

Cam-Clay model based on Borja et al. 1997

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Contents

1	Introduction	2
2	Quantities that are needed in a Uintah implementation	2
2.1	Elasticity	2
2.2	Plasticity	2
3	Why they are needed: Derivation of stress update based Rich Reguiero's notes	3
3.1	Elastic-plastic stress update	4
3.2	Newton iterations	6
3.3	Tangent calculation: elastic	8
3.4	Tangent calculation: elastic-plastic	9

1 Introduction

Introduce the equations and how they differ from Fossum-Brannon.

2 Quantities that are needed in a Uintah implementation

2.1 Elasticity

The elastic strain energy density in Borja's model has the form

$$W(\epsilon_v^e, \epsilon_s^e) = W_{\text{vol}}(\epsilon_v^e) + W_{\text{dev}}(\epsilon_v^e, V\epsilon_s^e)$$

where

$$W_{\text{vol}}(\epsilon_v^e) = -p_0 \tilde{\kappa} \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right)$$

$$W_{\text{dev}}(\epsilon_v^e, \epsilon_s^e) = \frac{3}{2} \mu (\epsilon_s^e)^2$$

where ϵ_{v0}^e is the volumetric strain corresponding to a mean normal compressive stress p_0 (tension positive), $\tilde{\kappa}$ is the elastic compressibility index, and the shear modulus is given by

$$\mu = \mu_0 + \frac{\alpha}{\tilde{\kappa}} W_{\text{vol}}(\epsilon_v^e) = \mu_0 - \alpha p_0 \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right).$$

The parameter α determines the extent of coupling between the volumetric and deviatoric responses. For consistency with isotropic elasticity, Rebecca Brannon suggests that $\alpha = 0$ (citation?).

The stress invariants p and q are defined as

$$p = \frac{\partial W}{\partial \epsilon_v^e} = p_0 \left[1 + \frac{3}{2} \frac{\alpha}{\tilde{\kappa}} (\epsilon_s^e)^2 \right] \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right) = p_0 \beta \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right)$$

$$q = \frac{\partial W}{\partial \epsilon_s^e} = 3 \left[\mu_0 - \alpha p_0 \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right) \right] \epsilon_s^e = 3\mu \epsilon_s^e.$$

The derivatives of the stress invariants are

$$\frac{\partial p}{\partial \epsilon_v^e} = -\frac{p_0}{\tilde{\kappa}} \left[1 + \frac{3}{2} \frac{\alpha}{\tilde{\kappa}} (\epsilon_s^e)^2 \right] \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right) = -\frac{p}{\tilde{\kappa}}$$

$$\frac{\partial p}{\partial \epsilon_s^e} = \frac{\partial q}{\partial \epsilon_s^e} = \frac{3\alpha p_0 \epsilon_s^e}{\tilde{\kappa}} \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right) = \frac{3\alpha p}{\beta \tilde{\kappa}} \epsilon_s^e$$

$$\frac{\partial q}{\partial \epsilon_s^e} = 3 \left[\mu_0 - \alpha p_0 \exp\left(-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\tilde{\kappa}}\right) \right] = 3\mu.$$

2.2 Plasticity

For plasticity we use a Cam-Clay yield function of the form

$$f = \left(\frac{q}{M} \right)^2 + p(p - p_c)$$

where M is the slope of the critical state line and the consolidation pressure p_c is an internal variable that evolves according to

$$\frac{1}{p_c} \frac{dp_c}{dt} = \frac{1}{\tilde{\lambda} - \tilde{\kappa}} \frac{d\epsilon_v^p}{dt}.$$

The derivatives of f that are of interest are

$$\frac{\partial f}{\partial p} = 2p - p_c$$

$$\frac{\partial f}{\partial q} = \frac{2q}{M^2}.$$

If we integrate the equation for p_c from t_n to t_{n+1} , we can show that

$$(p_c)_{n+1} = (p_c)_n \exp \left[\frac{(\epsilon_v^e)_{\text{trial}} - (\epsilon_v^e)_{n+1}}{\bar{\lambda} - \bar{\kappa}} \right].$$

The derivative of p_c that is of interest is

$$\frac{\partial p_c}{\partial (\epsilon_v^e)_{n+1}} = -\frac{(p_c)_n}{\bar{\lambda} - \bar{\kappa}} \exp \left[\frac{(\epsilon_v^e)_{\text{trial}} - (\epsilon_v^e)_{n+1}}{\bar{\lambda} - \bar{\kappa}} \right].$$

3 Why these quantities are needed: stress update based Rich Reguiero's notes

The volumetric and deviatoric components of the elastic strain ϵ^e are defined as follows:

$$\epsilon^e = \epsilon^e - \frac{1}{3} \epsilon_v^e \mathbf{1} = \epsilon^e - \frac{1}{3} \text{tr}(\epsilon^e) \mathbf{1} \quad \text{and} \quad \epsilon_s^e = \sqrt{\frac{2}{3}} \|\epsilon^e\| = \sqrt{\frac{2}{3}} \sqrt{\epsilon^e : \epsilon^e}.$$

The stress tensor is decomposed into a volumetric and a deviatoric component

$$\sigma = p \mathbf{1} + \sqrt{\frac{2}{3}} q \mathbf{n} \quad \text{with} \quad \mathbf{n} = \frac{\epsilon^e}{\|\epsilon^e\|} = \sqrt{\frac{2}{3}} \frac{\epsilon^e}{\epsilon_s^e}.$$

