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Multiphysics implementation of advanced soil mechanics models

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ABSTRACT

Using multiphysics computer codes has become a useful tool to solve systems of partial differential equations. However, these codes do not always allow for the free introduction of implicitly defined state functions when automatic differentiation is used to compute the iteration matrix. This makes it considerably more difficult to solve geomechanical problems using non-linear constitutive models. This paper proposes a method for overcoming this difficulty based on multiphysics capabilities. The implementation of the well-known Barcelona basic model is described to illustrate the application of the method. For this purpose, without including formulation details addressed by other authors, the fundamentals of its implementation in a finite element code are described. Examples that demonstrate the scope of the proposed methodology are also presented.

1. Introduction

In recent years, the application of numerical methods, particularly the finite element method (FEM), for solving boundary problems in soil mechanics has grown considerably, as illustrated by the high quality and large number of published papers on the subject. Among the noteworthy contributions to this area of research are those by Potts and Gens [1], Potts and Zdravkovic [2], Sheng et al. [3], Sheng et al. [4], Sheng et al. [5], Borja [6] and Gens and Potts [7]. The algorithms they propose have been implemented both in FEM codes developed primarily for research purposes [see 8,9 and 10] and in commercial FEM software [see, among others, 11–13], which include modules that facilitate the simulation of the behaviour of a large number of geotechnical structures (e.g., embankments and cuts, earth dams, retaining walls, slopes, tunnels and foundations).

The use of Multiphysics Partial Differential Equation Solvers (MPDES) emerges as a useful tool for the numerical solution of geotechnical problems [14]. With this class of solvers, the user defines the governing equations and models for the behaviour of the system. The code takes automatic control of assembling and solving the system of equations without it being necessary to redefine the memory storage structures or to implement the algorithms for its solution. The user focuses on the physics of the problem, which allows for the coupling of almost any physical or chemical process that could be described through Partial Differential Equations (PDEs). This coupling ability is one of the main advantages of MPDES. In addition, some MPDES include specific stress–strain models for geomaterials in their libraries. For instance, COMSOL Multiphysics (CM) [15], the multiphysics partial differential equation solver used as a reference in this work, introduces a variety of saturated geomechanic material models (modified Cam-Clay, Matsuoka–Nakai, Hoek–Brown, among others).

Although built-in models are of great use, ideally users would be able to implement any desired stress–strain model. In principle, MPDES interfaces are adapted to so. Their structure enables to define different constitutive models. However, an important difficulty may arise when non-linear models are used. Several MPDES include automatic differentiation modules [16–19]. This method of evaluating derivatives has experienced a rapid advance, becoming an efficient tool in computing technology [20,21]. Some codes, as CM, differentiate symbolically all expressions that contribute to the iteration matrix [22]. In such case, if there are state functions defined through implicit relationships (as it happens in non-linear constitutive models), their derivatives cannot be calculated. Thus, the iteration matrix cannot be defined, and the program fails to solve the problem. Therefore, elastoplastic models cannot be freely

Abbreviations: BBM, Barcelona basic model; CM, COMSOL Multiphysics; DODE, distributed ordinary differential equation; FEM, finite element method; MPDES, multiphysics partial differential equations solvers; PDE, partial differential equation; RRMSE, Relative Root Mean Square Error.

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implemented because they contain an implicit coupling between the stresses, plastic strains, and plastic variable increments. It is not possible either to implement simple models for non-linear elasticity, because both the volumetric and shear moduli are functions of stresses that must be calculated. This inability implies a very important limitation for the use of MPDES such as CM in the analysis of geomechanical boundary value problems.

This paper proposes a strategy for solving this problem using the multiphysics concept. A mixed method [see, for instance, 23] is proposed that identifies the stresses and plastic variables as main unknowns of the model. In this manner, users can freely introduce models with implicit couplings among the variables. To illustrate the application of the method, the Barcelona Basic Model (BBM) [24], a reference critical state model in unsaturated soil mechanics, has been implemented and analysed.

