Gradient Plasticity Modeling of Geomaterials in a Meshfree Environment

Majid T. Manzari* and Richard A. Regueiro+

*CEE Department, George Washington University
801 22nd Street, NW Washington, DC 20052.
manzari@gwu.edu

+Science Based Materials Modeling Department, Sandia National Laboratories
P.O. Box 969, MS 9405, Livermore, CA  94551-0969
raregue@sandia.gov

Abstract
Deformation and strength behavior of geomaterials in the pre- and post-failure regimes are of significant interest in various geomechanics applications. To address the need for development of a realistic constitutive framework, which allows for an accurate simulation of pre-failure response as well as an objective and meaningful post-failure response, a strain gradient plasticity model is formulated by incorporating the gradients of volumetric and deviatoric plastic strains on the evolution of damage in geomaterials. The resulting constitutive equations along with the balance of linear momentum for the continuum are cast into a coupled system of equations, with displacements and plastic multiplier appearing as the primary unknowns in the final governing integral equations. A finite element discretization of the governing equations requires the use of C-1 continuous elements, which are undesirable from an implementation point of view. This issue is naturally resolved when a meshfree discretization is used. Hence the developed model is formulated within the framework of a meshfree environment. The new constitutive model allows a thorough analysis of grain size effects on strength and dilatancy of rocks. The role and effectiveness of the new gradient terms on regularizing the underlying boundary value problems of geomechanics beyond the initiation of strain localization can also be assessed.

1. Introduction

With the ever-increasing speed of computers, significant advancements in numerical methods, and development of physically-based models of engineering materials in the past three decades, increasingly challenging problems of mechanics are now being tackled by the computational mechanics community. Among these challenging problems, the unified modeling of pre-failure deformations and post-failure response remains to be a highly desirable goal. As far as geomaterials are concerned, highly sophisticated and realistic constitutive models are now available. Many of these models are capable of providing accurate modeling of the pre-failure response. In many cases, these constitutive models also include useful ingredients for modeling material softening. However, since the unstable nature of softening leads to localization of strain, the initially local response of the material ceases to exit in the post localization regime and this
requires an account of the localized response, which is not possible with a local constitutive model. In the past few years, various techniques have been used to address this issue. Three of the most prominent techniques are: 1) the weak discontinuity approach via an enhanced finite element (Ortiz et al., 1987), 2) the strong discontinuity approach which allows a finite element with displacement discontinuity (Simo et al., 1993; Regueiro and Borja, 2001), and 3) a higher order continuum where nonlocal measures of stress or strain are used in the formulation of the constitutive law or a micropolar continuum that involves couple-stresses and rotations in addition to standard Cauchy stress tensor and the displacement vector. The first method has been used by several investigators (Ortiz et al, 1987) and has shown limited success in geomechanics problems (Manzari and Nour, 2000). The strong discontinuity approach has great potential in producing mesh-independent solutions and is being explored beyond classical constitutive models such as Von-Mises or Drucker-Prager plasticity models (Regueiro and Borja, 2001). Among nonlocal approaches, micropolar theory (Cosserat and Cosserat, 1909; Mindlin and Tiersten, 1963; Mindlin, 1964) provides an excellent means for considering scale effects and has successfully been used in the analysis of geotechnical systems undergoing severe shear localization (e.g., Manzari, 2004). However the use of micropolar theory is limited to the cases in which shear is the dominated mode of failure. Since pioneering work of Aifantis (1987) the strain gradient plasticity approach has received significant attention in recent years and it is being pursued by researchers in several fields of engineering mechanics because of its versatility in handling post failure conditions, particularly when tensile failure is involved. In addition to significant number of additional primary variables, another major drawback of the gradient plasticity approach is the need for C-1 continuity in the formulation of a finite element solution. This has been a significant impediment to further development of the method for application in realistic engineering problems. In a meshfree formulation, however, the C-1 continuity requirement does not pose a severe restriction on the shape functions as they naturally provide high order continuity. This unique feature of the meshfree environment is employed in this work to develop a realistic strain gradient plasticity model for geomaterials. An outline of the model and the meshfree formulation are discussed in the following sections.

