Advances in Discrete Element Method Applied to Soil, Rock and Concrete Mechanics

Frédéric V. Donzé  
Professor, Université Joseph Fourier – Grenoble Universités, France  
Frederic.Donze@hmg.inpg.fr

Vincent Richefeu  
Assistant Professor, Université Joseph Fourier – Grenoble Universités, France  
Vincent.Richefeu@hmg.inpg.fr

Sophie-Adélaïde Magnier  
Consulting Engineer, Geonum, France  
sam@geonum.com

ABSTRACT

The use of Discrete Element Methods (DEM) to investigate mechanical properties of geomaterials is growing fast and their applications in geotechnics have become almost systematic. Behind the generic name of DEM, different formulations exist and this paper focuses on recent developments in the Molecular Dynamics and Contact Dynamics-based approaches. After reviewing their formulation, a summary of their recent uses as numerical tools to investigate the mechanical behavior of soil, rock and concrete materials is given. Specific issues such as spherical discrete element packings, flow rules, capillarity effects, high-pressure loading response and high strain rate deformation are described in more details. The quantitative capabilities of DEM are also provided by comparing real experimental data to numerical models.

KEYWORDS: Discrete Element Method; Molecular dynamics; Contact dynamics; Soil mechanics; Rock mechanics; Concrete mechanics.
INTRODUCTION

Geomaterials, like soils, concretes or rocks, exhibit similar constitutive response when considering their yield strength dependencies or dilatancy processes. Their discontinuous and inhomogeneous nature leads to complex mechanical behaviors which can be difficult to tackle with classical numerical models. Among these complex features which need to be reproduced are cracks’ nucleation, interaction or their coalescence which gives way to a possible flow, diffuse or localized deformations.

Most of the numerical methods used in geotechnics have an implicit representation of the discontinuities, where only their influence on physical behavior, such as deformability or strength, are considered through constitutive laws of the discontinuities as equivalent continua. Since the joint elements introduced by Goodman in the FEM (Goodman 1976), continuum mechanics based methods are still progressing in the manner they deal with the propagation of various discontinuities, and the eXtended Finite Element Method (XFEM), (Belytschko and Black 1999; Waisman and Belytschko 2008), is one of the last achievement in this field. However, the continuous description encounters limitations when large-scale slip and opening of a large amount of fractures must be considered in 3D, limitations which become critical when fragmentation process and flow of material occur.

An alternative to these continuous approaches 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. The model then explicitly reproduces the discrete nature of the discontinuities, which are represented as the boundary of each element. The commonly adopted term for the numerical methods for discrete systems made of non deformable elements, is the “Discrete Element Method” (DEM) and it is particularly suitable to model granular materials.

Although many geomaterials, like rocks, do not look like granular materials, the discrete models however, are often applied to investigate their mechanical behavior, by assuming that the material can be approximated as assemblies of discrete elements bonded together by different models of cohesive forces or cementation effects; thus, the overall mechanical behavior can be evaluated through the collective contributions of these discrete elements under loading or unloading processes exhibiting motion, displacement, sliding, inter-element rotation and where de-bonding mimics the nucleation of cracks. Heating effects and fluid pressure are also included in some of these models and the Discrete Elements (DE) can be rigid (or eventually deformable), with smooth or rough surfaces of different shapes (Jing and Stephansson 2008).

There are different Discrete Element Methods used in the Geotechnical field, but we will consider only two of them in this review.

The first one is the classical Discrete (or Distinct) Element Method (DEM) pioneered by Cundall and Strack (Cundall and Strack 1979), which was the first approach proposed in the literature. Basically, the algorithm involves two stages. In the first one, interaction forces are computed when elements slightly interpenetrate each other: this force-displacement formulation is often referred to as a “Smooth contact” method or also as the “Force-Displacement” method. As pointed out in Cundall and Hart (1992), although it seems inappropriate that two discrete
elements can penetrate each other in a mathematical sense, what it really represents is the relative
deformation of the surface layers of the elements (especially when the surfaces are rough and
have asperities) rather than real interpenetration as such. In the second stage, Newton’s second
law is used to determine, for each DE, the resulting acceleration, which is then time integrated to
find the new element positions. This process is repeated until the simulation is achieved. This
simultaneous numerical solution of this system is also known as the Molecular Dynamics (MD)
formalism.

There are other discrete numerical methods which exclude possible interpenetration between
DE, i.e. they deal with unilateral contact. These methods are referred to as “non-smooth contact”
methods. Two main classes of numerical integrators exist for these methods: the event-driven
integrators also referred to as the Event-Driven Method (EDM) (Luding et al. 1996) and the so-
called time-stepping integrators, also referred to as the Contact Dynamics Method (CD) (Moreau

For EDM, a collision (or an “event”) occurs when two rigid elements touch each other and
the post-collisional velocities and angular velocities are prescribed by a collision operator
(Rapaport 1980; Walton and Braun 1986). Event-driven integrators are very accurate but, because
they treat only one force at a time, they are not suitable for systems with many contacts as
encountered in competent geomaterials as soils, rocks or concretes.

To overcome this limitation, the CD has a dedicated numerical scheme for mechanical
systems with many contacts. As the integrator work with the integral of the contact forces and not
with the forces itself, as in EDM, this method can handle both non-impulsive motion and
impulsive events such as impacts.

Since the DEM, EDM or CD often consider the discrete elements as non-deformable bodies
in time-explicit numerical schemes, they can offer limited performances when deformations and
stresses of the elements themselves must be considered in a static framework.

Then, the Discontinuous Deformation Analysis (DDA) (Shi and Goodman 1988) can be used.
It uses a finite element method to solve for stress and deformation filed inside the Discrete
Element, but it accounts for the interaction of independent elements along discontinuities.
However, since a continuous approach is used to describe the solid medium, DDA will not be
considered here. The interested reader is referred to Jing and Stephansson’s book (2008) for a
detailed and complete description of this method and its application to rock mechanics.

