

## Chapter 7

### INTEGRATION OF CONSTITUTIVE RELATIONS IN ELASTO(VISCO)PLASTICITY

#### OVERVIEW OF INTEGRATION METHODS FOR ELASTOPLASTICITY

Constitutive relations for elastoplasticity are generally expressed in incremental form, as described in an earlier chapter. The relation between incremental stress and incremental strain may be expressed in a general incremental form that incorporates the properties of elasticity, strain additivity, and plastic flow rule. For strain-controlled loading:

$$d\sigma_{ij} = D_{ijkl}^e \left( d\varepsilon_{kl} - \varphi \frac{\partial g}{\partial \sigma_{kl}} \right) \quad (7.1)$$

The evolution law for the hardening parameter  $q_\alpha$  is also typically described in incremental form:

$$dq_\alpha = \varphi h_\alpha \quad (7.2)$$

For a given loading step, the material behavior may be either fully elastic or elastoplastic. The loading–unloading criterion may be used to determine whether a material behaves elastically or elastoplastically. Expressed in Karush-Kuhn-Tucker form:

$$f(\sigma_{ij}, q_\alpha) \leq 0 \quad (7.3a)$$

$$\varphi \geq 0 \quad (7.3b)$$

$$f\varphi = 0 \quad (7.3c)$$

All equations of the loading-unloading criterion must be satisfied simultaneously. In words, the loading-unloading criterion state that the stress point must lie in legal stress space, on or within the yield surface, at all times; that because plastic deformation is irreversible, the plastic multiplier (which is proportional to plastic strain) for a load increment can only be non-negative; and that at least one of the two quantities, either the yield function and/or the plastic multiplier, must always equal zero. The consequence of the loading-unloading criterion is that material must deform elastically if the stress point is inside the yield surface, and that the stress point must lie on the yield surface during elastoplastic loading.

To be used in elastoplastic constitutive calculations, the incremental relations must be integrated over an imposed finite loading step. Ideally, the incremental constitutive relations could be integrated analytically for a given step. However, the general incremental form

represents a system of nonlinear equations that cannot be solved analytically. In practice, therefore, a numerical integration procedure must be used to obtain a solution for the system of constitutive equations.

The objective of an integration procedure is to use the incremental constitutive relations to obtain finite increments of the desired unknown quantities for finite increments of the known quantities; to use strain-controlled loading as an example, the objective is to find  $\Delta\sigma = \Delta\sigma(\Delta\varepsilon)$ . Note that the system of nonlinear equations which must be solved during the integration procedure typically depends on variables which take on different values for different combinations of stress and/or strain. If the value of a single variable in the governing system of constitutive equations is changed, a different solution for the system of equations is obtained. The variables in the constitutive equations are typically expressed as functions of stress and/or strain, and the values of stress and/or strain change during the loading step. Therefore, the variables in the constitutive equations evolve throughout the loading step. When using numerical integration procedures, each of the variables in the governing equations can take on a limited number of values (usually a single value), or be evaluated at a limited number of stress points or strain points. Different solutions to the equations are thus obtained when the variables are evaluated at different points. One of the defining characteristics of any specific integration procedure is the point throughout the stress or strain increment at which the variables are evaluated. This means that the solution to the system of equations varies as a function of the integration procedure used.

An integration procedure should satisfy three criteria: it should be robust, accurate, and efficient. These three criteria are defined as follows. Robustness refers to the ability of an integration procedure to obtain a stable, converged solution for all possible loading conditions. Accuracy of solution refers to the magnitude of relative error between the converged solution obtained using the integration procedure and the true, analytical solution. Efficiency refers to the tendency of the integration procedure to use the least possible resources (*i.e.*, computing power or computing time) during the solution process.

Different integration methods may be characterized by the following features:

- (1) The method by which the initial estimate of the solution is obtained;
- (2) The point(s) in the stress or strain interval at which the variables in the governing constitutive equations are evaluated;

- (3) The procedure by which the initial estimate of the solution is modified to a converged solution; and,
- (4) Procedures by which the accuracy of the solution is assessed or controlled.

Many different types of numerical methods are available to find approximate solutions to differential equations, systems of differential equations, and initial value problems. Several such methods which are used for integration of elastoplasticity will be discussed in the following sections. The methods discussed here include first-order (Euler) methods and higher-order Taylor series methods, including Runge-Kutta methods. A discussion of the Taylor series expansion and its use in numerical methods follows.

### Taylor Series Expansion

If the value of a function is known for given values of the arguments of the function, the value of the same function for different values of the function's arguments may be calculated using the Taylor series expansion of the function. The Taylor series expansion of a function is an infinite series. For a function of one variable:

$$f(x_0 + \Delta x) = f(x_0) + \left. \frac{\partial f}{\partial x} \right|_{x_0} \Delta x + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial x^2} \right|_{x_0} (\Delta x)^2 + \frac{1}{3!} \left. \frac{\partial^3 f}{\partial x^3} \right|_{x_0} (\Delta x)^3 + \dots \quad (7.4)$$

For a function of several variables, the Taylor series expansion includes more terms, including mixed derivatives with respect to several variables:

$$\begin{aligned} f(x_0 + \Delta x, y_0 + \Delta y) = & f(x_0, y_0) + \left. \frac{\partial f}{\partial x} \right|_{x_0, y_0} \Delta x + \left. \frac{\partial f}{\partial y} \right|_{x_0, y_0} \Delta y + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial x^2} \right|_{x_0, y_0} (\Delta x)^2 \\ & + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial x \partial y} \right|_{x_0, y_0} \Delta x \Delta y + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial y \partial x} \right|_{x_0, y_0} \Delta y \Delta x + \frac{1}{2!} \left. \frac{\partial^2 f}{\partial y^2} \right|_{x_0, y_0} (\Delta y)^2 + \dots \end{aligned} \quad (7.5)$$

Note that in order to obtain an exact answer for the value of the function using the Taylor series expansion, derivatives of all orders must be calculated. This makes the exact answer difficult to obtain for high-order functions using the Taylor series method if the exact function is not known, as is the case for the elastoplastic problem. Approximate answers can be obtained using the Taylor series expansion by arbitrarily truncating the Taylor series expansion.

The most common integration algorithms for elastoplastic constitutive relations use Taylor series expansion as described above. The two most common integration algorithms are

the elastic predictor-plastic corrector method and the explicit substepping method which are described later in this section.

### ***Euler Methods***

The most common numerical method used to solve the elastoplastic problem is the Euler method. The Euler method is a first-order method, meaning that the Taylor series expansion is truncated to include only the terms with first-order derivatives.

$$f(x_0 + \Delta x) \approx f(x_0) + \left. \frac{\partial f}{\partial x} \right|_{x_0} \Delta x \quad (7.6)$$

### ***Runge-Kutta Methods***

Runge-Kutta methods are higher-order Taylor series methods used to obtain solutions of increased accuracy. Typically, higher-order Taylor series methods have the shortcoming that higher-order derivatives must be calculated to obtain an estimate for the solution. Runge-Kutta methods were developed using Taylor series methods of the appropriate order such that the higher-order derivatives need not be calculated. Runge-Kutta methods have the advantage that the higher order derivatives need not be calculated; however, the first-order derivative must be evaluated at several points to maintain the same accuracy of solution as the corresponding Taylor method. The fourth-order Runge-Kutta method is the most popular of these methods, and calculates an approximate solution as follows:

$$f(x_0 + \Delta x) \approx f(x_0) + \frac{1}{6}(f_1 + 2f_2 + 2f_3 + f_4)\Delta x \quad (7.7)$$

where the components of the solution are:

$$f_1 = \left. \frac{\partial f}{\partial x} \right|_{(x_0, f(x_0))} \quad (7.8a)$$

$$f_2 = \left. \frac{\partial f}{\partial x} \right|_{(x_0 + \Delta x/2, f(x_0 + (\Delta x/2)f_1))} \quad (7.8b)$$

$$f_3 = \left. \frac{\partial f}{\partial x} \right|_{(x_0 + \Delta x/2, f(x_0 + (\Delta x/2)f_2))} \quad (7.8c)$$

$$f_4 = \left. \frac{\partial f}{\partial x} \right|_{(x_0 + \Delta x, f(x_0 + (\Delta x)f_3))} \quad (7.8d)$$

### **Integration Algorithms for Elastoplasticity: 1. Elastic Predictor-Plastic Corrector Method**

According to the constitutive relations of elastoplasticity, the elastic and plastic components of an elastoplastic loading step may be evaluated independently and then summed, using the operator split technique described by Simo and Ortiz (1985). If this approach is used, the loading step is assumed to be fully elastic, and the initial estimate for the solution uses the fully elastic constitutive matrix. If the resulting fully elastic stress increment causes the trial stress state to lie outside the initial yield surface, the loading step is then known to be elastoplastic and a second (*i.e.*, plastic) stress increment is added to the first. This method treats the stress increment as if it was a two-step process, with an elastic component followed by a plastic component. The elastic predictor-plastic corrector method uses a return algorithm, in which the initial estimate of the function (based on a fully elastic stress increment) is corrected by returning the stress point to the yield surface to meet the requirements for the solution, as illustrated in Figure 7.1. In the case of the elastoplastic loading problem, this means that the final stress point must lie on the final yield surface.

