$ ($\mathbf{v}$ is carried by the axis of rotation) and therefore $\Delta\mathbf{R}.\mathbf{v} = \Delta\omega\wedge\mathbf{v}$. The previous equation is therefore written as:

$$\Delta\omega\wedge\mathrm{v} = (1-\cos\theta)\Delta\mathrm{v} + \sin\theta(\Delta\mathrm{v})\wedge\mathrm{v}. \tag{33}$$

Let us take the cross product of this equation and the vector v; taking into account the formula of the double cross product, we obtain:

$$(\Delta\omega.\mathrm{v})\mathrm{v} - \Delta\omega = (1-\cos\theta)(\Delta\mathrm{v})\wedge\mathrm{v} - \sin\theta\Delta\mathrm{v}. \tag{34}$$

So we have both:

$$\begin{cases} (1-\cos\theta)\Delta\mathrm{v} + \sin\theta(\Delta\mathrm{v})\wedge\mathrm{v} = \Delta\omega\wedge\mathrm{v}\\ -\sin\theta\Delta\mathrm{v} + (1-\cos\theta)(\Delta\mathrm{v})\wedge\mathrm{v} = (\Delta\omega.\mathrm{v})\mathrm{v} - \Delta\omega \end{cases} \tag{35}$$

Solving this system with respect to the unknown quantity $\Delta\mathrm{v}$ and $(\Delta\mathrm{v})\wedge\mathrm{v}$ immediately gives:

$$\begin{aligned}
\Delta\mathrm{v} &= \frac{1}{2}\Delta\omega\wedge\mathrm{v} + \frac{\sin\theta}{2(1-\cos\theta)}\Delta\omega - \frac{\sin\theta}{2(1-\cos\theta)}(\Delta\omega.\mathrm{v})\mathrm{v}\\
&= \frac{1}{2}\Delta\omega\wedge\mathrm{v} + \frac{1+\cos\theta}{2\sin\theta}\Delta\omega - \frac{1+\cos\theta}{2\sin\theta}(\Delta\omega.\mathrm{v})\mathrm{v}
\end{aligned} \tag{36}$$

Note that we were thus able to evaluate $\Delta\mathbf{v}$ without calculating $\Delta\theta$. However, it is $\Delta\mathbf{V}$, and not $\Delta\mathbf{v}$, that we want to know; as $\mathbf{V} = \theta\mathbf{v}$, we have

$$\Delta\mathbf{V} = \Delta\theta \cdot \mathrm{v} + \theta\Delta\mathrm{v} = \frac{\Delta\theta}{\theta}\mathbf{V} + \frac{1}{2}\Delta\omega \wedge \mathbf{V} + \frac{\theta(1+\cos\theta)}{2\sin\theta}\Delta\omega - \frac{1+\cos\theta}{2\theta\sin\theta}(\Delta\omega.\mathbf{V})\mathbf{V}. \tag{37}$$

To calculate $\Delta\theta$ as a function of $\Delta\omega$, note that Eq.(18) implies that $\mathrm{tr}\,\mathbf{R} = 1 + 2\cos\theta$; thus, $\mathrm{tr}(\Delta\mathbf{R}) = -2\Delta\theta.\sin\theta$. But $\left(\Delta\mathbf{R}.\mathbf{R}^{-1}\right)_{\mathrm{ij}} = \Delta\Omega_{\mathrm{ij}} = \varepsilon_{\mathrm{ikj}}\Delta\omega_{\mathrm{k}}$. From there we get

$$\begin{aligned}
\Delta\mathrm{R}_{\mathrm{il}} &= \left(\Delta\mathbf{R}.\mathbf{R}^{-1}\right)_{\mathrm{ij}}\mathrm{R}_{\mathrm{j1}} = \varepsilon_{\mathrm{ikj}}\Delta\omega_{\mathrm{k}}\mathrm{R}_{\mathrm{j1}} \\
&\Rightarrow \mathrm{tr}(\Delta\mathbf{R}) = \Delta\mathrm{R}_{\mathrm{ii}} = \varepsilon_{\mathrm{ikj}}\Delta\omega_{\mathrm{k}}\left(\frac{1-\cos\theta}{\theta^2}\mathrm{V_jV_i} + \cos\theta\delta_{\mathrm{ji}} + \frac{\sin\theta}{\theta}\varepsilon_{\mathrm{jmi}}\mathrm{V_m}\right) \\
&= \varepsilon_{\mathrm{ikj}}\varepsilon_{\mathrm{jmi}}\frac{\sin\theta}{\theta}\Delta\omega_{\mathrm{k}}\mathrm{V_m} = -2\delta_{\mathrm{km}}\frac{\sin\theta}{\theta}\Delta\omega_{\mathrm{k}}\mathrm{V_m} = -2\frac{\sin\theta}{\theta}\Delta\omega.\mathbf{V};
\end{aligned} \tag{38}$$