The DEM method has been extensively applied to study flow of non-cohesive granular
materials (Cleary 2004, Cleary 2008), such as V-blender to mix monodisperse and bidisperse
powders (Moakher et al., 2000), Tumbling (ball) mills for polydisperse powders (Cleary and
Sawley, 1999; Rajamani et al. 2000), Helical ribbon mixer (Bertrand et al. 2003), Flat blade
mixer (Stewart et al., 2001), or Kenics static mixer (Szépvölgyi 2001). However, since the scope
of this article is the latest DEM’s developments in rock, soil and concrete mechanics, the flow of
non-cohesive granular materials will be ignored. The interested reader is referred to Cleary and
Sawley (2002) or Bierwisch et al. (2008).
In the following chapters, the choice for the Discrete Elements’ shape will be first presented. A short presentation of MD and CD will follow and finally, an overview on soil, rock and concrete models using DEM will be presented. Specific issues such as spherical discrete element packings, flow rules, capillarity effects, high-pressure loading response and high strain rate deformation will be described in more details.

MODELING GEOMATERIALS

Packings and shapes of Discrete Elements greatly contribute to the distribution of the interaction forces and their intensities (Voivret et al. 2009). In addition to the constitutive model, they must be able to represent the behavior of geomaterials observed in laboratory experiments and/or field observations. However, these models are theoretical approximations to what one observes in reality. Due to the extreme complexity of the physical behavior of geomaterials, and the limitation of currently available mathematical tools and computer methods, it is not possible to simulate every aspect of the physical behavior by mathematical models. Only the most important aspects of the overall behavior are usually considered when developing constitutive models.

In MD, constitutive models can be based on different types of contact laws. The simplest one is to assume linear contact laws for normal compression, and constant shear stiffness and friction angle for sliding. The other approaches assume the normal load–displacement response to be non-linearly elastic or to have force-dependent normal and shear stiffnesses. Moreover, a transmitted moment which produces a rolling resistance is now often used (Iwashita and Oda 1998; Iwashita and Oda 2000; Beleheine et al. 2008). These local interaction forces are controlled by a set of parameters, which contribute to the generation of very complex behaviors at the discrete system scale. This is why it is important to determine the respective role of these local parameters in order to identify the real underlying physical meaning of such a model.

In discrete models, forces and displacements are used as primary variables – rather than stresses and strains, as for the Finite Element Method. Therefore, homogenization is often needed to evaluate the overall behavior of particle systems if equivalent continua are required. Nevertheless, homogenization is often a difficult task because the parameters controlling the geometrical properties and the constitutive model do not always have, a clear physical meaning and/or they can exhibit cross dependencies.

Packing and shapes of the Discrete Elements

Most of the DEMs use disks in 2-D or spherical elements (in 3-D) because only a single value, the radius, is required to define the geometry of the particles and there is only one possible type of contact among particles, which can be detected easily. As a result, computer memory requirements and computer processing time are minimized with these particle shapes and in addition a large number of particles can be analyzed. However, it should be noted that disks and spheres tend to roll or rotate easily, which does not reflect the behavior of real geomaterials in case of large shear processes, for example.
Hence, more complex shapes such as ellipses (Ting et al. 1993), ellipsoids (Lin and Ng 1997), polygons (Issa and Nelson 1992; Matuttis et al. 2000; D’Addetta et al. 2002; Feng and Owen 2004), polyhedra (Hart et al. 1988; Cundall 1988; Ghaboussi et al. 1990) and superquadrics (Mustoe 1992; Hogue 1998) can provide more flexibility in particle characterization in the DEM (Williams and O’Connor 1995; Miyata et al. 2000) as shown in Figure 1. However these complex geometries, such as polygons and polyhedrons can be problematic because detecting contacts and calculating forces and torque in cases of edge-edge, edge-corner, corner-corner contacts, and extending from 2-D to 3-D and bonding particles together can be complicated and computationally expensive (Wang and Mora 2008).

Figure 1: a) clusters of inter penetrating spheres (Favier et al. 1999), b) clusters of non penetrating spheres (Salot et al. 2008), c) Superquadratic ellipsoid (Hogue 1998), d) Polyhedra

Another alternative solution to simulate more realistic grain shapes or contact surfaces, may be aggregates or clumps of disks and spheres bonded together (also called clusters, see Jensen et al. 1999) or clumps (Cho et al. 2007; Ning et al. 1997; Cheng et al. 2003; Lu et al. 2007, Salot et al. 2008). The disadvantage is that this method requires a larger number of elements and the contribution of the surface roughness becomes difficult to evaluate. However, in clusters, the contacts are more readily solved as compared to polyhedrons, and the calculation cost remains reasonable.

Polyhedra (or polygons in 2D) represent the only case for which space can be totally filled with the discrete elements without any voids, whereas, in all other cases, a geometrical porosity will be generated. Coupled with the constitutive models, this porosity will play a major role on the global response of the discrete system because it can have an influence on the average number of interaction forces per element and their orientations. Currently, the available algorithms to generate high density packing are classified as geometric or dynamic methods (see Jerier et al. 2008).

The dynamic method uses Newton’s second law of motion to determine the trajectory and the spheres’ final positions inside a container. The sphere packing is simulated by integrating different contact laws (Cheng et al. 2000; Yang et al. 2000; Salvat et al. 2005, Liu et al. 2000) which can be, for example, modeled by springs and dashpots between particles. A large variety of dynamic algorithms exists and they differ by the technique used: gravitational (Siiria and Ylioruusi 2007), uniaxial compaction (Dutt et al. 2005), isotropic compaction (Stroeven and Stroeven...
or radius expansion (Lubachevsky and Stillinger 1990). With these approaches, it is possible to control the packing properties. The dynamic method has the capability of generating isotropic packings with a high density value which is an undeniable advantage in geomaterial research. The numerous generation techniques and the different contact laws give a real flexibility to this method to model the desired packing. Nevertheless, the dynamic algorithms have drawbacks which cannot be ignored such as the residual overlaps, and a very time-consuming high packing preparation which becomes prohibitive when the packing holds more than 100000 spheres.

