Integration of 3D GTN model for Abaqus UMAT and VUMAT

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October 3, 2016

Contents

1 Nomenclature

Italic is used for scalars: g, Φ, K. Bold maths is used for rank 2 tensors: $\mathbf{I}$, $\boldsymbol{\sigma}$, $\boldsymbol{\epsilon}$. Script is used for rank 4 tensor: $\mathcal{C}$, $\mathcal{D}$, $\mathcal{I}$, $\mathcal{I}^{\text{sym}}$.

'$\cdot$' denotes dot product, single contraction: $\mathbf{T} = \boldsymbol{\sigma} \cdot \mathbf{n} \iff T^i_j = \sigma_{ij} n_i$ (surface traction).

':' denotes double product, double contraction: $\mathbf{S} : \mathbf{S} = S_{ij} S_{ij}$.

'$\otimes$' denotes tensor product: $\mathbf{I} \otimes \mathbf{I} = \delta_{ij}\delta_{kl}$.

Latin

A	void nucleation parameter
$c_{\alpha\beta}$	matrix of coefficients, $c^{-1}_{\alpha\beta} = \delta_{\alpha\beta} - \partial h_\alpha / \partial H_\beta$
$\mathcal{D}$	the linearisation moduli
f, f_c, f_f	void volume fraction; critical, and at fracture
f^*	bilinear function for void coalescence simulation
f^*_u	value of f^* at zero stress
f_N	fraction of void nucleating particles
G	shear modulus
g	flow potential
H_α	scalar state variables, $\alpha = 1, \dots, m$
$\mathbf{I}$	rank 2 identity tensor, δ_{ij}
J	Jacobian matrix of partial derivatives
$\mathcal{I}$	rank 4 identity tensor, $\delta_{ik}\delta_{jl}$
$\mathcal{I}^{\mathrm{sym}}$	symmetric rank 4 identity tensor, $\frac{1}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)$
K	compression modulus
$\mathcal{M}$	plastic tangent tensor, part of the linearisation moduli
m	number of solution dependent state variables
$\mathbf{n}$	normality tensor, $\mathbf{n} = \frac{3}{2q}\mathbf{S}$
q	von Mises equivalent stress, $q = \sqrt{\frac{3}{2}\mathbf{S} : \mathbf{S}} \to \partial q / \partial \boldsymbol{\sigma} = \mathbf{n}$
p	pressure, $p = -\frac{1}{3}\boldsymbol{\sigma} : \mathbf{I} \to \partial p / \partial \boldsymbol{\sigma} = -\frac{1}{3}\mathbf{I}$
p^e	elastic predictor pressure, $p^e = -\frac{1}{3}\boldsymbol{\sigma}^e : \mathbf{I}$
q_1, q_2, q_3	GTN fitted model 'material' parameters
s_N	standard deviation of the nucleation strain distribution
$\mathbf{S}$	stress deviator
$\mathbf{S}^e$	elastic predictor deviator

Greek

$\delta_{\alpha\beta}$	square unit matrix $m \times m$
$\boldsymbol{\epsilon}$	strain tensor
$\boldsymbol{\epsilon}^e$	elastic strain tensor
$\boldsymbol{\epsilon}^p$	plastic strain tensor, $\boldsymbol{\epsilon}^p = \varepsilon_q \mathbf{n} + \frac{1}{3}\varepsilon_p \mathbf{I}$
ε_p	volumetric strain
ε_q	equivalent plastic strain
ε_q^m	- equivalent plastic strain of the fully dense matrix
ε_N	mean of the nucleation strain distribution
Λ	plastic multiplier
$\boldsymbol{\sigma}$	stress tensor, $\boldsymbol{\sigma} = \mathbf{S} - p\mathbf{I}$
$\boldsymbol{\sigma}^e$	elastic predictor, $\boldsymbol{\sigma}^e = \mathbf{S}^e - p^e\mathbf{I}$
σ_0	flow stress of the fully dense matrix, $\sigma_0 = \sigma_0(\varepsilon_q^m)$
Φ	yield function

2 General analysis

2.1 Introduction

This work closely follows Beardsmore et al. (2006); Aravas (1987). Important misprints in Aravas (1987) are summarised in Table 1. The summation convention is used for Latin and Greek indices.

where	printed	must read
Appendix I, expression for A_{11}, third term	$\frac{\partial H^\alpha}{\Delta\varepsilon_p}$	$\frac{\partial H^\alpha}{\partial\Delta\varepsilon_p}$
Appendix I, expression for A_{12}, second and third terms	$\frac{\partial H^\alpha}{\partial\Delta\varepsilon_p}$	$\frac{\partial H^\alpha}{\partial\Delta\varepsilon_q}$
Appendix I, expression for A_{12}, third term	$+\Delta\varepsilon_p($	$+\Delta\varepsilon_q($
Appendix II, expression for A_{11}	$+\Delta\varepsilon_p$	$+\Delta\varepsilon_q$

Table 1: Misprints in Aravas (1987).

Finally $\partial H^\alpha/\partial\Delta\varepsilon_p$ and $\partial H^\alpha/\partial\Delta\varepsilon_q$ in Aravas (1987) must be understood as partial derivatives which take into account all implicit dependencies, i.e. derived from full differential. For this reason in this report the full differential notation is used instead: $dH_\alpha/d\Delta\varepsilon_p$ and $dH_\alpha/d\Delta\varepsilon_q$.

