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CONVERGENCE OF THE NEWTON–RAPHSON ALGORITHM IN ELASTIC–PLASTIC INCREMENTAL ANALYSIS

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SUMMARY

A spatially continuous, time discrete formulation of the loading of an elastic, perfectly plastic body governed by a von Mises yield condition is presented. It is assumed that incremental changes in strain occur along minimum work paths, which is equivalent to a backward difference implicit integration algorithm or the radial return method. This assumption permits the incremental problem to be formulated as a convex non-linear programming problem. The classical Newton–Raphson algorithm can be adopted to provide an iterative solution of the non-linear programming problem. It is shown that if an elastic or secant predictor modulus is used, the algorithm converges monotonically. However, if a tangent predictor is used, a line search algorithm must be included to ensure convergence.

INTRODUCTION

In recent work[1–5] the solution of the classical incremental problem in small displacement, stable plasticity has been discussed within the framework of a piecewise holonomic (or deformation theory) formulation. Essentially, this framework addresses time or load path discretization; the governing equations are satisfied only at discrete instants, and it is assumed that the strain follows a minimum work path between the discrete instants. This implies that, for each incremental problem, increments of stress and increments of strain can be related through a convex potential function. The existence of this relationship means that, over the increment, the material can be treated as holonomic or non-linear elastic; the essential path dependent nature of plasticity is reflected only in that the holonomic relations must be updated at the beginning of each time or load increment.

On the structural level, each incremental problem is equivalent to the solution of a problem in non-linear elasticity. A convex minimum principle can be formulated for each increment, and the solution of the incremental problem becomes a convex non-linear programming problem.

The piecewise holonomic framework can be shown[6] to be fully equivalent to symmetry preserving fully implicit algorithms in the more conventional approach to the integration of the elastic–plastic problem.[7,8] The conventional approach has been motivated by concern about the stability and accuracy of iterative methods of solution of the incremental problem,[9,10] and it is our purpose in this paper to explore whether the mechanically based piecewise holonomic formulation can provide insight into these concerns.

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The iterative procedures generally used in finite element analysis are based on Newton–Raphson techniques. Each iteration attempts to improve a trial solution, and is made up of two steps. The predictor step provides improvements in the trial displacement increments, and the corrector step computes the stresses associated with the new trial solution. It is attractive to attempt to link the Newton–Raphson algorithm to an iterative solution of the non-linear programming problem of the piecewise holonomic problem. Clearly, if conditions can be established which lead to a monotonic decrease in the value of the convex functional whose minimum is sought, conditions for stability and convergence of the Newton–Raphson algorithm can be given.

This question has been addressed previously.[1,4,11] It has been established that it is necessary for monotonic convergence to choose the elastic stiffness for the first iteration in the increment; this is associated with the possibility that the increment may lead to unloading at all points in the body. It has also been shown that the continual use of an elastic predictor leads to monotonic convergence. In practice, however, convergence is very slow. Firm conditions for convergence for tangent modulus predictors were not established.

In this paper we consider a body composed of an elastic, perfectly plastic material governed by a von Mises yield condition and subjected to some history of loading. Spatial discretization of the body will not be carried out; the essential principles are retained if we deal with a continuous body. The time domain will be discretized, and we shall be concerned with some generic interval.

The constitutive equations will be written in incremental form, together with the appropriate potential function, and the convex non-linear programming problem for the incremental structural problem will be formulated.

In considering a typical iteration in the solution algorithm, we start with a trial solution presented by a point on the convex functional whose least value is sought. We then approximate the non-linear functional by an unconstrained quadratic functional; finding the least value of this quadratic functional is a linear problem, corresponding to the predictor step. The state point defining the least value of the approximating quadratic functional is then identified on the original non-linear functional as the next trial solution, completing the iteration. This process involves the corrector step. Clearly, if the value of the non-linear functional associated with the new trial solution is less than the starting trial solution for any generic iteration, the algorithm converges.

We shall show how approximating quadratic functionals can be constructed corresponding to elastic, secant and consistent tangent predictors. We shall further show that the algorithm converges monotonically if the elastic predictor is used for the first step, and if any choice of the elastic or secant predictors is used for the second and subsequent steps. If the tangent predictor is used for the second and subsequent iterations, however, sufficient conditions for convergence cannot be established. We show that, if a line search algorithm is adopted, convergence can be guaranteed.

THE CONSTITUTIVE MODEL FOR AN ELASTIC–PERFECTLY PLASTIC VON MISES MATERIAL

Consider an elastic–perfectly plastic material with a von Mises yield condition. The strain tensor ε_{ij} can be decomposed into its hydrostatic and deviatoric components, ε_{kk} and e_{ij} respectively, such that

$$\varepsilon_{ij} = e_{ij} + \tfrac{1}{3}\varepsilon_{kk}\delta_{ij} \tag{1a}$$

Analogously, the stress tensor σ_{ij} can be decomposed into its hydrostatic and deviatoric components, σ_{kk} and s_{ij} respectively, such that

$$\sigma_{ij} = s_{ij} + \tfrac{1}{3}\sigma_{kk}\delta_{ij} \tag{1b}$$

The constitutive equations will be written directly in incremental form. We assume that, at the beginning of the nth increment, at time t_{n-1}, the stress σ_{ij}^{n-1}, the strain ε_{ij}^{n-1} and all other state parameters are known. At the end of the increment, at time t_n, the stress and strain are denoted by σ_{ij}^n and ε_{ij}^n. We seek a relationship between the stress σ_{ij}^n and the strain increment $\Delta\varepsilon_{ij}^n$, where

$$\Delta\varepsilon_{ij}^n = \varepsilon_{ij}^n - \varepsilon_{ij}^{n-1} \tag{2}$$

The volumetric behaviour is always elastic, and hence

$$\sigma_{kk}^n = \sigma_{kk}^{n-1} + 3K\,\Delta\varepsilon_{kk}^n \tag{3}$$

where K is the bulk modulus. The deviatoric strain increment is divided into elastic and plastic parts,

$$\Delta e_{ij}^n = \Delta e_{ij}^{en} + \Delta e_{ij}^{pn} \tag{4}$$

The von Mises yield condition is

$$\phi = \tfrac{1}{2}s_{ij}s_{ij} - k^2 \leqslant 0 \tag{5}$$

The yield surface, $\phi = 0$, is a hypersphere with its centre at the origin of the stress deviator space, shown diagrammatically in Figure 1.

