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Numerical integration of elasto-plastic constitutive models using the extrapolation method

W.T. Solowski & D. Gallipoli
Durham University, Durham, United Kingdom

ABSTRACT: Stress-strain integration algorithms are an important component of finite element codes. When they are robust, accurate and fast, the performance of a finite element code significantly improves, especially when advanced elasto-plastic constitutive models are used. This paper introduces a novel algorithm for the stress-strain integration of elasto-plastic soil models with automatic control of the integration error. The proposed algorithm is based on the extrapolation method used for the solution of ordinary differential equations. In this work the algorithm has been coded for the Barcelona Basic Model (a classic elasto-plastic volumetric hardening constitutive model for unsaturated soils) but its application can be easily extended to other categories of models. The efficiency and error properties of the extrapolation algorithm are assessed by integrating stresses over strain increments of different sizes and with different error tolerances. The performance of the algorithm is compared against alternative Runge-Kutta integration schemes with control of integration error.

1 INTRODUCTION

The numerical integration of stresses is an important part of any finite element code using elasto-plastic material models formulated as differential relationships between stresses and strains for which closed-form integration is not possible. In this case, stresses are numerically integrated over the corresponding strain increments after each load step of a finite element calculation. A wealth of alternative methods, usually divided between explicit and implicit schemes, have been proposed in the literature for the numerical integration of stresses (the interested reader can refer to Potts & Zdravkovic 1999 for further details). One well-known explicit integration scheme with automatic error control is the Modified Euler scheme proposed by Sloan (1987), which can be regarded as a second order Runge-Kutta method with a first order estimate of the integration error. In this paper, a new stress integration algorithm based on the extrapolation method is introduced and some initial comparisons with other commonly used algorithms, such as the Modified Euler and higher order Runge-Kutta schemes, are presented.

The extrapolation method is based on the concepts of Richardson extrapolation and Aitken-Neville interpolation (see e.g. Deuflhard & Bornemann 2002) and was developed, among others, by Gragg (1965). It is a method well-known for the numerical integration of ordinary differential equations and it has been used with some success for various problems, though not for stress integration. The extrapolation method has also been proven to be competitive against alternative methods for a wide range of accuracies (Deuflhard & Bornemann 2002).

The basic idea of the extrapolation method lies in calculating two different approximations of the integrated variable, both having lower estimated accuracy than required. Assuming that the power series expansions of the errors of these approximations have leading terms of the same order, it is then possible to eliminate such terms by linearly combining the two approximations. This yields a third (extrapolated) approximation that is more accurate than those two from which it has originated. Such approach can be repeated indefinitely using pairs of progressively more accurate approximations (i.e. pairs of approximations whose leading error terms have progressively higher order) until the estimated error of the extrapolated solution falls below a set tolerance. The method is exceptionally robust and has very good stability properties. It also allows for global error control over a given strain increment, which is computationally expensive to achieve when Runge-Kutta schemes with adaptive sub-stepping are used.

2 CONSTITUTIVE MODELS

The extrapolation scheme is quite general and any constitutive model that may be integrated explicitly, e.g. by the Modified Euler scheme, may be easily integrated by the extrapolation method. The general assumptions made in the formulation of the extrapolation algorithm are: a) the tangent elasto-plastic matrix $\mathbf{D}^{ep}$ of the constitutive model can be calculated, b) all the required model parameters (including the hardening parameters) can be computed directly after updating the stress state and c) the initial stress state $\boldsymbol{\sigma}_0$ lies on the yield locus and elasto-plastic loading occurs (additional algorithms are required for stress integration in the elastic region). In this paper, the extrapolation algorithm is applied to the integration of the Barcelona Basic Model (BBM) proposed by Alonso et al. (1990), which is a classic elasto-plastic model for unsaturated soils and reduces to the Modified Cam-Clay when the soil becomes saturated. Due to space limitation, the formulation of the elasto-plastic matrix $\mathbf{D}^{ep}$ for BBM is not presented here and will be published in a subsequent article by Solowski & Gallipoli (in prep.). Constitutive models for unsaturated soils, such as BBM, require in their formulations an additional scalar constitutive variable, which is usually soil suction (i.e. the difference between pore air pressure and pore water pressure). In the following treatment an extended strain vector $\boldsymbol{\varepsilon}$ is therefore used that includes the soil suction s as an additional seventh strain component:

$$\boldsymbol{\varepsilon} = \left\{ \varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, \varepsilon_{12}, \varepsilon_{13}, \varepsilon_{23}, s \right\} \tag{1}$$

The framework presented below is deliberately kept very general and it should not be difficult to adapt it for different constitutive models.

3 EXTRAPOLATION METHOD

In the extrapolation method an initial approximation of the stress $\Delta\boldsymbol{\sigma}_0^{(0)}$ is calculated by dividing the corresponding strain increment $\Delta\boldsymbol{\varepsilon}$ in a number N_0 of equal sub-increments $\delta\boldsymbol{\varepsilon} = \Delta\boldsymbol{\varepsilon}/N_0$ and by using an explicit scheme to integrate stresses over each of these sub-increments. Subsequently a second approximation of the stress increment $\Delta\boldsymbol{\sigma}_1^{(0)}$ over the same increment $\Delta\boldsymbol{\varepsilon}$ is calculated by using a number of sub-increments $N_1 > N_0$. The linear combination of these two approximations yields a more accurate extrapolated approximation $\Delta\boldsymbol{\sigma}_1^{(1)}$ (i.e. an approximation whose error series has a leading term of higher order than $\Delta\boldsymbol{\sigma}_0^{(0)}$ and $\Delta\boldsymbol{\sigma}_1^{(0)}$). The error estimate of such extrapolated approximation is then computed and, if such error is acceptable, the calculations are terminated. Otherwise another approximation of the stress increment $\Delta\boldsymbol{\sigma}_2^{(0)}$ is calculated with a number of sub-increments $N_2 > N_1$. Similarly as above, the linear combination of $\Delta\boldsymbol{\sigma}_2^{(0)}$ and $\Delta\boldsymbol{\sigma}_1^{(0)}$ yields the extrapolated approximation $\Delta\boldsymbol{\sigma}_2^{(1)}$, which is then combined again with the previous extrapolated approximation $\Delta\boldsymbol{\sigma}_1^{(1)}$ to yield an even more accurate extrapolated approximation $\Delta\boldsymbol{\sigma}_2^{(2)}$. If the error estimate is acceptable at this stage, calculations are terminated. Otherwise a new approximation of the stress increment $\Delta\boldsymbol{\sigma}_i^{(0)}$ is calculated by using a larger number of sub-increments $N_i > N_{i-1}$ and this approximation is used for calculating further extrapolated values. Such process continues until the error estimate becomes smaller than the set tolerance.

The scheme is summarized in the following table:

$$\begin{array}{lllllll}
N_0 & \Delta\boldsymbol{\sigma}_0^{(0)} & & & & & \\
N_1 & \Delta\boldsymbol{\sigma}_1^{(0)} & \Delta\boldsymbol{\sigma}_1^{(1)} & & & & \\
N_2 & \Delta\boldsymbol{\sigma}_2^{(0)} & \Delta\boldsymbol{\sigma}_2^{(1)} & \Delta\boldsymbol{\sigma}_2^{(2)} & & & \\
N_3 & \Delta\boldsymbol{\sigma}_3^{(0)} & \Delta\boldsymbol{\sigma}_3^{(1)} & \Delta\boldsymbol{\sigma}_3^{(2)} & \Delta\boldsymbol{\sigma}_3^{(3)} & & \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \\
N_i & \Delta\boldsymbol{\sigma}_i^{(0)} & \Delta\boldsymbol{\sigma}_i^{(1)} & \Delta\boldsymbol{\sigma}_i^{(2)} & \Delta\boldsymbol{\sigma}_i^{(3)} & \ldots & \Delta\boldsymbol{\sigma}_i^{(m)}
\end{array} \tag{2}$$

The first column of stresses in table (2) show the non-extrapolated approximation $\Delta\boldsymbol{\sigma}_i^{(0)}$ calculated by using an explicit integration scheme over N_i equal sized sub-increments $\delta\boldsymbol{\varepsilon}_i$ (i.e. $\delta\boldsymbol{\varepsilon}_i = \Delta\boldsymbol{\varepsilon}/N_i$).