2.2 Assumptions

2.2.1 Pressure-dependent plasticity

It is assumed that the yield function, Φ, and the flow potential, g, are independent of the third stress invariant. Accordingly it is assumed that both Φ and g are dependent on the first and the second stress invariants, represented by p and q, and on the limited number of scalar state variables, $H_\alpha, \alpha = 1, 2, \ldots, m$:

$$\Phi = \Phi(p, q, H_\alpha) \tag{2.1}$$

$$g = g(p, q, H_\alpha) \tag{2.2}$$

2.2.2 Associated flow rule

or associated plasticity or normality rule:

$$\dot{\boldsymbol{\epsilon}}^p = \dot{\Lambda}\frac{\partial g}{\partial \boldsymbol{\sigma}} \tag{2.3}$$

2.2.3 Strain rate decomposition

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^e + \dot{\boldsymbol{\epsilon}}^p \tag{2.4}$$

2.2.4 Linear elasticity

$$\boldsymbol{\sigma} = \mathcal{C} : \boldsymbol{\epsilon}^e \tag{2.5}$$

where

$$\mathcal{C} = 2G\mathcal{I}^{\text{sym}} + \left(K - \frac{2}{3}G\right)\mathbf{I} \otimes \mathbf{I} \tag{2.6}$$

or, in index notation:

$$C_{ijkl} = G(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \left(K - \frac{2}{3}G\right)\delta_{ij}\delta_{kl} \tag{2.7}$$

2.2.5 Evolution of state variables

$$\dot{H}_\alpha = h_\alpha\left(\dot{\boldsymbol{\epsilon}}^p, \boldsymbol{\sigma}, H_\beta\right) \tag{2.8}$$

2.3 Numerical integration

The aim is to calculate the new $\boldsymbol{\sigma}$ and update the state variables, given several values stored from the last increment.

From (2.5):

$$\boldsymbol{\sigma} = \mathcal{C} : (\boldsymbol{\epsilon}_t^e + \Delta\boldsymbol{\epsilon}^e) = \mathcal{C} : (\boldsymbol{\epsilon}_t^e + \Delta\boldsymbol{\epsilon} - \Delta\boldsymbol{\epsilon}^p) = \boldsymbol{\sigma}^e - \mathcal{C} : \Delta\boldsymbol{\epsilon}^p \tag{2.9}$$

or

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^e - \mathcal{C} : \left(\Delta\varepsilon_q \mathbf{n} + \frac{1}{3}\Delta\varepsilon_p \mathbf{I}\right) \tag{2.10}$$

where

$$\boldsymbol{\sigma}^e \stackrel{\text{def}}{=} \mathcal{C} : (\boldsymbol{\epsilon}_t^e + \Delta\boldsymbol{\epsilon}) = \boldsymbol{\sigma}_t + \mathcal{C} : \Delta\boldsymbol{\epsilon} \tag{2.11}$$

is elastic predictor.

(2.2)→(2.3):

$$\dot{\boldsymbol{\epsilon}}^p = \dot{\Lambda}\left(\frac{\partial g}{\partial q}\frac{\partial q}{\partial \boldsymbol{\sigma}} + \frac{\partial g}{\partial p}\frac{\partial p}{\partial \boldsymbol{\sigma}}\right) = \dot{\Lambda}\left(\frac{\partial g}{\partial q}\mathbf{n} - \frac{1}{3}\frac{\partial g}{\partial p}\mathbf{I}\right) \tag{2.12}$$

which shows that plastic strain deviator is $\parallel$ to $\mathbf{n}$, or more precisely, it is equal to $\varepsilon_q \mathbf{n}$. So:

$$\dot{\varepsilon_q} = \dot{\Lambda}\frac{\partial g}{\partial q} \tag{2.13}$$

$$\dot{\varepsilon_p} = -\dot{\Lambda}\frac{\partial g}{\partial p} \tag{2.14}$$

(2.13)/(2.14):

$$\dot{\varepsilon_p}\frac{\partial g}{\partial q} + \dot{\varepsilon_q}\frac{\partial g}{\partial p} = 0 \tag{2.15}$$

(2.6)→(2.10):

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^e - \left(2G\mathcal{I}^{\text{sym}} + \left(K - \frac{2}{3}G\right)\mathbf{I}\otimes\mathbf{I}\right) : \left(\Delta\varepsilon_q \mathbf{n} + \frac{1}{3}\Delta\varepsilon_p \mathbf{I}\right) \tag{2.16}$$

or

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^e - 2G\Delta\varepsilon_q \mathbf{n} - \frac{2}{3}G\Delta\varepsilon_p \mathbf{I} - \left(K - \frac{2}{3}G\right)\Delta\varepsilon_p \mathbf{I} \tag{2.17}$$

or finally

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^e - 2G\Delta\varepsilon_q \mathbf{n} - K\Delta\varepsilon_p \mathbf{I} \tag{2.18}$$

Splitting into spherical and deviatoric parts:

$$\mathbf{S} = \mathbf{S}^e - 2G\Delta\varepsilon_q \mathbf{n} \tag{2.19}$$

$$p = p^e + K\Delta\varepsilon_p \tag{2.20}$$

(2.19) means $\mathbf{S}^e \parallel \mathbf{n}$, hence:

$$\mathbf{n} = \frac{3}{2q^e}\mathbf{S}^e \tag{2.21}$$

(2.21)→(2.19):

$$q = q^e - 3G\Delta\varepsilon_q \tag{2.22}$$

The full system includes (2.15), (2.1), (2.20), (2.22), (2.8). In finite difference form:

$$\Omega = \Delta\varepsilon_p \frac{\partial g}{\partial q} + \Delta\varepsilon_q \frac{\partial g}{\partial p} = 0 \tag{2.23}$$

$$\Phi(p, q, H_\alpha) = 0 \tag{2.24}$$

$$p = p^e + K\Delta\varepsilon_p \tag{2.25}$$

$$q = q^e - 3G\Delta\varepsilon_q \tag{2.26}$$

$$\Delta H_\alpha = h_\alpha\left(\Delta\varepsilon_p, \Delta\varepsilon_q, p, q, H_\beta\right) \tag{2.27}$$

Following (Beardsmore et al., 2006) we solve the system (2.23),(2.24) and (2.27) simultaneously for $\Delta\varepsilon_p$, $\Delta\varepsilon_q$ and ΔH_α.