The time discretization requires that we introduce an assumption regarding the path followed in stress space as the stress deviator changes from s_{ij}^{n-1} to s_{ij}^n, or alternatively the path followed in strain space as the strain deviator changes from e_{ij}^{n-1} to e_{ij}^n. The path chosen is the minimum work path[3] or, equivalently, the maximum complementary work path. In deviator stress space, the stress path is elastic if s_{ij}^n lies within the yield surface, or an elastic path which terminates on the yield surface if $\phi(s_{ij}^n) = 0$, as shown in Figure 1. This implies that if Δe_{ij}^{pn} is not zero, it takes place

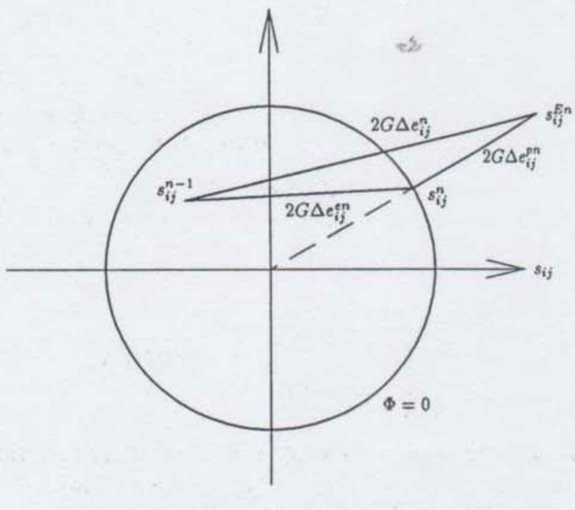

Figure 1. Yield condition in deviator stress space

at constant stress s^n_{ij}, and with a fixed direction. This path is identical to that adopted in the radial return algorithm.[6]

The increment in the elastic deviator strain Δe^{en}_{ij} is given by

$$\Delta e^{en}_{ij} = \frac{1}{2G}\Delta s^n_{ij} = \frac{1}{2G}(s^n_{ij} - s^{n-1}_{ij}) \tag{6}$$

where G is the shear modulus. The increment in the plastic deviator strain Δe^{pn}_{ij} is given by the flow rule,

$$\Delta e^{pn}_{ij} = \lambda \left.\frac{\partial \phi}{\partial s_{ij}}\right|_{s^n_{ij}}, \quad \phi(s^n_{ij}) = 0 \tag{7}$$

where λ is the plastic multiplier and is non-negative. Equation (7), for the von Mises yield function (equation (5)), becomes

$$\Delta e^{pn}_{ij} = \lambda s^n_{ij} \tag{8}$$

In view of equations (4), (6) and (8), Δe^n_{ij} can be written as

$$\Delta e^n_{ij} = \frac{1}{2G}\Delta s^n_{ij} + \lambda s^n_{ij} \tag{9}$$

Putting

$$s^{En}_{ij} = s^{n-1}_{ij} + 2G\,\Delta e^n_{ij} \tag{10}$$

we note that plastic deformation occurs only if the point corresponding to s^{En}_{ij} in the deviatoric stress space lies outside of the yield surface; otherwise, the path is elastic. In view of equation (10), equation (9) thus gives

$$s^n_{ij} = \frac{s^{En}_{ij}}{1 + 2G\lambda} \quad \text{for} \quad \phi(s^{En}_{ij}) > 0 \tag{11}$$

Since s^n_{ij} must lie on the yield surface whenever plastic deformations occur, substitution of equation (11) into the yield condition leads to

$$1 + 2G\lambda = \frac{1}{k}\left\{\frac{1}{2}s^{En}_{ij}s^{En}_{ij}\right\}^{1/2} \tag{12}$$

The full deviatoric incremental constitutive relations can now be written. From geometric considerations and from equations (11) and (12) for the plastic cases, we have

$$\left.\begin{aligned} s^n_{ij} &= s^{En}_{ij} \quad &(13\text{a})\\ \Delta e^{pn}_{ij} &= 0 \quad &(13\text{b})\end{aligned}\right\} \quad \text{if} \quad \tfrac{1}{2}s^{En}_{ij}s^{En}_{ij} \leqslant k^2$$

and

$$\left.\begin{aligned} s^n_{ij} &= \frac{k}{\{\frac{1}{2}s^{En}_{ij}s^{En}_{ij}\}^{1/2}}s^{En}_{ij} \quad &(14\text{a})\\ \Delta e^{pn}_{ij} &= \frac{1}{2G}(s^{En}_{ij} - s^n_{ij}) \quad &(14\text{b})\end{aligned}\right\} \quad \text{if} \quad \tfrac{1}{2}s^{En}_{ij}s^{En}_{ij} \geqslant k^2$$

Equation (14a) shows that the deviator stress s^n_{ij} at the end of the interval is proportional to s^{En}_{ij} defined by equation (10). It should be noted that equations (13a) and (14a) give the same relation between s^n_{ij} and s^{En}_{ij} when $\frac{1}{2}s^{En}_{ij}s^{En}_{ij} = k^2$.

The constitutive relations, represented by equations (13) and (14), give the deviator stress s_{ij}^n at the end of the interval as functions of Δe_{ij}^n, and they can be written in terms of a deviatoric potential function $W_n^d(\Delta e_{ij})$, as follows:

$$s_{ij}^n = \left.\frac{\partial W_n^d}{\partial \Delta e_{ij}}\right|_{\Delta e_{ij}^n} \tag{15}$$

where

$$W_n^d = \frac{1}{4G}(s_{ij}^{n-1} + 2G\,\Delta e_{ij})(s_{ij}^{n-1} + 2G\,\Delta e_{ij}) \quad \text{if} \quad \frac{1}{2}s_{ij}^E s_{ij}^E \leqslant k^2 \tag{16a}$$

$$W_n^d = \frac{k}{G}\left\{\frac{1}{2}(s_{ij}^{n-1} + 2G\Delta e_{ij})(s_{ij}^{n-1} + 2G\Delta e_{ij})\right\}^{1/2} - \frac{k^2}{2G} \quad \text{if} \quad \frac{1}{2}s_{ij}^E s_{ij}^E \geqslant k^2 \tag{16b}$$

and where

$$s_{ij}^E = s_{ij}^{n-1} + 2G\,\Delta e_{ij} \tag{16c}$$

The constitutive relations are completed by the addition of the volumetric relation (3), in the form

$$\sigma_{ij}^n = s_{ij}^n + \tfrac{1}{3}\sigma_{kk}^n\delta_{ij} \tag{17}$$

By introducing the potential function

$$W_n = W_n^v + W_n^d \tag{18}$$

where

$$W_n^v = \frac{1}{2}\frac{1}{9K}(\sigma_{kk}^{n-1} + 3K\,\Delta\varepsilon_{kk})^2 \tag{19}$$

is the volumetric part and W_n^d, given by equations (16a, b), is the deviatoric part, the full constitutive relations can be simply written in the form

$$\sigma_{ij}^n = \left.\frac{\partial W_n}{\partial \Delta\varepsilon_{ij}}\right|_{\Delta\varepsilon_{ij}^n} \tag{20}$$

THE MINIMUM PRINCIPLE FOR THE INCREMENTAL BOUNDARY VALUE PROBLEM

Consider a body with volume V and surface S. The body is loaded by tractions $P_i(x_i, t)$, with $0 \leqslant t \leqslant T$, acting on the unconstrained surface S_T, and is subject to imposed displacements on the constrained surface S_u, which are zero for simplicity. Body forces are also set equal to zero for simplicity: a generalization to include body forces and non-zero constrained displacements can easily be effected. The material of which the body is composed is elastic, perfectly plastic with a von Mises yield condition. The incremental formulation of the analysis problem is obtained by dividing the interval $[0, T]$, in which the loading history is defined, into sub-intervals. The problem in the nth interval $[t_{n-1}, t_n]$ is defined as follows: compute displacements $u_i^n(x_i)$, stresses $\sigma_{ij}^n(x_i)$, total strains $\varepsilon_{ij}^n(x_i)$ and deviator plastic strains $e_{ij}^{pn}(x_i)$ on V at t_n, given $u_i^{n-1}(x_i)$, $\sigma_{ij}^{n-1}(x_i)$, $\varepsilon_{ij}^{n-1}(x_i)$ and deviator plastic strains $e_{ij}^{p(n-1)}(x_i)$ on V at t_{n-1}.