2. A Two-Parameter Gradient Elastoplastic Model

2.1. Motivation
Pressure sensitivity and shear-induced dilatation are two important properties of soils, rocks, and almost all geomaterials and should carefully be addressed in a realistic constitutive model for geomaterials. Hence, when formulating a plasticity constitutive model for soils and rocks, at a minimum, two stress-invariants ($I$ and $\sqrt{J_2}$) are required in the mathematical structure. Moreover, while pressure sensitivity is a direct consequence of the presence of pore space (voids) in geomaterials, shear-induced dilatation is caused by interaction of grains over a characteristic length that is related to the average grain size. In soils, the average size of voids is usually well correlated with the average grain size. However in crystalline rocks, presence of pre-existing fissures, defects, and “foreign particles” inclusions may cause the overall compressibility to be identified with an average pore size (the pore size scale) that is different from the average grain size.
While the pore size scale is expected to affect the compressibility of the material, grain size scale would significantly influence shear-induced dilatation.

Motivated by the aforementioned difference between grain size scale and pore space scale and considering the difference between the volume change due to confining stress and the volume change due to shear, here we adopt a two-parameter gradient model for both elastic and plastic responses of the material. The first parameter is to mimic the pore space length scale, which affects the volume change of the first type \( l_v^e \), \( l_v^p \). The second parameter is to model the grain size length scale and its effect on shear resistance and shear induced dilatation \( l_s^e, l_s^p \).

2.2. Elastic Response
Motivated by the gradient elasticity theory proposed by Vardoulakis et al. (1996), a two-parameter gradient elasticity model is adopted here. In soils, it has been observed that shear modulus varies with mean effective stress. However, constant shear modulus is acceptable in rocks. Here we adopt a constant bulk and shear modulus.

\[
\begin{align*}
\dot{p} &= K(\varepsilon^e_v - l_v^2 \nabla^2 \varepsilon^e_v) \\
\dot{s} &= 2G(\varepsilon^e_s - l_s^2 \nabla^2 \varepsilon^e_s)
\end{align*}
\]

Equations (1) can be written as

\[
\dot{\sigma} = \mathbf{C} : \dot{\varepsilon} - \mathbf{C}^* : \nabla^2 \dot{\varepsilon}
\]

where

\[
\mathbf{C} = \lambda \mathbf{1} \otimes \mathbf{1} + 2G \mathbf{1} \\
\mathbf{C}^* = \lambda^* \mathbf{1} \otimes \mathbf{1} + 2G^* \mathbf{1}
\]

in which \( \mathbf{1} \) is the second order unit tensor and \( \mathbf{I} \) is the fourth order unit tensor and

\[
\lambda = K - \frac{2}{3} G; \quad \lambda^* = K^* - \frac{2}{3} G^* \\
G^* = l_s^2 G; \quad K^* = l_s^2 K
\]

In the above equations, length scales \( l_v^e \) and \( l_s^e \) relate to the volumetric and shear response of the material, respectively. This leads to a modified tensor of elastic moduli as shown in Eqn. 2.
2.3. Yield Function

Yield function is defined as

\[ f(\sigma, q) = \sqrt{\tau^2 + (c - \chi \tan \phi)^2} - (c - p \tan \phi) \]  

(6)

where:

\[ \tau = \left( \frac{1}{2} s : s \right)^{1/2}, \quad s = \sigma - \frac{1}{3} p I; \quad p = \frac{1}{3} \sigma_{ii} \]  

(7)

and \( q \) is a collection of four internal variables: \( \chi, c, \phi, \) and \( \psi \) which respectively represent tensile strength of the material, cohesion, friction angle, and dilation angle.

\[ q = \langle \chi, c \tan \phi, \tan \psi \rangle^T \]  