2.4 Linearisation moduli

This assumes backward Euler method. From (2.9):

$$\boldsymbol{\sigma} = \mathcal{C} : (\boldsymbol{\epsilon} - \boldsymbol{\epsilon}^p_t - \frac{1}{3}\Delta\varepsilon_p \mathbf{I} - \Delta\varepsilon_q \mathbf{n}) \tag{2.28}$$

$$\partial\boldsymbol{\sigma} = \mathcal{C} : \left(\partial\boldsymbol{\epsilon} - \frac{1}{3}\partial\Delta\varepsilon_p \mathbf{I} - \partial\Delta\varepsilon_q \mathbf{n} - \Delta\varepsilon_q \frac{\partial\mathbf{n}}{\partial\boldsymbol{\sigma}} : \partial\boldsymbol{\sigma}\right) \tag{2.29}$$

where it easy to show that:

$$\frac{\partial\mathbf{n}}{\partial\boldsymbol{\sigma}} = \frac{1}{q}\left(\frac{3}{2}\mathcal{I}^{\text{sym}} - \frac{1}{2}\mathbf{I}\otimes\mathbf{I} - \mathbf{n}\otimes\mathbf{n}\right) \tag{2.30}$$

Now $\partial\Delta\varepsilon_p$ and $\partial\Delta\varepsilon_q$ in terms of $\partial\boldsymbol{\sigma}$.
Using (2.23):

$$\partial\left(\Delta\varepsilon_p \frac{\partial g}{\partial q}\right) + \partial\left(\Delta\varepsilon_q \frac{\partial g}{\partial p}\right) = 0 \tag{2.31}$$

or

$$\partial\Delta\varepsilon_p \frac{\partial g}{\partial q} + \Delta\varepsilon_p \partial\frac{\partial g}{\partial q} + \partial\Delta\varepsilon_q \frac{\partial g}{\partial p} + \Delta\varepsilon_q \partial\frac{\partial g}{\partial p} = 0 \tag{2.32}$$

where using (2.2):

$$\partial\frac{\partial g}{\partial q}=\left(\frac{\partial^2 g}{\partial q\partial p}\frac{\partial p}{\partial \boldsymbol{\sigma}}+\frac{\partial^2 g}{\partial q^2}\frac{\partial q}{\partial \boldsymbol{\sigma}}\right):\partial\boldsymbol{\sigma}+\frac{\partial^2 g}{\partial q\partial H_\alpha}\partial H_\alpha \tag{2.33}$$

and

$$\partial\frac{\partial g}{\partial p}=\left(\frac{\partial^2 g}{\partial p^2}\frac{\partial p}{\partial \boldsymbol{\sigma}}+\frac{\partial^2 g}{\partial p\partial q}\frac{\partial q}{\partial \boldsymbol{\sigma}}\right):\partial\boldsymbol{\sigma}+\frac{\partial^2 g}{\partial p\partial H_\alpha}\partial H_\alpha \tag{2.34}$$

(2.33), (2.34)→ (2.32):

$$\begin{aligned}&\partial\Delta\varepsilon_p\frac{\partial g}{\partial q}+\Delta\varepsilon_p\left[\left(-\frac{1}{3}\frac{\partial^2 g}{\partial q\partial p}\mathbf{I}+\frac{\partial^2 g}{\partial q^2}\mathbf{n}\right):\partial\boldsymbol{\sigma}+\frac{\partial^2 g}{\partial q\partial H_\alpha}\partial H_\alpha\right]\\&+\partial\Delta\varepsilon_q\frac{\partial g}{\partial p}+\Delta\varepsilon_q\left[\left(-\frac{1}{3}\frac{\partial^2 g}{\partial p^2}\mathbf{I}+\frac{\partial^2 g}{\partial p\partial q}\mathbf{n}\right):\partial\boldsymbol{\sigma}+\frac{\partial^2 g}{\partial p\partial H_\alpha}\partial H_\alpha\right]=0\end{aligned} \tag{2.35}$$

∂(2.24):

$$\left(-\frac{1}{3}\frac{\partial\Phi}{\partial p}\mathbf{I}+\frac{\partial\Phi}{\partial q}\mathbf{n}\right):\partial\boldsymbol{\sigma}+\frac{\partial\Phi}{\partial H_\alpha}\partial H_\alpha=0 \tag{2.36}$$

Since $H_\alpha=H^t_\alpha+\Delta H_\alpha$, $\partial\Delta H_\alpha=\partial H_\alpha$. From (2.27):

$$\partial H_\alpha=\frac{\partial h_\alpha}{\partial\Delta\varepsilon_q}\partial\Delta\varepsilon_q+\frac{\partial h_\alpha}{\partial\Delta\varepsilon_p}\partial\Delta\varepsilon_p+\frac{\partial h_\alpha}{\partial q}\partial q+\frac{\partial h_\alpha}{\partial p}\partial p+\frac{\partial h_\alpha}{\partial H_\beta}\partial H_\beta \tag{2.37}$$

or

$$\partial H_\alpha=\frac{\partial h_\alpha}{\partial\Delta\varepsilon_q}\partial\Delta\varepsilon_q+\frac{\partial h_\alpha}{\partial\Delta\varepsilon_p}\partial\Delta\varepsilon_p+\frac{\partial h_\alpha}{\partial q}\mathbf{n}:\partial\boldsymbol{\sigma}-\frac{1}{3}\frac{\partial h_\alpha}{\partial p}\mathbf{I}:\partial\boldsymbol{\sigma}+\frac{\partial h_\alpha}{\partial H_\beta}\partial H_\beta \tag{2.38}$$

or

$$\partial H_\alpha-\frac{\partial h_\alpha}{\partial H_\beta}\partial H_\beta=\frac{\partial h_\alpha}{\partial\Delta\varepsilon_q}\partial\Delta\varepsilon_q+\frac{\partial h_\alpha}{\partial\Delta\varepsilon_p}\partial\Delta\varepsilon_p+\frac{\partial h_\alpha}{\partial q}\mathbf{n}:\partial\boldsymbol{\sigma}-\frac{1}{3}\frac{\partial h_\alpha}{\partial p}\mathbf{I}:\partial\boldsymbol{\sigma} \tag{2.39}$$