Together with the constitutive equations given by equation (20), the following equilibrium and compatibility equations must be satisfied at time t_n:

$$\frac{\partial \sigma_{ij}^n}{\partial x_j} = 0 \quad \text{on } V, \qquad \sigma_{ij}^n v_j = P_i^n \quad \text{on } S_T \tag{21a,b}$$

$$\Delta\varepsilon_{ij}^n = \frac{1}{2}\left(\frac{\partial \Delta u_i^n}{\partial x_j} + \frac{\partial \Delta u_j^n}{\partial x_i}\right) \quad \text{on } V, \qquad \Delta u_i^n = 0 \quad \text{on } S_u \tag{22a,b}$$

where v_j is the outward normal vector at a point on S and $\Delta u_i^n = u_i^n - u_i^{n-1}$.

The problem defined by equations (20), (21) and (22) is time independent in the sense that the parameter t simply measures the order of the events and not the real time.

The problem in the nth interval has the same characteristics as the deformation theory problem.[3] In fact, because of the straight line path assumption for the deviator plastic strain components in the generic interval, there is a one-to-one relation between the total strain increment $\Delta\varepsilon_{ij}^n$ and the stress σ_{ij}^n. Hence, in each interval the elastic–plastic problem is equivalent to a non-linear elastic problem.

We now introduce the functional

$$U_n = \int_V W_n(\Delta\varepsilon_{ij})\,\mathrm{d}V - \int_V \sigma_{ij}^{n-1}\,\Delta\varepsilon_{ij}\,\mathrm{d}V - \int_{S_T} \Delta P_i^n\,\Delta u_i\,\mathrm{d}S \tag{23}$$

where $\Delta P_i^n = P_i^n - P_i^{n-1}$ is the load increment in the nth interval. From the principle of virtual work, assuming that equation (21) holds at time t_{n-1}, we may write

$$\int_V \sigma_{ij}^{n-1}\,\Delta\varepsilon_{ij}^n\,\mathrm{d}V = \int_{S_T} P_i^{n-1}\,\Delta u_i\,\mathrm{d}S \tag{24}$$

The functional U_n may thus be written as

$$U_n = \int_V W_n(\Delta\varepsilon_{ij})\,\mathrm{d}V - \int_{S_T} P_i^n\,\Delta u_i\,\mathrm{d}S \tag{25}$$

The problem defined by equations (20), (21) and (22) can be shown by standard variational arguments to be equivalent to finding the least value of U_n as defined in equation (25), subject to the condition that $\Delta\varepsilon_{ij}$ and Δu_i must be compatible, i.e. they must satisfy equation (22). Thus the least value of $U_n(\Delta\varepsilon_{ij}, \Delta u_i)$ is given by $U_n(\Delta\varepsilon_{ij}^n, \Delta u_i^n)$.

THE ITERATIVE SOLUTION ALGORITHM

The minimization of U_n in the nth time interval requires an iterative procedure. Guided by the conventional Newton–Raphson technique, we consider a two-step iterative algorithm.

At the beginning of the generic ith iteration, we assume that we are given $\Delta u_i^{n(i-1)}$, $\Delta e_{ij}^{n(i-1)}$, $\Delta\varepsilon_{kk}^{n(i-1)}$, $s_{ij}^{n(i-1)}$, $\sigma_{kk}^{n(i-1)}$ and we seek new estimates $\Delta u_i^{(i)}$, $\Delta e_{ij}^{n(i)}$, $\Delta\varepsilon_{kk}^{n(i)}$, $s_{ij}^{n(i)}$, $\sigma_{kk}^{n(i)}$. In the first step of the algorithm, which we shall refer to as the *predictor step*, we replace W_n^{d}, which is the only problematic term in U_n, by a quadratic approximation. This leads to the minimization of a quadratic function, or a linear problem, which provides $\Delta u_i^{(i)}$, $\Delta e_{ij}^{n(i)}$ and $\Delta\varepsilon_{kk}^{n(i)}$.

In the second step, which we shall refer to as the *corrector step*, we apply equations (3), (13) and (14) to compute $s_{ij}^{n(i)}$, $\Delta e_{ij}^{pn(i)}$, $\sigma_{kk}^{n(i)}$ from $\Delta e_{ij}^{n(i)}$, $\Delta\varepsilon_{kk}^{n(i)}$. This completes the iteration. For the purpose of the predictor step in the ith iteration, it is convenient to assign each material point in the body to either of two subregions, $V_{\mathrm{e}}^{(i)}$ or $V_{\mathrm{p}}^{(i)}$. The subregion $V_{\mathrm{e}}^{(i)}$ contains all points for which $\Delta e_{ij}^{\mathrm{p}n(i-1)} = 0$, $s_{ij}^{\mathrm{E}n(i-1)} s_{ij}^{\mathrm{E}n(i-1)} \leqslant 2k^2$, while the subregion $V_{\mathrm{p}}^{(i)}$ contains all points for which $\Delta e_{ij}^{\mathrm{p}n(i-1)} \neq 0$, $s_{ij}^{\mathrm{E}n(i-1)} s_{ij}^{\mathrm{E}n(i-1)} > 2k^2$. Note that $V_{\mathrm{e}}^{(i)}$, $V_{\mathrm{p}}^{(i)}$ have no significance in the application of the corrector step.

In the first iteration, we shall set $\Delta u_i^{n(0)} = 0$, $\Delta e_{ij}^{n(0)} = 0$, $\Delta\varepsilon_{kk}^{n(0)} = 0$, $s_{ij}^{\mathrm{E}n(0)} = s_{ij}^{n-1}$ and $\Delta e_{ij}^{\mathrm{p}n(0)} = 0$. This implies that for the first iteration all points in the body lie in $V_{\mathrm{e}}^{(1)}$, while $V_{\mathrm{p}}^{(1)}$ is empty.

Again, for the purposes of the predictor step in the ith iteration, it is convenient to introduce the differences $\Delta\hat{e}_{ij}$, $\Delta\hat{u}_i$, defined by

$$\Delta e_{ij} = \Delta e_{ij}^{n(i-1)} + \Delta\hat{e}_{ij}, \quad \Delta u_i = \Delta u_i^{n(i-1)} + \Delta\hat{u}_i \tag{26a,b}$$

The predictor step is then phrased in terms of the determination of the fields $\Delta\hat{e}_{ij}$, $\Delta\hat{u}_i$.