The geometric algorithms generate sphere packings which use geometric functions applied on spheres. Different geometric algorithms were developed to generate sphere assemblies in cylindrical (Mueller 2005), cubical (Jodrey and Tory 1985) or conical (Kadushinikov and Nurkanov 2001) containers. For example, the ballistic deposition algorithm (Mueller 2005; Jullien and Meakin 2000) assures a high speed of the packing generation. With this one by one element placement, the size distribution is controlled and the use of a stability criterion induces a high coordination number. The advantage of using geometric methods rather than dynamic methods to generate dense polydisperse packings is to lower the computation time. In the past few years, the interest for the geometric method has increased with new, more efficient algorithms as the one developed by Al-Raoush et al (2007). New geometric algorithms based on tetrahedral meshes to generate dense isotropic arrangements of non-overlapping spheres of different sizes have been recently developed (Jérier et al. 2008). The method consists in first filling in a tetrahedral mesh with spheres in contact (i.e. hard-sphere clusters). Then, they can increase the packing density value by detecting the large empty spaces and filling them with new spheres (see Figure 2). These kind of geometric algorithms are not only very fast but they can also generate composite media (see Figure 3).

Besides particle shapes, deformability of the particle themselves has also been considered for DEM modeling for granular materials. Thornton and Zhang (2003) considered elastic particles to investigate particle stress and deformation effects on shear-band behaviors of granular assemblies. However, the main thrust of development in this direction is the combined discrete and finite element methods, such as reported in different papers (Munjiza et al. 1995; Owen et al. 2002; Bangash and Munjiza 2003). The reader is referred to Munjiza’s book (2004) for a detailed and complete description of a possible method to couple FEM and DEM.

![Figure 2: 3D mesh made of unstructured tetrahedra (left) and its corresponding polydisperse sphere packing (right) (Jérier et al. 2008)]
Figure 3: 3D mesh made of unstructured tetrahedra which includes a preexisting line of spherical discrete elements (left) and its corresponding polydisperse sphere packing around the preexisting line of discrete elements (right) (Jérier et al. 2008)

MD AND CD FORMULATIONS

From the original work of the DEM for granular materials for geomechanics and civil engineering applications reported in the series of papers by Cundall and Strack (1979) or Cundall and Strack (1982), which was based on an earlier work by Cundall (1971) to the application of parallel computing to solve large problems, like Meegoda (1997), the reader can find a complete history of the DEM in the book of Jing and Stephansson (2008).

Since Cundall and Hart (1992) made the distinction between hard contacts and soft contacts, the objective of this chapter is to present the key points of these different approaches by selecting two common formulations used to study geomaterials. The reader is invited to read the referenced articles to see the details of the numerical formulations.

Molecular Dynamics (MD)

Since the realistic modeling of the deformations of the elementary units is much too costly from a calculation point of view, in MD the interaction force is related to the overlap $u$ of two elements, as in Figure 4. Note that the evaluation of the inter-element forces based on the overlap may not be sufficient to account for the inhomogeneous stress distribution inside the particles. Consequently, numerical results are of the same quality as the simple assumptions about the force-overlap relation. As seen in the previous paragraph, discrete elements can have different geometries. This aspect must be considered in the formulation, as the formalism becomes heavier with increasing geometrical complexity. In order to keep the formalism as simple as possible, we have chosen to present the fundamental equations only for the spherical geometry. For tetrahedrons, one can read the book of Munjinza (2004), for super-quadratic elements (Hogue 1998) and for clusters or clumps of spheres the reader is referred to (Cho et al. 2007; Nicot et al. 2007; Salot et al. 2008).

Basic interaction law for geomaterials

When considering $(i)$ perfectly smooth particles (i.e. without roughness), $(ii)$ isotropic elastic constitutive equations for the particles, $(iii)$ the non influence of the tangential component of the contact force on the normal component, and $(iv)$ a negligible interpenetration when compared
with the surface contact, Hertz’ law (Maugis 1999) exhibits a non-linear relation between the elastic contact force and the maximum overlap $u_n$. The elastic contact force reads:

$$f^e_n = \frac{4}{3} \left( \frac{1 - v_A^2}{E_A} + \frac{1 - v_B^2}{E_B} \right)^{-1} \sqrt{R} u_n^{3/2},$$

(1)

Where $R = R_A R_B / (R_A + R_B)$ is the equivalent radius of particles $A$ and $B$, $E_A$ and $E_B$ are their Young’s modulus, and $v_A$ and $v_B$ are their Poisson coefficients. This model of the contact behavior is absolutely necessary for certain issues such as wave propagation in granular matters.

Figure 4: Interacting spherical discrete elements

For small deformation, dense geomaterials exhibit a linear elastic response. To reproduce this behavior, linear elastic interaction forces between the discrete elements are generally sufficient and lead to smaller simulation times. However, using only a local “spring” model with a unique elastic stiffness can be insufficient to reproduce the basic elastic properties of an isotropic and homogeneous geomaterial; similarly to Hertz’ law, two distinct elastic stiffnesses need to be defined locally. Thus, the interaction force $f$ which represents the action of element $A$ on element $B$ may be decomposed into an elastic normal force $f^e_n$ and an incremental shear force $f_t$ (Figure 1) which may be classically linked to relative normal and incremental shear displacements respectively, through normal and secant tangential stiffnesses, $K_n$ and $K_t$, (Hart et al. 1988; Walton 1993) such that,

$$f^e_n = K_n u_n,$$  

(2)

$$f_t = \{f_t\}_{\text{updated}} - K_t \Delta u_t,$$  

(3)

where $\Delta u_t$ is the incremental displacement projected in the plane tangent to the contact normal vector. The incremental shear force is reset to zero (i.e. $\{f_t\}_{\text{updated}} = 0$) if a threshold value
depending on the normal force is reached, then the particle can slip. A local criterion of rupture similar to the Mohr-Coulomb criterion is generally considered for this purpose:

$$|f_t| < \mu f_n + C$$  \hspace{1cm} (4)

where $C$ is the local cohesion and $\mu$ is the friction coefficient. Moreover, when the simulated geomaterial exhibits maximum traction strength, it is possible to use local maximum traction strength, for which,

$$f_n = K_n u_n < -T, \text{ then, } f_n = f_r = 0,$$

which simulates the breaking of a cohesive link (Figure 5).

The realism of DEM simulations is fully dependent on the underlying model of the interactions. So in addition to the basic laws previously described, several authors have introduced more complex interaction laws such as capillary cohesion (Soulié et al. 2006; Richefeu et al. 2007; Scholtès et al. 2009a), solid cohesion (Delenne et al. 2004; Jiang et al. 2006b), plasticity (Shiu 2008) with temperature and relaxation (Luding et al. 2005), and moment transfer (Iwashita and Oda 1998; Iwashita and Oda 2000; Belheine et al., 2009).