or

$$c^{-1}_{\alpha\beta}\partial H_\beta=\frac{\partial h_\alpha}{\partial\Delta\varepsilon_q}\partial\Delta\varepsilon_q+\frac{\partial h_\alpha}{\partial\Delta\varepsilon_p}\partial\Delta\varepsilon_p+\frac{\partial h_\alpha}{\partial q}\mathbf{n}:\partial\boldsymbol{\sigma}-\frac{1}{3}\frac{\partial h_\alpha}{\partial p}\mathbf{I}:\partial\boldsymbol{\sigma} \tag{2.40}$$

where

$$c^{-1}_{\alpha\beta}=\delta_{\alpha\beta}-\frac{\partial h_\alpha}{\partial H_\beta} \tag{2.41}$$

Finally

$$\partial H_\alpha=c_{\alpha\beta}\left(\frac{\partial h_\beta}{\partial\Delta\varepsilon_q}\partial\Delta\varepsilon_q+\frac{\partial h_\beta}{\partial\Delta\varepsilon_p}\partial\Delta\varepsilon_p+\left(\frac{\partial h_\beta}{\partial q}\mathbf{n}-\frac{1}{3}\frac{\partial h_\beta}{\partial p}\mathbf{I}\right):\partial\boldsymbol{\sigma}\right) \tag{2.42}$$

(2.42)→ (2.35),(2.36) the following system is obtained:

$$A_{11}\partial\Delta\varepsilon_p + A_{12}\partial\Delta\varepsilon_q = (B_{11}\mathbf{I} + B_{12}\mathbf{n}) : \partial\boldsymbol{\sigma} \tag{2.43}$$

$$A_{21}\partial\Delta\varepsilon_p + A_{22}\partial\Delta\varepsilon_q = (B_{21}\mathbf{I} + B_{22}\mathbf{n}) : \partial\boldsymbol{\sigma} \tag{2.44}$$

where

$$A_{11} = \frac{\partial g}{\partial q} + \left(\Delta\varepsilon_p \frac{\partial^2 g}{\partial q \partial H_\alpha} + \Delta\varepsilon_q \frac{\partial^2 g}{\partial p \partial H_\alpha}\right) c_{\alpha\beta} \frac{\partial h_\beta}{\partial \Delta\varepsilon_p} \tag{2.45}$$

$$A_{12} = \frac{\partial g}{\partial p} + \left(\Delta\varepsilon_p \frac{\partial^2 g}{\partial q \partial H_\alpha} + \Delta\varepsilon_q \frac{\partial^2 g}{\partial p \partial H_\alpha}\right) c_{\alpha\beta} \frac{\partial h_\beta}{\partial \Delta\varepsilon_q} \tag{2.46}$$

$$A_{21} = \frac{\partial \Phi}{\partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial \Delta\varepsilon_p} \tag{2.47}$$

$$A_{22} = \frac{\partial \Phi}{\partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial \Delta\varepsilon_q} \tag{2.48}$$

$$\begin{aligned} B_{11} &= \frac{1}{3}\Delta\varepsilon_p \left(\frac{\partial^2 g}{\partial q \partial p} + \frac{\partial^2 g}{\partial q \partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial p}\right) \\ &\quad + \frac{1}{3}\Delta\varepsilon_q \left(\frac{\partial^2 g}{\partial p^2} + \frac{\partial^2 g}{\partial p \partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial p}\right) \end{aligned} \tag{2.49}$$

$$\begin{aligned} B_{12} &= -\Delta\varepsilon_p \left(\frac{\partial^2 g}{\partial q^2} + \frac{\partial^2 g}{\partial q \partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial q}\right) \\ &\quad - \Delta\varepsilon_q \left(\frac{\partial^2 g}{\partial p \partial q} + \frac{\partial^2 g}{\partial p \partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial q}\right) \end{aligned} \tag{2.50}$$

$$B_{21} = \frac{1}{3}\left(\frac{\partial \Phi}{\partial p} + \frac{\partial \Phi}{\partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial p}\right) \tag{2.51}$$

$$B_{22} = -\left(\frac{\partial \Phi}{\partial q} + \frac{\partial \Phi}{\partial H_\alpha} c_{\alpha\beta} \frac{\partial h_\beta}{\partial q}\right) \tag{2.52}$$

The system (2.43)-(2.44) has the following solution:

$$\partial\Delta\varepsilon_p = (M_{pI}\mathbf{I} + M_{pn}\mathbf{n}) : \partial\boldsymbol{\sigma} \tag{2.53}$$

$$\partial\Delta\varepsilon_q = (M_{qI}\mathbf{I} + M_{qn}\mathbf{n}) : \partial\boldsymbol{\sigma} \tag{2.54}$$

where

$$M_{pI} = \frac{A_{22}B_{11} - A_{12}B_{21}}{\det A} \tag{2.55}$$

$$M_{pn} = \frac{A_{22}B_{12} - A_{12}B_{22}}{\det A} \tag{2.56}$$

$$M_{qI} = \frac{A_{11}B_{21} - A_{21}B_{11}}{\det A} \tag{2.57}$$

$$M_{qn} = \frac{A_{11}B_{22} - A_{21}B_{12}}{\det A} \tag{2.58}$$

and

$$\det A = A_{11}A_{22} - A_{12}A_{21} \tag{2.59}$$

(2.53),(2.54) →(2.29):

$$\partial\boldsymbol{\sigma} = \mathcal{C} : \left(\partial\boldsymbol{\epsilon} - \frac{1}{3}(M_{pI}\mathbf{I} + M_{pn}\mathbf{n}) : \partial\boldsymbol{\sigma} \otimes \mathbf{I} \right.$$
$$\left. -(M_{qI}\mathbf{I} + M_{qn}\mathbf{n}) : \partial\boldsymbol{\sigma} \otimes \mathbf{n} - \Delta\varepsilon_q \frac{\partial\mathbf{n}}{\partial\boldsymbol{\sigma}} : \partial\boldsymbol{\sigma}\right) \tag{2.60}$$

