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COMPUTATIONAL STUDY USING DISCRETE ELEMENT METHOD FOR STRESS-STRAIN RESPONSE OF GEOMATERIALS

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Abstract. Relevant geomaterials, like soils, concretes or rocks, exhibit similar constitutive response when considering their yield strength dependencies or dilatancy processes. The continuous description of these geomaterials encounters limitations when large-scale slip and opening of a large amount of fractures. Discrete-based methods represent the material as an assemblage of independent elements interacting with one another and can be reproduce the discrete nature of the discontinuities, which are represented as the boundary of each element. In this case, for each particle, the interaction law is used in conjunction with the momentum balance principle so as to specify a set of governing equations to describe its interactions and motion. By solving these equations, we obtain the final state of rest of these particles. The constitutive stress-strain response is obtained in an uniaxial compression experiment were a sample of geomaterial is slowly compressed by a piston until failure occurs. The peak stress at which failure of the sample occurs is known as Unconfined Compressive Strength (UCS). This work studies these responses in geomaterials samples using Discrete Element Method (DEM). In our numeric simulation, a set of particles is placed between two piston walls which are compressed at constant speed. Then, we monitor the position and forces for construct a curve by each sample. Interactions incorporate translational and rotational degrees of freedom to rotate relative to each other when in frictional contact. Analytical relationship between the microphysical parameters and the macroscopic properties can be obtained by conducting a series of computational simulations to tune the microphysical parameters until desired macroscopic properties. To simulate elastic-brittle failure of material, a Mohr-Coulomb criterion is employed. These data are used to measure some elastic properties of the particle model such as Young's modulus, wall forces, broken bond and the UCS himself. Results shows that possible obtain significant values for different geomaterials such as some specific concretes and rocks.

Keywords: Computational Geomechanics, Uniaxial Compression Simulation, Stress-strain response, Geomaterials, Discrete Elements

1 Introduction

We believe that the study of geomaterials is very broad and covers many topics. This research seeks to understand the behavior of rocks and related materials such as concrete, soil and porous materials. Their discontinuous and inhomogeneous nature leads to complex mechanical behaviors which can be difficult to capture with standard numerical models as finite or boundary elements, as related by Donzé et al. [1]. On the other hand continuous description of geomaterials encounters limitations when large-scale slip and opening of a large amount of fractures.

An alternative is to use discrete-based methods which represent the material as an assemblage of independent elements (also called units, particles or grains), interacting with one another. Such models explicitly reproduce the discrete nature of the discontinuities, which are represented as the boundary of each element. The Discrete Element Method (DEM) is a numerical method for discrete systems made of non-deformable elements and particularly suitable to model granular materials. This method was initially described by Cundall and Strack [2] and has been widely used in dynamic numerical analyses from an engineering perspective. The scheme is a *Lagrangian* approach where individual particles are calculated on the basis of *Newton's* second law of motion. Discrete elements enable us to investigate the dynamic characteristics of particles and their motion precisely. For example, DEM application in a discontinuous medium was accomplished by Hoang Tran [3] that demonstrated the method efficiency in modeling the behavior of granular soil domains in microscopic scale.

In this work, we will investigate a geomaterial sample using uniaxial compression simulation with DEM. According to Weatherley et al. [4] the simulations measure the equivalent macroscopic properties of synthetic geomaterials samples and can be an important tool for calibrating discrete element models. In fact, a quasi-static uniaxial compression test of a geomaterial sample is a common laboratory technique for measuring the macroscopic properties such as *Young's* modulus and the Unconfined Compressive Strength (UCS). The last property is an important measure of the strength of a geomaterial and is associated to the peak stress at which failure of the sample occurs. The *Young's* modulus and the UCS were obtained from a stress-strain curve. *Young's* modulus is defined as the slope of the linear section of the stress-strain curve, whilst the UCS is the corresponding peak value. Equally important, the number of broken bonds is a useful quantity to monitor in elastic-brittle simulations, as measures of amount of damage the geomaterial sample has suffered due to the external load. Time-series of the number of broken bonds are presented along with the wall force time-series for comparison. Recent results presented by Sanches et al. [5] show that is difficult to establish an analytical relationship between the microphysical parameters and the macroscopic properties of the material. To overcome this, one more time will realize a procedure to conduct uniaxial compression simulations to fine tune the microphysical parameters until suitable macroscopic properties are obtained.