A variety of forms of the predictor step may be obtained by choosing different quadratic approximations of W_n^{d}. We shall limit consideration to approximations $W_n^{\mathrm{d}i}$ which conform to the following basic structure:

$$\begin{aligned} W_n^{\mathrm{d}i}(\Delta\hat{e}_{ij}) &= W_n^{\mathrm{d}}(\Delta e_{ij}^{n(i-1)}) + \left.\frac{\partial W_n^{\mathrm{d}}}{\partial \Delta e_{ij}}\right|_{\Delta e_{ij}^{n(i-1)}} \Delta\hat{e}_{ij} + \frac{1}{2} D_{ijkl}\Delta\hat{e}_{ij}\Delta\hat{e}_{kl} \\ &= W_n^{\mathrm{d}}(\Delta e_{ij}^{n(i-1)}) + s_{ij}^{n(i-1)}\Delta\hat{e}_{ij} + \frac{1}{2} D_{ijkl}\Delta\hat{e}_{ij}\Delta\hat{e}_{kl} \end{aligned} \tag{27}$$

The first two terms on the right hand side of equation (27) can be recognized as the zeroth and first order terms of a Taylor series expansion of $W_n^{\mathrm{d}}(\Delta e_{ij}^{n(i-1)} + \Delta\hat{e}_{ij})$ about $\Delta e_{ij}^{n(i-1)}$. The only choice which can be made in equation (27) to distinguish one predictor from another is the fourth order tensor D_{ijkl}, which we will refer to as the predictor modulus. It will be assumed that in all choices D_{ijkl} is symmetric and positive semi-definite.

We observe first that for points in $V_{\mathrm{e}}^{(i)}$, where $s_{ij}^{\mathrm{E}n(i-1)} s_{ij}^{\mathrm{E}n(i-1)} \leqslant 2k^2$, W_n^{d} given in equation (16a) is quadratic, and thus the choice for D_{ijkl} is unambiguous: we set

$$D_{ijkl} = D_{ijkl}^{\mathrm{E}} = 2G\,\delta_{ik}\delta_{jl} \quad \text{in } V_{\mathrm{e}}^{(i)} \tag{28a}$$

in which case

$$\tfrac{1}{2} D_{ijkl}^{\mathrm{E}}\Delta\hat{e}_{ij}\Delta\hat{e}_{kl} = G\,\Delta\hat{e}_{ij}\Delta\hat{e}_{ij} \tag{28b}$$

We shall refer to D_{ijkl}^{E} as the elastic predictor modulus. Since in the first iteration $V_{\mathrm{p}}^{(1)}$ is empty, this implies that the elastic predictor modulus is used in all points in V in the first iteration whatever other choices are made regarding D_{ijkl}. This is consistent with the possibility that the load increment may lead to general unloading in the body, in which case the behaviour of the body is elastic.

The choice of D_{ijkl} is thus confined to a choice in $V_{\mathrm{p}}^{(i)}$. The first option is to choose the *elastic predictor*, i.e. we put

$$D_{ijkl} = D_{ijkl}^{\mathrm{E}} = 2G\,\delta_{ik}\delta_{jl} \quad \text{in } V_{\mathrm{p}}^{(i)} \tag{29}$$

The second option we shall consider is the *secant predictor*;[12] in this case

$$\begin{aligned} D_{ijkl} &= D_{ijkl}^{\mathrm{S}} \\ &= \frac{k}{\{\frac{1}{2} s_{ij}^{\mathrm{E}n(i-1)} s_{ij}^{\mathrm{E}n(i-1)}\}^{1/2}}\, 2G\,\delta_{ik}\delta_{jl} \quad \text{in } V_{\mathrm{p}}^{(i)} \end{aligned} \tag{30}$$

The third choice is the *consistent tangent predictor*,[10] where D_{ijkl} in $V_{\mathrm{p}}^{(i)}$ is chosen as the second order term in the Taylor series expansion of $W_n^{\mathrm{d}}(\Delta e_{ij}^{n(i-1)} + \Delta\hat{e}_{ij})$ about $\Delta e_{ij}^{n(i-1)}$, with W_n^{d} given by equation (16b). Thus we put

$$D_{ijkl} = D_{ijkl}^{\mathrm{C}} = \left.\frac{\partial^2 W_n^{\mathrm{d}}}{\partial \Delta e_{ij}\partial \Delta e_{kl}}\right|_{\Delta e_{ij}^{n(i-1)}} \quad \text{in } V_{\mathrm{p}}^{(i)} \tag{31a}$$

On differentiating equation (16b), after some manipulation, we find

$$D^{\mathrm{C}}_{ijkl} = \frac{k}{\{\frac{1}{2}s^{\mathrm{E}n(i-1)}_{ij}s^{\mathrm{E}n(i-1)}_{ij}\}^{1/2}}\quad 2G\left\{\delta_{ik}\delta_{jl} - \frac{1}{2k^2}s^{n(i-1)}_{ij}s^{n(i-1)}_{kl}\right\} \tag{31b}$$

Finally, we may choose what we shall refer to as the *first order tangent predictor*, which is still used in some finite element codes. The first order tangent predictor arises from truncating the Taylor series expansion of $W^{\mathrm{d}}_n(\Delta e^{n(i-1)}_{ij} + \Delta\hat{e}_{ij})$ after the first order term; thus we put

$$\begin{aligned} D_{ijkl} &= D^{\mathrm{T}}_{ijkl} \\ &= 0 \quad \text{in } V^{(i)}_{\mathrm{p}} \end{aligned} \tag{32}$$

To complete the formulation of the predictor step, we substitute the approximate quadratic function $W^{\mathrm{d}i}_n$ (equation (27)) for W^{d}_n in the expression for U_n (equation (25)), leading to an approximate potential U^i_n. For convenience, we shall put

$$U^i_n(\Delta\hat{\varepsilon}_{ij}, \Delta\hat{u}_i) = U_n(\Delta\varepsilon^{n(i-1)}_{ij}, \Delta u^{n(i-1)}_i) + \hat{U}^i_n(\Delta\hat{\varepsilon}_{ij}, \Delta\hat{u}_i) \tag{33}$$

Noting our definitions of $V^{(i)}_{\mathrm{e}}$ and $V^{(i)}_{\mathrm{p}}$, and the choice of D^{E}_{ijkl} in $V^{(i)}_{\mathrm{e}}$, after some straightforward manipulation we find that

$$\begin{aligned} \hat{U}^i_n(\Delta\hat{\varepsilon}_{ij}, \Delta\hat{u}_i) = &\int_{V^{(i)}_{\mathrm{e}}} G\,\Delta\hat{e}_{ij}\Delta\hat{e}_{ij}\,\mathrm{d}V + \int_{V^{(i)}_{\mathrm{p}}} \frac{1}{2}D_{ijkl}\Delta\hat{e}_{ij}\Delta\hat{e}_{kl}\,\mathrm{d}V \\ &+ \int_V \frac{1}{2}K\,\Delta\hat{\varepsilon}^2_{kk}\,\mathrm{d}V + \int_V \sigma^{n(i-1)}_{ij}\,\Delta\hat{\varepsilon}_{ij}\,\mathrm{d}V - \int_{S_T} P^n_i\,\Delta\hat{u}_i\,\mathrm{d}S \end{aligned} \tag{34}$$

In this expression

$$\Delta\hat{\varepsilon}_{kk} = \Delta\varepsilon_{kk} - \Delta\varepsilon^{n(i-1)}_{kk} \tag{35}$$

The least value of $\hat{U}^i_n$, subject to the compatibility constraint

$$\Delta\hat{\varepsilon}_{ij} = \frac{1}{2}\left(\frac{\partial\Delta\hat{u}_i}{\partial x_j} + \frac{\partial\Delta\hat{u}_j}{\partial x_i}\right) \tag{36}$$

gives values $\Delta\hat{u}^{(i)}_i$, $\Delta\hat{e}^{(i)}_{ij}$, $\Delta\hat{\varepsilon}^{(i)}_{kk}$, and the new estimates are then

$$\begin{aligned} \Delta u^{n(i)}_i &= \Delta u^{n(i-1)}_i + \Delta\hat{u}^{(i)}_i \\ \Delta e^{n(i)}_{ij} &= \Delta e^{n(i-1)}_{ij} + \Delta\hat{e}^{(i)}_{ij} \\ \Delta\varepsilon^{n(i)}_{kk} &= \Delta\varepsilon^{n(i-1)}_{kk} + \Delta\hat{\varepsilon}^{(i)}_{kk} \end{aligned} \tag{37}$$

We can make any of the choices referred to above for D_{ijkl} in the second term on the right hand side of equation (34).