![Figure 5: Local rupture criterion](image)

Equations of motion

At a given time step, the total force $F_i$ and the total moment $M_i$ acting on the mass center of the $i^{th}$ discrete element are known. They result either from other elements, from boundaries or from volume forces (such as the force due to gravity). In classical DEM, the problem is reduced to the integration of Newton's equations of motion for the translational and rotational degrees of freedom:
\[ m_i \ddot{x}_i = F_i + m_i g \]
\[ I_i \ddot{\omega}_i = M_i \]

(6)

where \( m_i \) is the mass of \( i^{th} \) element, \( \ddot{x}_i \) is its translational acceleration, \( F_i = \sum_k f_i^k \) is the total force applied on this element due to the \( k \) interactions with other elements or with the boundaries, \( g \) is the acceleration due to volume forces like gravity, \( I_i \) is the moment of inertia of the spherical particles (which corresponds to a scalar value in the case of a spherical particle), \( \ddot{\omega}_i \) is its angular velocity and \( M_i = \sum_k (l_i^k \times F_i^k + q_i^k) \) is the total moment, where \( q_i^k \) are the moments at interaction points other than those due to a tangential force.

The equations of motion are thus a system of coupled ordinary differential equations to be solved in 3 dimensions. The time integration method is usually based on the “Velocity-Verlet” finite-difference algorithm, but many other algorithms can be used as described in textbooks such as (Allen et al. 1987; Rapaport 1995).

To obtain a proper integration of the particle movement, the time step must be chosen carefully. By analogy between a contact (with stiffness \( K_n \)) and an oscillating mass \( m \), it can be shown that the time step must be chosen as a small portion (typically a twentieth to a tenth) of the half period given by \( \pi \sqrt{K_n / m} \). In addition, numerical stability can be enhanced with viscosity at the contact level, larger masses of the particles or moderation of particle velocities (so called non viscous damping).

If rotation is involved, integration of rotational equations should also be considered, including updating angular velocities and updating the orientation degree of freedom (Dullweber et al. 1997; Kol et al. 1997; Omelyan 1998a; Omelyan 1998b; Buss et al. 2000; Miller et al. 2002; Munjiza et al. 2003; Krysl et al. 2005; Wang et al. 2007).

**Contact dynamics (CD)**

The contact dynamics (CD) method, introduced later, provides an alternative approach based on a ‘nonsmooth’ formulation of mutual exclusion and dry friction between elements (Moreau 1994; Jean 1999). This method has been successfully used for several geomechanical problems (Rafiee et al. 2008; Silvani et al. 2008). However, as we shall see in the following, the CD method is much more difficult to implement than the MD. This partially explains the small number of codes based on contact dynamics.

In the CD method, the equations of motion are expressed as differential inclusions and the accelerations are replaced by velocity jumps. Strangely, no elastic contact law is required. In fact, at a given time step, all kinematic constraints implied by enduring contacts and possible rolling of elements over one another are simultaneously taken into account in order to determine all velocities and contact forces. This point will be developed in the next sections.
**Basic kinematic constraints**

In the generic CD algorithm, an iterative process is used to compute forces and velocities. It consists of solving a single contact problem with all other contact forces kept constant, and iteratively updating the forces until a given convergence criterion is fulfilled. The CD method implies in its generic formulation two basic kinematic constraints when the discrete elements are in contact:

1. The *Signorini conditions* stating that the normal force $f_n$ is positive (repulsive) or null when the distance $\delta_n$ between two particles is zero. Otherwise, $f_n = 0$. Figure 6(a) shows a representation of this condition. It is important to remark that, strictly speaking, these conditions do not represent a force law (i.e. bijective force-displacement relation). Besides, a kinematic constraint is added for persistent contact ($\delta_n = 0$): the normal force is positive if the relative velocity $v_n = \dot{\delta}_n$ is non null and vanishes otherwise.

2. The *Coulomb's friction law* gives a relationship between the sliding velocity and the friction force $f_t$. If the sliding velocity $v_s$ is nonzero, then the friction force $f_t = f_t(v_s/|v_s|)$ resists sliding and its value is given by the coefficient of friction $\mu$ times the normal force $f_n$. If, on the other hand, $v_s$ is zero (non-sliding contact), then $f_t$ can take any value in the interval $[-\mu f_n, \mu f_n]$. This is illustrated in Figure 6(b) as a graph.

![Graph illustrating the Signorini condition in velocity](a)
![Graph illustrating the Coulomb friction law](b)

**Figure 6:** (a) Graph illustrating the Signorini condition in velocity; (b) Graph illustrating the Coulomb friction law.

These two basic laws can also be completed with a ‘rolling friction’ law that introduces a moment resistance (Bratberg et al. 2002; Taboada et al. 2006). This may have different microscopic origins such as the presence of cement between particles or plastic deformation in the area of contact. This additional law may also be used to mimic non-spherical particles.
Both Signorini’s conditions and Coulomb’s friction law are ‘nonsmooth’ in the sense that the two conjugate variables \((v_n, f_n)\) or \((v_t, f_t)\) belong to a continuous set of possible values.

Within the scope of CD, the time resolution is much larger than the collision characteristic time (unlike the MD approach). Instead, the time step represents a unit of time during which collisions can occur causing velocity jumps. This gives another meaning to the term ‘nonsmooth’. The challenge of the problem is to predict, from the current configuration, the contact forces and particle velocities at the following moment. Due to the coarse-grained time stepping, the kinematic constraints are used with formal velocities corresponding to weighted average velocities between two moments:

\[
v_d = \eta_d v_d^- + (1 - \eta_d) v_d^+,
\]

Where, \(d\) stand for normal (n) or tangential (t) direction, \(\eta_d\) are the weights, \(v_d^-\) and \(v_d^+\) correspond to the relative velocities at the beginning and the end of a time step. For binary collisions \(\eta_d\) can be expressed as a function of the restitution coefficients \(e_d = \frac{v_d^+}{v_d^-}\):

\[
\eta_d = \frac{e_d}{(1 + e_d)}.
\]