2 The Discrete Element Method

Classic DEM is considered an explicit solution for the dynamic equilibrium of individual particles rather than solving the entire system [2]. The equations governing the translational and rotational dynamic equilibrium of a particle i with mass m_i is

$$\frac{d^2 x_i(t)}{dt^2} = \ddot{x}_i(t) = \frac{F_{xi}(t)}{m_i}, \quad \frac{d^2\theta(t)}{dt^2} = \ddot{\theta}_i(t) = \dot{\omega}_i(t) = \frac{T_i(t) + M_i(t)}{I_i}. \tag{1}$$

where $\ddot{x}_i$ is the acceleration vector for *ith* particle, F_{xi} are the contact forces, m_i is the particle mass, $\dot{\omega}_i$ is the angular velocity vector, T_i is the torque, M_i is the resultant moment acting through the centroid of the particle i and I_i is the moment of inertia. For a circular particle the moment of inertia is equal to $\rho \pi r_i^4 / 2$ where r_i is the radius and ρ is the density.

From the dynamic equilibrium equations of particles and knowing the resulting forces acting on them, it is possible to calculate the accelerations for *ith* particle. Particularly, if the translation motion, can be isolated, we have:

$$m_i a_i^t = F_i^t . \tag{2}$$

where m_i is the inertia (mass) matrix, $a_i^t = \ddot{u}_i^t$ is the acceleration vector at time t, and F_i^t is the resultant force vector. To update such parameters it is necessary to implement integration methods, i.e. given by their first and second derivatives with respect to time. The relationship between the acceleration and velocity vector is:

$$a_i^t = \frac{1}{\Delta t}\left(v_i^{t+\Delta t/2} - v_i^{t-\Delta t/2}\right). \tag{3}$$

where $v_i^{t-\Delta t/2}$, $v_i^{t+\Delta t/2}$ are the velocity at t - $\Delta t/2$ and t + $\Delta t/2$ respectively for the *ith* particle.

Equation (3) is also known as the position *Verlet* time integration scheme, and the velocity at time $t + \Delta t/2$ is then calculated as:

$$v_i^{t+\Delta t/2} = v_i^{t-\Delta t/2} + \Delta t \frac{1}{m_i}\left(F_i^t\right). \tag{4}$$

The velocity at time $t + \Delta t/2$ is equal to the average velocity within the interval from t to $t + \Delta t$. Then, we can calculate the updated particle position as:

$$x_i^{t+\Delta t} = x_i^t + \Delta t \times v_i^{t+\Delta t/2} . \tag{5}$$

Particle position vector x gives the particle *Cartesian* coordinates and the total rotation about the principal axis (for the 3D case). In two dimensions there is no coupling between the three degrees of rotational freedom. Additionally, the force F_n denotes the normal component of the contact force, while the tangential (shear) component is denoted by F_t. According to O'Sullivan [6], the contact normal and shear forces can be calculated as:

$$F_n = F_N - c_n v_n , \quad F_t = F_T - c_t v_t . \tag{6}$$

where F_N is the elastic part of the normal interaction, c_n is the normal interaction damping coefficient, $v_n = (v \cdot n)n$ if n is the unit vector in the interaction between the centers of the two particles, v is the particle translational velocity vector and the contact damping force proportional to the tangential component of the relative velocity, $v_t = v \times n$ and c_t is the tangential interaction damping coefficient.

Particularly, in the tangential interaction, the frictional component of which is given by

$$F_T = \mu F_N \left(1 - \left(1 - |\delta_t| / \delta_{máx}\right)^{3/2}\right). \tag{7}$$

where δ_t is the total tangential displacement between the two surfaces from the point where they initially came into contact. If $|\delta_t| > \delta_{máx}$ then gross sliding is deemed to have started and the frictional force assumes a constant value given by *Amonton's* law, $F_T = \mu F_N$, where μ is the friction coefficient.

2.1 Geomaterials failure

To simulate geomaterials failure under compressive loads, we need to integrate some additional techniques to traditional DEM such as: 1) Implementation of cementations (rotational) elastic-brittle bonds and rotational friction interactions and 2) Moving walls. The model adopted consists of a rectangular prism of particles sandwiched between two piston walls, which are compressed at constant speed. Simulation results are then used to measure the macroscopic elastic properties of the particle model. A typical particle interactions model is designed for only three (translational) degrees of freedom configuration and is suitable for granular flow of individual particles or aggregates. To simulate elastic-brittle failure of geomaterials, more sophisticated particle-pair interactions are

required. In particular, a particle-pair interaction that incorporates both translational and rotational degrees of freedom is required**.** Then, two bonded particles may undergo normal and shear forces, as well as bending and twisting moments.

According to Weatherley et al. [4], bonds designed to impart such forces and moments are known as cementations bonds. In order to properly simulate elastic-brittle failure, bonds require a failure threshold criterion. In this work a *Mohr-Coulomb* failure criterion is employed. A bond will fail if the shear stress within the bond exceeds its shear strength τ, given by:

$$\tau = C + \sigma_N \tan\left(\varphi_f\right). \tag{8}$$

where C is the cohesive strength of the bond for zero normal stress σ_N and φ_f is the internal angle of friction of the bond.