The models used to determine p and q are

$$p = p_0 \beta \exp \left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}} \right] \quad \text{with} \quad \beta = 1 + \frac{3}{2} \frac{\alpha}{\bar{\kappa}} (\epsilon_s^e)^2$$

$$q = 3\mu \epsilon_s^e.$$

The strains are updated using

$$\epsilon^e = \epsilon_{\text{trial}}^e - \Delta \gamma \frac{\partial f}{\partial \sigma} \quad \text{where} \quad \epsilon_{\text{trial}}^e = \epsilon_n^e + \Delta \epsilon = \epsilon_n^e + (\epsilon - \epsilon_n).$$

Remark 1: The interface with MPMICE, among other things in Uintah, requires the computation of the quantity dp/dJ . Since J does not appear in the above equation we proceed as explained below.

$$J = \det(\mathbf{F}) = \det(\mathbf{1} + \nabla_0 \mathbf{u}) = \det(\mathbf{1} + \epsilon)$$

$$= 1 + \text{tr} \epsilon + \frac{1}{2} [(\text{tr} \epsilon)^2 - \text{tr}(\epsilon^2)] + \det(\epsilon). \quad = 1 + \epsilon_v + \frac{1}{2} [\epsilon_v^2 - \text{tr}(\epsilon^2)] + \det(\epsilon).$$

Also,

$$J = \frac{\rho_0}{\rho} = \frac{V}{V_0} \quad \text{and} \quad \epsilon_v = \frac{V - V_0}{V_0} = \frac{V}{V_0} - 1 = J - 1.$$

We use the relation $J = 1 + \epsilon_v$ while keeping in mind that this is *true only for infinitesimal strains and plastic incompressibility* for which ϵ_v^2 , $\text{tr}(\epsilon^2)$, and $\det(\epsilon)$ are zero. Under these conditions

$$\frac{\partial p}{\partial J} = \frac{\partial p}{\partial \epsilon_v} \frac{\partial \epsilon_v}{\partial J} = \frac{\partial p}{\partial \epsilon_v} \quad \text{and} \quad \frac{\partial p}{\partial \rho} = \frac{\partial p}{\partial \epsilon_v} \frac{\partial \epsilon_v}{\partial J} \frac{\partial J}{\partial \rho} = -\frac{J}{\rho} \frac{\partial p}{\partial \epsilon_v}.$$

Remark 2: MPMICE also needs the density at a given pressure. For the Borja model, with $\epsilon_v = J - 1 = \rho_0/\rho - 1$, we have

$$\rho = \rho_0 \left[1 + \epsilon_{v0} + \bar{\kappa} \ln \left(\frac{p}{p_0 \beta} \right) \right]^{-1}.$$

Remark 3: The quantity q is related to the deviatoric part of the Cauchy stress, s as follows:

$$q = \sqrt{3J_2} \quad \text{where} \quad J_2 = \frac{1}{2} s : s.$$

The shear modulus relates the deviatoric stress s to the deviatoric strain ϵ^e . We assume a relation of the form

$$s = 2\mu \epsilon^e.$$

Note that the above relation assumes a linear elastic type behavior. Then we get the Borja shear model:

$$q = \sqrt{\frac{3}{2} s : s} = \sqrt{\frac{3}{2}} (2\mu) \sqrt{\epsilon^e : \epsilon^e} = \sqrt{\frac{3}{2}} (2\mu) \sqrt{\frac{3}{2} \epsilon_s^e} = 3\mu \epsilon_s^e.$$

3.1 Elastic-plastic stress update

For elasto-plasticity we start with a yield function of the form

$$f = \left(\frac{q}{M}\right)^2 + p(p - p_c) \leq 0 \quad \text{where} \quad \frac{1}{p_c} \frac{dp_c}{dt} = \frac{1}{\bar{\lambda} - \bar{\kappa}} \frac{d\epsilon_v^p}{dt}.$$

Integrating the ODE for p_c with the initial condition $p_c(t_n) = (p_c)_n$, at $t = t_{n+1}$,

$$(p_c)_{n+1} = (p_c)_n \exp \left[\frac{(\epsilon_v^p)_{n+1} - (\epsilon_v^p)_n}{\bar{\lambda} - \bar{\kappa}} \right].$$

From the additive decomposition of the strain into elastic and plastic parts, and if the elastic trial strain is defined as

$$(\epsilon_v^e)_{\text{trial}} := (\epsilon_v^e)_n + \Delta \epsilon_v$$

we have

$$\epsilon_v^p = \epsilon_v - \epsilon_v^e \implies (\epsilon_v^p)_{n+1} - (\epsilon_v^p)_n = (\epsilon_v)_{n+1} - (\epsilon_v^e)_{n+1} - (\epsilon_v)_n + (\epsilon_v^e)_n = \Delta \epsilon_v + (\epsilon_v^e)_n - (\epsilon_v^e)_{n+1} = (\epsilon_v^e)_{\text{trial}} - (\epsilon_v^e)_{n+1}.$$

Therefore we can write

$$(p_c)_{n+1} = (p_c)_n \exp \left[\frac{(\epsilon_v^e)_{\text{trial}} - (\epsilon_v^e)_{n+1}}{\bar{\lambda} - \bar{\kappa}} \right].$$

The flow rule is assumed to be given by

$$\frac{\partial \epsilon^p}{\partial t} = \gamma \frac{\partial f}{\partial \sigma}.$$

Integration of the PDE with backward Euler gives

$$\epsilon_{n+1}^p = \epsilon_n^p + \Delta t \gamma_{n+1} \left[\frac{\partial f}{\partial \sigma} \right]_{n+1} = \epsilon_n^p + \Delta \gamma \left[\frac{\partial f}{\partial \sigma} \right]_{n+1}.$$

This equation can be expressed in terms of the trial elastic strain as follows.