2. Formulation of the problem

To simplify the description of the methodology when analysing the mechanical behaviour of unsaturated soils, a soil consisting of three species, soil skeleton, water and air is considered in three phases: solid, liquid and gas. The presence of solids dissolved in the water is not considered, whereas the presence of dissolved air is considered according to Henry's law. The gas is formed by a mixture of dry air and water vapour. The presence of vapour mixed with air in the gas phase is considered in accordance with the psychometric law. Because of this consideration, and assuming a displacement finite element approach, the solid displacements $\mathbf{u}$, liquid pressure P_L and gas pressure P_G are the 'main unknowns' (state or primary variables) of the problem, and the mass balance of the species (soil, water and gas) and the equilibrium equation are the PDEs to solve. Isothermal conditions are assumed. Thus, no enthalpy balance is solved, and the temperature remains constant. The mass-balance equations implemented in the solver have been described in detail by Navarro and Alonso [9] and Alonso et al. [25].

The equilibrium equation is formulated in terms of the total stress tensor $\boldsymbol{\sigma}_{TOT}$ as follows:

$$\nabla\boldsymbol{\sigma}_{TOT} + \rho g\mathbf{k} = \mathbf{0} \tag{1}$$

where '$\nabla\cdot$' is the divergence operator, ρ is the average soil density, g is the gravitational acceleration, and $\mathbf{k}$ is a unit vector in the direction of gravity. The total stress tensor $\boldsymbol{\sigma}_{TOT}$ is different from the constitutive stress $\boldsymbol{\sigma}$ used in the constitutive model. In this work, $\boldsymbol{\sigma}$ is assumed equal to the net stress ($\boldsymbol{\sigma} = \boldsymbol{\sigma}_{TOT} - P_G\cdot\mathbf{m}$, where $\mathbf{m}$ is the vector form of the Kronecker delta), and the mechanical behaviour of the soil is described by the pair of net stress and matric suction $s = P_G - P_L$ [26]. Thus, using the notation of Solowski and Gallipoli [27], the general constitutive relation is obtained as follows:

$$d\boldsymbol{\sigma} = \mathbf{D}^{el}d\boldsymbol{\varepsilon}^{el,\sigma} = \mathbf{D}^{el}(d\boldsymbol{\varepsilon} - (d\boldsymbol{\varepsilon}^{pl} + d\boldsymbol{\varepsilon}^{el,s})) \tag{2}$$

where $\mathbf{D}^{el}$ is the elastic matrix, and $d\boldsymbol{\varepsilon}^{el,\sigma}$ is the elastic strain associated with changes in the constitutive stresses. This latter term is the difference between the strain $d\boldsymbol{\varepsilon}$ (obtained by spatial differentiation of $\mathbf{u}$) and the sum of the plastic strain $d\boldsymbol{\varepsilon}^{pl}$ and elastic strain due to suction changes $d\boldsymbol{\varepsilon}^{el,s}$.

Introducing the definition for the plastic potential and the hardening law, the following relation is obtained [28]:

$$d\boldsymbol{\sigma} = \mathbf{D}^{ep,\varepsilon}d\boldsymbol{\varepsilon} + \mathbf{D}^{ep,s}ds \tag{3}$$

where $\mathbf{D}^{ep,\varepsilon}$ is a 6×6 (three-dimensional problem) matrix defined as follows [27]:

$$\mathbf{D}^{ep,\varepsilon} = \mathbf{D}^{el} - \frac{\mathbf{D}^{el}\mathbf{g}\left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{el}}{\left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{e}\mathbf{g} - \frac{\partial F}{\partial p_0^*}\frac{\partial p_0^*}{\partial\varepsilon_V^{pl}}\mathbf{m}^{T}\mathbf{g}} \tag{4}$$