2.2 Viscous damping

Uniaxial compression experiments are usually conducted in the so-called quasi-static regime, *i. e.*, external loads are applied slowly compared with the compressional wave speed of the sample. To simulate these conditions, it is also necessary to incorporate two body forces designed to attenuate translational and rotational oscillations. The viscosity coefficients are chosen to be small so that damping has little effect on the elastic response of the simulated geomaterial sample but it is sufficient to attenuate unwanted oscillations.

2.3 Macroscopic elastic properties

Macroscopic elastic properties as *Young's* modulus and Unconfined Compressive Strength (UCS) can be obtained from a stress-strain curve. To measure these quantities in a simulation, it is necessary construct the stress-strain curve for the geomaterial.

Therefore, suppose the net restoring forces (at time t) that particles apply to the top and bottom walls are $F^{(t)}(t)$ and $F^{(b)}(t)$ respectively, and the unit normal vector of the walls is $n^{(t/b)}$. The stress exerted on the walls by the particle assembly is:

$$\sigma_{YY}(t) = \frac{F^{(t)} \cdot n^{(t)} + F^{(b)} \cdot n^{(b)}}{2A_c}. \tag{9}$$

where A_c is contact area between a wall and the particle assembly. Since the peak stress is reached for relatively small axial strain, the contact area can be approximated by the undeformed area at particle assembly base.

It is also relatively straightforward to accounting for the total strain. Let $X(t)(t)$ and $X(b)(t)$ be the positions of the top and bottom walls at time t. The strain $\varepsilon_{YY}(t)$ is given by:

$$\varepsilon_{YY}(t) = \frac{\left[\left(X^{(t)}(0) - X^{(b)}(0)\right) - \left(X^{(t)}(t) - X^{(b)}(t)\right)\right] \cdot y}{\left[\left(X^{(t)}(0) - X^{(b)}(0)\right)\right] \cdot y}, \tag{10}$$

or

$$\varepsilon_{YY}(t) = 1 - \frac{\left[\left(X^{(t)}(t) - X^{(b)}(t)\right)\right] \cdot y}{\left[\left(X^{(t)}(0) - X^{(b)}(0)\right)\right] \cdot y}. \tag{11}$$

where y is the unit vector normal to the bottom wall.

To compute the stress-strain curve, we use the net force acting on each wall and their position at each simulation time step.

2.4 Uniaxial compression simulation

To simulate uniaxial compression it is necessary add two walls in the numerical model, which serve as pistons for compressing the geomaterial sample. One of them is added below the sample (the bottom wall) and another a top the sample (the top wall). It is worth mentioning that simply adding walls to the simulation is insufficient, we also have to define interactions between the walls and particles. For basic uniaxial compression simulations, repulsive elastic interactions are enough. If the interest were in tensile loading, one would need to bond the walls to particles at the base and top of the model. Herein, the following particle-wall interactions are sufficient to carry out simulations. Finally, only one component remains to be added to the uniaxial compression simulation: a method to move the two walls at constant speed. In this case, the wall speed is linearly increased from zero to the desired value over a few hundred time-steps. The top wall will move downwards and the bottom wall upwards.

3 Computational implementation

Numerical processes include domain clearing, particle registration, wall registration, collision detection, contact force calculation, and particle updating. Thus, there are three computational steps: internal force evaluation, in which the contact forces are calculated; integration of equations of motion, where the displacements of elements are computed; and contact detection, where new contacts are identified and broken contacts are removed. The interaction of the elements is treated as a dynamic process that alternates between applying Newton's second law and evaluating a force-displacement law on contacts. This law gives the acceleration of an element resulting from the forces acting on it, including gravitational forces, external forces prescribed by boundary conditions, and internal forces developed at inter-element contacts. Acceleration is then integrated to obtain speed and displacement. The force displacement law is used to find contact forces of known displacements. The equations of motion are then integrated in time. Once the calculated particles are recorded, they are stored in memory using a linked structure. This computational effectiveness is particularly important for large discretization. The efficiency of contact force estimation by a force calculation method is increased with parallel computing.

The computational model is based on multi-core processing, according to Weatherley et al. [4]. A modular open source object-oriented simulation code written in C^{++} was tested. In the DEM simulation, spatial domain decomposition (in sub-domains) is implemented using a master slave strategy with inter process communications using the Message Passing Interface (MPI). For this, a *Verlet* list neighbor search algorithm for detecting neighboring particles and an explicit first-order finite difference time integration scheme is employed. Besides, a simple Application Programming Interface (API) allows evaluating simulations via scripts written in Python programming language. During all iterations and loading step, each DEM ensemble runs independently. The parallelization is achieved by decomposing the problem domain into sub-domains, where the interface of each sub-domain needs to be duplicated for information to be passed between two neighboring sub-domains.