The other columns of table (2) contain the extrapolated approximation $\Delta\boldsymbol{\sigma}_i^{(m)}$ (with $m > 0$), which can be calculated as a linear combination of the approximations $\Delta\boldsymbol{\sigma}_i^{(m-1)}$ and $\Delta\boldsymbol{\sigma}_{i-1}^{(m-1)}$ according to the following two alternative rules

$$\Delta\boldsymbol{\sigma}_i^{(m)} = \Delta\boldsymbol{\sigma}_i^{(m-1)} + \frac{\Delta\boldsymbol{\sigma}_i^{(m-1)} - \Delta\boldsymbol{\sigma}_{i-1}^{(m-1)}}{\left(\dfrac{N_i}{N_{i-m}}\right)^2 - 1} \tag{3}$$

or

$$\Delta\boldsymbol{\sigma}_i^{(m)} = \Delta\boldsymbol{\sigma}_i^{(m-1)} + \frac{\Delta\boldsymbol{\sigma}_i^{(m-1)} - \Delta\boldsymbol{\sigma}_{i-1}^{(m-1)}}{\left(\dfrac{N_i}{N_{i-m}}\right) - 1} \tag{4}$$

where $i,m = 1, 2, 3 \ldots$

It can be shown that equations (3) and (4) provide extrapolated approximations whose error expansion series have leading terms of progressively higher order and therefore converge towards the true solution (see, for example, Gragg 1965). The extrapolation rule of equation (3) is used when the error expansion series of the approximation $\Delta\boldsymbol{\sigma}_i^{(0)}$ contains only even power terms such as:

$$\Delta\boldsymbol{\sigma} = \Delta\boldsymbol{\sigma}_i^{(0)} + a_1\left(\frac{\Delta\boldsymbol{\varepsilon}}{N_i}\right)^2 + a_2\left(\frac{\Delta\boldsymbol{\varepsilon}}{N_i}\right)^4 + a_3\left(\frac{\Delta\boldsymbol{\varepsilon}}{N_i}\right)^6 + \ldots \tag{5}$$

Equation (4) is instead used when the error expansion series of the approximation $\Delta\boldsymbol{\sigma}_i^{(0)}$ contains both odd and even power terms such as:

$$\Delta\boldsymbol{\sigma} = \Delta\boldsymbol{\sigma}_i^{(0)} + a_1\left(\frac{\Delta\boldsymbol{\varepsilon}}{N_i}\right)^2 + a_2\left(\frac{\Delta\boldsymbol{\varepsilon}}{N_i}\right)^3 + a_3\left(\frac{\Delta\boldsymbol{\varepsilon}}{N_i}\right)^4 + \ldots \quad (6)$$

If the error expansion of the approximation $\Delta\boldsymbol{\sigma}_i^{(0)}$ has the form of equation (5) and equation (3) can therefore be used, the algorithm converges faster as each subsequent extrapolation increases by two the order of the leading term in the series.

Note that the superscript $^{(m)}$ in the approximation $\Delta\sigma_i^{(m)}$ represents the number of subsequent extrapolations used to calculate that particular approximation. Thus those approximations with the same superscript $^{(m)}$ have leading terms of the error series of the same order. The subscript $_i$ in the approximation $\Delta\sigma_i^{(m)}$ identifies instead those approximations that belong to the same sequence of extrapolations (i.e. those approximations that are on the same row of table (2)).