The term

$$R^i = \int_{S_T} P^n_i\,\Delta\hat{u}_i\,\mathrm{d}S - \int_V \sigma^{n(i-1)}_{ij}\,\Delta\hat{\varepsilon}_{ij}\,\mathrm{d}V \tag{38}$$

which appears in equation (34) plays the role of a *residual*. If $R^i = 0$ for arbitrary $\Delta\hat{\varepsilon}_{ij}$, $\Delta\hat{u}_i$, the principle of virtual work tells us that $\sigma^{n(i-1)}_{ij}$, P^n_i satisfy the equilibrium equations (26a, b). Further, if $R^1 = 0$ and D_{ijkl} is positive definite, the least value of $\hat{U}^i_n$ is given by $\Delta\hat{e}_{ij} = \Delta\hat{\varepsilon}_{kk} = 0$, $\Delta\hat{u}_i = 0$, and the iterative process can be terminated.

In the corrector step, the values $\Delta e^{n(i)}_{ij}$, $\Delta\varepsilon^{n(i)}_{kk}$ are substituted into equations (13), (14) and (3) to obtain $s^{n(i)}_{ij}$, $\Delta e^{\mathrm{p}n(i)}_{ij}$ and $\sigma^{n(i)}_{kk}$. The iteration has now been completed, and we proceed to the next iteration.

It should be noted that the predictor step is equivalent to the solution of a linear structural problem, whereas the corrector step involves local calculations at each point in the body.

SUFFICIENT CONDITIONS FOR MONOTONIC CONVERGENCE

In applying the iterative algorithm described in the previous section, two issues are of significance; whether convergence occurs, and the rate at which convergence takes place. In finite element applications, it is known that the rate of convergence for the elastic and secant predictors is slow, whereas faster convergence occurs for the tangent predictors. The quadratic convergence normally associated with the full Newton–Raphson algorithm requires the use of the consistent tangent predictor.

However, we are not assured that convergence will occur in all circumstances, and our purpose is to investigate this aspect within the framework of the non-linear programming problem. We shall be concerned with sufficient conditions for monotonic convergence. We ask whether, for the generic ith iteration, the new estimates $\Delta u_i^{n(i)}$, $\Delta \varepsilon_{ij}^{n(i)}$ are improvements on the previous estimates $\Delta u_i^{n(i-1)}$, $\Delta \varepsilon_{ij}^{n(i-1)}$. To answer this question, we consider the difference

$$\Delta U_n^i = U_n(\Delta u_i^{n(i)}, \Delta \varepsilon_{ij}^{n(i)}) - U_n(\Delta u_i^{n(i-1)}, \Delta \varepsilon_{ij}^{n(i-1)}) \tag{39}$$

Clearly, if $\Delta U_n^i < 0$ for each iteration, the iterative process will converge monotonically in that each iteration will take us closer to the least value of U_n.

In the two-step process, we first minimize the quadratic function U_n^i (equation (33)) to find $\Delta u_i^{n(i)}$, $\Delta \varepsilon_{ij}^{n(i)}$, and then compute $U_n(\Delta u_i^{n(i)}, \Delta \varepsilon_{ij}^{n(i)})$. It is evident from equations (33) and (34) that

$$\begin{aligned} U_n^i(\Delta \varepsilon_{ij}^{n(i-1)}, \Delta u_i^{n(i-1)}) &= U_n^i(\Delta \hat{\varepsilon}_{ij} = 0, \Delta \hat{u}_i = 0) \\ &= U_n(\Delta \varepsilon_{ij}^{n(i-1)}, \Delta u_i^{n(i-1)}) \end{aligned} \tag{40}$$

Furthermore, since $\Delta \varepsilon_{ij}^{n(i)}$, $\Delta u_i^{n(i)}$ are associated with the least value of $\hat{U}_n^i$, and hence U_n^i, it follows that

$$U_n^i(\Delta \varepsilon_{ij}^{n(i)}, \Delta u_i^{n(i)}) \leqslant U_n^i(\Delta \varepsilon_{ij}^{n(i-1)}, \Delta u_i^{n(i-1)}) \tag{41}$$

with equality occurring if and only if $R^i = 0$. Hence, from (40) and (41),

$$U_n^i(\Delta \varepsilon_{ij}^{n(i)}, \Delta u_i^{n(i)}) \leqslant U_n(\Delta \varepsilon_{ij}^{n(i-1)}, \Delta u_i^{n(i-1)}) \tag{42}$$

We now consider the difference

$$\Delta I = U_n(\Delta \varepsilon_{ij}^{n(i)}, \Delta u_i^{n(i)}) - U_n^i(\Delta \varepsilon_{ij}^{n(i)}, \Delta u_i^{n(i)}) \tag{43}$$

Evidently, if $\Delta I \leqslant 0$, then $\Delta U_n^i \leqslant 0$, with equality only if $R^i = 0$, and convergence is assured.

The difference ΔI defined in equation (43) involves only the functions W_n^d (equation (16)) and W_n^{di} (equation (27)) since all other terms in U_n and U_n^i are identical. Hence

$$\Delta I = \int_V \{ W_n^d(\Delta e_{ij}^{n(i)}) - W_n^{di}(\Delta e_{ij}^{n(i)}) \} \, dV \tag{44}$$

Again it is evident that if the integrand in equation (44) is non-positive at each material point, $\Delta I \leqslant 0$. Hence we consider

$$\Delta W = W_n^d(\Delta e_{ij}) - W_n^{di}(\Delta e_{ij}) \tag{45}$$

We shall show that $\Delta W \leqslant 0$ for all material points in $V_e^{(i)}$, and for material points in $V_p^{(i)}$ when the elastic or secant predictors are used. This implies that sufficient conditions for monotonic convergence are met for these predictors.