4 Numerical results

Considering the computational implementation, at initialization, particles are randomly inserted and bond together. For geomaterials breakage simulations, the best results are obtained using blocks of particles with variable radii and random locations. The reference simulation scenario generates a rectangular prism of particles whose radii lie in the range 0.4 until 2.0 mm. Two more ranges were considered using double and the half of the particle radii. The prism adopted is 10 x 20 x 10 mm in size with the center of the base at the origin. Each particle pair is tagged with a bond tag that specifies the type of interactions between bonded particles. Next, two walls are added to the simulation scenario. As previously said, these walls serve as pistons for compressing the geomaterial sample

which are positioned below (bottom wall) and above the sample (top wall). Then, interactions between the walls and particles are defined: repulsive elastic interactions are sufficient for basic uniaxial compression simulations under study. However, we would need to bond the walls to particles at the base and top of the model to assess tensile loading. The elastic stiffness (a single microphysical parameter) specifies the elastic repulsion between sample particles and walls. For this simulation we set the standard elastic stiffness equal to 100,000.0 and 102,000.0 N/mm^2 generating two result sets plus some point variations.

To simulate elastic-brittle failure, more sophisticated particle-pair interactions are required. In particular, particle-pair interactions that incorporate translational and rotational degrees of freedom. Then, two bonded particles may undergo normal and shear forces, as well as bending and twisting moments. Bonds designed to impart such forces and moments are known as cementations bonds. Rotational frictional interactions are defined by a microscopic *Young's* modulus equal to 100,000.0 N/mm^2 and *Poisson's* ratio equal to 0.25 and two microscopic coefficients of friction. Typically the *Young's* and *Poisson's* for friction interactions are set equal to their brittle counterparts. The static μ coefficient of friction is set 0.6 and applied when two particles are in static frictional contact, i.e., prior to the first time the frictional sliding criterion is met. Thereafter the dynamic μ_d coefficient of friction equals 0.4 is applied. By setting dynamic μ_d < static μ, one can simulate the physical observation that the frictional force required to maintain sliding is less than the force necessary to initiate sliding. A viscosity coefficient equal to 0.002 is chosen small so that damping has little effect on the sample elastic response, but is still sufficient to attenuate unwanted oscillations. In the uniaxial compression simulation, we move the two walls at constant speed. It is best to gradually increase the wall speed from zero to the desired value over a few hundred timesteps. The velocity of the wall increases linearly over that number of timesteps. In addition, the two walls move in opposite directions both at a speed of 0.125 m/s. Although this rate is significantly higher than typically used in laboratory uniaxial compression experiments, it is sufficiently small to maintain quasi-static conditions in our simulations. The piston speeds are approximately 20000× lower than the compressional wave speed of the simulated geomaterial sample. The initial acceleration of the walls from zero to the desired speed also helps ensure the sample is loaded quasi-statically, as shown by Weatherley et al. [4].

The Figure 1 and 2, show evaluate time series evolution of the broken bonds in the connected particles considering the initial stiffness. First, it is evident that a significant fraction of bonds breaks down before the peak stress is reached. In other words, the sample undergoes significant irreversible internal damage before reaching UCS. The second interesting observation presented by Figure 2 is that the total number of broken links after the peak stress is reached is approximately 30 until 40% of the initial number of connections. The values varies when we consider the particle at twice or half the radius. Considering only the results with range 0.4 until 2.0 mm was observed that apparently the geomaterial sample remains largely intact even after the post-peak stress. This is exactly what one would expect in laboratory uniaxial compression experiments.

It is also feasible to determine the time series force exerted on the rigid wall (Figures 3 and 4). Figure 3 shows that the maximum force on the bottom wall occurs between 15000 and 20000 step increments (loading and unloading). Figure 4 show that the maximum force on the top wall occurs in step increments bigger. Besides this, the maximum force value slightly increases on the bottom wall and most significantly on top (about 25%).

Finally, the *Young's* modulus and UCS was obtained from a stress–strain curve, as shown in Figures 5 and 6. Considering magnitude the values, we believe it is possible to relate this sample of geomaterial analyzed with some rock material or a few high resistance concrete. The analysis was made considering an increase and decrease in the particle size of the material (ranging of 0.2 until 1.0 mm, 0.4 until 2.0 mm and 0.8 until 4.0 mm, respectively for the three graphs presented). A variation of the UCS about 180 until 300 MPa and the *Young's* modulus (E) about 120 until 190 GPa can be observed in Figures 5 and 6 for these three ranges. We believe that the geomaterial sample no longer remains intact as before when we increase the particle size. Apparently, this is less expected in uniaxial compression laboratory experiments. Additionally, we see that the total number of broken bonds after reaching the maximum force undergoes a reasonable variation from the initial number of connections.