Different sequences of sub-increment N_i can be used in table (2). The most common ones are:

$$N_i = 2(i+1) \Rightarrow \mathbf{N} = \{2,4,6,8,10,12,14,\ldots\} \quad (7)$$

(Deuflhard 1983, 2002)

$$N_i = 2N_{i-2} \Rightarrow \mathbf{N} = \{2,4,6,8,12,16,24,32,48,64,\ldots\} \quad (8)$$

(Stoer & Bulirch 2002, Lambert 1973)

$$N_i = 2^i \Rightarrow \mathbf{N} = \{2,4,8,16,32,64,128,\ldots\} \quad (9)$$

(Lambert 1973)

In this paper the following sequence was used:

$$\mathbf{N} = \begin{Bmatrix} 32,48,64,96,128,160,192,256, \\ 320,384,448,512,608,736,992 \end{Bmatrix} \quad (10)$$

This sequence performed best for the fairly large strain increments $\Delta\boldsymbol{\varepsilon}$ used in this work, although for smaller increments the sequences given in (7) or (8) are advantageous. It was also observed that the choice of the sequence of sub-increments may seriously influence the quality of the results and the computational time required for integration.

The extrapolation method does not have a fixed order as, for example, Runge-Kutta schemes. In the extrapolation method the order of the approximation depends on the number of subsequent extrapolations, i.e. on the number of columns in table (2). Each subsequent column has another term eliminated in the error series and thus gives a higher order approximation.

An estimate E of the integration error over the strain $\Delta\boldsymbol{\varepsilon}$ is obtained as (see Deuflhard & Bornemann 2002, Stoer & Bulirsch 2002):

$$E = \left|\Delta\boldsymbol{\sigma}_i^{(m)} - \Delta\boldsymbol{\sigma}_i^{(m-1)}\right| \quad (11)$$

In equation (11) $\Delta\boldsymbol{\sigma}_i^{(m)}$ denotes the most accurate value in the extrapolation table (2) and $\Delta\boldsymbol{\sigma}_i^{(m-1)}$ is the second most accurate value on the same row.

Two different criteria may be used to check convergence, namely the "error per step" (EPS) criterion and the "error per unit step" (EPUS) criterion. The former criterion assumes convergence when the estimated error becomes smaller than the set tolerance:

$$\left|\Delta\boldsymbol{\sigma}_i^{(m)} - \Delta\boldsymbol{\sigma}_i^{(m-1)}\right| \le \text{Tolerance} \quad (12)$$

A modified version of the EPS criterion was used by Sloan (1987) where the tolerance is scaled according to the current stress state:

$$\left|\frac{\Delta\boldsymbol{\sigma}_i^{(m)} - \Delta\boldsymbol{\sigma}_i^{(m-1)}}{\boldsymbol{\sigma}_0 + \Delta\boldsymbol{\sigma}_i^{(m)}}\right| \le \text{Tolerance} \quad (13)$$

The latter criterion assumes convergence when the estimated error normalized by the integrated stress increment becomes smaller than the set tolerance:

$$\left|\frac{\Delta\boldsymbol{\sigma}_i^{(m)} - \Delta\boldsymbol{\sigma}_i^{(m-1)}}{\Delta\boldsymbol{\sigma}_i^{(m)}}\right| \le \text{Tolerance} \quad (14)$$

Thus the EPUS criterion ensures that the integration error is maintained within a certain percentage of the computed stress change. Note that the use of the EPUS criterion requires particular care when the stress increment $\Delta\boldsymbol{\sigma}_i^{(m)}$ approaches zero.

Different choices of the norm in equations (12), (13) and (14) are also possible. In the present work the maximum norm of all stress components was used as this satisfies the convergence criterion for each individual stress component. This however may result rather expensive computationally in comparison to other choices, e.g. Cartesian norm.