$$\epsilon_{n+1}^p - \epsilon_{n+1}^e = \epsilon_n^p - \epsilon_n^e + \Delta \gamma \left[\frac{\partial f}{\partial \sigma} \right]_{n+1}$$

or

$$\epsilon_{n+1}^e = \Delta \epsilon + \epsilon_n^e - \Delta \gamma \left[\frac{\partial f}{\partial \sigma} \right]_{n+1} = \epsilon_{\text{trial}}^e - \Delta \gamma \left[\frac{\partial f}{\partial \sigma} \right]_{n+1}.$$

In terms of the volumetric and deviatoric components

$$(\epsilon_v^e)_{n+1} = \text{tr}(\epsilon_{n+1}^e) = \text{tr}(\epsilon_{\text{trial}}^e) - \Delta \gamma \text{tr} \left[\frac{\partial f}{\partial \sigma} \right]_{n+1} = (\epsilon_v^e)_{\text{trial}} - \Delta \gamma \text{tr} \left[\frac{\partial f}{\partial \sigma} \right]_{n+1}$$

and

$$\mathbf{e}_{n+1}^e = \mathbf{e}_{\text{trial}}^e - \Delta \gamma \left[\left(\frac{\partial f}{\partial \sigma} \right)_{n+1} - \frac{1}{3} \text{tr} \left(\frac{\partial f}{\partial \sigma} \right)_{n+1} \mathbf{1} \right].$$

With $\mathbf{s} = \boldsymbol{\sigma} - p\mathbf{1}$, we have

$$\frac{\partial f}{\partial \sigma} = \frac{\partial f}{\partial \mathbf{s}} : \frac{\partial \mathbf{s}}{\partial \sigma} + \frac{\partial f}{\partial p} \frac{\partial p}{\partial \sigma} = \frac{\partial f}{\partial \mathbf{s}} : [\mathbf{I}^{(s)} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1}] + \frac{\partial f}{\partial p} \mathbf{1} = \frac{\partial f}{\partial \mathbf{s}} - \frac{1}{3} \text{tr} \left[\frac{\partial f}{\partial \mathbf{s}} \right] \mathbf{1} + \frac{\partial f}{\partial p} \mathbf{1}$$

and

$$\frac{1}{3} \text{tr} \left[\frac{\partial f}{\partial \sigma} \right] \mathbf{1} = \frac{1}{3} \left(\text{tr} \left[\frac{\partial f}{\partial \mathbf{s}} \right] - \text{tr} \left[\frac{\partial f}{\partial \mathbf{s}} \right] + 3 \frac{\partial f}{\partial p} \right) \mathbf{1} = \frac{\partial f}{\partial p} \mathbf{1}.$$

Remark 4: Note that, because $\sigma = \sigma(p, q, p_c)$ the chain rule should contain a contribution from p_c :

$$\frac{\partial f}{\partial \sigma} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial \sigma} + \frac{\partial f}{\partial p} \frac{\partial p}{\partial \sigma} + \frac{\partial f}{\partial p_c} \frac{\partial p_c}{\partial \sigma}.$$

However, the Borja implementation does not consider that extra term. Also note that for the present model

$$\sigma = \sigma(p(\varepsilon_v^e, \varepsilon_s^e, \varepsilon_v^p, \varepsilon_s^p), s(\varepsilon_v^e, \varepsilon_s^e, \varepsilon_v^p, \varepsilon_s^p), p_c(\varepsilon_v^p))$$

Therefore, for situations where $\text{tr}(\partial f / \partial s) = \mathbf{0}$, we have

$$\frac{\partial f}{\partial \sigma} - \frac{1}{3} \text{tr} \left[\frac{\partial f}{\partial \sigma} \right] \mathbf{1} = \frac{\partial f}{\partial s} - \frac{1}{3} \text{tr} \left[\frac{\partial f}{\partial s} \right] \mathbf{1} = \frac{\partial f}{\partial s}.$$

The deviatoric strain update can be written as

$$\mathbf{e}_{n+1}^e = \mathbf{e}_{\text{trial}}^e - \Delta \gamma \left(\frac{\partial f}{\partial s} \right)_{n+1}$$

and the shear invariant update is

$$(\varepsilon_s^e)_{n+1} = \sqrt{\frac{2}{3}} \sqrt{\mathbf{e}_{n+1}^e : \mathbf{e}_{n+1}^e} = \sqrt{\frac{2}{3}} \sqrt{\mathbf{e}_{\text{trial}}^e : \mathbf{e}_{\text{trial}}^e - 2\Delta \gamma \left[\frac{\partial f}{\partial s} \right]_{n+1} : \mathbf{e}_{\text{trial}}^e + (\Delta \gamma)^2 \left[\frac{\partial f}{\partial s} \right]_{n+1} : \left[\frac{\partial f}{\partial s} \right]_{n+1}}$$

The derivative of f can be found using the chain rule (for smooth f):

$$\frac{\partial f}{\partial \sigma} = \frac{\partial f}{\partial p} \frac{\partial p}{\partial \sigma} + \frac{\partial f}{\partial q} \frac{\partial q}{\partial \sigma} = (2p - p_c) \frac{\partial p}{\partial \sigma} + \frac{2q}{M^2} \frac{\partial q}{\partial \sigma}.$$