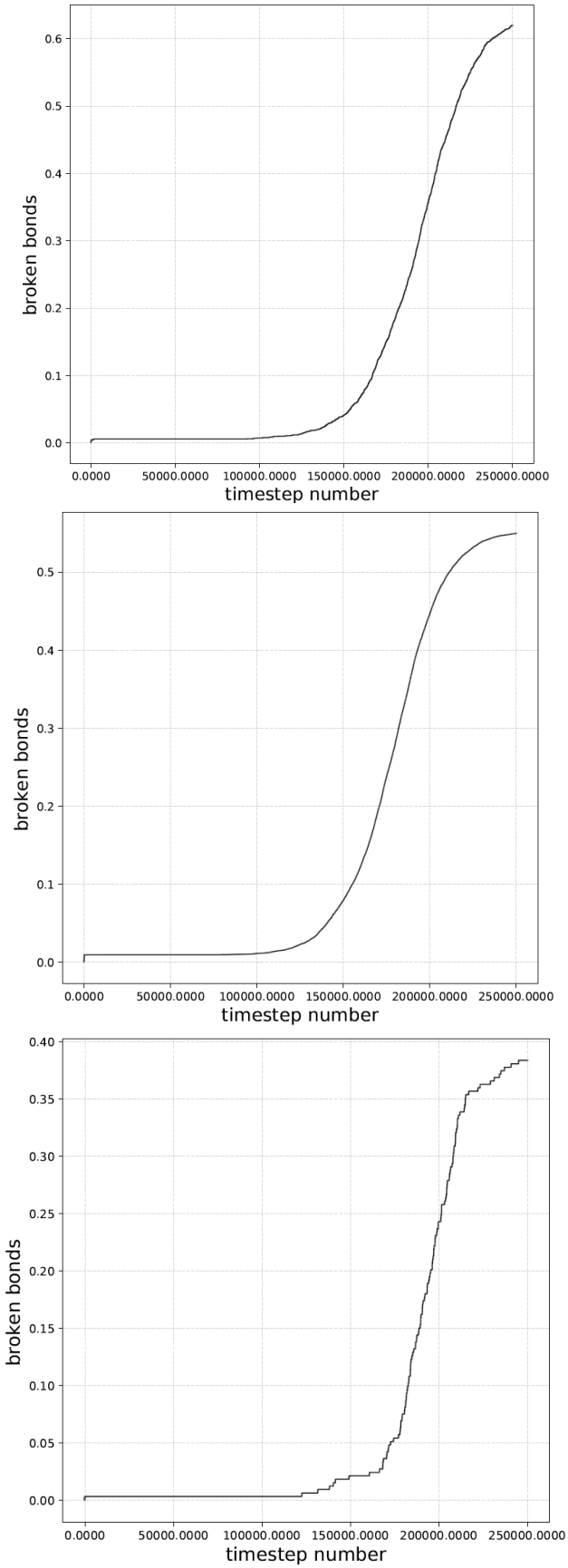

Figure 1. Number of broken bonds

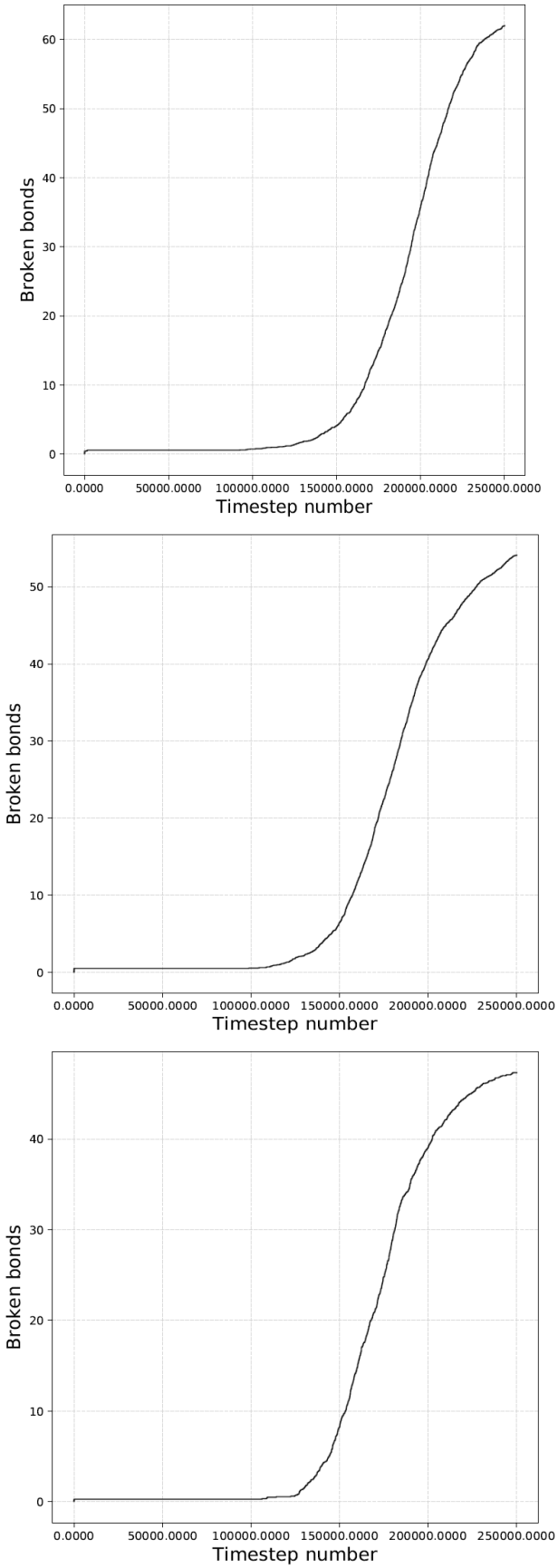

Figure 2. Broken bonds - percentage (%)