Several different return algorithms have been proposed. These return algorithms may be generally classified according to the direction in which the plastic stress increment occurs. As stated earlier, the solution for the elastoplastic strain increment depends in the general case on the point at which the variables in the constitutive equations are evaluated. If these variables have constant values for all stress points, the solution will also have a constant value independent of the stress point at which the derivatives are evaluated; but the variables do not have constant values throughout an interval in the general case.

There are two general methods used to evaluate the derivatives. The first method evaluates the variables at a single point, and is called the generalized midpoint rule; the second method evaluates the variables at two points, and is called the generalized trapezoidal rule.

Specific applications of these two rules are the explicit and implicit methods. Explicit algorithms which use the Euler method are called forward Euler algorithms. Implicit algorithms which use the Euler method are called backward Euler algorithms. The explicit method evaluates the variables for the initial conditions (*i.e.*, at the stress point when fully elastic behavior ends

and elastoplastic behavior begins). The implicit method evaluates the variables for the final conditions at the end of the loading interval. These methods are illustrated in Figure 7.1. Each of these two methods has its advantages and disadvantages, as described below.

When explicit methods are used, the values of the variables are known, since the initial conditions are known. Since initial conditions are known, the value of the function can be calculated only by changing the value of the plastic multiplier until the consistency condition is satisfied. However, a solution is not assumed or known to exist when using explicit methods. These methods may exhibit divergence for highly nonlinear functions.

When implicit methods are used, a solution is implicitly assumed to exist. Therefore, a solution should be obtained for any step size. However, the values of the variables in the constitutive equations change as the value of the function changes, and the value of the function changes as the values of the variables change. The solution must therefore be obtained using an iterative procedure. Convergence and stability of the solution depends on the iterative procedure used.

### ***Initial Estimate for Solution***

Prager's consistency condition was developed so that the change in the yield function equals zero for a given loading step, and is usually written as:

$$df = \frac{\partial f}{\partial \sigma_{ij}} d\sigma_{ij} + \frac{\partial f}{\partial q_\alpha} dq_\alpha = 0 \quad (7.9)$$

Due to nonlinearities in the yield function in stress space and/or in stress-plastic hardening parameter space, use of Prager's consistency condition generally does not satisfy the consistency condition  $f=0$ . However, for iterative methods, Prager's consistency condition may be used in conjunction with the equations for strain additivity, incremental elasticity, plastic flow rule, and plastic hardening rule, to obtain an initial estimate for the solution to the final stress point and plastic hardening parameters.

$$\frac{\partial f}{\partial \sigma_{ij}} D_{ijkl}^e \left( d\varepsilon_{kl} - \varphi \frac{\partial g}{\partial \sigma_{kl}} \right) + \frac{\partial f}{\partial q_\alpha} \varphi h_\alpha = 0 \quad (7.10)$$

Equation (7.10) may be rearranged to obtain an initial estimate of the plastic multiplier  $\varphi$ :

$$\varphi = \frac{\frac{\partial f}{\partial \sigma_{ij}} D_{ijkl}^e d\varepsilon_{kl}}{\frac{\partial f}{\partial \sigma_{mn}} D_{mnpq}^e \frac{\partial g}{\partial \sigma_{pq}} - \frac{\partial f}{\partial q_\alpha} h_\alpha} \quad (7.11)$$

If the initial stress state is not at yield, a more accurate estimate for  $\varphi$  is found using:

$$\varphi = \frac{f^{tr}}{\frac{\partial f}{\partial \sigma_{mn}} D_{mnpq}^e \frac{\partial g}{\partial \sigma_{pq}} - \frac{\partial f}{\partial q_\alpha} h_\alpha} \quad (7.12)$$

where  $f^{tr}$  is the value of the yield function at the trial stress point. The final stress point is then determined by subtracting the stress correction from the trial stress:

$$\sigma_{ij}^f = \sigma_{ij}^{tr} - d\sigma_{ij} = \sigma_{ij}^{tr} - \varphi D_{ijkl}^e \frac{\partial g}{\partial \sigma_{kl}} = \sigma_{ij}^{tr} - \frac{f^{tr}}{\frac{\partial f}{\partial \sigma_{mn}} D_{mnpq}^e \frac{\partial g}{\partial \sigma_{pq}} - \frac{\partial f}{\partial q_\alpha} h_\alpha} D_{ijkl}^e \frac{\partial g}{\partial \sigma_{kl}} \quad (7.13)$$

while the plastic hardening parameter  $q_\alpha$  is updated using the same value of  $\varphi$ :

$$q_\alpha = q_{\alpha 0} + \varphi h_\alpha = q_{\alpha 0} + \frac{f^{tr}}{\frac{\partial f}{\partial \sigma_{mn}} D_{mnpq}^e \frac{\partial g}{\partial \sigma_{pq}} - \frac{\partial f}{\partial q_\alpha} h_\alpha} h_\alpha \quad (7.14)$$

The gradients to the yield surface are evaluated at the initial stress point, while the gradient to the plastic potential surface is evaluated at the stress point appropriate to the integration method, as described in the previous section. One option is to initially evaluate the gradients at the trial stress point, which Jeremic and Sture (1997) call the “semi-Backward Euler starting point”. Another option is to estimate  $\varphi$  using the gradients to the yield surface at the initial stress point, which Jeremic and Sture (1997) call the “forward Euler starting point”.

### ***Correction of Initial Estimate and Convergence to Solution***

Usually, the initial estimate of the stress increment will not satisfy the consistency condition. If satisfaction of this condition is desired, the initial estimate for the solution must be modified. The procedure by which the initial estimate is corrected is typically called a return algorithm.

Various stress corrections were evaluated by Potts and Gens (1985), who concluded that the theoretically correct return method applies the correction in the “no additional strain”

direction. This means that elastic strains which occur during the stress correction are exactly counterbalanced by equal but opposite plastic strains.

Because the plastic multiplier for the stress correction is determined using only the first-order (*i.e.*, linear) terms of the gradient to the yield surface, the final stress point resulting from this estimate of  $\varphi$  will lie on the plane tangent to the yield surface at the initial stress point. Therefore, the final stress point will only satisfy the consistency condition if the yield function, plastic potential function, and hardening function are all linear functions. In other cases, iterative methods must be used to determine the final stress point and final yield surface. Typically, Newton-Raphson methods are used in the iteration process. When using Newton-Raphson methods, the derivative (*i.e.*, slope) of the unknown function at a point is used to estimate the next value of the argument of the function.

Figure 7.2 shows the Newton-Raphson procedure for a function of one variable. The goal is to find the value  $x_{n+1}$  which satisfies  $f(x_{n+1}) = 0$ . The value  $x_{n+1}^i$  is the trial value of  $x_{n+1}$  for the  $i$ th iteration. At each trial point  $x_{n+1}^i$ , the following trial value  $x_{n+1}^{i+1}$  is found using the slope at  $x_{n+1}^i$ :

$$x_{n+1}^{i+1} = x_{n+1}^i + \Delta x = x_{n+1}^i - \left[ \frac{df}{dx} \Big|_{x_{n+1}^i} \right]^{-1} f(x_{n+1}^i) \quad (7.15)$$

This process continues until the function takes a value at which the equation is considered solved, within the specified tolerance.

Two of the most common Newton-Raphson-type methods in multi-variable systems of equations of the type encountered in elastoplasticity are the closest point projection method (CPPM) and the cutting plane method.

The CPPM is implemented by continuously minimizing the residual values  $R$  of the constitutive equations and the consistency condition by updating the values of the variables  $U$  in those equations:

$$\{U_{n+1}^{i+1}\} = \{U_{n+1}^i\} + \{\Delta U\} = \{U_{n+1}^i\} - \left[ \frac{\partial R}{\partial U} \Big|_{U_{n+1}^i} \right]^{-1} \{R_{n+1}^i\} \quad (7.16)$$

where the residuals are equal to the difference between the value of a variable calculated using the constitutive equations and the current value of that variable. The final solution is obtained when the residuals are reduced to zero within a specified tolerance. Examples of CPPM



implementation include the use of Modified Cam-clay with an implicit procedure (Borja and Lee, 1990), with an implicit procedure including implicit treatment of nonlinear elasticity (Borja, 1991), and for bounding surface plasticity (Borja et al., 2001).