The extrapolation method relies on the explicit integration of stresses and the final extrapolated approximation $\Delta\boldsymbol{\sigma}_i^{(m)}$ in table (2) can therefore drift away from the yield locus resulting in an inconsistent stress state. As a result, it might be necessary to map the final extrapolated approximation $\Delta\boldsymbol{\sigma}_i^{(m)}$ back on the yield locus (see e.g. Potts & Zdravkovic 1999 for further details on drift correction). In the examples presented in this work such correction was very rarely employed because the observed drift was not significant.

4 EXPLICIT INTEGRATION SCHEME

As mentioned earlier, the extrapolation algorithm relies on an initial (i.e. non-extrapolated) approximation $\Delta\boldsymbol{\sigma}_i^{(0)}$ calculated by using explicit integration over a number N_i of equal sub-increments $\delta\boldsymbol{\varepsilon}_i$ (where $\delta\boldsymbol{\varepsilon}_i = \Delta\boldsymbol{\varepsilon}/N_i$). The explicit method of choice is the modified midpoint method (see e.g. Press et al. 2002 and Deuflhard & Bornemann 2002) because it has been proven (see e.g. Deuflhard & Bornemann 2002) to possess an error series containing only even power terms similar to equation (5).

In this work, however, the midpoint method rather than the modified midpoint method was used because of convergence problems encountered with the modified midpoint method. It was also assumed that the midpoint method possesses an error series containing only even power terms (similarly to the modified midpoint method) and therefore the extrapolation rule of equation (3) was used.

The midpoint method can be regarded as a second order Runge–Kutta integration scheme. The increment $\Delta\boldsymbol{\varepsilon}$ is divided into N_i equal sized sub-increments $\delta\boldsymbol{\varepsilon}_i$. For the generic nth sub-increment of strain the two corresponding sub-increments of stress $\delta\boldsymbol{\sigma}(0)$ and $\delta\boldsymbol{\sigma}(0.5)$ are calculated as follows:

$$\delta\boldsymbol{\sigma}(0) = \mathbf{D}^{ep}\left(\boldsymbol{\varepsilon}_{n-1}, \boldsymbol{\sigma}_{n-1}, p^*_{0,n-1}\right)\frac{\delta\boldsymbol{\varepsilon}_i}{2} \tag{15}$$

$$\delta\boldsymbol{\sigma}(0.5) = \mathbf{D}^{ep}\left(\boldsymbol{\varepsilon}_{n-0.5}, \boldsymbol{\sigma}_{n-0.5}, p^*_{0,n-0.5}\right)\delta\boldsymbol{\varepsilon}_i \tag{16}$$

where:

$$\boldsymbol{\varepsilon}_{n-0.5} = \boldsymbol{\varepsilon}_{n-1} + 0.5\,\delta\boldsymbol{\varepsilon}_i \tag{17}$$

$$\boldsymbol{\sigma}_{n-0.5} = \boldsymbol{\sigma}_{n-1} + \delta\boldsymbol{\sigma}(0) \tag{18}$$

$$p^*_{0,n-0.5} = p^*_{0,n-1} + \delta p^*_0(0) \tag{19}$$

Note that p_0^* is the hardening parameter of the BBM, and $\delta p_0^*(0)$ is the sub-increment of this parameter over $\delta\boldsymbol{\varepsilon}_i/2$.

Following each sub-increment, the updated stress and strain are given by:

$$\boldsymbol{\sigma}_n = \boldsymbol{\sigma}_{n-1} + \delta\boldsymbol{\sigma}(0.5) \tag{20}$$

$$\boldsymbol{\varepsilon}_n = \boldsymbol{\varepsilon}_{n-1} + \delta\boldsymbol{\varepsilon}_i \tag{21}$$

After calculating equations (15)–(21) N_i times with $n = 1, 2, 3, \ldots, N_i$ respectively, the stress approximation $\Delta\boldsymbol{\sigma}_i^{(0)}$ of table (2) is computed as:

$$\Delta\boldsymbol{\sigma}_i^{(0)} = \boldsymbol{\sigma}_{N_i} - \boldsymbol{\sigma}_0 \tag{22}$$

Table 1. Error in mean stress p and shear stress q in oedometric test, for 5% volumetric strain increment.