Now, with $p = 1/3 \text{tr}(\sigma)$ and $q = \sqrt{3/2} \mathbf{s} : \mathbf{s}$, we have

$$\begin{aligned} \frac{\partial p}{\partial \sigma} &= \frac{\partial}{\partial \sigma} \left[\frac{1}{3} \text{tr}(\sigma) \right] = \frac{1}{3} \mathbf{1} \\ \frac{\partial q}{\partial \sigma} &= \frac{\partial}{\partial \sigma} \left[\sqrt{\frac{3}{2}} \mathbf{s} : \mathbf{s} \right] = \sqrt{\frac{3}{2}} \frac{1}{\sqrt{\mathbf{s} : \mathbf{s}}} \frac{\partial \mathbf{s}}{\partial \sigma} : \mathbf{s} = \sqrt{\frac{3}{2}} \frac{1}{\|\mathbf{s}\|} \left[\mathbf{I}^{(s)} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} \right] : \mathbf{s} = \sqrt{\frac{3}{2}} \frac{\mathbf{s}}{\|\mathbf{s}\|}. \end{aligned}$$

Therefore,

$$\frac{\partial f}{\partial \sigma} = \frac{2p - p_c}{3} \mathbf{1} + \sqrt{\frac{3}{2}} \frac{2q}{M^2} \frac{\mathbf{s}}{\|\mathbf{s}\|}.$$

Recall that

$$\sigma = p \mathbf{1} + \sqrt{\frac{2}{3}} q \mathbf{n} = p \mathbf{1} + \mathbf{s}.$$

Therefore,

$$\mathbf{s} = \sqrt{\frac{2}{3}} q \mathbf{n} \quad \text{and} \quad \|\mathbf{s}\| = \sqrt{\mathbf{s} : \mathbf{s}} = \sqrt{\frac{2}{3}} q^2 \mathbf{n} : \mathbf{n} = \sqrt{\frac{2}{3}} q^2 \frac{\mathbf{e}^e : \mathbf{e}^e}{\|\mathbf{e}^e\|^2} = \sqrt{\frac{2}{3}} q^2 = \sqrt{\frac{2}{3}} q.$$

So we can write

$$\frac{\partial f}{\partial \sigma} = \frac{2p - p_c}{3} \mathbf{1} + \sqrt{\frac{3}{2}} \frac{2q}{M^2} \mathbf{n}. \quad (1)$$

Using the above relation we have

$$\frac{\partial f}{\partial p} = \frac{1}{3} \text{tr} \left[\frac{\partial f}{\partial \sigma} \right] = 2p - p_c \quad \text{and} \quad \frac{\partial f}{\partial s} = \frac{\partial f}{\partial \sigma} - \frac{\partial f}{\partial p} \mathbf{1} = \sqrt{\frac{3}{2}} \frac{2q}{M^2} \mathbf{n}.$$

The strain updates can now be written as

$$\begin{aligned} (\varepsilon_v^e)_{n+1} &= (\varepsilon_v^e)_{\text{trial}} - \Delta \gamma [2p_{n+1} - (p_c)_{n+1}] \\ \mathbf{e}_{n+1}^e &= \mathbf{e}_{\text{trial}}^e - \sqrt{\frac{3}{2}} \Delta \gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) \mathbf{n}_{n+1} \\ (\varepsilon_s^e)_{n+1} &= \sqrt{\frac{2}{3}} \sqrt{\mathbf{e}_{\text{trial}}^e : \mathbf{e}_{\text{trial}}^e - \sqrt{6} (\Delta \gamma)^2 \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) \mathbf{n}_{n+1} : \mathbf{e}_{\text{trial}}^e + \frac{3}{2} (\Delta \gamma)^4 \left(\frac{2q_{n+1}}{M_{n+1}^2} \right)^2}. \end{aligned}$$

From the second equation above,

$$\mathbf{n}_{n+1} : \mathbf{e}_{\text{trial}}^e = \mathbf{n}_{n+1} : \mathbf{e}_{n+1}^e + \sqrt{\frac{3}{2}} \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) \mathbf{n}_{n+1} : \mathbf{n}_{n+1} = \frac{\mathbf{e}_{n+1}^e : \mathbf{e}_{n+1}^e}{\|\mathbf{e}_{n+1}^e\|} + \sqrt{\frac{3}{2}} \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) = \|\mathbf{e}_{n+1}^e\| + \sqrt{\frac{3}{2}} \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right).$$

Also notice that

$$\mathbf{e}_{\text{trial}}^e : \mathbf{e}_{\text{trial}}^e = \mathbf{e}_{n+1}^e : \mathbf{e}_{n+1}^e + 2 \sqrt{\frac{3}{2}} \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) \mathbf{e}_{n+1}^e : \mathbf{n}_{n+1} + \left[\sqrt{\frac{3}{2}} \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) \right]^2$$

or,

$$\|\mathbf{e}_{\text{trial}}^e\|^2 = \left[\|\mathbf{e}_{n+1}^e\| + \sqrt{\frac{3}{2}} \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) \right]^2.$$

Therefore,

$$\mathbf{n}_{n+1} : \mathbf{e}_{\text{trial}}^e = \|\mathbf{e}_{\text{trial}}^e\|$$

and we have

$$(\varepsilon_s^e)_{n+1} = \sqrt{\frac{2}{3}} \sqrt{\|\mathbf{e}_{\text{trial}}^e\|^2 - \sqrt{6} (\Delta\gamma)^2 \left(\frac{2q_{n+1}}{M_{n+1}^2} \right) \|\mathbf{e}_{\text{trial}}^e\| + \frac{3}{2} (\Delta\gamma)^4 \left(\frac{2q_{n+1}}{M_{n+1}^2} \right)^2} = \sqrt{\frac{2}{3}} \|\mathbf{e}_{\text{trial}}^e\| - \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right).$$