or rearranging:

$$\left(\mathcal{C} : \left(\frac{1}{3}M_{pI}\mathbf{I}\otimes\mathbf{I} + \frac{1}{3}M_{pn}\mathbf{I}\otimes\mathbf{n} + M_{qI}\mathbf{n}\otimes\mathbf{I} + M_{qn}\mathbf{n}\otimes\mathbf{n} + \Delta\varepsilon_q\frac{\partial\mathbf{n}}{\partial\boldsymbol{\sigma}}\right) + \mathcal{I}\right) : \partial\boldsymbol{\sigma}$$
$$= \mathcal{C} : \partial\boldsymbol{\epsilon} \tag{2.61}$$

or

$$(\mathcal{M} + \mathcal{C}^{-1}) : \partial\boldsymbol{\sigma} = \partial\boldsymbol{\epsilon} \tag{2.62}$$

so

$$\mathcal{D} = \left(\mathcal{M} + \mathcal{C}^{-1}\right)^{-1} \tag{2.63}$$

where

$$\mathcal{M} = \frac{1}{3}M_{pI}\mathbf{I}\otimes\mathbf{I} + \frac{1}{3}M_{pn}\mathbf{I}\otimes\mathbf{n} + M_{qI}\mathbf{n}\otimes\mathbf{I} + M_{qn}\mathbf{n}\otimes\mathbf{n} + \Delta\varepsilon_q\frac{\partial\mathbf{n}}{\partial\boldsymbol{\sigma}} \tag{2.64}$$

or, expanding the last term, and replacing $\mathcal{I}^{sym}$ with $\mathcal{I}$, since both sides in (2.62) are symmetric:

$$\mathcal{M} = \left(\frac{1}{3}M_{pI} - \frac{\Delta\varepsilon_q}{2q}\right)\mathbf{I}\otimes\mathbf{I} + \frac{1}{3}M_{pn}\mathbf{I}\otimes\mathbf{n} + M_{qI}\mathbf{n}\otimes\mathbf{I} + \left(M_{qn} - \frac{\Delta\varepsilon_q}{q}\right)\mathbf{n}\otimes\mathbf{n} + \frac{3\Delta\varepsilon_q}{2q}\mathcal{J} \tag{2.65}$$

3 GTN model

3.1 GTN yield function and state variables

The flow potential and the yield function of the GTN model are:

$$\Phi = g = \left(\frac{q}{\sigma_0}\right)^2 + 2q_1 f \cosh\left(\frac{3}{2}\frac{q_2 p}{\sigma_0}\right) - (1 + q_3 f^2) = 0 \tag{3.1}$$

where

$$\sigma_0 = \sigma_0(\varepsilon_q^m) \tag{3.2}$$

is the flow stress of the fully dense matrix as a function of the equivalent plastic strain of the fully dense matrix, ε_q^m. As shown by Aravas (1987) $\varepsilon_q^m \neq \varepsilon_q$. ε_q is a macroscopic characteristic of material related to macroscopic plastic strain rate tensor, used in the flow rule, whereas ε_q^m is a microscopic property.

Accordingly there are two state variables in the GTN model - void volume fraction, f, and ε_q^m.

The equivalent plastic work principle:

$$(1-f)\sigma_0\dot{\varepsilon}_q^m = \boldsymbol{\sigma} : \dot{\boldsymbol{\epsilon}}^p \tag{3.3}$$

or

$$\dot{\varepsilon}_q^m = \frac{-p\dot{\varepsilon_p} + q\dot{\varepsilon_q}}{(1-f)\sigma_0} \tag{3.4}$$

Also after Aravas (1987):

$$\dot{f} = \dot{f}_{gr} + \dot{f}_{nucl} \tag{3.5}$$

where $\dot{f}_{gr}$ is void volume rate due to growth of existing voids:

$$\dot{f}_{gr} = (1-f)\dot{\varepsilon_p} \tag{3.6}$$

and $\dot{f}_{nucl}$ is void volume rate due to nucleation of new voids:

$$\dot{f}_{nucl} = A\dot{\varepsilon}_q^m \tag{3.7}$$

$$A = \frac{f_N}{s_N\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\varepsilon_q^m - \varepsilon_N}{s_N}\right)^2\right] \tag{3.8}$$

$$A' = -\frac{f_N(\varepsilon_q^m - \varepsilon_N)}{s_N^3\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{\varepsilon_q^m - \varepsilon_N}{s_N}\right)^2\right] = -\frac{\varepsilon_q^m - \varepsilon_N}{s_N^2}A \tag{3.9}$$

f_N is a volume fraction of void nucleating particles. No void nucleation is assumed for compressive stress, $p > 0$. This seems to be what `Abaqus`' `*VOID NUCLEATION` option is doing.

In finite difference form the evolution of state variables is:

$$\Delta H_1 \equiv \Delta\varepsilon_q^m = \frac{-p\Delta\varepsilon_p + q\Delta\varepsilon_q}{(1-f)\sigma_0} \equiv h_1 \tag{3.10}$$

$$\Delta H_2 \equiv \Delta f = (1-f)\Delta\varepsilon_p + A\Delta\varepsilon_q^m \equiv h_2 \tag{3.11}$$

(3.10),(3.11) complete the full system of equations for GTN case. The full system thus consists of 4 equations (2.23),(2.24),(3.10),(3.11), where p and q are defined by (2.25),(2.26).