The CPPM and other Newton-Raphson methods evaluate the gradients to the plastic potential surface in illegal stress space (*i.e.*, outside the yield surface) and therefore may exhibit divergence in areas of stress space where the functions for the governing equation become highly nonlinear. An example of such a region in stress space is illustrated in Figure 7.3 at a rounded corner of the yield surface. Several different improvements to the CPPM have been proposed. Macari et al. (1997) improved the performance of the CPPM in these areas by using Picard iteration and adaptive order inverse interpolation on the hardening parameters. Crisfield (1991) described the line search techniques in which the step-size is reduced until the new value of the function decreases when the reduced-size step is applied. The line search procedure guarantees that a Newton-Raphson step proceeds in the direction towards convergence, as illustrated in Figure 7.4. It may be seen in Figure 7.4 that use of the full step-size  $\Delta x$  and trial argument  $x_{n+1}^1$  (*trial*) leads to a value of  $f(x_{n+1}^1)$  that is greater than the previous value of  $f(x_{n+1}^0)$ , which indicates that the updated stress point is moving away from the updated yield surface and divergence may occur. The line search uses a reduced step-size of  $\Delta x/2$  and argument  $x_{n+1}^1$ . The value of the function  $f(x_{n+1}^1)$  is less than the previous value and is therefore in a convergent direction. The next Newton-Raphson step may then proceed. Jeremic (2001) described an improved line search technique in which the reduced step-size is based on the minimization of residuals for the unknown variables.

Perez-Fouget and Armero (2002) improved the traditional, Newton CPPM using a primal CPPM which uses a line search procedure, and a dual (staggered) CPPM in which two different CPPM calculations are performed, separately, for the plastic multiplier  $\phi$  and the other constitutive variables (*e.g.*, stress components, plastic hardening parameters).

The cutting plane method was first described by Ortiz and Simo (1986) and later elaborated by Jeremic and Sture (1997). The cutting plane method is similar to the CPPM, except that an increment to the plastic multiplier  $\Delta\phi$  is calculated in the same way as the initial estimate for  $\phi$ :

$$\Delta\varphi_{n+1}^{i+1} = \frac{f_{n+1}^i}{\frac{\partial f}{\partial \sigma_{ij}} D_{ijkl}^e \frac{\partial g}{\partial \sigma_{kl}} - \frac{\partial f}{\partial q_\alpha} h_\alpha} \quad (7.17)$$

where  $f_{n+1}^i$  is the value of the yield function after the  $i$ th iteration, and all derivatives are evaluated at the current estimate of the stress point (Figure 7.5). The stresses and plastic hardening parameter are then updated to reflect the new value of  $\varphi$ . Similar to the CPPM, the cutting plane method may exhibit divergence in highly nonlinear regions of stress space. Jeremic and Sture (1997) describe an improvement to the cutting plane method in which second derivatives to the plastic potential function are used to improve the search direction and convergence performance for  $\Delta\varphi$ . As for the CPPM, line search techniques may be used to improve the convergence of the cutting plane method.

Manzari and Prachathananukit (2001) evaluated the CPPM and cutting plane method and concluded that one of the weaknesses of the cutting plane method is that the consistency condition is not rigorously satisfied. However, it is possible to correct the updated yield function to satisfy this condition. Manzari and Prachathananukit (2001) also point out that fewer calculations are required when using the cutting plane method than the CPPM.

## **Integration Algorithms for Elastoplasticity: 2. Explicit Substepping Method**

When using this method, the elastoplastic constitutive matrix  $D^{ep}$  is calculated before a loading step. The elastoplastic stress increment is then determined, and the final stress may be corrected to the final yield surface if desired. If this approach is used, the loading step is known or assumed to be elastoplastic, and both the elastic and plastic components are incorporated into the calculation of the constitutive matrix. The stress increment calculated using the elastoplastic constitutive matrix may not lie on the final yield surface due to “drift” or nonlinearity in the stress-strain behavior which is not taken into account during calculation of  $D^{ep}$ . Therefore, the final stress point calculated using this method may need to be corrected to the final yield surface to satisfy the consistency condition. If the final correction is made, the algorithm is called a plastic predictor-plastic corrector method.

### Solution Procedure

In elastoplastic calculations for strain-controlled loading, the unknown quantities are the stress increments  $\Delta\sigma_{ij}$ . The first derivative, which relates strain increments to stress increments, is the elastoplastic constitutive matrix  $D^{ep}$ . This matrix may be calculated by substituting equation (7.11) into equation (7.1):

$$D_{ijkl}^{ep} = \frac{\partial\sigma_{ij}}{\partial\varepsilon_{kl}} = D_{ijkl}^e - \frac{D_{ijmn}^e \frac{\partial f}{\partial\sigma_{mn}} \frac{\partial g}{\partial\sigma_{pq}} D_{pqkl}^e}{\frac{\partial f}{\partial\sigma_{rs}} D_{rstu}^e \frac{\partial g}{\partial\sigma_{tu}} - \frac{\partial f}{\partial q_\alpha} h_\alpha} \quad (7.18)$$

Then the truncated Taylor series expansion used for the Euler method becomes:

$$\sigma_{ij,f} \approx \sigma_{ij,0} + \frac{\partial\sigma_{ij}}{\partial\varepsilon_{kl}} d\varepsilon_{kl} \approx \sigma_{ij,0} + D_{ijkl}^{ep} d\varepsilon_{kl} \quad (7.19)$$

The plastic hardening parameter  $q_\alpha$  is updated using the value of  $\varphi$  which was used to form  $D^{ep}$ :

$$q_\alpha = q_{\alpha 0} + \varphi h_\alpha = q_{\alpha 0} + \frac{\frac{\partial f}{\partial\sigma_{ij}} D_{ijkl}^e d\varepsilon_{kl}}{\frac{\partial f}{\partial\sigma_{mn}} D_{mnpq}^e \frac{\partial g}{\partial\sigma_{pq}} - \frac{\partial f}{\partial q_\alpha} h_\alpha} h_\alpha \quad (7.20)$$

This is an explicit method; therefore, all derivatives should be evaluated at the initial stress point.

Higher-order Taylor series expansion may be used with this method to attain more accurate solutions (Sloan, 1987). The modified Euler method (Sloan, 1987) is a second-order method similar to the first. Two equally sized steps are performed consecutively:

$$\left(D_{ijkl}^{ep}\right)_0 = D_{ijkl}^{ep}\left(\sigma_{ij,0}\right) \quad (7.21a)$$

$$\left(\sigma_{ij,f}\right)_1 \approx \sigma_{ij,0} + \left(\Delta\sigma_{ij}\right)_1 = \sigma_{ij,0} + \left(D_{ijkl}^{ep}\right)_0 \Delta\varepsilon_{kl} \quad (7.21b)$$

$$\left(D_{ijkl}^{ep}\right)_1 = D_{ijkl}^{ep}\left(\sigma_{ij,f}\right)_1 \quad (7.21c)$$

$$\left(\sigma_{ij,f}\right)_2 \approx \left(\sigma_{ij,f}\right)_1 + \left(\Delta\sigma_{ij}\right)_2 = \left(\sigma_{ij,f}\right)_1 + \left(D_{ijkl}^{ep}\right)_1 \Delta\varepsilon_{kl} \quad (7.21d)$$

and the final stress is estimated using one-half of the sum of the two successive stress increments:

$$\sigma_{ij,f} \approx \sigma_{ij,0} + \frac{(\Delta\sigma_{ij})_1 + (\Delta\sigma_{ij})_2}{2} \quad (7.22)$$

When using the Modified Euler method, the hardening parameter  $q_\alpha$  should be updated twice using the value of  $\phi$  which is calculated for each reduced stress increment.

The fourth-order Runge-Kutta method can also be used with the explicit substepping method using the rules for Runge-Kutta arithmetic as described above. For the elastoplastic problem, the first derivative  $\frac{\partial f}{\partial x}$  is the elastoplastic matrix  $D^{ep}$  and the increment  $\Delta x$  to the argument of the function is the strain increment  $d\varepsilon$ . The plastic hardening parameter is also updated using a fourth-order method. As for the Euler method, the plastic hardening parameter updates for each component of the solution use the value of  $\phi$  which was used to form the corresponding  $D^{ep}$ . See Sloan (1987) for details.

### ***Error Estimates and Substepping Algorithms***

Note that according to theory, the local truncation error resulting from use of the Euler method is second-order in the step size  $\Delta x$ , which for elastoplasticity is the strain increment  $\Delta\varepsilon$ :

$$f(x_0 + \Delta x) = f(x_0) + \left. \frac{\partial f}{\partial x} \right|_{x_0} \Delta x + \frac{M_2 (\Delta x)^2}{2} = f(x_0) + \left. \frac{\partial f}{\partial x} \right|_{x_0} \Delta x + O((\Delta x)^2) \quad (7.23)$$

$$\sigma_{ij,f} = \sigma_{ij,0} + D_{ijkl}^{ep} \Delta\varepsilon_{kl} + \frac{M_2 (d\varepsilon_{kl})^2}{2} = \sigma_{ij,0} + D_{ijkl}^{ep} \Delta\varepsilon_{kl} + O((\Delta\varepsilon_{kl})^2) \quad (7.24)$$

where  $M_2$  is the maximum value of the second derivative of the function over the interval of solution:

$$M_2 = \max \left\| \frac{\partial^2 f}{\partial x^2} \right\|_{x_0}^{x_f} \quad \text{or} \quad M_2 = \max \left\| \frac{\partial^2 \sigma}{\partial \varepsilon^2} \right\|_{\sigma_0}^{\sigma_f} \quad (7.25)$$

and  $O(\cdot)$  represents an error term. However, calculation of the second derivative  $\frac{\partial^2 \sigma}{\partial \varepsilon^2}$  is difficult

or impossible when the stress and strain increments represent vector quantities. Sloan and Booker (1992), and Sloan et al. (2001) used Richardson extrapolation as a method used to

estimate the local truncation error for integration methods. A description of Richardson extrapolation for the Euler method follows.