The elastic strain can therefore be updated using

$$\begin{aligned} (\varepsilon_v^e)_{n+1} &= (\varepsilon_v^e)_{\text{trial}} - \Delta\gamma [2p_{n+1} - (p_c)_{n+1}] \\ (\varepsilon_s^e)_{n+1} &= (\varepsilon_s^e)_{\text{trial}} - \Delta\gamma \left(\frac{2q_{n+1}}{M_{n+1}^2} \right). \end{aligned}$$

The consistency condition is needed to close the above equations

$$f = \left(\frac{q_{n+1}}{M} \right)^2 + p_{n+1} [p_{n+1} - (p_c)_{n+1}] = 0.$$

The unknowns are $(\varepsilon_v^e)_{n+1}$, $(\varepsilon_s^e)_{n+1}$ and $\Delta\gamma$. Note that we can express the three equations as

$$\begin{aligned} (\varepsilon_v^e)_{n+1} &= (\varepsilon_v^e)_{\text{trial}} - \Delta\gamma \left[\frac{\partial f}{\partial p} \right]_{n+1} \\ (\varepsilon_s^e)_{n+1} &= (\varepsilon_s^e)_{\text{trial}} - \Delta\gamma \left[\frac{\partial f}{\partial q} \right]_{n+1} \\ f_{n+1} &= 0. \end{aligned} \tag{2}$$

3.2 Newton iterations

The three nonlinear equations in the three unknowns can be solved using Newton iterations for smooth yield functions. Let us define the residual as

$$\underline{\mathbf{r}}(\underline{\mathbf{x}}) = \begin{bmatrix} (\varepsilon_v^e)_{n+1} - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma \left[\frac{\partial f}{\partial p} \right]_{n+1} \\ (\varepsilon_s^e)_{n+1} - (\varepsilon_s^e)_{\text{trial}} + \Delta\gamma \left[\frac{\partial f}{\partial q} \right]_{n+1} \\ f_{n+1} \end{bmatrix} =: \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} \quad \text{where} \quad \underline{\mathbf{x}} = \begin{bmatrix} (\varepsilon_v^e)_{n+1} \\ (\varepsilon_s^e)_{n+1} \\ f_{n+1} \end{bmatrix} =: \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}.$$

The Newton root finding algorithm is :

To code the algorithm we have to find the derivatives of the residual with respect to the primary variables. Let's do the terms one by one. For the first row,

$$\begin{aligned} \frac{\partial r_1}{\partial x_1} &= \frac{\partial}{\partial \varepsilon_v^e} [\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma (2p - p_c)] = 1 + \Delta\gamma \left(2 \frac{\partial p}{\partial \varepsilon_v^e} - \frac{\partial p_c}{\partial \varepsilon_v^e} \right) \\ \frac{\partial r_1}{\partial x_2} &= \frac{\partial}{\partial \varepsilon_s^e} [\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma (2p - p_c)] = 2\Delta\gamma \frac{\partial p}{\partial \varepsilon_s^e} \\ \frac{\partial r_1}{\partial x_3} &= \frac{\partial}{\partial \Delta\gamma} [\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}} + \Delta\gamma (2p - p_c)] = 2p - p_c = \frac{\partial f}{\partial p} \end{aligned}$$

Require: $\underline{\mathbf{x}}^0$

$k \leftarrow 0$

while $\underline{\mathbf{r}}(\underline{\mathbf{x}}^k) \neq 0$ **do**

$$\underline{\mathbf{x}}^{k+1} \leftarrow \underline{\mathbf{x}}^k - \left[\left(\frac{\partial \underline{\mathbf{r}}}{\partial \underline{\mathbf{x}}} \right)^{-1} \right]_{\underline{\mathbf{x}}^k} \cdot \underline{\mathbf{r}}(\underline{\mathbf{x}}^k)$$

$k \leftarrow k + 1$

end while

where

$$\begin{aligned} \frac{\partial p}{\partial \varepsilon_v^e} &= -\frac{p_0 \beta}{\widetilde{\kappa}} \exp \left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\widetilde{\kappa}} \right] = \frac{p}{\widetilde{\kappa}} \quad , \quad \frac{\partial p_c}{\partial \varepsilon_v^e} = \frac{(p_c)_n}{\widetilde{\kappa} - \widetilde{\lambda}} \exp \left[\frac{\varepsilon_v^e - (\varepsilon_v^e)_{\text{trial}}}{\widetilde{\kappa} - \widetilde{\lambda}} \right] \quad \text{and} \\ \frac{\partial p}{\partial \varepsilon_s^e} &= \frac{3 p_0 \alpha \varepsilon_s^e}{\widetilde{\kappa}} \exp \left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\widetilde{\kappa}} \right]. \end{aligned}$$

For the second row,

$$\begin{aligned} \frac{\partial r_2}{\partial x_1} &= \frac{\partial}{\partial \varepsilon_v^e} \left[\varepsilon_s^e - (\varepsilon_s^e)_{\text{trial}} + \Delta \gamma \frac{2q}{M^2} \right] = \frac{2\Delta \gamma}{M^2} \frac{\partial q}{\partial \varepsilon_v^e} \\ \frac{\partial r_2}{\partial x_2} &= \frac{\partial}{\partial \varepsilon_s^e} \left[\varepsilon_s^e - (\varepsilon_s^e)_{\text{trial}} + \Delta \gamma \frac{2q}{M^2} \right] = 1 + \frac{2\Delta \gamma}{M^2} \frac{\partial q}{\partial \varepsilon_s^e} \\ \frac{\partial r_2}{\partial x_3} &= \frac{\partial}{\partial \Delta \gamma} \left[\varepsilon_s^e - (\varepsilon_s^e)_{\text{trial}} + \Delta \gamma \frac{2q}{M^2} \right] = \frac{2q}{M^2} = \frac{\partial f}{\partial q} \end{aligned}$$

where

$$\frac{\partial q}{\partial \varepsilon_v^e} = -\frac{3p_0 \alpha \varepsilon_s^e}{\widetilde{\kappa}} \exp \left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\widetilde{\kappa}} \right] = \frac{\partial p}{\partial \varepsilon_s^e} \quad \text{and} \quad \frac{\partial q}{\partial \varepsilon_s^e} = 3\mu_0 + 3p_0 \alpha \exp \left[-\frac{\varepsilon_v^e - \varepsilon_{v0}^e}{\widetilde{\kappa}} \right] = 3\mu.$$