where

$$\Delta\theta = \frac{1}{\theta}\Delta\omega.\mathbf{V} \tag{39}$$

Transferring this result to the previous expression of $\Delta\mathbf{V}$, we finally get

$$\Delta\mathbf{V} = \frac{1}{2}\Delta\omega \wedge \mathbf{V} + \frac{\theta(1+\cos\theta)}{2\sin\theta}\Delta\omega + \left[\frac{1}{\theta^2} - \frac{1+\cos\theta}{2\theta\sin\theta}\right](\Delta\omega.\mathbf{V})\mathbf{V}. \tag{40}$$

This formula allows the incrementation of the vector $\mathbf{V}$. If, after the incrementation, the norm of this vector exceeds π, we correct this last modulo $2\pi\mathbf{v}$, i.e. we perform the substitution

$$\mathbf{V} \to \mathbf{V} - 2\pi\mathbf{v} = \left(1 - \frac{2\pi}{||\mathbf{V}||}\right)\mathbf{V} \tag{41}$$

(which is equivalent to replacing θ by $2\pi - \theta$ and $\mathbf{v}$ by - $\mathbf{v}$).

5. Example: simple shear

We consider the typical example of a rigid plastic material, with linear kinematic work hardening, subjected to a stress of simple shear. The relations between the initial coordinates $\mathrm{X_i}$ and current coordinates $\mathrm{x_i}$ are written, for this load.

$$\begin{cases} \mathrm{x_1} = \mathrm{X_1} + \gamma\mathrm{X_2} \\ \mathrm{x_2} = \mathrm{X_2} \\ \mathrm{x_3} = \mathrm{X_3} \end{cases} \tag{42}$$

The expression of the shear stress $\tau \equiv \Sigma_{12}$ as a function of the deformation parameter γ is given by FRESSEENEAS and MOLINARI [2].

$$\tau = \frac{\Sigma_0}{\sqrt{3}} + \frac{h}{3}\left[\frac{2\gamma}{1+\gamma^2/4}\ln\left(1+\gamma^2/4\right) + \frac{1-\gamma^2/4}{1+\gamma^2/4}\left(-\gamma + 4\,\mathrm{Arctg}\,\frac{\gamma}{2}\right)\right], \tag{43}$$

where Σ_0 and h denotes the initial elastic limit and the slope of work hardening in a simple tensile test.

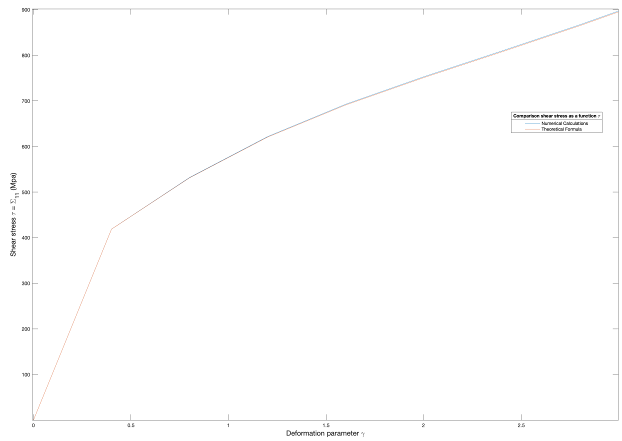

Figure 1: Shear stress as a function of the deformation parameter

Fig.(1) shows the comparison of the results obtained numerically (with $\Sigma_0 = 500$, $\mathrm{h} = 1000$ and $\mathrm{E} = 2000000$: quasi-rigid material) and those deduced from the formula Eq.(43). The agreement is excellent.

We also compared the theoretical and numerical values of Σ_{11}; the agreement is again excellent. The above comparison is for the two-dimensional option; a comparable agreement is obtained in the three-dimensional option, but not shown here.

References

[1] Fressengeas, C and Molinari A. (1983). Modèle d'écrouissage cinématique en grande deformation, *C.R.A.S.*, **297 II**, 93.

[2] Fressengeas, C and Molinari A. (1983). Représentation du comportement plastique anisotrope aux grandes deformations, Arch. Mech. **36** , 483.