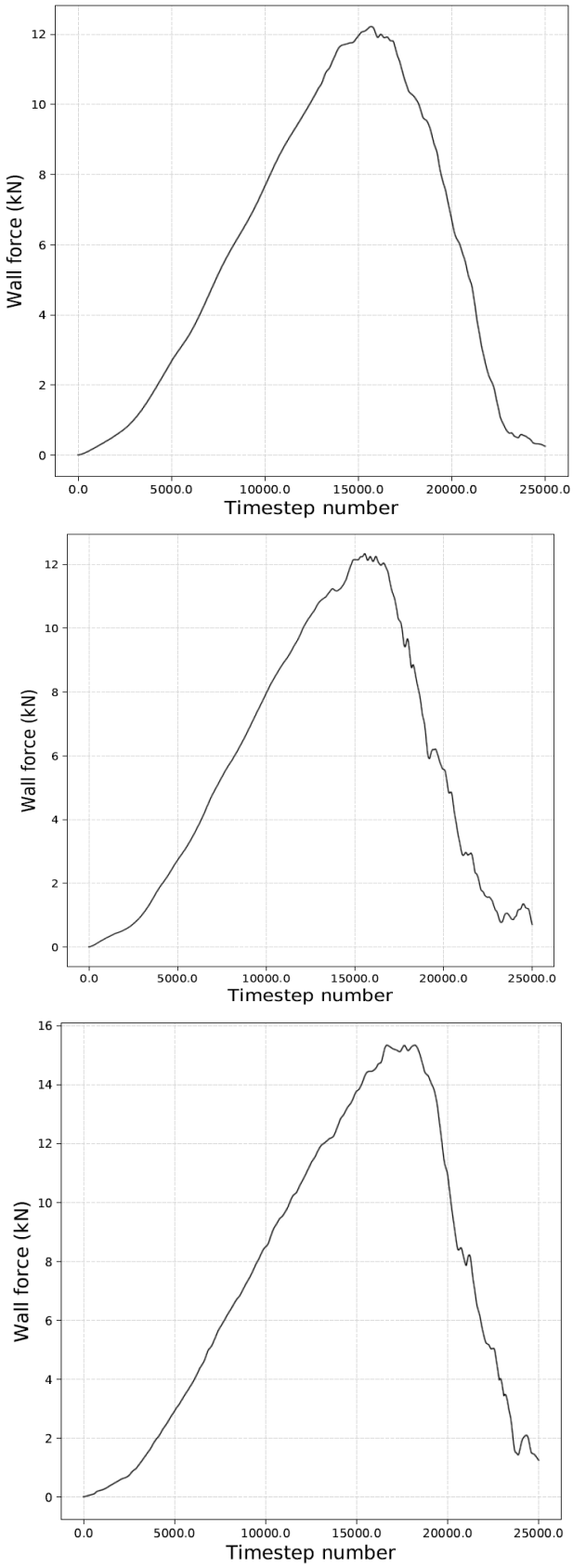

Figure 3. Wall force - bottom

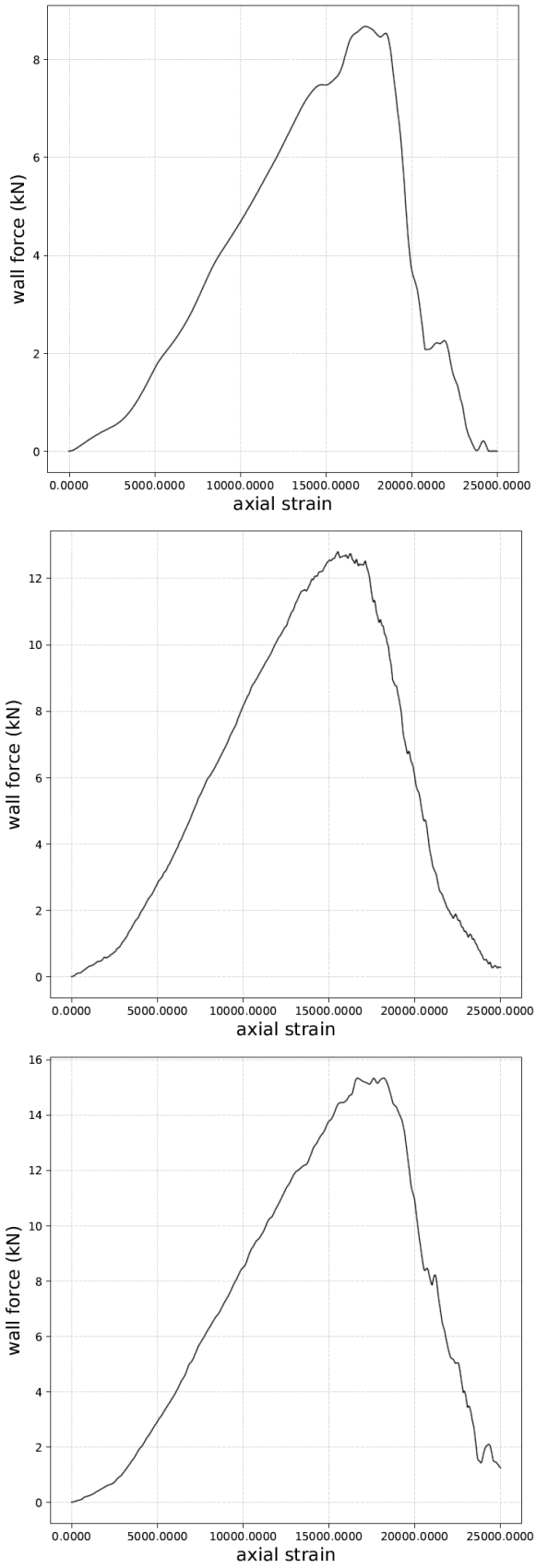

Figure 4. Wall force - top

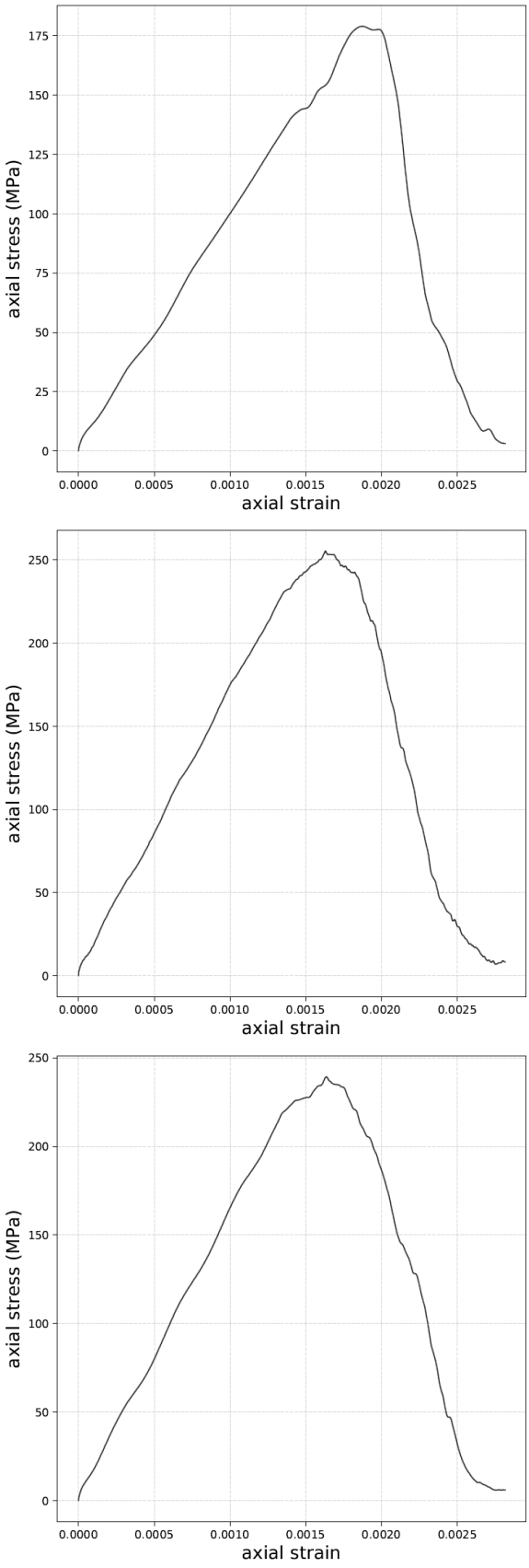

Figure 5. Stress-strain - initial stiffness

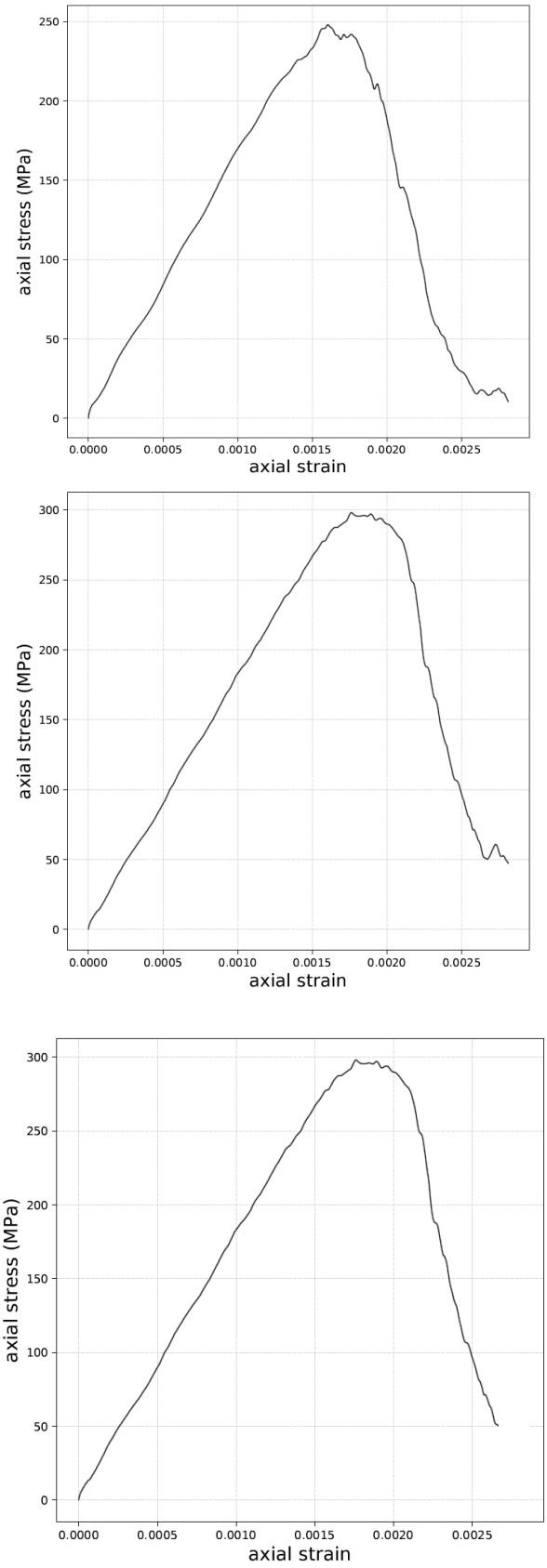

Figure 6. Stress-strain - slightly higher stiffness

5 Conclusions

Discrete elements has been shown to be a powerful numerical technique for modeling the static and dynamic mechanical behavior of geomaterials. When used properly, it allows the simulation of fairly complex nonlinear and interaction problems in geotechnical engineering. Based on simulations of standard geotechnical laboratory tests such as the one dimensional compression or direct simple shear tests, can be observed behavior non-linear, stress-strain and strength. This work aimed to describe the modeling of macroscopic properties in a standard geomaterials samples using this discrete