For the third row,

$$\begin{aligned} \frac{\partial r_3}{\partial x_1} &= \frac{\partial}{\partial \varepsilon_v^e} \left[\frac{q^2}{M^2} + p(p - p_c) \right] = \frac{2q}{M^2} \frac{\partial q}{\partial \varepsilon_v^e} + (2p - p_c) \frac{\partial p}{\partial \varepsilon_v^e} - p \frac{\partial p_c}{\partial \varepsilon_v^e} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial \varepsilon_v^e} + \frac{\partial f}{\partial p} \frac{\partial p}{\partial \varepsilon_v^e} - p \frac{\partial p_c}{\partial \varepsilon_v^e} \\ \frac{\partial r_3}{\partial x_2} &= \frac{\partial}{\partial \varepsilon_s^e} \left[\frac{q^2}{M^2} + p(p - p_c) \right] = \frac{2q}{M^2} \frac{\partial q}{\partial \varepsilon_s^e} + (2p - p_c) \frac{\partial p}{\partial \varepsilon_s^e} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial \varepsilon_s^e} + \frac{\partial f}{\partial p} \frac{\partial p}{\partial \varepsilon_s^e} \\ \frac{\partial r_3}{\partial x_3} &= \frac{\partial}{\partial \Delta \gamma} \left[\frac{q^2}{M^2} + p(p - p_c) \right] = 0. \end{aligned}$$

We have to invert a matrix in the Newton iteration process. Let us see whether we can make this quicker to do. The Jacobian matrix has the form

$$\frac{\partial \underline{\mathbf{r}}}{\partial \underline{\mathbf{x}}} = \begin{bmatrix} \frac{\partial r_1}{\partial x_1} & \frac{\partial r_1}{\partial x_2} & \frac{\partial r_1}{\partial x_3} \\ \frac{\partial r_2}{\partial x_1} & \frac{\partial r_2}{\partial x_2} & \frac{\partial r_2}{\partial x_3} \\ \frac{\partial r_3}{\partial x_1} & \frac{\partial r_3}{\partial x_2} & \frac{\partial r_3}{\partial x_3} \end{bmatrix} = \begin{bmatrix} \underline{\mathbf{A}} & \underline{\mathbf{B}} \\ \underline{\mathbf{C}} & 0 \end{bmatrix}$$

where

$$\underline{\mathbf{A}} = \begin{bmatrix} \frac{\partial r_1}{\partial x_1} & \frac{\partial r_1}{\partial x_2} \\ \frac{\partial r_2}{\partial x_1} & \frac{\partial r_2}{\partial x_2} \end{bmatrix}, \quad \underline{\mathbf{B}} = \begin{bmatrix} \frac{\partial r_1}{\partial x_3} \\ \frac{\partial r_2}{\partial x_3} \end{bmatrix}, \quad \text{and} \quad \underline{\mathbf{C}} = \begin{bmatrix} \frac{\partial r_3}{\partial x_1} & \frac{\partial r_3}{\partial x_2} \end{bmatrix}.$$

We can also break up the $\underline{\mathbf{x}}$ and $\underline{\mathbf{r}}$ matrices:

$$\Delta \underline{\mathbf{x}} = \underline{\mathbf{x}}^{k+1} - \underline{\mathbf{x}}^k = \begin{bmatrix} \Delta \underline{\mathbf{x}}^{vs} \\ \Delta x_3 \end{bmatrix}, \quad \underline{\mathbf{r}} = \begin{bmatrix} \underline{\mathbf{r}}^{vs} \\ r_3 \end{bmatrix} \quad \text{where} \quad \underline{\mathbf{r}}^{vs} = \begin{bmatrix} r_1 \\ r_2 \end{bmatrix} \quad \text{and} \quad \Delta \underline{\mathbf{x}}^{vs} = \begin{bmatrix} \Delta x_1 \\ \Delta x_2 \end{bmatrix}.$$

Then

$$\begin{bmatrix} \Delta \underline{\mathbf{x}}^{vs} \\ \Delta x_3 \end{bmatrix} = - \begin{bmatrix} \underline{\mathbf{A}} & \underline{\mathbf{B}} \\ \underline{\mathbf{C}} & 0 \end{bmatrix}^{-1} \begin{bmatrix} \underline{\mathbf{r}}^{vs} \\ r_3 \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} \underline{\mathbf{A}} & \underline{\mathbf{B}} \\ \underline{\mathbf{C}} & 0 \end{bmatrix} \begin{bmatrix} \Delta \underline{\mathbf{x}}^{vs} \\ \Delta x_3 \end{bmatrix} = - \begin{bmatrix} \underline{\mathbf{r}}^{vs} \\ r_3 \end{bmatrix}$$

or

$$\underline{\underline{\mathbf{A}}} \Delta \underline{\underline{\mathbf{x}}}^{vs} + \underline{\underline{\mathbf{B}}} \Delta x_3 = -\underline{\underline{\mathbf{r}}}^{vs} \quad \text{and} \quad \underline{\underline{\mathbf{C}}} \Delta \underline{\underline{\mathbf{x}}}^{vs} = -r_3.$$