Richardson extrapolation compares the answers for an order  $n$  estimate of the solution to an order  $n+1$  estimate of the solution. For the case which an order-one solution is compared to an order-two solution, an initial estimate for the solution is first obtained using the forward Euler method for the full step-size  $\Delta x$  or  $\Delta \varepsilon_{ij}$ :

$$\left(D_{ijkl}^{ep}\right)_0 = D_{ijkl}^{ep}\left(\sigma_{ij,0}\right) \quad (7.26a)$$

$$\left(\sigma_{ij,f}\right)_1 \approx \sigma_{ij,0} + \left(\Delta\sigma_{ij}\right)_1 = \sigma_{ij,0} + \left(D_{ijkl}^{ep}\right)_0 \Delta\varepsilon_{kl} \quad (7.26b)$$

A second estimate for the solution is obtained by using a two-step process which uses the forward Euler method to estimate the value of the function using half of the original step-size ( $\Delta x/2$  or  $\Delta \varepsilon_{ij}/2$ ), then recalculates the derivative at the new midpoint estimate ( $\sigma_{ij,m}$ ) and uses the forward Euler method again for half of the original step-size:

$$\left(D_{ijkl}^{ep}\right)_0 = D_{ijkl}^{ep}\left(\sigma_{ij,0}\right) \quad (7.27a)$$

$$\sigma_{ij,m} \approx \sigma_{ij,0} + \frac{1}{2}\left(\Delta\sigma_{ij}\right)_1 = \sigma_{ij,0} + \left(D_{ijkl}^{ep}\right)_0 \left(\Delta\varepsilon_{kl} / 2\right) \quad (7.27b)$$

$$\left(D_{ijkl}^{ep}\right)_1 = D_{ijkl}^{ep}\left(\sigma_{ij,m}\right) \quad (7.27c)$$

$$\left(\sigma_{ij,f}\right)_2 \approx \sigma_{ij,m} + \frac{1}{2}\left(\Delta\sigma_{ij}\right)_2 = \sigma_{ij,m} + \left(D_{ijkl}^{ep}\right)_1 \left(\Delta\varepsilon_{kl} / 2\right) \quad (7.27d)$$

The total stress increments for the one-step process and two-step processes are then the full stress increment for the one-step estimate  $\left(\Delta\sigma_{ij}\right)_1$  and the average of the stress increments  $\left(\Delta\sigma_{ij}\right)_1$  and  $\left(\Delta\sigma_{ij}\right)_2$  which result from the two-step estimate, respectively:

$$\text{One-step estimate: } \Delta\sigma_{ij} = \left(\Delta\sigma_{ij}\right)_1 \quad (7.28a)$$

$$\text{Two-step estimate: } \Delta\sigma_{ij} = \frac{1}{2}\left(\left(\Delta\sigma_{ij}\right)_1 + \left(\Delta\sigma_{ij}\right)_2\right) \quad (7.28b)$$

The local truncation error  $e_l$  may be estimated as the difference between the two estimates for the stress increment or the final stress:

$$e_l \approx \frac{\frac{1}{2}\left(\left(\Delta\sigma_{ij}\right)_2 - \left(\Delta\sigma_{ij}\right)_1\right)}{1 - 2^{-p}} = \frac{\left(\sigma_{ij,f}\right)_2 - \left(\sigma_{ij,f}\right)_1}{1 - 2^{-p}} \quad (7.29)$$

where  $p$  is the order of accuracy for the method. Since  $p = 1$  for the Euler method,

$$e_l \approx (\Delta\sigma_{ij})_2 - (\Delta\sigma_{ij})_1 = 2((\sigma_{ij,f})_2 - (\sigma_{ij,f})) \quad (7.30)$$

A similar procedure can be used for the fourth-order Runge-Kutta method, using the original step size and comparing the answer to the solution which used two steps, each with half of the original step size. Since  $p = 4$  for the fourth-order Runge-Kutta method, the local truncation error is estimated as

$$e_l \approx \frac{16}{15}((\sigma_{ij,f})_2 - (\sigma_{ij,f})) \quad (7.31)$$

Truncation error for Runge-Kutta methods can also be estimated using the Runge-Kutta-England, Runge-Kutta-Fehlberg, or Runge-Kutta-Dormand-Prince schemes which use Richardson extrapolation (Sloan, 1987; Sloan and Booker, 1992; Sloan et al., 2001).

One advantage of calculating these error estimates is that the error resulting from nonlinearity in the function can be controlled by limiting the step size. Although reducing the size of a single loading step into several sequential “substeps” to improve convergence performance and reduce error was introduced years earlier (Nayak and Zienkiewicz, 1972; Owen and Hinton, 1980), Sloan (1987) introduced the idea of using “substepping” to control local truncation error. The concept was updated by Sloan and Booker (1992) for use with Tresca and Mohr-Coulomb yield surfaces, and then extended to the general case of elastoplastic models with non-linear elasticity by Sloan et al. (2001). Note that all substepping schemes can be classified as explicit methods.

The error for a load increment may be controlled by dividing a load into a suitable number of substeps. The error in each load increment is desired to be less than some tolerance  $\delta$ . The maximum absolute error in magnitude of the stress is approximately:

$$e_l \approx \frac{\|(\sigma_f)_2 - (\sigma_f)_1\|}{1 - 2^{-p}} \quad (7.32)$$

where  $\|(\sigma_f)_2 - (\sigma_f)_1\|$  is the difference in magnitude between the predicted stresses using one full step and two half-steps for the method of interest. The relative error  $E_l$  can be calculated using the total magnitude of the stresses, and should be less than the tolerable error:

$$E_l \approx \frac{\|(\sigma_f)_2 - (\sigma_f)_1\|}{(1-2^{-p})\|(\sigma_f)_2\|} \leq \delta \quad (7.33)$$

Since the answer for a  $p$ -order method should be accurate to  $(\Delta h)^p$  where  $\Delta h$  is the step size, dividing the increment into  $N$  equal substeps each of length  $(\Delta h / N)$  reduces the relative error to:

$$E_l \approx \frac{\|(\sigma_f)_2 - (\sigma_f)_1\|}{N^p (1-2^{-p})\|(\sigma_f)_2\|} \quad (7.34)$$

Then if the error is to be less than the tolerable error, the number of substeps required is:

$$N \geq \left[ \frac{\|(\sigma_f)_2 - (\sigma_f)_1\|}{\delta (1-2^{-p})\|(\sigma_f)_2\|} \right]^{\frac{1}{p}} \quad (7.35)$$

It is possible also to use substeps of variable size, as by Sloan (1987) or Sloan and Booker (1992). For a given substep, this type of analysis requires comparing answers obtained by methods of order  $p$  and order  $p+1$  (e.g., the order 1 Euler method and the order 2 modified Euler method, or one of the modified Runge-Kutta schemes which produces answers of order 4 and order 5). The relative error between these two answers is:

$$E \approx \frac{\|(\sigma_f)_{p+1} - (\sigma_f)_p\|}{\|(\sigma_f)_{p+1}\|} \quad (7.36)$$

where  $(\sigma_f)_p$  and  $(\sigma_f)_{p+1}$  are the final stresses calculated using methods of orders  $p$  and  $p+1$ , respectively. If a given substep  $n$  is of size  $\Delta h_n$ , the next substep  $n+1$  will be of the size

$$\Delta h_{n+1} = q \Delta h_n \quad (7.37)$$

The factor  $q$  can be calculated as a function of the tolerance and the relative error estimated by comparing the answers obtained above:

$$q = \left[ \frac{\delta}{E_n} \right]^{\frac{1}{p+1}} \quad (7.38)$$

although it has been recommended to use in practice a reduced value of  $0.8q$  (Sloan, 1987) or  $0.9q$  (Sloan and Booker, 1992). Sloan also recommends that  $q$  should be between 0.01 and 2.

Sloan and Booker (1992) tested various substepping procedures for Tresca and Mohr-Coulomb models, and Sloan et al. (2001) tested these methods for various constitutive models including generalized critical state models. They concluded that although the Runge-Kutta-type methods and variable-size-substep-type methods are computationally expensive, the performance of these methods becomes competitive and even more efficient than Euler methods as error tolerance is reduced.