3.2 Simulation of void coalescence

Following Tvergaard and Needleman (1984):

$$\Phi = g = \left(\frac{q}{\sigma_0}\right)^2 + 2q_1 f^* \cosh\left(\frac{3q_2 p}{2\sigma_0}\right) - (1 + q_3 f^{*2}) = 0 \tag{3.12}$$

where

$$f^* = \begin{cases} f & f \leqslant f_c \\ f_c + (f - f_c)(f_u^* - f_c)/(f_f - f_c) & f > f_c \end{cases} \tag{3.13}$$

f_c is the critical value of the void volume fraction, and f_f is the void volume fraction at fracture (no load bearing capacity), f_u^* is the value of f^* at zero stress:

$$f_u^* = \frac{q_1 + \sqrt{q_1^2 - q_3}}{q_3} \tag{3.14}$$

If $q_3 = q_1^2$ then $f_u^* = 1/q_1$. This is the case originally proposed by Tvergaard and Needleman (1984). If $q_3 = 0$ then $f_u^* = 1/2q_1$.

3.3 GTN partial derivatives

In the following the f^* form of the flow potential and the yield function is assumed as in (3.12). If one does not want to use f^* function then one has to use $f_c \geqslant 1$. In that case $f^* \equiv f$.

$$a = \frac{3q_2 p}{2\sigma_0} \tag{3.15}$$

$$\frac{df^*}{df} = \begin{cases} 1 & f \leqslant f_c \\ \frac{f_u^* - f_c}{f_f - f_c} & f > f_c \end{cases} \tag{3.16}$$

$$\frac{\partial g}{\partial p} = \frac{3q_1 q_2 f^*}{\sigma_0} \sinh a \tag{3.17}$$

$$\frac{\partial g}{\partial q} = \frac{2q}{\sigma_0^2} \tag{3.18}$$

$$\frac{\partial^2 g}{\partial p^2} = \frac{9q_1 q_2^2 f^*}{2\sigma_0^2} \cosh a \tag{3.19}$$

$$\frac{\partial^2 g}{\partial q^2} = \frac{2}{\sigma_0^2} \tag{3.20}$$

$$\frac{\partial^2 g}{\partial p \partial q} = 0 \tag{3.21}$$

$$\frac{\partial^2 g}{\partial p \partial H_1} = \frac{\partial^2 g}{\partial p \partial \Delta\varepsilon_q^m} = -\frac{3q_1 q_2 f^* \sigma_0'}{\sigma_0^2}(\sinh a + a \cosh a) \tag{3.22}$$

$$\frac{\partial^2 g}{\partial p \partial H_2} = \frac{\partial^2 g}{\partial p \partial \Delta f} = \frac{3q_1 q_2}{\sigma_0} \sinh a \frac{df^*}{df} \tag{3.23}$$

$$\frac{\partial^2 g}{\partial q \partial H_1} = \frac{\partial^2 g}{\partial q \partial \Delta\varepsilon_q^m} = -\frac{4q}{\sigma_0^3}\sigma_0' \tag{3.24}$$

$$\frac{\partial^2 g}{\partial q \partial H_2} = \frac{\partial^2 g}{\partial q \partial \Delta f} = 0 \tag{3.25}$$

$$\frac{\partial g}{\partial H_1} = \frac{\partial g}{\partial \Delta\varepsilon_q^m} = -\frac{\sigma_0'}{\sigma_0^2}\left(\frac{2q^2}{\sigma_0} + 3q_1 q_2 f^* p \sinh a\right) \tag{3.26}$$

$$\frac{\partial g}{\partial H_2} = \frac{\partial g}{\partial \Delta f} = 2(q_1 \cosh a - q_3 f^*)\frac{df^*}{df} \tag{3.27}$$

$$\frac{\partial h_1}{\partial H_1} = \frac{p\Delta\varepsilon_p - q\Delta\varepsilon_q}{(1-f)\sigma_0^2}\sigma_0' \tag{3.28}$$

$$\frac{\partial h_1}{\partial H_2} = \frac{-p\Delta\varepsilon_p + q\Delta\varepsilon_q}{(1-f)^2\sigma_0} \tag{3.29}$$

$$\frac{\partial h_2}{\partial H_1} = A + A'\Delta\varepsilon_q^m \tag{3.30}$$

$$\frac{\partial h_2}{\partial H_2} = -\Delta\varepsilon_p \tag{3.31}$$

$$\frac{\partial h_1}{\partial p} = -\frac{\Delta\varepsilon_p}{(1-f)\sigma_0} \tag{3.32}$$

$$\frac{\partial h_1}{\partial q} = \frac{\Delta\varepsilon_q}{(1-f)\sigma_0} \tag{3.33}$$

$$\frac{\partial h_1}{\partial \Delta\varepsilon_p} = -\frac{p}{(1-f)\sigma_0} \tag{3.34}$$

$$\frac{\partial h_1}{\partial \Delta\varepsilon_q} = \frac{q}{(1-f)\sigma_0} \tag{3.35}$$

$$\frac{\partial h_2}{\partial p} = 0 \tag{3.36}$$

$$\frac{\partial h_2}{\partial q} = 0 \tag{3.37}$$

$$\frac{\partial h_2}{\partial \Delta\varepsilon_p} = 1 - f \tag{3.38}$$

$$\frac{\partial h_2}{\partial \Delta\varepsilon_q} = 0 \tag{3.39}$$

3.4 Jacobian

Most numerical algorithms will use jacobian to calculate the next approximation. If the time step is small (explicit dynamic analysis) the forward difference approximation of jacobian is enough for a quick convergence. However, for large time increments (quasi static analysis, implicit solvers) this approximation is too inaccurate. Hence jacobian must be provided. Here we derive the GTN jacobian.