(8)

2.4. Flow Rule

Magnitude and direction of plastic deformations are described by a non-associative flow rule:

\[ \dot{\varepsilon} = \dot{\lambda} \frac{\partial Q}{\partial \sigma} = \dot{\lambda} m \]  

(9)

where \( \dot{\lambda} \) is known as plastic multiplier and \( Q \) is the plastic potential defined as follows:

\[ Q(\sigma, q) = \sqrt{\tau^2 + (c - \chi \tan \psi)^2} - (c - p \tan \psi) \]  

(10)

2.5. Hardening laws

The key feature of this constitutive model is the presence of gradient of plastic multiplier in the hardening law defining the evolution of internal variables, \( q \).

\[ q = \dot{\lambda} h(\sigma, q, m) - \nabla^2 \dot{\lambda} g(\sigma, q, m) \]  

(11)

where \( h \) and \( g \) are chosen to be of the following forms:

\[ h = \begin{bmatrix} h_\chi \\ h_c \\ h_\phi \\ h_\psi \end{bmatrix} = \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \\ 0 & A_3 \\ 0 & A_4 \end{bmatrix} \begin{bmatrix} B_1 & B_2 \\ 0 & B_3 \end{bmatrix} \begin{bmatrix} 1 - \int^p \nabla^2 \frac{\partial Q}{\partial \sigma} \\ 1 - \int^p \nabla^2 \frac{\partial Q}{\partial s} \end{bmatrix} \]  

(12)

and
\[
g = \begin{bmatrix}
g_{\chi} \\
g_{c} \\
g_{\phi} \\
g_{y}
\end{bmatrix} =
\begin{bmatrix}
A_1 & 0 \\
0 & A_2 \\
0 & A_3 \\
0 & A_4
\end{bmatrix}
\begin{bmatrix}
B_1^* \\
B_2^* \\
B_3^*
\end{bmatrix}
\begin{bmatrix}
\frac{\partial Q}{\partial p} \\
\frac{\partial Q}{\partial s}
\end{bmatrix}
\] (13)

in which:
\[
A_1 = -\alpha_{x}(\chi - \chi_r); \quad A_2 = -\alpha_{c}(c - c_r) \\
A_3 = -\alpha_{\phi}(\tan \phi - \tan \phi_r); \quad A_4 = -\alpha_{\psi}\tan \psi
\] (14)

where \(\chi_r, \ c_r, \ \phi_r\) are residual values of \(\chi, \ c, \ \phi\) as a steady state response is attained in shear loading. Parameters \(\alpha_{x}, \ \alpha_{c}, \ \alpha_{\phi}, \ \text{and} \ \alpha_{\psi}\) are model constants that allow the pace of variation of internal variables \(\chi, \ c, \ \phi, \ \text{and} \ \psi\) to be set as desired. Variable \(B_1\) and matrices \(B_2, B_3, \text{and} \ \mathbf{B}^*_2, \text{and} \ \mathbf{B}^*_3\) are defined as:
\[
B_1^* = l^p_2 B_1 = l^p_2 \frac{p}{G_f'} \\
B_2^* = l^p_2 B_2 = l^p_2 \frac{s}{G_f'}; \quad B_3^* = l^p_2 B_3 = l^p_2 \frac{s}{G''_f}
\] (15)
in which \(G_f'\) and \(G''_f\) are the fracture energy corresponding to mode I (tensile) and Mode II (shear) failure, respectively.