### **Performance of Integration Procedures**

The accuracy, stability, and efficiency of the various integration procedures have been evaluated and reported in the literature with mixed results. Potts and Ganendra (1994) reported that substepping procedures yield more accurate results than implicit, return-algorithm-type approaches for the Modified Cam-clay model. Wathugala and Pal (1999) compared four methods (elastic predictor-plastic corrector method, plastic predictor-plastic corrector method, implicit method, and modified Euler method) for a hierarchical single-surface constitutive model. They reported that the modified Euler method experienced some accuracy and stability problems near failure or critical state with large strain increments, and that the implicit method also became unstable near failure when large strain increments are used. Also, the elastic predictor-plastic corrector method and plastic predictor-plastic corrector method were the most efficient in terms of CPU time. Manzari and Prachathananukit (2001) evaluated the CPPM, cutting plane method, and substepping method for a complex bounding surface sand model. They concluded that the substepping approach is more accurate than the CPPM and cutting plane method when small strain increments are used, but that the CPPM outperforms the other two methods as strain increments increase in size. Efficiency of the CPPM was less than that of the cutting plane method in terms of CPU time during the early stages of a cyclic loading simulation, but the CPPM could continue the analysis longer during post-peak behavior. The substepping method failed early using this complicated constitutive model.



## **AN INTERNALLY CONSISTENT INTEGRATION METHOD FOR CRITICAL STATE MODELS**

See Appendix A for article submitted to *International Journal for Numerical and Analytical Methods in Geomechanics* in June 2004 and accepted for publication in August 2004.

### **MODIFICATIONS TO THE NEW INTEGRATION METHOD FOR THE RATE-DEPENDENT CHALK MODEL**

The integration method proposed in the previous section has many computational strengths. However, it is important to recognize that while chalk behaves very much like a material which can be described by the rate-independent Modified Cam-Clay (MCC) model, several differences exist between the chalk model described in Chapter 6 and the MCC model. These differences include the following:

1. MCC assumes bulk modulus is a function of mean stress  $p$  and of a constant recompression coefficient  $\kappa$ , while the chalk model uses a constant bulk modulus;
2. The origin of the elliptical yield surface is at  $p = 0$  in MCC, while the origin is offset by a value equal to the attraction  $a$  such that the origin is at  $p = -a$ ;
3. The center of the elliptical yield surface is always located halfway between the origin and the preconsolidation stress  $p_c$  in MCC (*i.e.*,  $R = 0.5$ ), while the chalk model can use other values for  $R$ ;
4. MCC is rate-independent, while the chalk model incorporates rate-dependence;
5. The elliptical yield surface accommodates all values of shear stress ratio  $\eta$  in MCC, while the chalk model truncates the elliptical yield surface at the adjusted failure shear stress ratio  $\bar{\eta}_f$ ; and,
6. Provisions must also be made to account for third-invariant effects.

These discrepancies create differences in the constitutive equations between the chalk model and MCC, and necessitate modifications to the integration method proposed in the previous section. In this section, the changes which must be made to apply the proposed integration method to the chalk model are described.

The first change is related to the calculation of the recompression parameter  $\kappa$  for the chalk model, which is characterized by a constant bulk modulus  $K$ . For MCC, the bulk modulus is calculated at the starting stress point using the nonlinear relation for Cam-Clay:

$$K = \frac{p(1+e)}{\kappa} \quad (7.39)$$

where  $\kappa$  has a constant value, and  $p$  and  $e$  are the values at the start of the loading step. If the effects of nonlinear elasticity are considered, a secant value of bulk modulus is calculated for each iteration:

$$\bar{K} = \frac{p_0(1+e_0) + p_f(1+e_f)}{2\kappa} \quad (7.40)$$

where the subscripts 0 and  $f$  refer to the initial and final states of the material, respectively.

A similar procedure is used for the chalk model. For this model and its constant value of bulk modulus, the tangent value of  $\kappa$  is different for each value of mean stress:

$$\kappa = \frac{p(1+e_{eq})}{K} \quad (7.41)$$

where  $e_{eq}$  is the equivalent void ratio for hydrostatic conditions, and is defined as in Chapter 5:

$$e_{eq} = \frac{1+e}{\exp\left(\frac{p_{eq}-p}{K}\right)} - 1 \quad (7.42)$$

The secant value of  $\kappa$  is required for many calculations using the new method. The secant value of  $\kappa$  between any two stress points, with mean stresses  $p_1$  and  $p_2$ , may be calculated as follows:

$$\bar{\kappa} = \frac{\sqrt{p_1 p_2 (1+e_{eq,1})(1+e_{eq,2})}}{K} \quad (7.43)$$

where  $e_1$  and  $e_2$  are the equivalent void ratios for hydrostatic conditions corresponding to the two stress points of interest.

A second difference is the effect of the attraction  $a$  and the offset of the origin of the elliptical cap. As described in Chapter 6, the model may then be formulated in transformed  $(\bar{p}, q)$  space where  $\bar{p} = p + a$ . All quantities originally defined in  $(p, q)$  space are so transformed: preconsolidation stress  $p_c$  becomes  $\bar{p}_c = p_c + a$  and so on. All integration calculations are then carried out in transformed  $(\bar{p}, q)$  space.

A third difference is the incorporation of the eccentricity parameter  $R$  into the chalk model. As explained in Chapter 5, this difference changes the equation of the viscoplastic potential surface from:

$$g = q^2 - M^2 \bar{p} (\bar{p}_{eq} - \bar{p}) \quad (7.44)$$

to:

$$g = q^2 - M^2 R^2 \bar{p}_{eq}^2 + M_2^2 R^2 (\bar{p} - R \bar{p}_{eq})^2 \quad (7.45)$$

where  $M_2 (= \frac{MR}{1-R})$ . This new equation changes the gradients to the viscoplastic potential and also their derivatives. The new equations are given below.

The most significant change from MCC is the consideration of rate-dependent behavior in the chalk model. The rate-dependent behavior in the chalk model depends on the volumetric age of the chalk, which in turn is described by the time-lines model in Chapter 5. As described in Chapter 5, all time-lines within a given meridional section (*i.e.*, constant Lode angle  $\theta$ ) appear as similar ellipses in  $p$ - $q$  space. Each time-line is described by an equivalent hydrostatic stress  $p_{eq}$  as described in Chapter 5.

The result of the time-lines formulation is that all equations originally written in terms of the isotropic preconsolidation stress  $p_c$  for integration of the rate-independent MCC model must now be written in terms of the equivalent hydrostatic stress  $p_{eq}$ . The effects of volumetric age must also be considered when integrating the constitutive equations. The key equations are given below.

The final change between MCC and the chalk model is that the chalk model truncates the elliptical viscoplastic potential surfaces where intersected by the shear failure surface. Therefore, the maximum adjusted shear stress ratio permitted in the chalk model is the adjusted failure shear stress ratio  $\bar{\eta}_f$ . Any shear stress ratios greater than this limiting value are automatically reduced to the failure shear stress ratio.

The modified equations used for integration of the rate-dependent chalk model given in the following paragraphs. Recall that the equations for integration of rate-independent cap models are expressed in terms of the ratio  $(\bar{p}_c / \bar{p})$ :

$$\bar{p}_c = \exp\left[\frac{N - e_f + \kappa \ln(\bar{p}_c/\bar{p})}{\lambda}\right] \quad (7.46)$$

$$\bar{p} = \frac{\bar{p}}{\bar{p}_c} \exp\left[\frac{N - e_f + \kappa \ln(\bar{p}_c/\bar{p})}{\lambda}\right] \quad (7.47)$$

$$q = \frac{\bar{\eta}\bar{p}}{\bar{p}_c} \exp\left[\frac{N - e_f + \kappa \ln(\bar{p}_c/\bar{p})}{\lambda}\right] \quad (7.48)$$

The same equations may be used for integration of the rate-dependent chalk model. As stated above, all the relations in terms of  $\bar{p}_c/\bar{p}$  included in section 7.2 are reformulated in terms of  $\bar{p}_{eq}/\bar{p}$ . Fortunately, there is a relation between  $\bar{p}_c$  and  $\bar{p}_{eq}$  in the rate-dependent model:

$$\frac{\bar{p}_c}{\bar{p}_{eq}} = \left(\frac{t_v}{t_{v,\min}}\right)^{\frac{\psi}{\lambda-\kappa}} \quad (7.49)$$

while the ratio  $\bar{p}_{eq}/\bar{p}$  may be expressed as:

$$\frac{\bar{p}_{eq}}{\bar{p}} = \frac{G_0 M_2^2 - \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2 (M^2 - M_2^2)}}{G_0 R (M_2^2 - M^2)} \quad (7.50)$$

where  $G_0$  is the William-Warnke third-invariant scaling parameter. The quantity  $\bar{p}_c/\bar{p}$  in equations (7.46)-(7.48) then becomes:

$$\frac{\bar{p}_c}{\bar{p}} = \frac{G_0 M_2^2 - \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2 (M^2 - M_2^2)}}{G_0 R (M_2^2 - M^2)} \left(\frac{t_v}{t_{v,\min}}\right)^{\frac{\psi}{\lambda-\kappa}} \quad (7.51)$$

For integration of the rate-independent model, the only unknown parameter to be solved for is the adjusted shear stress ratio  $\bar{\eta}$ . For the three-dimensional rate-dependent model, the number of unknowns is three (only two for models with deviatoric coaxiality): the adjusted shear stress ratio  $\bar{\eta}$ , the volumetric age  $t_v$ , and for models with deviatoric normality, the William-Warnke scaling parameter  $G_0$ .