The 4 equations of a GTN step are (2.23), (3.12),(3.10), (3.11):

$$f_1 = \Delta\varepsilon_p \frac{\partial g}{\partial q} + \Delta\varepsilon_q \frac{\partial g}{\partial p} = 0 \tag{3.40}$$

$$f_2 = g = \left(\frac{q}{\sigma_0}\right)^2 + 2q_1 f^* \cosh\left(\frac{3q_2 p}{2\sigma_0}\right) - (1 + q_3 f^{*2}) = 0 \tag{3.41}$$

$$f_3 = \Delta\varepsilon_q^m (1-f)\sigma_0 + p\Delta\varepsilon_p - q\Delta\varepsilon_q = 0 \tag{3.42}$$

$$f_4 = \Delta f - (1-f)\Delta\varepsilon_p - A\Delta\varepsilon_q^m = 0 \tag{3.43}$$

and the variables are $x_1 = \Delta\varepsilon_p$, $x_2 = \Delta\varepsilon_q$, $x_3 = \Delta\varepsilon_q^m$, $x_4 = \Delta f$. With that the jacobian is $J_{ij} = \partial f_i / \partial x_j$.

(3.17),(3.18)→(3.40):

$$f_1 = \Delta\varepsilon_p \frac{2q}{\sigma_0} + 3q_1 q_2 f^* \Delta\varepsilon_q \sinh a = 0, \tag{3.44}$$

a is defined by (3.15), so:

$$\frac{\partial a}{\partial \Delta\varepsilon_p} = \frac{3q_2 K}{2\sigma_0} \tag{3.45}$$

$$\frac{\partial a}{\partial \Delta\varepsilon_q^m} = -\frac{3q_2 p}{2\sigma_0^2}\sigma_0' \tag{3.46}$$

$$J_{11} = \frac{\partial f_1}{\partial x_1} = \frac{\partial f_1}{\partial \Delta\varepsilon_p} = \frac{1}{\sigma_0}\left(2q + \frac{9}{2} q_1 q_2^2 f^* K \Delta\varepsilon_q \cosh a\right) \tag{3.47}$$

$$J_{12} = \frac{\partial f_1}{\partial x_2} = \frac{\partial f_1}{\partial \Delta\varepsilon_q} = -\frac{6G\Delta\varepsilon_p}{\sigma_0} + 3q_1 q_2 f^* \sinh a \tag{3.48}$$

$$J_{13} = \frac{\partial f_1}{\partial x_3} = \frac{\partial f_1}{\partial \Delta\varepsilon_q^m} = -\frac{\sigma_0'}{\sigma_0^2}\left(2q\Delta\varepsilon_p + \frac{9}{2} q_1 q_2^2 f^* p \Delta\varepsilon_q \cosh a\right) \tag{3.49}$$

$$J_{14} = \frac{\partial f_1}{\partial x_4} = \frac{\partial f_1}{\partial \Delta f} = 3q_1 q_2 \Delta\varepsilon_q \sinh a \frac{df^*}{df} \tag{3.50}$$

$$J_{21} = \frac{\partial f_2}{\partial x_1} = \frac{\partial f_2}{\partial \Delta\varepsilon_p} = K\frac{\partial g}{\partial p} = \frac{3Kq_1 q_2 f^*}{\sigma_0} \sinh a \tag{3.51}$$

$$J_{22} = \frac{\partial f_2}{\partial x_2} = \frac{\partial f_2}{\partial \Delta\varepsilon_q} = -3G\frac{\partial g}{\partial q} = -\frac{6Gq}{\sigma_0^2} \tag{3.52}$$

$$J_{23} = \frac{\partial f_2}{\partial x_3} = \frac{\partial f_2}{\partial \Delta\varepsilon_q^m} = -\frac{\sigma_0'}{\sigma_0^2}\left(\frac{2q^2}{\sigma_0} + 3q_1 q_2 f^* p \sinh a\right), \text{ as in (3.26)} \tag{3.53}$$

$$J_{24} = \frac{\partial f_2}{\partial x_4} = \frac{\partial f_2}{\partial \Delta f} = 2(q_1 \cosh a - q_3 f^*)\frac{df^*}{df}, \text{ as in (3.27)} \tag{3.54}$$

$$J_{31} = \frac{\partial f_3}{\partial x_1} = \frac{\partial f_3}{\partial \Delta \varepsilon_p} = K\Delta\varepsilon_p + p \tag{3.55}$$

$$J_{32} = \frac{\partial f_3}{\partial x_2} = \frac{\partial f_3}{\partial \Delta \varepsilon_q} = 3G\Delta\varepsilon_q - q \tag{3.56}$$

$$J_{33} = \frac{\partial f_3}{\partial x_3} = \frac{\partial f_3}{\partial \Delta \varepsilon_q^m} = (1-f)(\sigma_0 + \Delta\varepsilon_q^m \sigma_0') \tag{3.57}$$

$$J_{34} = \frac{\partial f_3}{\partial x_4} = \frac{\partial f_3}{\partial \Delta f} = -\Delta\varepsilon_q^m \sigma_0 \tag{3.58}$$

$$J_{41} = \frac{\partial f_4}{\partial x_1} = \frac{\partial f_4}{\partial \Delta \varepsilon_p} = -(1-f) \tag{3.59}$$

$$J_{42} = \frac{\partial f_4}{\partial x_2} = \frac{\partial f_4}{\partial \Delta \varepsilon_q} = 0 \tag{3.60}$$

$$J_{43} = \frac{\partial f_4}{\partial x_3} = \frac{\partial f_4}{\partial \Delta \varepsilon_q^m} = -A'\Delta\varepsilon_q^m - A \tag{3.61}$$

$$J_{44} = \frac{\partial f_4}{\partial x_4} = \frac{\partial f_4}{\partial \Delta f} = 1 + \Delta\varepsilon_p \tag{3.62}$$

3.5 Solution step by step

$\boldsymbol{\sigma}_t, \sigma_0(t), f_t, \varepsilon_q^m(t)$ must be saved from the previous increment.