3. Integration of Constitutive Equations and its Relationship with Global Solution

Given the presence of gradient of plastic multiplier \((\nabla^2 \lambda)\) in the hardening law (Eqn. 11), the consistency condition \((\dot{f} = 0)\) leads to a differential equation in terms of plastic multiplier \(\dot{\lambda}\). Hence a closed form solution for \(\dot{\lambda}\) does not exit and the consistency condition should be enforced in a weak sense and can be solved simultaneously with an integral form of the equation of linear momentum. To this end, a variational form of the aforementioned equations at step \(n+1\) \((t_{n+1})\) of the incremental solution can be written as follows:

\[
\mathcal{A}_{n+1} = \int_{\Omega} \nabla^\prime \mathbf{w} : \mathbf{\sigma} \ d\Omega - \int_{\Omega} \mathbf{w} \cdot \mathbf{b} \ d\Omega - \int_{\Gamma_s} \mathbf{w} \cdot \mathbf{t} \ d\Omega = 0
\]

\[
\mathcal{F}_{n+1} = \int_{\Omega} \eta f \ d\Omega = 0
\] (16)

where \(\mathbf{w} = \delta \mathbf{u}\) and \(\eta = \delta \lambda\), with the appropriate boundary conditions imposed on \(\mathbf{u}\) and \(\lambda\). It should be noted that defining appropriate boundary conditions for \(\lambda\) is still an open research problem. To proceed further, we need to determine the stress tensor, \(\mathbf{\sigma}\), and the
vector of internal variables, $q$, at $t_{n+1}$. This is achieved by using a backward Euler integration scheme. Equations 2 and 9 can be combined to obtain

$$
\dot{\sigma} = C : \ddot{\varepsilon}^e - C^e : \nabla^2 \dot{\varepsilon}^e = \\
C : \dot{\mathbf{e}} - \dot{\mathbf{C}} : \mathbf{m} - C^e : \nabla^2 \dot{\varepsilon} + C^e : \mathbf{m} \nabla^2 \dot{\lambda}
$$

(17)

Now given the converged values of $\sigma$ and $q$ from the previous time step ($t_n$), we can write:

$$
\sigma = \sigma_n + C : \Delta \varepsilon - \Delta \lambda C : \mathbf{m} - C^e : \nabla^2 (\Delta \varepsilon) + \nabla^2 (\Delta \lambda) C^e : \mathbf{m} \\
q = q_n + \Delta \lambda h - \nabla^2 (\Delta \lambda) g
$$

(18)

Equations (16) and (18) are used a two-step iterative solution leading to the determination of $u$ and $\lambda$ at the current time step and the update of stress tensor and internal variables. First, nonlinear equations (16) are solved for nodal values of $u$ and $\lambda$. Then using the nodal values of $u$ and $\lambda$, updated values of $\sigma$ and $q$ are determined from the backward Euler integration calculations conducted at each integration point.

4. Meshfree Formulation

In the meshfree formulation, we use the following interpolation functions for $u$ and $\lambda$:

$$
u^h = \Psi^h_I U_I \quad (I = 1 : N_p^u)$$
$$\lambda^h = \Psi^h_I \Gamma_I \quad (I = 1 : N_p^\lambda)
$$

(19)

where $N_p^u$ and $N_p^\lambda$ are, respectively, the number of nodal points that are used in interpolation of $u$ and $\lambda$. Using Equation (19) we find:

$$
\varepsilon^h = B^h_I U_I; \quad \nabla^2 \varepsilon^h = B^h_I \Gamma_I; \quad \nabla^2 \lambda^h = B^h_I \Gamma_I
$$

(20)

Similarly

$$
w^h = \Psi^h_J W_J; \quad \nabla^* w^h = B^h_J W_J; \quad \eta^h = \Psi^h_J H_J
$$

(21)

Substituting in the linearized form of Equations (16) leads to:

$$
W_J : \{F^h_J + K_{uum} \delta U_I + K_{um}^{ij} \delta \Gamma_I \} = 0 \\
H_J : \{F^h_J + K_{uum} \delta U_I + K_{um}^{ij} \delta \Gamma_I \} = 0
$$

(22)

Summing over all particles, we find:
In the incremental solution, using the solution of Eqn. 23, \( \delta d = \left\{ \delta U \right\} \), solution at iteration \( k+1 \) is obtained as \( \delta d^{k+1} = \delta d^k + \delta d \). We will then check for convergence of the global solution by computing the residuals defined in Eqn. (16) and comparing them to a desirable tolerance.