We shall demonstrate the results geometrically. First, we note that it will be convenient to write W_n^{d} and $W_n^{\mathrm{d}i}$ as functions of

$$s_{ij}^{\mathrm{E}} = s_{ij}^{(n-1)} + 2G\Delta e_{ij} \tag{46}$$

so that

$$s_{ij} = 2G\frac{\partial W_n^{\mathrm{d}}}{\partial s_{ij}^{\mathrm{E}}}$$

The function W_n^{d} (equations (16a) and (16b)) can thus be written as

$$W_n^{\mathrm{d}} = \frac{1}{4G}s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}} \qquad \text{for} \quad \frac{1}{2}s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}} \leqslant k^2 \tag{47a}$$

$$W_n^{\mathrm{d}} = \frac{k}{G}\left\{\frac{1}{2}s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}}\right\}^{1/2} - \frac{k^2}{G} \quad \text{for} \quad \frac{1}{2}s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}} \geqslant k^2 \tag{47b}$$

In s_{ij}^{E} space, equation (47a) represents a symmetric paraboloid with its least value at the origin. Equation (47b) represents a symmetric cone with its apex at $s_{ij}^{\mathrm{E}} = 0$. A two-dimensional representation of W_n^{d} is shown in Figure 2. The paraboloid and the cone touch along the hypercircle $s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}} = 2k^2$ with a common tangent. It is seen that the paraboloid lies within the cone.

For material points in $V_{\mathrm{e}}^{(i)}$, $D_{ijkl} = 2G\,\delta_{ik}\delta_{jl}$ (equation (28a)), and we see through straightforward algebra that, from equation (27),

$$W_n^{\mathrm{d}i} = \frac{1}{4G}s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}} \tag{48}$$

This is simply the paraboloid that makes up part of W_n^{d} (equation (47a)). Hence it follows that

$$W_n^{\mathrm{d}}(s_{ij}^{\mathrm{E}}) \leqslant W_n^{\mathrm{d}i}(s_{ij}^{\mathrm{E}}) \tag{49}$$

for any choice of s_{ij}^{E}, and hence of Δe_{ij}, for material points in $V_{\mathrm{e}}^{(i)}$.

Now consider material points in $V_{\mathrm{p}}^{(i)}$, where

$$(s^{\mathrm{E}n(i-1)})^2 = \tfrac{1}{2}s_{ij}^{\mathrm{E}n(i-1)}s_{ij}^{\mathrm{E}n(i-1)} > k^2 \tag{50}$$

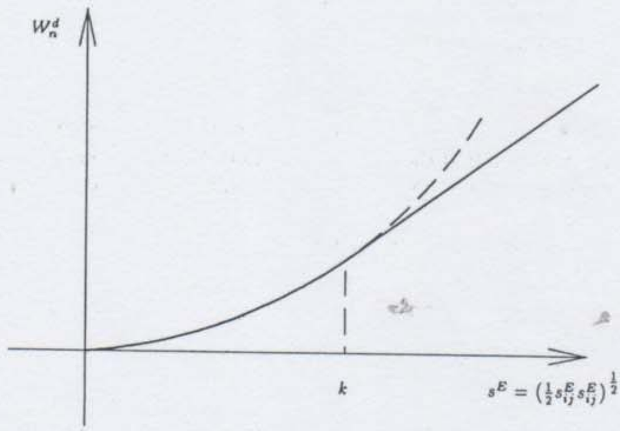

Figure 2. Deviator potential function

For the choice of the elastic predictor, $D_{ijkl} = 2G\,\delta_{ik}\,\delta_{jl}$. Substituting into equation (27), we find that

$$W_n^{\mathrm{d}i} = W_n^{\mathrm{d}}(s_{ij}^{\mathrm{E}n(i-1)}) + \left.\frac{\partial W_n^{\mathrm{d}}}{\partial s_{ij}^{\mathrm{E}}}\right|_{s_{ij}^{\mathrm{E}n(i-1)}} (s_{ij}^{\mathrm{E}} - s_{ij}^{\mathrm{E}n(i-1)})$$
$$+ \frac{1}{4G}(s_{ij}^{\mathrm{E}} - s_{ij}^{\mathrm{E}n(i-1)})(s_{ij}^{\mathrm{E}} - s_{ij}^{\mathrm{E}n(i-1)}) \tag{51}$$

With some tedious but straightforward manipulation, which we shall not give in detail for the sake of brevity, we can show that equation (51) can be recast in the form

$$W_n^{\mathrm{d}i} = \frac{k}{G}(s^{\mathrm{E}n(i-1)} - k)$$
$$+ \frac{1}{4G}\left[s_{ij}^{\mathrm{E}} - \left(1 - \frac{k}{s^{\mathrm{E}n(i-1)}}\right)s_{ij}^{\mathrm{E}n(i-1)}\right]\left[s_{ij}^{\mathrm{E}} - \left(1 - \frac{k}{s^{\mathrm{E}n(i-1)}}\right)s_{ij}^{\mathrm{E}n(i-1)}\right] \tag{52}$$

In this form, we can see that $W_n^{\mathrm{d}i}$ is a paraboloid of precisely the same shape and size as that given by equation (47a), but displaced upwards by a distance $k(s^{\mathrm{E}n(i-1)} - k)/G$, and with its least value located at the point $(1 - k/s^{\mathrm{E}n(i-1)})\,s_{ij}^{\mathrm{E}n(i-1)}$. The displaced paraboloid touches the cone of equation (47b) at the point $s_{ij}^{\mathrm{E}n(i-1)}$ with a common tangent plane. A two-dimensional representation, in the plane containing the W axis and the point $s_{ij}^{\mathrm{E}n(i-1)}$, is shown in Figure 3. It is thus seen that the paraboloid lies within the cone, and within the parabolic part of W_n^{d}, and hence

$$W_n^{\mathrm{d}}(s_{ij}^{\mathrm{E}}) \leqslant W_n^{\mathrm{d}i}(s_{ij}^{\mathrm{E}}) \tag{53}$$

for any choice of s_{ij}^{E} or Δe_{ij}.

For the choice of the secant predictor, D_{ijkl} is given by equation (30). Substituting into equation (27), we can write

$$W_n^{\mathrm{d}i} = W_n^{\mathrm{d}}(s_{ij}^{\mathrm{E}n(i-1)}) + \left.\frac{\partial W_n^{\mathrm{d}}}{\partial s_{ij}^{\mathrm{E}}}\right|_{s_{ij}^{\mathrm{E}n(i-1)}} (s_{ij}^{\mathrm{E}} - s_{ij}^{\mathrm{E}n(i-1)})$$
$$+ \frac{1}{4G\,s^{\mathrm{E}n(i-1)}}(s_{ij}^{\mathrm{E}} - s_{ij}^{\mathrm{E}n(i-1)})(s_{ij}^{\mathrm{E}} - s_{ij}^{\mathrm{E}n(i-1)}) \tag{54}$$