As for integration of the rate-independent models, the solution for the chalk model is solved by iteratively minimizing the residual between the current estimate for  $\bar{\eta}$  and a ‘consistent’ value between the trial stress point, final stress point, and gradient to the viscoplastic

potential. For the chalk model, however, three sequential Newton-Raphson calculations are performed during each iteration to minimize the residuals for all three unknown variables.

The residual  $r_1$  which applies to the volumetric age is formed in exactly the same way as described in Chapter 5 for the one-dimensional model:

$$r_1 = \bar{p} - \left[ \bar{p}_{tr} - K \frac{\Psi}{(1 + e_{eq}) \bar{t}_v} \frac{\Delta t}{\bar{t}_v} \right] \quad (7.52)$$

where  $\bar{t}_v$  is the secant volumetric age as described in Chapter 5:

$$\bar{t}_v = \sqrt{t_{v0} t_{vf}} \quad (7.53)$$

The increment to the final volumetric age is determined using Newton-Raphson iteration, as follows:

$$\Delta t_{vf} = \frac{-r_1}{\partial r_1 / \partial t_{vf}} \quad (7.54)$$

In equation (7.54), the value of the derivative  $\partial r_1 / \partial t_{vf}$  is given as follows:

$$\frac{\partial r_1}{\partial t_v} = -K \frac{\Psi}{(1 + e_{eq}) \bar{t}_v^2} \frac{\Delta t}{\bar{t}_v} \frac{\partial \bar{t}_v}{\partial t_{vf}} - \frac{\bar{p}}{t_{vf}} \frac{\Psi}{(\lambda - \kappa)} = -\frac{K}{2} \frac{\Psi}{(1 + e_{eq}) \bar{t}_v^2} \frac{\Delta t}{\sqrt{t_{v0}}} + \frac{\bar{p}}{t_{vf}} \frac{\Psi}{(\kappa - \lambda)} \quad (7.55)$$

The residual  $r_2$  which applies to the adjusted shear stress ratio is formed in a similar way as described in the previous section for the rate-independent model:

$$r_2 = \frac{q - q_{tr}}{\bar{p} - \bar{p}_{tr}} - \frac{3G}{K} \frac{(\partial g / \partial q)_{\sigma_f}}{(\partial g / \partial \bar{p})_{\sigma_f}} \quad (7.56)$$

where the derivatives are evaluated at the final stress point  $\sigma_f$ . The increment to the final adjusted shear stress ratio is also determined using Newton-Raphson iteration:

$$\Delta \bar{\eta} = \frac{-r_2}{\partial r_2 / \partial \bar{\eta}} \quad (7.57)$$

The derivative  $\partial r_2 / \partial \bar{\eta}$  is given as follows:

$$\frac{\partial r_2}{\partial \bar{\eta}} = \frac{(\bar{p} - \bar{p}_{tr}) \left[ \bar{p} + \bar{\eta} \bar{p}_{eq} \frac{\partial(\bar{p}/\bar{p}_{eq})}{\partial \bar{\eta}} + \bar{\eta} \frac{\bar{p}}{\bar{p}_c} \frac{\partial \bar{p}_c}{\partial \bar{\eta}} \right] - (q - q_{tr}) \left[ \bar{p}_{eq} \frac{\partial(\bar{p}/\bar{p}_{eq})}{\partial \bar{\eta}} + \frac{\bar{p}}{\bar{p}_c} \frac{\partial \bar{p}_c}{\partial \bar{\eta}} \right]}{(\bar{p} - \bar{p}_{tr})^2} \quad (7.58)$$

$$- \frac{3G}{K} \frac{\partial[(\partial g/\partial q)/(\partial g/\partial \bar{p})]}{\partial \bar{\eta}} - \frac{\partial g/\partial q}{\partial g/\partial \bar{p}} \frac{\partial(3G/K)}{\partial \bar{\eta}}$$

The required quantities in equation (7.58) for the case  $R \neq 0.5$  follow:

$$\frac{\partial(\bar{p}/\bar{p}_{eq})}{\partial \bar{\eta}} = - \frac{\bar{p}}{\bar{p}_{eq}} \frac{\bar{\eta}(M_2^2 - M^2)}{\sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} \left[ G_0 M_2^2 - \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} \right]} \quad (7.59)$$

$$\frac{\partial \bar{p}_c}{\partial \bar{\eta}} = \bar{p}_c \frac{\kappa}{\lambda} \frac{\bar{\eta}(M_2^2 - M^2)}{\sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} \left[ G_0 M_2^2 - \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} \right]} \quad (7.60)$$

$$\frac{\partial g/\partial q}{\partial g/\partial \bar{p}} = \frac{\bar{\eta}(M_2^2 - M^2)}{G_0 M_2^2 \left[ \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} - G_0 M_2^2 \right]} \quad (7.61)$$

$$\frac{\partial[(\partial g/\partial q)/(\partial g/\partial \bar{p})]}{\partial \bar{\eta}} = \frac{M^2(M^2 - M_2^2) \left[ \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} - G_0 M_2^2 \right]}{M_2^2 \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} \left[ \sqrt{G_0^2 M^2 M_2^2 + \bar{\eta}^2(M^2 - M_2^2)} - G_0 M_2^2 \right]^2} \quad (7.62)$$

while these quantities are simplified if  $R = 0.5$ :

$$\frac{\partial(\bar{p}/\bar{p}_{eq})}{\partial \bar{\eta}} = - \frac{\bar{p}}{\bar{p}_{eq}} \frac{2\bar{\eta}}{(G_0^2 M^2 + \bar{\eta}^2)} \quad (7.63)$$

$$\frac{\partial \bar{p}_c}{\partial \bar{\eta}} = \bar{p}_c \frac{\kappa}{\lambda} \frac{2\bar{\eta}}{(G_0^2 M^2 + \bar{\eta}^2)} \quad (7.64)$$

$$\frac{\partial g/\partial q}{\partial g/\partial \bar{p}} = \frac{2\bar{\eta}}{G_0^2 M^2 - \bar{\eta}^2} \quad (7.65)$$

$$\frac{\partial[(\partial g/\partial q)/(\partial g/\partial \bar{p})]}{\partial \bar{\eta}} = \frac{2(G_0^2 M^2 + \bar{\eta}^2)}{(G_0^2 M^2 - \bar{\eta}^2)^2} \quad (7.66)$$

For the chalk model ( $v = \text{constant}$ ), the derivative in equation (7.58) becomes:

$$\frac{\partial(3G/K)}{\partial\bar{\eta}} = 0 \quad (7.67)$$

The residual  $r_3$  which applies to the Lode angle uses the William-Warnke scaling parameter  $G_0$  and is formed as follows:

$$r_3 = \theta - \left[ \theta_{tr} - \frac{(q_{tr} - q)}{q^2} \frac{\partial g / \partial \theta}{\partial g / \partial q} \right] \quad (7.68)$$

where  $\partial g / \partial \theta$  is obtained using the chain-rule:

$$\frac{\partial g}{\partial \theta} = \frac{\partial g}{\partial G_0} \frac{\partial G_0}{\partial \theta} \quad (7.69)$$

As for the other desired parameters, the increment to the final Lode angle is also determined using Newton-Raphson iteration:

$$\Delta\theta = \frac{-r_3}{\partial r_3 / \partial \theta} \quad (7.70)$$

The derivative  $\partial r_3 / \partial \theta$  is given as follows:

$$\frac{\partial r_3}{\partial \theta} = 1 + \frac{(q_{tr} - q)}{q^2} \frac{1}{\partial g / \partial q} \frac{\partial^2 g}{\partial \theta^2} = 1 + \frac{(q_{tr} - q)}{q^2} \frac{1}{\partial g / \partial q} \left( \frac{\partial g}{\partial \theta} \frac{\partial^2 G_0}{\partial \theta^2} + \frac{\partial^2 g}{\partial G_0^2} \frac{\partial G_0}{\partial \theta} \right) \quad (7.71)$$

The various derivatives in equations (7.69) and (7.71) are obtained as shown. For  $R \neq 0.5$ :

$$\frac{\partial g}{\partial G_0} = 2G_0 \left[ M_2^2 (\bar{p} - R\bar{p}_{eq})^2 - M^2 R^2 \bar{p}_{eq}^2 \right] \quad (7.72)$$

$$\frac{\partial^2 g}{\partial G_0^2} = 2 \left[ M_2^2 (\bar{p} - R\bar{p}_{eq})^2 - M^2 R^2 \bar{p}_{eq}^2 \right] \quad (7.73)$$

while for  $R = 0.5$ :

$$\frac{\partial g}{\partial G_0} = 2G_0 M^2 \bar{p} (\bar{p} - \bar{p}_{eq}) \quad (7.74)$$

$$\frac{\partial^2 g}{\partial G_0^2} = 2M^2 \bar{p} (\bar{p} - \bar{p}_{eq}) \quad (7.75)$$