ε_V^{pl} being the plastic volumetric strain, 'T' the transpose operator, and F the yield function. $\mathbf{D}^{ep,s}$ is a 6×1 array defined as:

$$\mathbf{D}^{ep,s} = \mathbf{D}^{el}\left(\mathbf{g}\frac{\frac{\partial F}{\partial s} - \left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{el}\mathbf{b}}{\left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{el}\mathbf{g} - \frac{\partial F}{\partial p_0^*}\frac{\partial p_0^*}{\partial\varepsilon_V^{p}}} - \mathbf{b}\right) \tag{5}$$

where, if the BBM is used, the 6×1 array $\mathbf{b}$ is given by the expression [27]:

$$\mathbf{b} = \frac{1}{3}\frac{\kappa_s}{(P_{ATM} + s)(1+e)}\mathbf{m} \tag{6}$$

being κ_s the elastic modulus for changes in suction, P_{ATM} the atmospheric pressure, and e the void ratio (assumed to be 100 kPa). As in other critical state models [29], the preconsolidation pressure p_0^* in Eqs. (4) and (2) is the model hardening parameter, defined in Fig. 1, where the 'hardening direction' $\mathbf{g}$ is also defined. For simplicity, in this work, $\mathbf{g}$ is taken as normal to F in the s = constant plane, but it is simple to adapt the formulation to introduce a different flow rule. The variation of p_0^* with respect to ε_V^{pl} constitutes the hardening law, which is formulated according to the expression [27]:

$$dp_0^* = \mathbf{H}^{\varepsilon}d\boldsymbol{\varepsilon} + H^{s}ds \tag{7}$$

where the vector $\mathbf{H}^{\varepsilon}$ (6×1) and scalar H^s are defined as:

$$\mathbf{H}^{\varepsilon} = \frac{\partial p_0^*}{\partial\varepsilon_V^{p}}\frac{\mathbf{m}^{T}\mathbf{g}\left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{el}}{\left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{el}\mathbf{g} - \frac{\partial F}{\partial p_0^*}\frac{\partial p_0^*}{\partial\varepsilon_V^{p}}} \tag{8}$$

$$H^{s} = \frac{\partial p_0^*}{\partial\varepsilon_V^{p}}\frac{\mathbf{m}^{T}\mathbf{g}\left(\frac{\partial F}{\partial s} - \left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{el}\mathbf{b}\right)}{\left(\frac{\partial F}{\partial\boldsymbol{\sigma}}\right)^{T}\mathbf{D}^{el}\mathbf{g} - \frac{\partial F}{\partial p_0^*}\frac{\partial p_0^*}{\partial\varepsilon_V^{p}}} \tag{9}$$

Therefore, if both a 'generalised' (or 'enhanced', in keeping with the notation of Solowski and Gallipoli [27]) strain vector $\boldsymbol{\varepsilon}_{enh} = (\boldsymbol{\varepsilon}, s)$, which includes strain and suction, and an 'enhanced' stress vector $\boldsymbol{\sigma}_{enh} = (\boldsymbol{\sigma}, p_0^*)$, which includes the constitutive stress and the hardening parameter, are defined, the following equation is obtained:

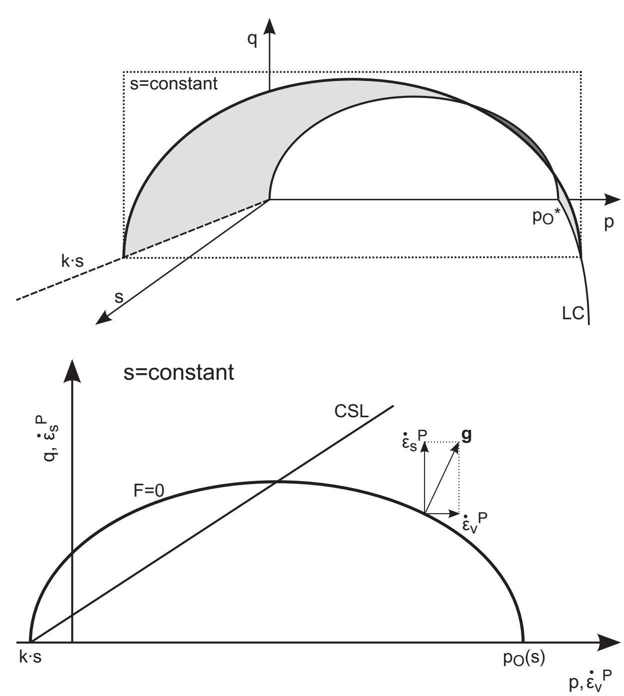

Fig. 1. General form of the yield function. CSL is the Critical State Line.