Matrices and vectors in Eqn. (23) are given below:

\[
\begin{bmatrix}
K^{uu} & K^{u\lambda} \\
K^{\lambda u} & K^{\lambda\lambda}
\end{bmatrix}
\left\{ \delta U \right\} = -\left\{ F^{u} \right\}
\]  

\[\text{(23)}\]

\( F^{u}_j = \int_{\Omega^h} (B^j)^T \sigma(d^k) \, d\Omega - \int_{\Omega^h} \Psi^j \, b \, d\Omega - \int_{\Omega^h} \Psi^j \, t \, d\Omega \) \hspace{1cm} \[\text{(24-a)}\]

\( F^{\lambda}_j = \int_{\Omega^h} \Psi^{\lambda}_j \, f \, (d^k) \, d\Omega \) \hspace{1cm} \[\text{(24-b)}\]

\( K^{uu}_{ji} = \int_{\Omega^h} (B^j)^T \, k^u_i \, d\Omega; \quad k^u_i = B^{-1}(C : B^j - C' : B^j) \) \hspace{1cm} \[\text{(24-c)}\]

\( K^{u\lambda}_{ji} = \int_{\Omega^h} (B^j)^T \, k^{\lambda}_i \, d\Omega; \) \hspace{1cm} \[\text{(24-d)}\]

\( K^{\lambda u}_{ji} = \int_{\Omega^h} B^j \cdot k^u_i \, d\Omega; \quad B^j = \Psi^j (\frac{df}{d\sigma} + \frac{df}{d\gamma} \, a) \) \hspace{1cm} \[\text{(24-e)}\]

\( K^{\lambda\lambda}_{ji} = \int_{\Omega^h} B^j \cdot k^{\lambda}_i \, d\Omega \) \hspace{1cm} \[\text{(24-f)}\]

The following matrices are used in Eqn. (24):

\( k^u_i = B^{-1}(-C : m \Psi^u_j - C' : m B^j) \)

\( -(\Delta \lambda C - \nabla^2 (\Delta \lambda) C') : \frac{\partial m}{\partial q} \cdot A^{-1}.(h \Psi^u_j - g B^j) \) \hspace{1cm} \[\text{(25-a)}\]

\( A = 1 - \Delta \lambda \bigg( \frac{\partial h}{\partial q} \cdot \frac{\partial m}{\partial q} + \nabla^2 (\Delta \lambda) \frac{\partial g}{\partial q} \bigg) \) \hspace{1cm} \[\text{(25-b)}\]

\( a = A^{-1} \left[ (\Delta \lambda \bigg( \frac{\partial h}{\partial \sigma} \cdot \frac{\partial m}{\partial \sigma} + \nabla^2 (\Delta \lambda) \frac{\partial g}{\partial \sigma} \bigg) \right] \) \hspace{1cm} \[\text{(25-c)}\]

\( B = I + (\Delta \lambda C - \nabla^2 (\Delta \lambda) C') : \bigg( \frac{\partial m}{\partial \sigma} + \frac{\partial m}{\partial q} \cdot a \bigg) \) \hspace{1cm} \[\text{(25-d)}\]

5. Concluding Remarks

Based on the characteristic behavior of geomaterials, particularly rocks, it is argued that it is necessary to account for the distinct roles of pre-existing fissures, distributed pore space, and grain size in compressibility and shear-induced dilatation of geomaterials. Hence, a two-parameter gradient plasticity model for geomaterials is formulated. This
amounts to introduction of two different length scales: one for volume change behavior and one for shear deformations. Integration of the constitutive model and details of the global formulation in a meshfree environment are discussed. The meshfree formulation is particularly suitable due to its flexibility in accommodating derivatives of higher order. Numerical simulations demonstrating the performance of the formulation presented in this paper are the subject of authors’ current research and will be the subject of forthcoming publications.

6. References