From the first equation above,

$$\Delta \underline{\underline{\mathbf{x}}}^{vs} = -\underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{r}}}^{vs} - \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{B}}} \Delta x_3.$$

Plugging in the second equation gives

$$r_3 = \underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{r}}}^{vs} + \underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{B}}} \Delta x_3.$$

Rearranging,

$$\Delta x_3 = x_3^{k+1} - x_3^k = \frac{-\underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{r}}}^{vs} + r_3}{\underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{B}}}}.$$

Using the above result,

$$\Delta \underline{\underline{\mathbf{x}}}^{vs} = -\underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{r}}}^{vs} - \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{B}}} \left(\frac{-\underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{r}}}^{vs} + r_3}{\underline{\underline{\mathbf{C}}} \underline{\underline{\mathbf{A}}}^{-1} \underline{\underline{\mathbf{B}}}} \right).$$

We therefore have to invert only a 2×2 matrix.

3.3 Tangent calculation: elastic

We want to find the derivative of the stress with respect to the strain:

$$\frac{\partial \sigma}{\partial \epsilon} = \mathbf{1} \otimes \frac{\partial p}{\partial \epsilon} + \sqrt{\frac{2}{3}} \mathbf{n} \otimes \frac{\partial q}{\partial \epsilon} + \sqrt{\frac{2}{3}} q \frac{\partial \mathbf{n}}{\partial \epsilon}. \quad (3)$$

For the first term above,

$$\frac{\partial p}{\partial \epsilon} = p_0 \exp \left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}} \right] \frac{\partial \beta}{\partial \epsilon} - p_0 \frac{\beta}{\bar{\kappa}} \exp \left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}} \right] \frac{\partial \epsilon_v^e}{\partial \epsilon} = p_0 \exp \left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}} \right] \left(\frac{\partial \beta}{\partial \epsilon} - \frac{\beta}{\bar{\kappa}} \frac{\partial \epsilon_v^e}{\partial \epsilon} \right).$$

Now,

$$\frac{\partial \beta}{\partial \epsilon} = \frac{3\alpha}{\bar{\kappa}} \epsilon_s^e \frac{\partial \epsilon_s^e}{\partial \epsilon}.$$

Therefore,

$$\frac{\partial p}{\partial \epsilon} = \frac{p_0}{\bar{\kappa}} \exp \left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}} \right] \left(3\alpha \epsilon_s^e \frac{\partial \epsilon_s^e}{\partial \epsilon} - \beta \frac{\partial \epsilon_v^e}{\partial \epsilon} \right).$$

We now have to figure out the other derivatives in the above expression. First,

$$\frac{\partial \epsilon_s^e}{\partial \epsilon} = \sqrt{\frac{2}{3}} \frac{1}{\sqrt{e^e : e^e}} \frac{\partial e^e}{\partial \epsilon} : e^e = \sqrt{\frac{2}{3}} \frac{1}{\|e^e\|} \left(\frac{\partial \epsilon^e}{\partial \epsilon} - \frac{1}{3} \mathbf{1} \otimes \frac{\partial \epsilon_v^e}{\partial \epsilon} \right) : e^e.$$

For the special situation where all the strain is elastic, $\epsilon = \epsilon^e$, and (see Wikipedia article on tensor derivatives)

$$\frac{\partial \epsilon^e}{\partial \epsilon} = \frac{\partial \epsilon}{\partial \epsilon} = \mathbf{I}^{(s)} \quad \text{and} \quad \frac{\partial \epsilon_v^e}{\partial \epsilon} = \frac{\partial \epsilon_v}{\partial \epsilon} = \mathbf{1}.$$

That gives us

$$\frac{\partial \epsilon_s^e}{\partial \epsilon} = \sqrt{\frac{2}{3}} \frac{1}{\|e^e\|} \left(\mathbf{I}^{(s)} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} \right) : e^e = \sqrt{\frac{2}{3}} \frac{1}{\|e^e\|} \left[e^e - \frac{1}{3} \text{tr}(e^e) \mathbf{1} \right].$$

But $\text{tr}(e^e) = 0$ because this is the deviatoric part of the strain and we have

$$\boxed{\frac{\partial \epsilon_s^e}{\partial \epsilon} = \sqrt{\frac{2}{3}} \frac{e^e}{\|e^e\|} = \sqrt{\frac{2}{3}} \mathbf{n}} \quad \text{and} \quad \boxed{\frac{\partial \epsilon_v^e}{\partial \epsilon} = \mathbf{1}}.$$

Using these, we get

$$\frac{\partial p}{\partial \epsilon} = \frac{p_0}{\bar{\kappa}} \exp \left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}} \right] \left(\sqrt{6} \alpha \epsilon_s^e \mathbf{n} - \beta \mathbf{1} \right). \quad (4)$$

The derivative of q with respect to ϵ can be calculated in a similar way, i.e.,

$$\frac{\partial q}{\partial \epsilon} = 3\mu \frac{\partial \epsilon_s^e}{\partial \epsilon} + 3\epsilon_s^e \frac{\partial \mu}{\partial \epsilon} = 3\mu \frac{\partial \epsilon_s^e}{\partial \epsilon} - 3\frac{p_0}{\bar{\kappa}} \alpha \epsilon_s^e \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] \frac{\partial \epsilon_v^e}{\partial \epsilon}.$$