**Rigid-body dynamics**

For convex particles, starting from force and moment balance equations, it is possible to formalize the problem for a given contact \(\alpha\) as follows:

\[
\mathbf{M}^\alpha \cdot \begin{pmatrix} f_n^\alpha \\ f_t^\alpha \end{pmatrix} = \begin{pmatrix} 1 + e^- \alpha v_n^\alpha + a_n^\alpha \\ 1 + e^- \alpha v_t^\alpha + a_t^\alpha \end{pmatrix},
\]

where, \(a_n^\alpha\) and \(a_t^\alpha\) depend on the relative velocities \(v_n^-\) and \(v_t^-\) at the beginning of the time step and the forces of the preceding iteration (within a time step), \(\mathbf{M}^\alpha\) is a symmetric matrix with constant and positive components. For sake of simplicity, the expression of the matrix components and coefficients \(a_n^\alpha\) and \(a_t^\alpha\) are not given in this review. For details, the reader may refer to the references dedicated exclusively to the CD method (Jean 1999; Radjai and Richefeu 2009). Note also that a relation with formal relative rolling velocity must be added if a moment transfer is taken into account.

As we can see in Equation 9, the normal and tangential forces \(f_n^\alpha\) and \(f_t^\alpha\) are affine functions of the formal velocities \(v_n^\alpha\) and \(v_t^\alpha\). These functions define a set of solutions compatible with the equations of dynamics. The kinematics constraints presented in the previous section are thus used to obtain a finite solution: it corresponds to the points \((v_n^\alpha, f_n^\alpha)\) and \((v_t^\alpha, f_t^\alpha)\) that belong to both the sets of acceptable solutions (affine functions) and the kinematics constraints (see Figure 7).
Figure 7: Single contact Solution of the equations of dynamics in normal (a) and tangential (b) directions. The dashed lines represent the set of dynamically plausible solutions. The force solutions, shown by round dots, are restricted by the Signorini condition (in velocity) for normal forces, and by the friction law for tangential forces.

The solution for all forces and velocities in a granular system by this method implies performing the above-mentioned intersections simultaneously at all contacts. Since the forces at each contact depend on other forces acting on the elements, the numerical implementation requires an iteration scheme within each time step. The ‘Gauss-Seidel’ numerical scheme is generally used for this purpose because it is robust and can easily be parallelized. A numerical scheme based on projected conjugate gradient can also be used. It is more efficient than Gauss-Seidel for linear problems and can be parallelized as well (Renouf and Alart 2005). The iterative numerical scheme has to stop when a given criterion of convergence is satisfied. A classical criterion is the measure of force stability for each contact compared to the previous iteration. A less strict criterion defined from averaged values of forces nevertheless gives satisfactory convergence in most cases.

APPLICATION TO SOIL MECHANICS

The structure of a soil is the combined effects between the geometrical arrangement of grains, their shapes, their composition, the interaction forces and pore spaces. Water and air are generally found in macro-pores and micro-pores, and they play an important role in the soil behavior. Although soils are in essence discrete materials, they are usually treated as continuum material in theoretical, constitutive modeling and numerical analyses within continuum mechanics. This method plays an important role and is widely used in geotechnical engineering. However, the behavior of soils is so complex that it is a difficult task to reproduce it with a continuum constitutive law, and such laws tend to contain many ad hoc parameters and no particular model or theory has received universal acceptance yet (Jiang & Yu 2005).

Since DEM exhibits the same discrete nature as soils, it can capture quite naturally complex behaviors like nonlinear stress/strain response, dilation related to mean stress, transition from brittle to ductile behavior, hysteresis, nonlinear strength envelopes, acoustic emissions, etc., (Cundall 2002). To get such results, the basic Mohr–Coulomb criterion can be used to control
shear behavior at contacts between the discrete elements. However, there is extensive work on the constitutive modeling used in DEM to study soils. Cundall and Strack (1982) and Taylor and Preece (1992) used Hertzian contact theory as well as Mindlin and Deresiewich's (1953) approach, to obtain the value of the parameters. Another method is based on the elastic properties (Young’s modulus and Poisson's ratio) of the bulk material and the relations between the stress tensor that acts on a representative volume of particles and the forces between the particles in this volume (Cundall and Strack 1982; Walton 1987; Chang et al. 2003). Assuming an elastic bulk material, Liao and Chan (1997) developed a method to determine the bounds of the spring constant between two particles. The upper bound is given by Voigt’s hypothesis (uniform strain occurred in all the particles) and the lower bound by Reuss’ hypothesis (uniform stress accrued in all the particles). It should be emphasized that the analytical theories are limited to spherical particles of homogenous properties.

In the absence of an analytical approach or other robust methodology to determine the soil parameters, many authors use trial-and-error (Asaf et al. 2006). Some authors suggest using numerical testing procedures for drained triaxial tests (Figure 8) to calibrate the DEM parameters (Belheine et al. 2009).

**Figure 8: From left to right, three different deformation stages of a numerical triaxial test (Scholtès et al., 2009a) performed using YADE (Kozicki and Donzé 2008)**

For example, the main input parameters in the numerical model, can be: the normal and tangential contact stiffnesses, rolling contact stiffness (as developed by Oda et al. 1982; Oda et al. 1998; Oda and Iwashita 2000; Schlangen et al. 1997; Iwashita and Oda 1998; Iwashita and Oda 2000; Tordesillas and Walsh 2002; Kuhn and Bagi 2004), local friction and the plastic limit of rolling. Several parametric studies can be done to evaluate the influence of each of the above on the output macro parameters such as Poisson’s ratio, Young’s modulus (Figure 9), the dilatancy angle, the peak and the post peak strength. It was found that the elastic response is mainly governed by the normal contact stiffness and the ratio of shear to normal contact stiffnesses.

Secondly, a coupled effect was found between the local friction (see Figure 10, for example), the rolling stiffness on the peak stress and a plastic moment on the post peak stress of the sand. In addition, the observed deformation depends strongly on local friction.