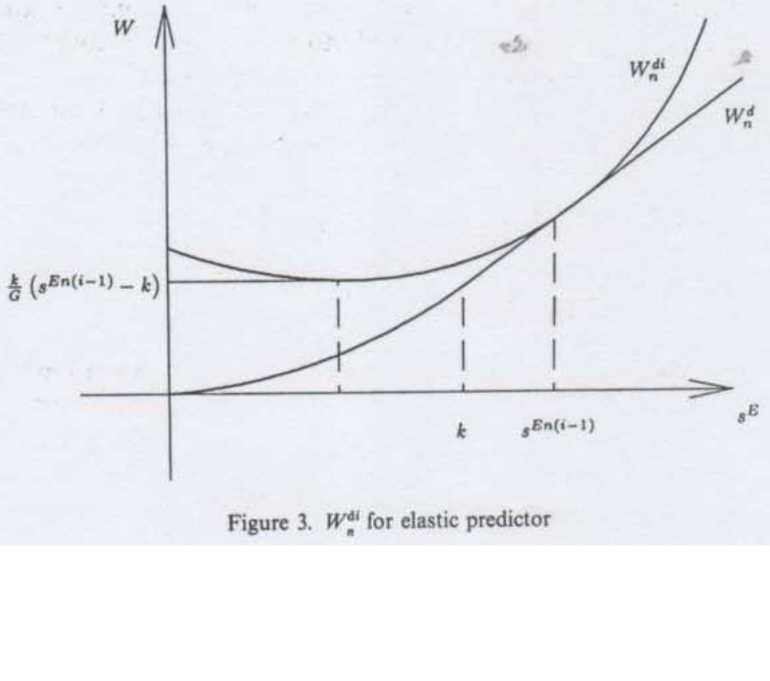

Figure 3. $W_n^{\mathrm{d}i}$ for elastic predictor

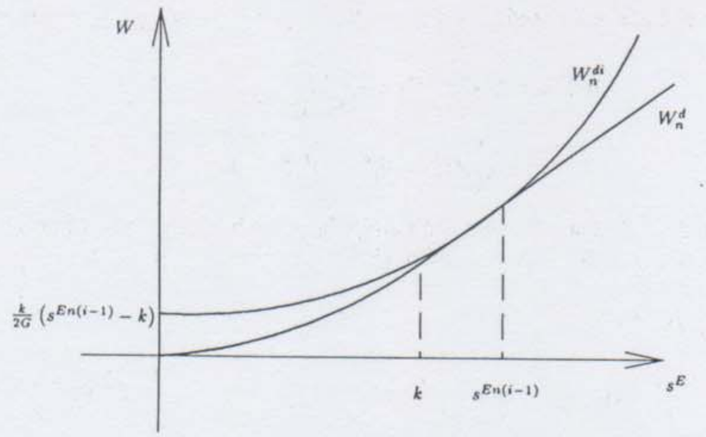

Figure 4. W_n^{di} for secant predictor

Again, after some manipulation which we shall not give in detail, we can show that equation (54) can be written as

$$W_n^{\mathrm{d}i} = \frac{k}{4G\, s^{\mathrm{E}n(i-1)}} s_{ij}^{\mathrm{E}} s_{ij}^{\mathrm{E}} + \frac{k}{2G}(s^{\mathrm{E}n(i-1)} - k) \tag{55}$$

In this form, $W_n^{\mathrm{d}i}$ is a paraboloid which has the value $k(s^{\mathrm{E}n(i-1)} - k)/2G$ at $s_{ij}^{\mathrm{E}} = 0$ and which touches the cone of equation (47b) along the hypercircle $s_{ij}^{\mathrm{E}} s_{ij}^{\mathrm{E}} = 2(s^{\mathrm{E}n(i-1)})^2$. A two-dimensional representation is shown in Figure 4. Again, $W_n^{\mathrm{d}i}$ lies within W_n^{d}, and hence

$$W_n^{\mathrm{d}} \leqslant W_n^{\mathrm{d}i} \tag{56}$$

for all s_{ij}^{E} and hence Δe_{ij}.

It follows then that monotonic convergence is assured for the elastic and secant predictors. since ΔW (equation (45)) is non-positive for all points in V. This result was given, although in a different form, by Martin *et al.*[1] and Bird and Martin.[12] It should be noted that the increment size is not limited in any way, and thus convergence is unconditional.

In the case of the tangent predictors, we cannot show that equation (56) holds for material points in $V_{\mathrm{p}}^{(i)}$. Indeed, for the case of the first order tangent predictor, where $D_{ijkl} = 0$ in $V_{\mathrm{p}}^{(i)}$,

$$\begin{aligned} W_n^{\mathrm{d}i} &= W_n^{\mathrm{d}}(s_{ij}^{\mathrm{E}n(i-1)}) + \left.\frac{\partial W_n^{\mathrm{d}}}{\partial s_{ij}^{\mathrm{E}}}\right|_{s_{ij}^{\mathrm{E}n(i-1)}} (s_{ij}^{\mathrm{E}} - s_{ij}^{\mathrm{E}n(i-1)}) \\ &= \frac{k}{2G\, s^{\mathrm{E}n(i-1)}} s_{ij}^{\mathrm{E}} s_{ij}^{\mathrm{E}n(i-1)} - \frac{k^2}{2G} \end{aligned} \tag{57}$$

In this case $W_n^{\mathrm{d}i}$ is a hyperplane which touches the cone defined by equation (47b) in the plane which contains the W axis and $s_{ij}^{\mathrm{E}n(i-1)}$, as shown diagrammatically in Figure 5. For this case,

$$W_n^{\mathrm{d}} \geqslant W_n^{\mathrm{d}i} \tag{58}$$

for all s_{ij}^{E} and hence Δe_{ij}.

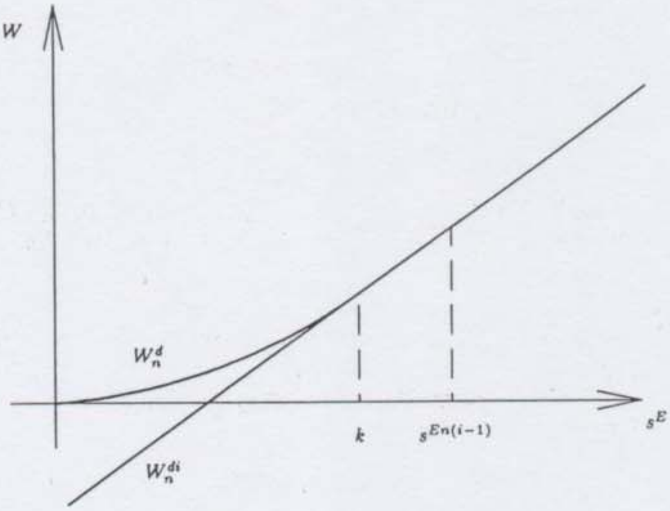

Figure 5. W_n^{di} for tangent predictor

For the consistent tangent predictor we can shown, after some manipulation, that we can write

$$W_n^{\mathrm{d}i} = \frac{k}{2G\,s^{\mathrm{E}n(i-1)}}\left(\frac{1}{2}s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}}\right) - \frac{k}{2G\,s^{\mathrm{E}n(i-1)}}\left[\frac{1}{s^{\mathrm{E}n(i-1)}}\left(\frac{1}{2}s_{ij}^{\mathrm{E}}s_{ij}^{\mathrm{E}n(i-1)} - s^{\mathrm{E}n(i-1)}\right)\right]^2 - \frac{k^2}{2G} + \frac{k\,s^{\mathrm{E}n(i-1)}}{2G} \tag{59}$$

We cannot demonstrate conclusively the relation between W_n^{d} and $W_n^{\mathrm{d}i}$ in this case. Nevertheless, it is clear that $W_n^{\mathrm{d}i}$ for the consistent tangent problem is identical to that for the first order tangent predictor in the plane containing the W axis and the point $s_{ij}^{\mathrm{E}n(i-1)}$ (Figure 5). Hence

$$W_n^{\mathrm{d}} \geqslant W_n^{\mathrm{d}i} \tag{60}$$

for some s_{ij}^{E} and hence Δe_{ij}.