1. $\boldsymbol{\sigma}^e = \boldsymbol{\sigma}_t + \mathcal{C} : \Delta\boldsymbol{\epsilon}$
2. $p^e, \mathbf{S}^e, q^e, \mathbf{n}$ (2.21); f^* (3.13)
3. $\Delta\varepsilon_p = \Delta\varepsilon_q = \Delta\varepsilon_q^m = \Delta f = 0$
4. σ_0, σ_0' - user defined law
5. Solve (2.23),(2.24),(3.10),(3.11). Use `DNSQ` (Hiebert, 1980*b*) or `DNLS1` (Hiebert, 1980*a*).
6. $p = p^e + K\Delta\varepsilon_p$; $q = q^e - 3G\Delta\varepsilon_q$;
7. $f = f_t + \Delta f$; $\varepsilon_q^m = \varepsilon_q^m(t) + \Delta\varepsilon_q^m$
8. $\Delta\boldsymbol{\epsilon}^p = \Delta\varepsilon_q \mathbf{n} + \frac{1}{3}\Delta\varepsilon_p \mathbf{I}$; $\Delta\boldsymbol{\epsilon}^e = \Delta\boldsymbol{\epsilon} - \Delta\boldsymbol{\epsilon}^p$; $\boldsymbol{\epsilon}^e = \boldsymbol{\epsilon}^e_t + \Delta\boldsymbol{\epsilon}^e$; $\boldsymbol{\epsilon}^p = \boldsymbol{\epsilon}^p_t + \Delta\boldsymbol{\epsilon}^p$

9. $\mathbf{S} = \frac{2q}{3}\mathbf{n}$; $\boldsymbol{\sigma} = \mathbf{S} - p\mathbf{I}$

For UMAT only:

10. (3.15)-(3.39), (2.41), (2.45)-(2.52), (2.59), (2.55)-(2.58).

11. $\mathcal{M}$, $\mathcal{D}$ (2.64),(2.63)

3.6 Numerical solution

I tried to use the Levenberg-Marquardt (Moré, 1978; Hiebert, 1980*a*) and the Powell dog leg (Powell, 1970; Hiebert, 1980*b*) algorithms. We use the matrix notation in this section: $\mathbf{x} \equiv x_i, \mathbf{f} \equiv f_i, \mathbf{J} \equiv J_{ij}$.

3.7 Levenberg-Marquardt algorithm

The LM implementation available in `Slatec` library as `DNLS1` routine (Hiebert, 1980*a*) requires the user to supply the functions, $\mathbf{f}$, and the Jacobian, $\mathbf{J}$ (we are discussing a situattion of large time steps where the forward difference approximation of Jacobian is not accurate enough). In LM algorithm we are searching for a local minimiser of $||\mathbf{f}(\mathbf{x})||^2$. If $\mathbf{x}^*$ is the exact solution to $\mathbf{f} = 0$, then we are looking to find a solution $\mathbf{x}$, which is close enough to $\mathbf{x}^*$, or such that $||\mathbf{f}(\mathbf{x}^*)||^2$ is close enough to $||\mathbf{f}(\mathbf{x})||^2$. Accordingly the two convergence criteria in `DNLS1` are:

$$\Delta \leqslant \epsilon_x ||\mathbf{D}\mathbf{x}|| \tag{3.63}$$

$$|r_a| \leqslant \epsilon_f \text{ and } r_p \leqslant \epsilon_f \text{ and } \frac{r_a}{r_p} \leqslant 2 \tag{3.64}$$

If $\mathbf{p}$ is the current step, then the actual reduction is

$$r_a = 1 - \left(\frac{||\mathbf{f}(\mathbf{x}+\mathbf{p})||}{||\mathbf{f}(\mathbf{x})||} \right)^2 \tag{3.65}$$

and the predicted reduction is

$$r_p = \left(\frac{||\mathbf{J}\mathbf{p}||}{||\mathbf{f}||} \right)^2 + 2 \left(\lambda^{1/2} \frac{||\mathbf{D}\mathbf{p}||}{||\mathbf{f}||} \right)^2 \tag{3.66}$$

$\mathbf{D}$ is the diagonal matrix of scaling factors. λ is the Levenberg-Marquardt parameter, found from the least squares solution of:

$$\begin{pmatrix} \mathbf{J} \\ \lambda^{1/2}\mathbf{D} \end{pmatrix} \mathbf{p} = - \begin{pmatrix} \mathbf{f} \\ 0 \end{pmatrix}, \tag{3.67}$$

subject to constraint that $\lambda = 0$ if $||\mathbf{D}\mathbf{p}|| \leqslant \Delta$, or $\lambda > 0$ if $||\mathbf{D}\mathbf{p}|| = \Delta$, where Δ is the trust region (Moré, 1978). Note that in `DNLS1` (actually in `DMPAR`, its subsidiary routine) the constraint is implemented slightly differently: $\lambda = 0$ if $||\mathbf{Dp}|| - \Delta \leqslant 0.1\Delta$, or $\lambda > 0$ if $|(||\mathbf{Dp}|| - \Delta)| \leqslant 0.1\Delta$.

Initially, $\Delta = \mathrm{k}||\mathbf{Dx}||$ if $||\mathbf{Dx}|| \neq 0$ and $\Delta = \mathrm{k}$ otherwise. k is a user specified factor, typically $\mathrm{k} \in (0.1, 100)$. On the following iterations, Δ is updated based on the success of the previous iteration, as measured by the gain function,

Because on each call of UMAT/VUMAT $\mathbf{x}$ is unpredictable, I always start from $\mathbf{x} = 0$. Hence initially $\Delta = \mathrm{k}$. I choose $\mathrm{k} = 100$. Either too small or too large k can be fatal for the algorithm.

3.8 Powell dog leg algorithm

As in LM, functions and the Jacobian must be supplied. Two convergence criteria are implemented: (1) the exact answer is found (within machine tolerance), i.e. $||\mathbf{f}|| = 0$, and (2) criterion (3.63), where Δ and $\mathbf{D}$ have the same meaning as in LM.

3.9 Books

Useful books for non-linear optimisation: Rabinowitz (1970); Gill and Murray (1974); Fletcher (1980); Gill et al. (1981); Powell (1982); Scales (1985); Nocedal and Wright (1999).

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