However, the soil parameters measured in the lab are usually based on remolded soil and do not necessarily represent the soil in-situ. Thus, the model may result in an erroneous prediction. Asaf et al. (2007) suggested recently the determination of DEM parameters based on in-situ field tests, which consisted of sinkage tests performed with different penetration tools. In order to
minimize the difference between the observed and simulation results, an inverse solution technique using the Nelder–Mead optimization algorithm has been proposed (Asaf et al. 2007). Although formulated for a 2D model, this approach seems very promising.

**Figure 9:** Young's modulus (a) and Poisson’s ratio (b) for $K' = 35\,\text{MN/m}^2$ (from Plassiard et al. 2008)

**Figure 10:** Triaxial tests for different values of $\mu$. Differential stress (left) and volumetric strain (right) are plotted versus axial strain (from Plassiard et al. 2008)

**Failure criterion and plastic flow rule**

Over the years, a large number of formulations have been developed to describe yield conditions, plastic potentials, and failure state of soils. Dozens of rupture criteria for geomaterials (such as the Mohr-Coulomb criterion, or its circular version the Druker-Prager criterion or others) have been developed over the past forty years and DEM models exhibit behaviors which are in good agreement with these.
Since there is no strong agreement within the engineering and applied mechanics community as to which flow rule is most appropriate, the DEM can bring some interesting insight, as it is a direct representation of the granular state of the material and it does not introduce any “a priori” flow rule.

Authors using direct DEM simulation (Sibille et al. 2007; Bardet 1994; Calvetti et al. 2003) have shown that when the material is loaded in axisymmetric conditions, its response can be satisfactorily interpreted in terms of classical plasticity with a single mechanism, provided that a non associated flow rule is adopted (see for example Figure 11). It was specifically shown that, the direction of plastic flow, depends on the current stress state and loading history but is independent of the stress increment direction. It is worth noting that DEM stress probing simulations on the deviatoric plane, indicate that the behavior under more general loading conditions is fully incrementally non-linear (Calvetti et al. 2002; Calvetti et al. 2003).

**Figure 11:** On the left, equilibrium states (A), (B), (C) and (D) for a numerical sample with a confining pressure of $\sigma_3 = 100 \ kPa$, and on the right, plastic flow direction $\%_p$ versus stress increment direction $\alpha_{\text{dr}}$ for initial equilibrium states (C) and (D) (from Plassiard et al. 2008)

While localized failure has been extensively studied, (Bardet and Proubet 1991; Anandarajah 1994; Ng and Doby 1994; Iwashita and Oda 1998; Iwashita and Oda 2000; Oda and Kazama 1998; Oda and Iwashita 2000; Thornton 2000; Thornton and Zhang 2003; Thornton and Zhang 2006; McDowell and Harireche 2002; Cheng et al. 2003; Jiang et al. 2006), diffuse failure modes are still not characterized from an experimental point of view and not described by proper criteria from a theoretical point of view. Because of the non-associative character of geomaterials plastic strains, many bifurcations leading to various failure mechanisms exist strictly inside the plastic limit condition (Darve and Lambert 2004). The contribution of the DEM method is very interesting in this special case, where loose geomaterials are generally considered, because it has been seen that a bifurcation domain according to Hill’s condition (Hill 1958) exists whichever DEM approach was considered (MD or CD). For each approach, the bifurcation domain is strictly included inside the plastic limit condition (see Figure 12).
Generally speaking, this is the case for non-associated material for which stress increment directions and strain increment directions can be strongly uncorrelated before reaching the plastic limit condition. Thus, the description of sudden collapses, inside the plastic limit condition, as observed by (Gajo et al. 2000; Chu and Leong 2003) by considering Hill’s sufficient condition of stability is possible with DEM.

**DEM and unsaturated soils**

Unsaturated soils are subjected to capillary effects, which can be related to the presence of water menisci between neighboring grains. The effects of these forces depend on the degree of saturation of the medium. For low water content levels corresponding to disconnected liquid bridges between grains, capillary theory allows the force induced by those bridges to be linked to the local geometry of the grains and to the matrix suction or capillary pressure inside the medium. As long as the water does not percolate, it is interesting to use DEM to simulate the water effects in the pendular regime, by adding extra forces between the discrete elements which represent the presence of capillary menisci at contacts and study their consequences in terms of force and water volume. Note that the pendular regime starts when the water phase is no longer continuous (see Figure 13). In the DEM, each liquid bridge is assumed to connect only two particles.

![Figure 12: Synthesis of cones of unstable stress directions in the axisymmetric plane of stresses computed from a loose specimen; full circles represent stress probes for which no vanishing or negative values of second order work were found (from Sibille et al. 2007)](image)

Therefore, two types of forces coexist within the granular medium. For dry contacts, a contact force develops between contacting discrete elements. This repulsive force, which is a function of the relative motion between the contacting grains, is usually well described by an elastoplastic contact model. For water bonded particles, a specific attractive force exists. This water-induced
attractive interaction can be described by a resulting capillary force, and is a function of the bridge volume, of the size of particles, and of the fluid nature.

\[ F_{\text{cap}} = 2\pi y_0 \gamma + \pi y_0^2 \Delta \mu, \]  

(10)

where \( \gamma \) is the surface tension of the liquid phase and \( \Delta \mu \) is the capillarity pressure. Triaxial compression test simulations have well reproduced the increase of the shear strength due to capillary effects (Figure 14) and their influence on the Mohr-Coulomb failure criterion (Figure 15). The results also suggest that, in partially saturated materials within the pendular regime, the effects of pore fluid are adequately represented by a discrete distribution of forces rather than by an averaged pressure in the fluid phase. Indeed, as a representative quantity of the pore fluid distribution inside unsaturated materials, this suction associated stress tensor indicates that pore fluid has its own fabric which is inherently anisotropic and strongly dependent on the combined loading and hydric history of the material. This tensorial nature of water in unsaturated material implies suction to produce shear effects on the solid phase. This suction-induced shear effect consequently makes it difficult to associate an isotropic quantity to water as expressed in Bishop’s effective stress. Pore pressure is no longer an isotropic stress in unsaturated soil, and therefore, cannot be considered as an equivalent continuum medium (Scholtès et al. 2009a). DEM analyses also confirm that suction is a pore-scale concept, and that stress definitions for unsaturated soils should also include microscopic intergrain stresses as the ones resulting from capillary forces (Scholtès et al., 2009b). The DEM appears to be a pertinent complementary tool for the study of unsaturated soil mechanics. More precisely, discrete methods should convey a new insight into the discussion about the controversial concept of generalized effective stress by relating basic physical aspects to classical phenomenological views.
Figure 14: Deviatoric stress and volumetric strain versus axial strain curves obtained from triaxial tests at different saturation degrees under a constant confining pressure (10 kPa) (from Scholtes et al., 2008a)