Tolerance [%]	Error in the most accurate midpoint method approximation [%]		Error in the extrapolation method approximation [%]	
	p	q	p	q
0.5	0.11	0.13	0.04	0.05
0.1	0.05	0.06	0.02	0.025
0.01	0.013	0.014	0.00033	0.0013
0.001	0.0033	0.0029	0.00027	0.00054

where σ_0 is the initial stress state, corresponding to the initial strain state $\boldsymbol{\varepsilon}_0$ before the increment $\Delta\boldsymbol{\varepsilon}$.

5 VERIFICATION AND RESULTS

The performance of the extrapolation method was assessed against analytical solutions as well as various Runge-Kutta schemes. The results presented here refer to the integration of the Barcelona Basic Model (BBM) proposed by Alonso et al. (1990). The BBM parameters were taken from Gallipoli (2000) as follows: elastic shear modulus $G = 20$ MPa, elastic swelling index for changes in mean net stress $\kappa = 0.02$, elastic swelling index for changes in suction $\kappa_s = 0.008$, atmospheric pressure $p_{atm} = 100$ kPa, rate of increase in cohesion with suction $k = 0.6$, normal compression slope at zero suction $\lambda(0) = 0.2$, parameter defining the change of normal compression slope with suction $\beta = 0.00001$, reference stress $p_c = 10$ kPa, specific volume on normal compression line at mean net stress equal to p^c and zero suction $N(0) = 1.9$, critical state line slope $M = 0.5$ and ratio of normal compression line slopes at infinite and zero suctions $r = 0.75$. The initial values of hardening parameter p_0^* and suction were 200 kPa and 100 kPa respectively. An associated flow rule was adopted and the EPUS convergence criterion (14) was used.

5.1 *Comparison against analytical solution*

Comparisons against analytical solutions were performed for the integration of three different types of strain increments, i.e. isotropic compression, oedometric compression and wetting under constant volume. The soil was initially in a virgin isotropic stress state with a mean net stress $p = 350$ kPa. Here, for the sake of brevity, only the integration of oedometric strain increments is presented but the results for all cases were similar. The extrapolation algorithm showed very good convergence, even when a very stringent tolerance and a large strain increment of 5% were used as indicated in Table 1.

Table 2. Error in mean stress p and shear stress q in oedometric test, for 0.5% volumetric strain increment.

Tolerance [%]	Error in the most accurate midpoint method approximation [%]		Error in the extrapolation method approximation [%]	
	p	q	p	q
3	0.43	1.70	0.58	1.22
0.3	0.155	0.66	0.0051	0.046
0.01	0.078	0.34	0.0026	0.0125
0.001	0.017	0.078	0.00033	0.0012

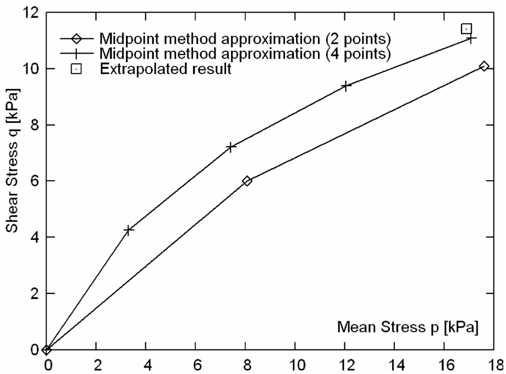

Figure 1. Calculated stress increment for an oedometric strain increment of 0.5% and tolerance of 3%. Only the elasto-plastic part of the increment is shown.

Table 2 shows similar results to Table 1 but for a smaller strain increment of 0.5%, where the largest part of non-linearity occurs. For such small strain increment the sequence of sub-increments of equation (8) was used.