elements. In a uniaxial compression experiments, a sample of geomaterial is slowly compressed by a piston until failure occurs. The numerical model sought to reproduce the experimental procedure. The corresponding number of broken bonds and the wall force time-series in bottom and top of the wall was been determined. Interesting results were found when we analyzed the resistance of the sample. The constitutive stress-strain responses shown the *Young's* modulus varying about 120 until 190 GPa and also the Unconfined Compressive Strength varying about 180 until 300 MPa for two little different particle stiffness. These results comprise a considerable resistance range when compared to materials used in practice. So it seems possible to model materials with different resistance behaviors. Additionally, was also observed that analytical relationship between the microphysical parameters and the macroscopic properties can be obtained by conducting a simulation campaign to fine tune these parameters so as to obtain suitable macroscopic properties.

It was likewise observed that the standard geomaterial sample remains largely intact even after the post-peak stress for a pre-set particle radius. This is exactly what one would expect in laboratory uniaxial compression experiments. Seemingly the sample becomes more susceptible to damage by increasing the particle size. This is less expected in uniaxial compression laboratory experiments. Anyway, considering the magnitude of the values encountered in the simulations we think that it is possible to relate the sample of geomaterial analyzed with a specific rock material or a high strength concrete. Future investigations will ca be examine this different types of geomaterials samples such as rocks porous and particular high resistance concretes.

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