Using the expressions in the boxes above,

$$\frac{\partial q}{\partial \epsilon} = \sqrt{6}\mu n - 3\frac{p_0}{\bar{\kappa}} \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] \alpha \epsilon_s^e \mathbf{1}. \quad (5)$$

Also,

$$\frac{\partial n}{\partial \epsilon} = \sqrt{\frac{2}{3}} \left[\frac{1}{\epsilon_s^e} \frac{\partial \mathbf{e}^e}{\partial \epsilon} - \frac{1}{(\epsilon_s^e)^2} \mathbf{e}^e \otimes \frac{\partial \epsilon_s^e}{\partial \epsilon} \right].$$

Using the previously derived expression, we have

$$\frac{\partial n}{\partial \epsilon} = \sqrt{\frac{2}{3}} \frac{1}{\epsilon_s^e} \left[\mathbf{I}^{(s)} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} - \sqrt{\frac{2}{3}} \frac{1}{\epsilon_s^e} \frac{\mathbf{e}^e \otimes \mathbf{e}^e}{\|\mathbf{e}^e\|} \right]$$

or

$$\frac{\partial n}{\partial \epsilon} = \sqrt{\frac{2}{3}} \frac{1}{\epsilon_s^e} \left[\mathbf{I}^{(s)} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} - n \otimes n \right]. \quad (6)$$

Plugging the expressions for these derivatives in the original equation, we get

$$\begin{aligned} \frac{\partial \sigma}{\partial \epsilon} = & \frac{p_0}{\bar{\kappa}} \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] \left(\sqrt{6} \alpha \epsilon_s^e \mathbf{1} \otimes n - \beta \mathbf{1} \otimes \mathbf{1} \right) + 2\mu n \otimes n - \sqrt{6} \frac{p_0}{\bar{\kappa}} \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] \alpha \epsilon_s^e n \otimes \mathbf{1} + \\ & \frac{2}{3} \frac{q}{\epsilon_s^e} \left[\mathbf{I}^{(s)} - \frac{1}{3} \mathbf{1} \otimes \mathbf{1} - n \otimes n \right]. \end{aligned}$$

Reorganizing,

$$\begin{aligned} \frac{\partial \sigma}{\partial \epsilon} = & \frac{\sqrt{6} p_0 \alpha \epsilon_s^e}{\bar{\kappa}} \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] (\mathbf{1} \otimes n + n \otimes \mathbf{1}) - \left(\frac{p_0 \beta}{\bar{\kappa}} \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] + \frac{2}{9} \frac{q}{\epsilon_s^e} \right) \mathbf{1} \otimes \mathbf{1} + \\ & 2 \left(\mu - \frac{1}{3} \frac{q}{\epsilon_s^e} \right) n \otimes n + \frac{2}{3} \frac{q}{\epsilon_s^e} \mathbf{I}^{(s)}. \end{aligned} \quad (7)$$

3.4 Tangent calculation: elastic-plastic

From the previous section recall that

$$\frac{\partial \sigma}{\partial \epsilon} = \mathbf{1} \otimes \frac{\partial p}{\partial \epsilon} + \sqrt{\frac{2}{3}} n \otimes \frac{\partial q}{\partial \epsilon} + \sqrt{\frac{2}{3}} q \frac{\partial n}{\partial \epsilon}$$

where

$$\begin{aligned} \frac{\partial p}{\partial \epsilon} = & \frac{p_0}{\bar{\kappa}} \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] \left(3\alpha \epsilon_s^e \frac{\partial \epsilon_s^e}{\partial \epsilon} - \beta \frac{\partial \epsilon_v^e}{\partial \epsilon} \right), \quad \frac{\partial q}{\partial \epsilon} = 3\mu \frac{\partial \epsilon_s^e}{\partial \epsilon} - 3\frac{p_0}{\bar{\kappa}} \alpha \epsilon_s^e \exp\left[-\frac{\epsilon_v^e - \epsilon_{v0}^e}{\bar{\kappa}}\right] \frac{\partial \epsilon_v^e}{\partial \epsilon} \quad \text{and} \\ \frac{\partial n}{\partial \epsilon} = & \sqrt{\frac{2}{3}} \left[\frac{1}{\epsilon_s^e} \frac{\partial \mathbf{e}^e}{\partial \epsilon} - \frac{1}{(\epsilon_s^e)^2} \mathbf{e}^e \otimes \frac{\partial \epsilon_s^e}{\partial \epsilon} \right]. \end{aligned}$$

The total strain is equal to the elastic strain for the purely elastic case and the tangent is relatively straightforward to calculate. For the elastic-plastic case we have

$$\epsilon_{n+1}^e = \epsilon_{\text{trial}}^e - \Delta\gamma \left[\frac{\partial f}{\partial \sigma} \right]_{n+1}.$$

Dropping the subscript $n + 1$ for convenience, we have

$$\frac{\partial \epsilon^e}{\partial \epsilon} = \frac{\partial \epsilon_{\text{trial}}^e}{\partial \epsilon} - \frac{\partial f}{\partial \sigma} \otimes \frac{\partial \Delta\gamma}{\partial \epsilon} - \Delta\gamma \frac{\partial}{\partial \epsilon} \left[\frac{\partial f}{\partial \sigma} \right] = \mathbf{I}^{(s)} - \left[\frac{2p - p_c}{3} \mathbf{1} + \sqrt{\frac{2}{3}} \frac{2q}{M^2} n \right] \otimes \frac{\partial \Delta\gamma}{\partial \epsilon} - \Delta\gamma \frac{\partial}{\partial \epsilon} \left[\frac{2p - p_c}{3} \mathbf{1} + \sqrt{\frac{2}{3}} \frac{2q}{M^2} n \right].$$