It follows then that we cannot establish sufficient conditions for monotonic convergence for the tangent predictors in the same sense as for the elastic and secant predictors. The criterion for convergence, however, is that $\Delta U_n^{(i)}$ (equation (39)) should be negative in each iteration. This can hold even when we cannot be certain that ΔW (equation (45)) is non-positive for each material point. There are various possible approaches to this equation, and we shall consider one in the following section.

6. CONDITIONS FOR CONVERGENCE FOR THE TANGENT PREDICTIONS

We begin with the conclusion that we do not have sufficient conditions for monotonic convergence when either the first order tangent predictor or the consistent or second order tangent predictor is used. We shall consider, as an alternative approach, the line search algorithm of Crisfield[13] and Simo and Taylor.[10] In this approach, we replace equations (37), which produce the new estimates, by

$$\begin{aligned} \Delta u_n^{(i)} &= \Delta u_n^{(i-1)} + a\,\Delta\hat{u}_n^{(i)} \\ \Delta e_{ij}^{n(i)} &= \Delta e_{ij}^{n(i-1)} + a\,\Delta\hat{e}_{ij}^{n(i)} \\ \Delta\varepsilon_{kk}^{n(i)} &= \Delta\varepsilon_{kk}^{n(i-1)} + a\,\Delta\hat{\varepsilon}_{kk}^{n(i)} \end{aligned} \tag{61}$$

where $\Delta\hat{u}_n^{(i)}$, $\Delta\hat{e}_{ij}^{n(i)}$, $\Delta\hat{\varepsilon}_{kk}^{n(i)}$ are obtained, as before, through the minimization of $\hat{U}_n^i$ (equation (34)) with D_{ijkl} chosen as either D_{ijkl}^{T} (equation (32)) or D_{ijkl}^{C} (equation (31b)) for points in $V_p^{(i)}$, and

$$a \geqslant 0 \tag{62}$$

The new estimates given by equation (61) are first substituted into equation (34), to give

$$\begin{aligned} \hat{U}_n^i(a) = a^2\Bigg[&\int_{V_e^{(i)}} G\,\Delta\hat{e}_{ij}^{n(i)}\,\Delta\hat{e}_{ij}^{n(i)}\,\mathrm{d}V + \int_{V_p^{(i)}} \frac{1}{2} D_{ijkl}\,\Delta\hat{e}_{ij}^{n(i)}\,\Delta\hat{e}_{ij}^{n(i)}\,\mathrm{d}V \\ &+ \int_V \frac{1}{2} K(\Delta\hat{\varepsilon}_{kk}^{n(i)})^2\,\mathrm{d}V\Bigg] + a\Bigg[\int_V \sigma_{ij}^{n(i-1)}\,\Delta\hat{\varepsilon}_{ij}^{n(i)}\,\mathrm{d}V - \int_{S_T} P_i^n\,\Delta\hat{u}_i^{n(i)}\,\mathrm{d}S\Bigg] \end{aligned} \tag{63}$$

The function $\hat{U}_n^i$ may be plotted as a function of a, as shown in Figure 6. The least value of $\hat{U}_n^i(a)$ occurs for $a = 1$, while $\hat{U}_n^i(a = 0)$ and $\hat{U}_n^i(a = 2)$ are each equal to zero.

From the definition of the new estimates given by equations (61), we may also plot

$$\begin{aligned} \Delta U_n^i(a) = {} & U_n(\Delta u_i^{n(i-1)} + a\,\Delta\hat{u}_i^{n(i)}, \Delta e_{ij}^{n(i-1)} + a\,\Delta\hat{\varepsilon}_{ij}^{n(i)}) \\ & - U_n(\Delta u_i^{n(i-1)}, \Delta e_{ij}^{n(i-1)}) \end{aligned} \tag{64}$$

The first observations we make are that

$$\Delta U_n^i(a = 0) = 0 \tag{65a}$$

and

$$\left.\frac{\mathrm{d}\Delta U_n^i}{\mathrm{d}a}\right|_{a=0} = \left.\frac{\mathrm{d}\hat{U}_n^i}{\mathrm{d}a}\right|_{a=0} \tag{65b}$$

for either the first order or second order tangent predictor, in view of equation (27).

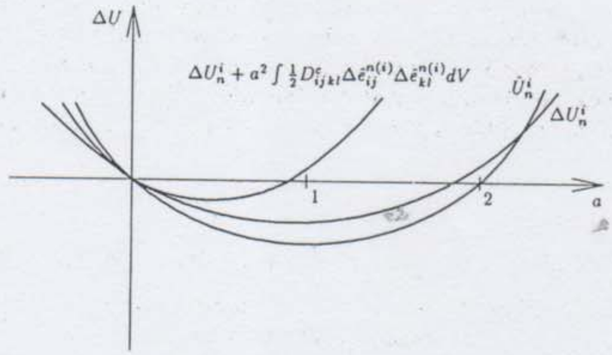

Figure 6. Variation of ΔU_n^i and $\Delta\hat{U}_n^i$ with a

Second, in view of equation (58), we can write

$$\Delta U_n^i(a) + a^2 \int \frac{1}{2} D^{\mathrm{C}}_{ijkl} \, \Delta \hat{e}_{ij}^{n(i)} \, \Delta \hat{e}_{kl}^{n(i)} \, \mathrm{d}V \geqslant \hat{U}_n^i(a) \tag{66}$$

Note that when the first order tangent predictor is used, inequality (66) applies with $D^{\mathrm{C}}_{ijkl} = 0$. When the second order tangent predictor is used, the relationship between $\Delta U_n^i(a)$ and $\hat{U}_n^i(a)$ cannot be determined at this level of generality, except insofar as the information given in equations (65). The function $\Delta U_n^i(a)$ is also plotted in Figure 6.

The geometry of the function $\Delta U_n^i(a)$ permits us to reach two conclusions. First, the least value of $\Delta U_n^i(a)$ will occur for $a > 0$, and will be negative. Thus, when the line search algorithm is used in conjunction with the Newton–Raphson algorithm, monotonic convergence is assured. It appears clear that fastest rate of convergence, in the sense of determining the greatest improvement which can be obtained after the calculation of $\Delta \hat{u}_i^{n(i)}$, $\Delta \hat{e}_i^{n(i)}$ in each iteration, is achieved when the line search algorithm is employed. The value of a which gives the least value of $\Delta U_n^i(a)$ may be larger or smaller than unity. Second, if the line search algorithm is not used routinely, $\Delta U_n^i(a = 1)$ may be either positive or negative. If $\Delta U_n^i(a = 1) < 0$, the iteration will provide an improved solution. If, on the other hand, $\Delta U_n^i(a = 1) > 0$, the geometry of Figure 6 shows us that there exists a value a', $0 < a' < 1$, for which $\Delta U_n^i(a') < 0$. Thus, monotonic convergence can be assured if a modified line search algorithm is used for iterations in which the choice $a = 1$ gives a tendency to divergence. In practical terms, this tendency can be identified by examining the residual, or by computing the function $\Delta U_n^i(a = 1)$ directly.

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