Figure 1 shows the two non-extrapolated approximations obtained by the midpoint method using 2 and 4 sub-increments respectively together with the extrapolated approximation. Note that Figure 1 corresponds to a rather large tolerance of 3% and only one extrapolation is therefore necessary to achieve the required accuracy.

5.2 *Error map*

The error map shown in Figure 2 was created by using a grid of 101 × 101 equally spaced integration points corresponding to different combinations of shear and volumetric strain increments ranging between zero and 5% together with a uniform suction decrease of 50 kPa. Each point represents a triaxial strain increment with respect to an initial virgin triaxial stress state with mean net stress p = 309.7 kPa, shear stress

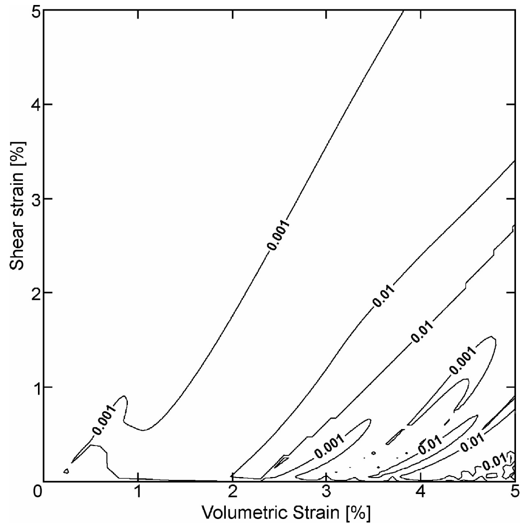

Figure 2. Error map for triaxial strain increments (error in %) The error shown in Figure 2 is the maximum value of the normalized errors E_{ij} calculated for each stress component as follows.

q = 227.1 kPa and suction s = 100 kPa (i.e. the initial stress state lies on the wet side of the yield locus).

$$E_{ij} = \frac{\left|\Delta\sigma_{ij,calc} - \Delta\sigma_{ij,true}\right|}{\Delta\sigma_{ij,abs}} \quad i, j = 1,2,3 \tag{23}$$

In equation (23) $\Delta\sigma_{ij,calc}$ is the approximation of the stress increment calculated by the extrapolation method, $\Delta\sigma_{ij,true}$ is the true stress increment and $\Delta\sigma_{ij,abs}$ is the sum of the absolute values of the stress sub-increments calculated according to equation (16) over the strain increment $\Delta\boldsymbol{\varepsilon}$. This means that, if the stress increment increases from zero to a maximum value $\Delta\sigma_{ij,max}$ and subsequently falls back to zero (over the strain increment $\Delta\boldsymbol{\varepsilon}$), the value of $\Delta\sigma_{ij,abs}$ is equal to $2\Delta\sigma_{ij,max}$. Note that the true stress increment $\Delta\sigma_{ij,true}$ in equation (23) was calculated numerically by a fifth order Runge-Kutta method with a very large number of sub-increments to ensure that the error was negligible.

The tolerance used for the integration of the strain increments in Figure 2 was equal to 0.1%. Inspection of Figure 2 indicates that this tolerance is significantly larger than the error observed for all combinations of shear and volumetric strains, suggesting that the extrapolation method is capable of providing good error control.

5.3 *Integration of random strain increments*

The extrapolation method was used to integrate a set of 6000 large random strain increments. The initial stress

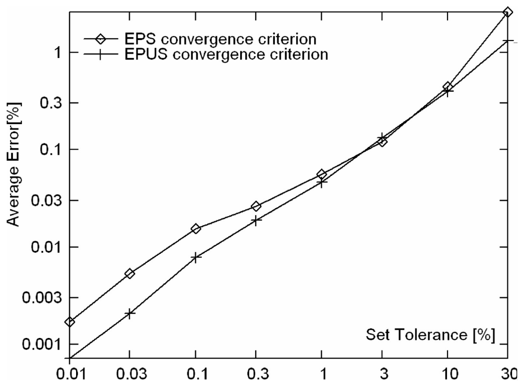

Figure 3. Average error against set tolerance for extrapolation method with different convergence criteria.