Figure 15: Mohr–Coulomb failure criterion under dry and unsaturated conditions (from Scholtes et al., 2008a)

DEM and saturated soils

In saturated soils, interaction with fluid influences the way solid particles move through fluid. The fluid equations of motion are usually solved by standard Computational Fluid Dynamics (CFD) models (Tsuji et al. 1993), in the form of either finite difference based techniques or finite volume based techniques (Munjinza 2004). Both finite volume and finite difference techniques use discretization of the spatial domain to approximately satisfy the governing equations in integral form. Finite difference and finite volume based CFD techniques are based on Eulerian formulation (Kawagushi et al. 1998).
Figure 16: Continuum-discrete model (from Zeghal and Shamy 2008)

The essence of this formulation is that the grid is fixed in space and does not move with particles of fluid. The CFD grid comprises grid points fixed in space and fluid particles moving relative to these grid points, while the Discrete Element Method comprises grid points moving together with solid particles (Figure 16). The coupling of the two, requires a Lagrangian grid to be superimposed over the Eulerian grid. As the solid particles are by definition loosely packed, and most of the domain is filled by the fluid, the primary grid is the Eulerian CFD grid. As a consequence, the primary solver is the Eulerian CFD solver. Thus, these are in essence CFD problems. The influence of fluid on the motion of solid particles is obtained through transferring the fluid pressure and drag forces onto the discrete elements. There are two approaches available to take into account the influence of solid particles on the CFD model:

- Resolving the interaction of each individual particle with the fluid.
- Averaging the interaction between solid particles and the fluid through introduction of solid ‘density’ (see Munjinza (2004) for more details).

Coupled continuum-discrete hydro-mechanical models are for example used to analyze the liquefaction of saturated granular soils in loose and cemented deposits. Recent numerical simulations were conducted to investigate the response of saturated granular deposits when subjected to a dynamic base excitation (El Shamy and Zeghal 2007), see Figure 17. It was shown that in a case of a loose granular deposit and from a micro-mechanical point of view, the liquefaction process started near the surface and propagated downward. Moreover, in case of a weakly cemented granular deposit, which is a commonly used configuration to mitigate site liquefaction hazard, it was seen that the medium did not liquefy even when the pore pressure ratio approached 1.0 in view of the cohesion provided by the interaction forces acting between the discrete elements.
APPLICATION TO ROCK MECHANICS

Fracturation process

Although rocks do not look like granular materials, within DEM this material is represented as an assembly of discrete elements linked together by cohesive frictional forces with a tensile threshold. The basic idea is to reproduce the brittle behavior of rocks by simulating the initiation, propagation and interaction of local cracks. These cracks are initiated when the interaction force between two discrete elements exceeds its tensile or shear strength, depending on the local stress conditions. When local cracks coalesce, they form a large discontinuity (which can be defined as a macro-crack), which can propagate when new micro-cracks occur at its tips (see Figure 18). One of the major advantages of DEM is that the fracturing process occurring within the rock mass can be modeled without any assumptions where and how cracks may appear.

Using a 2D DEM model, Potyondy and Cundall (2004), simulated biaxial and Brazilian tests of Lac du Bonnet granite and showed that the DEM was capable of reproducing many features of rock behavior, including elasticity, fracturing, damage accumulation producing material anisotropy, hysteresis, dilation, post-peak softening and strength increase with confinement.
Figure 18: Stress–strain response and damage patterns formed during biaxial tests at confinements of 0.1, 10 and 70 MPa, using a 2D granite model: (a) Stress-strain response; (b) Post-peak crack distribution, $\sigma_3 = 0.1$ MPa; (c) Post-peak crack distribution, $\sigma_3 = 10$ MPa; (d) Post-peak crack distribution, $\sigma_3 = 70$ MPa (from Potyondy and Cundall 2004).

However, the model presented some limitations. The material strength matches that of Lac du Bonnet granite only for stresses near the uniaxial state—i.e., the tensile strength was too high, and the slope of the strength envelope as a function of confining stress was too low. An explanation given by the authors was that “there is evidence to support the postulate that including complex-shaped, breakable grains of a size comparable to that of the rock will remove this limitation” (Potyondy and Cundall 2004).

Thus, a key point concerns the discrete element size effect. It was found in 2D (Potyondy and Cundall 2004), that the fracture roughness depends on the radius of the discrete elements. This implies that when modeling damage processes, for which macroscopic fractures form, the particle size and model properties should be chosen to match the material fracture toughness as well as the unconfined compressive strength. Indeed, for a 2D cubically packed model, the mode-I fracture toughness was found to be:

$$K_{IC} = \sigma'_t \sqrt{\pi R},$$  \hspace{1cm} (11)

where the tensile strength of the model is $\sigma'_t = \phi_n / 2Rt$, with $\phi_n$ being the contact-bond tensile strength, $R$ the Discrete element size and $t = 1$ for a 2D problem. This poses a severe limitation on the size of a region that can be represented with this kind of model, because the present micro-
property characterization is such that the particle size must be chosen to be of the same order as
the grain size. However, in 3D, this limitation disappears, since $t=R$, leading to a fracture
roughness $K_I$ expression which would be independent of the discretization size (Shiu et al. 2008).
However, further investigations need to be done to confirm this independency. Note that a general
approach to measure fracture toughness under random packing of non-uniform size particles, has
been developed recently (Moon et al. 2006), where the energy balance approach and the
collocation method, were introduced to determine fracture toughness. In solving the critical
equilibrium state of a circular disc with a central crack, the results of both methods are in
agreement with the critical stress intensity factor obtained by Yarema & Krestin (1966).