The other required derivatives are:

$$\frac{\partial g}{\partial q} = 2q \quad (7.76)$$

$$G_\theta = \frac{c_1 \cos(\theta^*) + \sqrt{c_2(c_3 + c_4)}}{c_2 + c_4} \quad (7.77)$$

$$\frac{\partial G_\theta}{\partial \theta} = \frac{[-c_1(c_2 + c_4)\sin(\theta^*)] \left[ 1 + \frac{2c_2 \cos(\theta^*)}{\sqrt{c_2(c_3 + c_4)}} \right] + [4c_1 \cos(\theta^*)\sin(\theta^*)][c_1 \cos(\theta^*) + \sqrt{c_2(c_3 + c_4)}]}{(c_2 + c_4)^2} \quad (7.78)$$

$$\begin{aligned} \frac{\partial^2 G_\theta}{\partial \theta^2} = & \frac{-8c_1^2 \cos(\theta^*)\sin(\theta^*) \left[ \sin(\theta^*) + \frac{2c_2 \cos(\theta^*)\sin(\theta^*)}{\sqrt{c_2(c_3 + c_4)}} \right]}{(c_2 + c_4)^2} \\ & + [c_1 \cos(\theta^*) + \sqrt{c_2(c_3 + c_4)}] \left\{ \frac{16c_4 \sin^2(\theta^*) + [2c_4 - 4c_1 \sin^2(\theta^*)](c_2 + c_4)}{(c_2 + c_4)^3} \right\} \\ & + \frac{c_2(c_3 + c_4)[2c_1c_2 \sin^2(\theta^*) - c_2c_4] - c_1[c_2(c_3 + c_4)]^{1.5} \cos(\theta^*) - 2c_1c_2^2c_4 \sin^2(\theta^*)}{(c_2 + c_4)[c_2(c_3 + c_4)]^{1.5}} \end{aligned} \quad (7.79)$$

where  $c_1 = 2(1 - k^2)$

$$c_2 = (2k - 1)^2$$

$$c_3 = k(5k - 4)$$

$$c_4 = 2c_1 \cos^2(\theta - \pi/6)$$

$k$  = William-Warnke parameter

A converged solution is obtained when the three following conditions are satisfied:

$$\begin{aligned} r_1 < \text{TOLER}_1 \quad \text{OR} \quad t_v = t_{v,\min} \\ r_2 < \text{TOLER}_2 \quad \text{OR} \quad \bar{\eta} = \bar{\eta}_f \\ r_3 < \text{TOLER}_3 \end{aligned} \quad (7.80)$$

where  $\text{TOLER}_i$  is the specified tolerance for residual  $r_i$ .



## REFERENCES

- Borja, R.I. (1991). Cam-clay plasticity, part II: Implicit integration of constitutive equations based on a nonlinear elastic stress predictor. *Computer Methods in Applied Mechanics and Engineering*, 88, 225-240.
- Borja, R.I. and Lee, S.R. (1990). Cam-clay plasticity, part I: Implicit integration of elasto-plastic constitutive relations. *Computer Methods in Applied Mechanics and Engineering*, 78, 49-72.
- Borja, R.I., Lin, C.-H., and Montans, F.J. (2001). Cam-clay plasticity, part IV: Implicit integration of anisotropic bounding surface model with nonlinear hyperelasticity and ellipsoidal loading function. *Computer Methods in Applied Mechanics and Engineering*, 190, 3293-3323.
- Jeremic, B. (2001). Line Search Techniques for Elasto-Plastic Finite Element Computations in Geomechanics. University of California-Davis Report no. UCD/CGM-01/04.
- Jeremic, B. and Sture, S. (1997). Implicit integrations in elastoplastic geotechnics. *Mechanics of Cohesive-Frictional Materials*, 2, 165-183.
- Macari, E.J., Weihe, S., and Arduino, P. (1997). Implicit integration of elastoplastic constitutive models for frictional materials with highly non-linear hardening functions. *Mechanics of Cohesive-Frictional Materials*, 2, 1-29.
- Manzari, M.T. and Prachathananukit, R. (2001). *International Journal for Numerical and Analytical Methods in Geomechanics*, 25, 525-549.
- Nayak, G.C., and Zienkiewicz, O.C. (1972). Elastoplastic stress analysis: a generalization for various constitutive relations including strain softening. *International Journal for Numerical Methods in Engineering*, 5, 113-135.
- Ortiz, M. and Simo, J.C. (1986). An analysis of a new class of integration algorithms for elastoplastic constitutive relations. *International Journal for Numerical Methods in Engineering*, 23, 353-366.
- Owen, D.R.J., and Hinton, E. (1980). *Finite Elements in Plasticity: Theory and Practice*. Pineridge Press, Swansea, Wales, 594 p.
- Perez-Fouget, A. and Armero, F. (2002). On the formulation of closest-point projection algorithms in elastoplasticity – part II: Globally convergent schemes. *International Journal for Numerical Methods in Engineering*, 53, 331-374.
- Potts, D.M. and Ganendra, D. (1994). An evaluation of substepping and implicit stress point algorithms. *Computer Methods and Applied Mechanics in Engineering*, 119, 341-354.
- Potts, D.M. and Gens, A. (1985). A critical assessment of methods of correcting for drift from the yield surface in elasto-plastic finite element analysis. *International Journal for Numerical and Analytical Methods in Geomechanics*, 9, 149-159.

Simo, J.C., and Ortiz, M. (1985). A unified approach to finite deformation elastoplastic analysis based on the use of hyperelastic constitutive equations. *Computer Methods in Applied Mechanics and Engineering*, 49, 221-245.

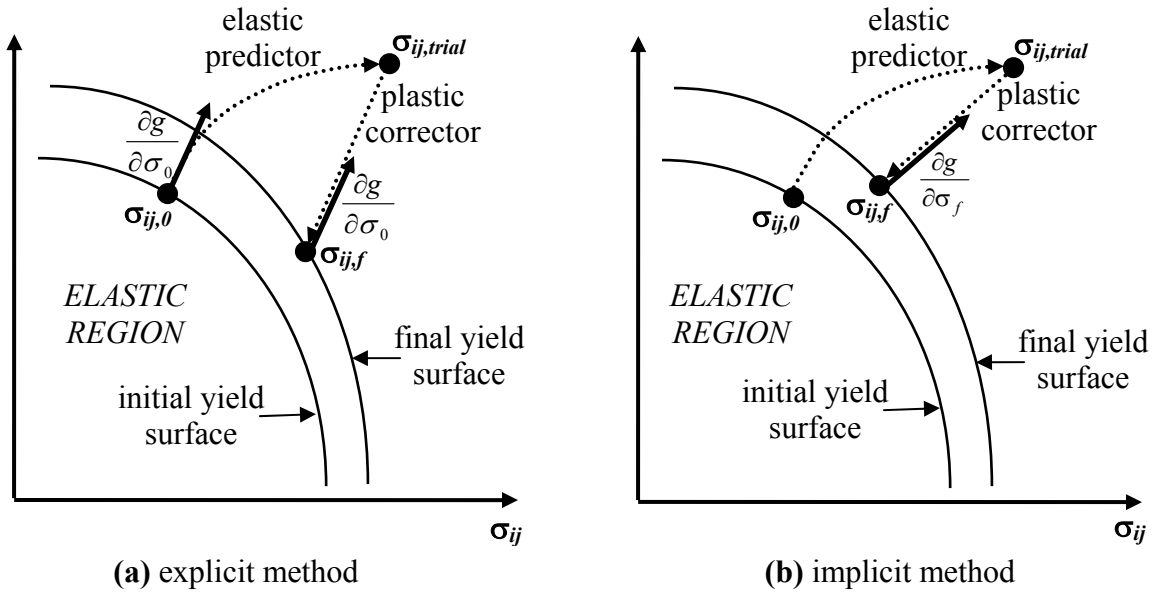
Simo, J.C. and Taylor, R.L. (1985). Consistent tangent operators for rate-independent elastoplasticity. *Computer Methods in Applied Mechanics in Engineering*, 48, 101-118.

Sloan, S.W. (1987). Substepping schemes for the numerical integration of elastoplastic stress-strain relations. *International Journal for Numerical Methods in Engineering*, 24, 893-911.