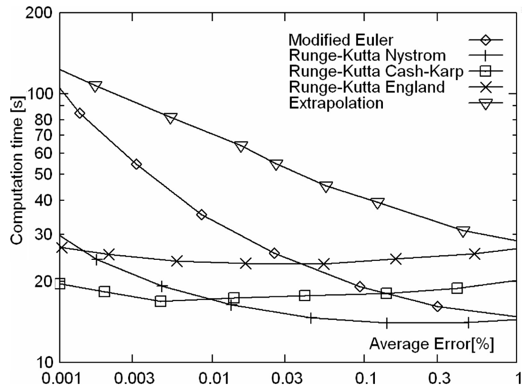

Figure 4. Comparison between extrapolation and Runge-Kutta methods (EPS convergence criterion).

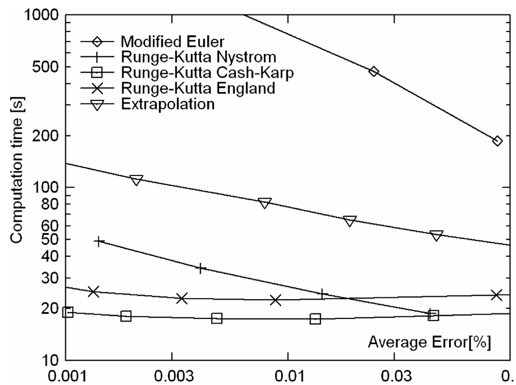

Figure 5. Comparison between extrapolation and Runge-Kutta methods (EPUS convergence criterion).

state was the same as in section 5.2. An average error E_{Av} was defined as:

$$E_{Av} = \frac{1}{6000}\sum_k E_k \quad k = 1,2,3,...,6000 \tag{24}$$

where E_k is the error for each strain increment calculated as the average of the errors E_{ij} for each stress component. Note that E_{ij} is calculated according to equation (23).

Figure 3 shows the relationship between the set tolerance and the average error calculated according to equation (24). Inspection of Figure 3 indicates that a reasonable linear relationship is observed between set tolerance and average error especially when the EPUS convergence criterion is used. This means that the average error of the extrapolation method tends to change proportionally with the value of the set tolerance. Inspection of Figure 3 also indicates that the average error is well below the set tolerance as already observed from Figure 2.

The same set of 6000 strain increments was also integrated by using various Runge-Kutta methods. Figures 4 and 5 compare the computational time required by the extrapolation method and the Runge-Kutta schemes when using the EPS criterion (13) and the EPUS criterion (14) respectively. As expected, computational time tends to increase with decreasing average error and the extrapolation method tends to be slower than Runge-Kutta schemes. It can also be seen that the computational time of the extrapolation method scales linearly with the average error and avoids the non-linear increase of Runge-Kutta schemes when high accuracy is set.

A detailed description of Runge-Kutta schemes for stress integration and further discussions on their efficiency will be presented in a subsequent publication by Solowski & Gallipoli (in prep.).

6 CONCLUSIONS

The extrapolation method is very stable and offers excellent error control, practically guaranteeing that the integration error is kept below the set tolerance. Unfortunately, it tends to be slower than alternative Runge-Kutta schemes (Deuflhard & Bornemann 2002) but it remains competitive when robustness and error control are more important than speed.

In contrast with classical Runge-Kutta schemes using sub-stepping for error control, the extrapolation method has the advantage of providing an estimate of the global error over the whole interval of integration $\Delta\boldsymbol{\varepsilon}$.

Future research will concentrate on increasing the efficiency of the extrapolation method and possibly implementing adaptive sub-stepping as proposed by Deuflhard (1983) or similar. Sub-stepping should increase the efficiency of the algorithm but the code is likely to become more complex and one would have to rely on local error control. Another possible line of future research focuses on developing extrapolation methods for higher order explicit Runge-Kutta schemes.

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