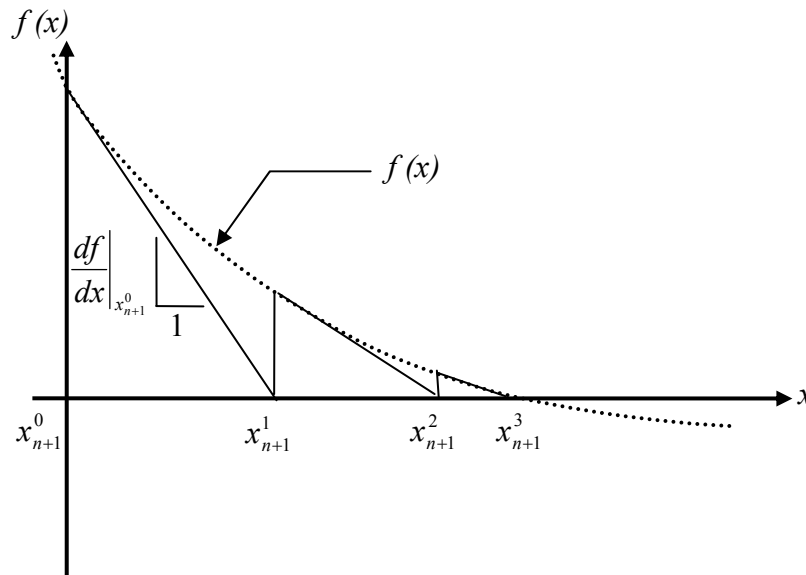
Sloan, S.W., Abbo, A.J., and Sheng, D. (2001). Refined explicit integration of elastoplastic models with automatic error control. *Engineering Computations*, 18 (1/2), 121-154.

Sloan, S.W. and Booker, J.R. (1992). Integration of Tresca and Mohr-Coulomb constitutive relations in plane strain elastoplasticity. *International Journal for Numerical Methods in Engineering*, 33, 163-196.

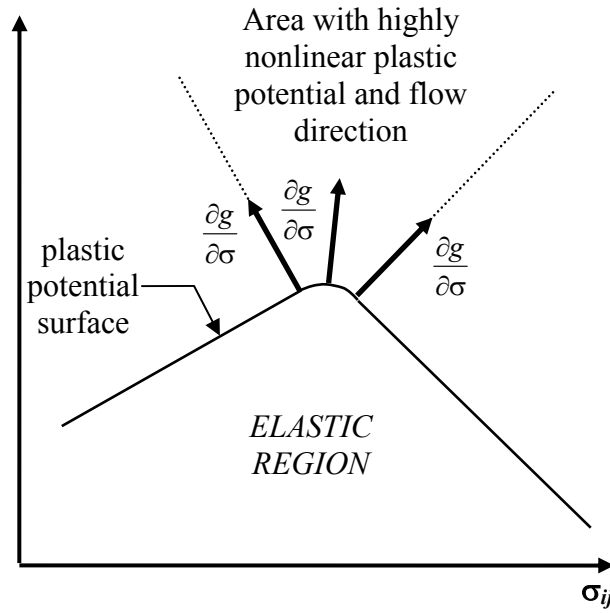
Wathugala, G.W. and Pal, S. (1999). Comparison of different implementation algorithms for HiSS constitutive models in FEM. *International Journal of Solids and Structures*, 36, 4941-4962.



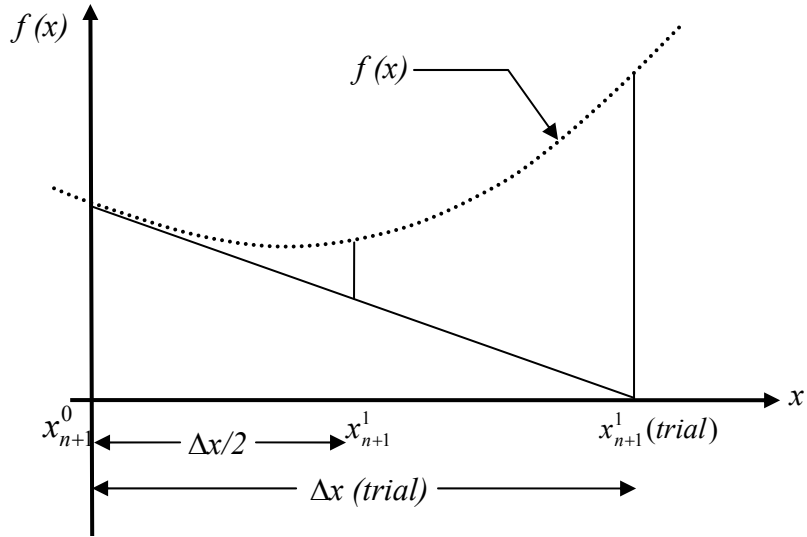
**Figure 7.1. Illustration of the elastic predictor-plastic corrector as a return algorithm: (a) explicit procedure – gradients are evaluated at initial stress point; (b) implicit method – gradients are evaluated at final stress point. Plastic predictor – plastic corrector algorithms work the same way.**



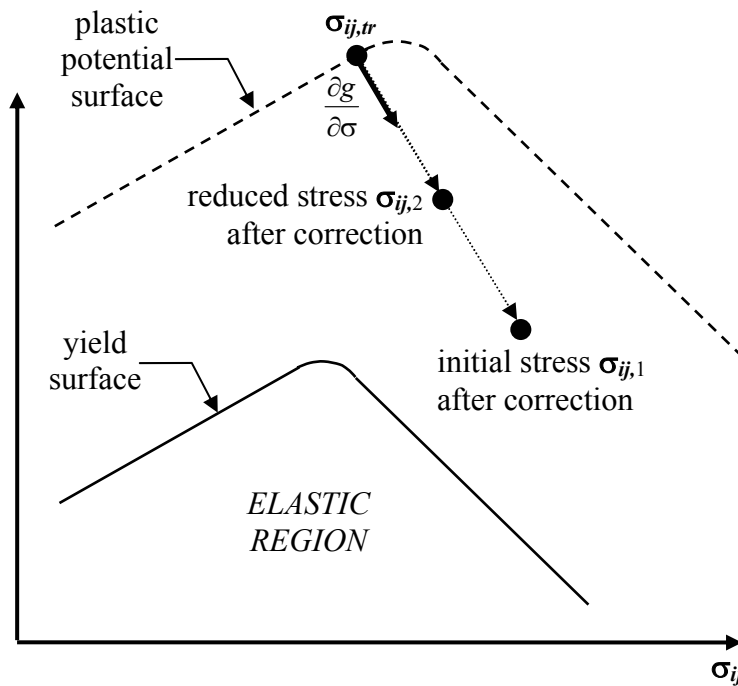
**Figure 7.2. Use of the Newton-Raphson method for a function of one variable.**



**Figure 7.3. Illustration of potentially non-convergent region in stress space. In the “transition area” near a rounded corner, the plastic flow direction changes rapidly, potentially leading to non-convergence.**



(a)

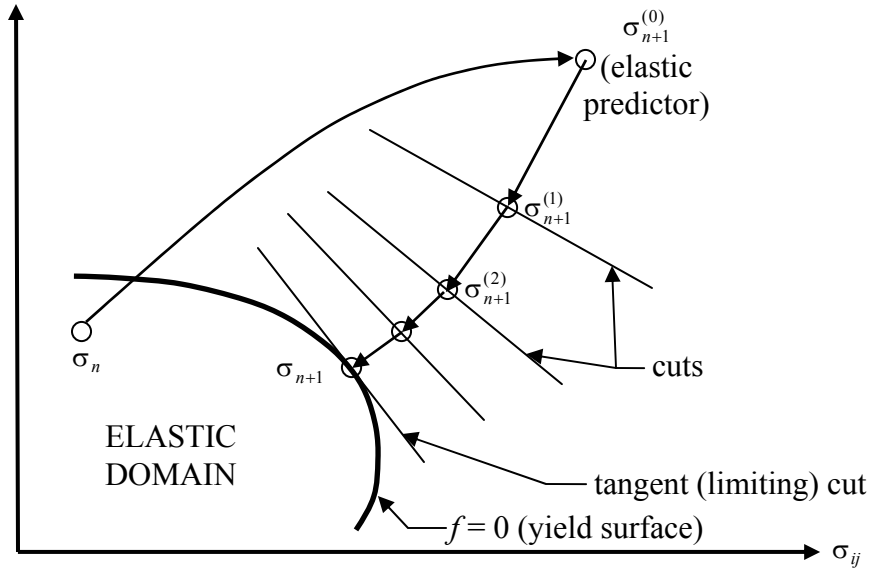


$$f(\sigma_{ij,1}) > f(\sigma_{ij,tr})$$

$$f(\sigma_{ij,2}) < f(\sigma_{ij,tr})$$

(b)

Figure 7.4. Use of the line search procedure to limit incremental corrector step lengths (a) for a 1-D function; (b) in stress space near a nonlinear plastic potential surface. The stress corrector is reduced so the incrementally corrected stress is closer to the final yield surface.



**Figure 7.5. Illustration of the cutting plane method for a nonhardening yield surface. The elastic predictor is returned iteratively to the yield surface. The updated stresses are projected onto a straight “cut” defined as the trace of the plane  $f = 0$  on the linearized yield function about the estimate of the stresses for the current iteration. (Ortiz and Simo, 1986)**