Rather than just following the stress or strain responses of DEM models, a possible
evaluation of the capability of the DEM to reproduce the fracturation process in stiff rocks is to
use the Acoustic Emissions (AE) recorded during laboratory testing of rock samples. This can
provide significant information on the local-mechanics of failure processes (Lockner 1993).
Information about the onset and propagation of micro-cracking and fracture in rock samples
subjected to different stress regimes can be determined by recording the time and location of AE
during the test. Using the DEM, any bond breakage is identified as a micro-crack. The location of
the crack is assumed to be the contact point between two discrete elements, and the crack
orientation is assumed to be perpendicular to the line joining the particle centers. Doing so,
Hazzard and Young (2004), have shown that in the case of the 3D axial compression numerical
test to simulate Lac du Bonnet granite, AE were located randomly throughout the sample prior
to the peak stress but localized along inclined planes as the sample failed. This mechanical process
agrees with the observations from laboratory carried out on the same rock material.

Fractured rocks

When the rock mass exhibits pre-existing fractured patterns, the model needs to deal with
numerous internal discontinuities. The influence of sliding and separation along these joints is
difficult to tackle with equivalent continuum models, thus deformation characteristics cannot be
modeled realistically where joint sliding is a dominating factor for rocks (Wittke 1990, Sitharam
and Madhavi Latha 2002). Discrete modeling, which enables to model the rock mass as intact
rock and joints, have been widely used for example, to simulate tunneling through blocky rock
masses (Bhasin and Hoeg 1997a; Bhasin and Hoeg 1997b; Shen and Barton 1997; Ferrero et al.
2004). The behavior of the blocky rock mass can be evaluated considering joint sliding, opening
and detachment of blocks. In the discrete element numerical simulations, the properties of the
discontinuities are directly considered and this provides a better way to assess the global response
of the fractured rock mass. For example, it has been seen that the deformation patterns and failure
mechanisms around tunnels are generally found to be in good agreement with the orientation and
strength properties of discontinuities (Solak 2008).
Figure 19: Stability assessment of South East / East rock corner slope of the Acropolis Hill in Athens, using 3DEC. On the left, topography of the corner, including the main wall; on the right, planar segments correspond to the main discontinuities observed at surface where the A and B blocks might fall (Stefanou and I. Vardoulakis 2005).

When using DEM to study the stability of 3D fractured rock masses, usually a continuum block is considered and it is cut into a number of discrete blocks by faults or joints the geometry of which is defined by piecewise planar segments (see Figure 19 as an example). These segments are then assigned constitutive properties. External boundary conditions can be applied to the assemblage while internal block boundary conditions are calculated from the interactions at their contacts, which allow pre-existing faults to be modeled explicitly. Since DEM approach an explicit finite difference time scheme to solve equations of motion, these equations need to be damped to compute a static equivalent stress field. To do so, very small time steps are used to move blocks according to unbalanced force gradients and a new equilibrium is reached when unbalanced forces are reduced to zero. The time step is selected to maintain numerical stability during this process and does not correspond to an absolute time period. In conventional static models, the equilibrium condition is reached using constant initial boundary conditions and this solution scheme is used to obtain the block displacements, and hence stress state. Here, when the state of stress needs to be determined for joints at the limit of stability, the generally used solution scheme is: after hydrostatic loading, boundaries are moved and fault slip occurs when stresses resolved on fault segments exceed joint strength. This pseudo-static equilibrium is maintained by adjusting the boundary block velocities to maintain the maximum block unbalanced forces within a low range (Baird and McKinnon 2007). This approach can be used for engineering-scale problems such as mine design or slope stability, e.g. McKinnon and Garrido de la Barra (2003).

An alternative to the finite difference procedure and one-by-one relaxation sequence, is to use the Discontinuous Deformation Analysis (DDA), which is based on block theory and the minimum energy principle. Originated by Shi and Goodman (1985), it was further developed for coupled stress-flow problems (Jing et al. 2001). The method uses standard Finite Element Method meshes over blocks and the contacts are processed using the penalty method. Note that similar approaches were also developed, see for example Barbosa and Ghaboussi (1990), which uses four-noded blocks as the standard element, and was called the discrete finite element method.
Another similar development, called the combined finite-discrete element method (Munjiza et al., 1999), considers not only the block deformation but also fracturing and fragmentation of the rocks. However, in terms of development and application, the DDA occupies the front position for rock engineering (Jiao et al. 2007). DDA, which is an implicit method, has two advantages over the explicit DEM: relatively larger time steps; and closed-form integrations for the stiffness matrices of elements. An existing FEM code can also be readily transformed into a DDA code while retaining all the advantageous features of the FEM (Jing and Hudson 2002). The DDA was also extended to handle three-dimensional block system analysis (Shi 2001). The code development has reached a certain level of maturity with applications focusing mainly on tunneling, caverns, fracturing and fragmentation processes of geological and structural materials and earthquake effects (Jing and Hudson 2002).

Similar to the DEM, but without considering block deformation and motion, is the Key Block approach, initiated independently by Warburton (1993) and Goodman and Shi (1985), with a more rigorous topological treatment of block system geometry in the latter. This is a special method for analysis of stability of rock structures dominated by the geometrical characteristics of the rock blocks and hence the fracture systems. It does not utilize any stress and deformation analysis, but identifies the ‘key blocks’ or ‘keystones’, which are formed by intersecting fractures and excavated free surfaces in the rock mass which have the potential for sliding and rotation in certain directions. Key block theory, or simply block theory, and the associated code development have applications in rock engineering, with further developments using Monte Carlo simulations and probabilistic predictions (Mauldon 1993; Hattzor, 1993) or water effects (Karaca and Goodman, 1993). Predictably, the major applications are in the field of tunnel and slope stability analysis, as reported by Lee et al., (2000) or Jing and Hudson (2002).

**Fractured rocks with circulating fluid**

Water plays a major role in the behavior of rocks. Its contribution has been under discussion for a long time (Logan 1992), but despite intensive numerical developments, the interpretation of the field observations remains difficult. Usually, the problems of fluid flow through fractured rocks are most often dealt with by discrete approaches such as combinations of DFN with classical DEM (see Figure 20) (Baghbanan and Jing 2008) or DDA methods (Jing & Stephansson 2008). However, there is also the case where, fracturing and fragmentation is the result of the interaction of a fluid with a fracturing rock. A typical example of this type of problem is the hydro-fracturation. The fluid exerts pressure onto the free surface of the solid, causing the solid to accelerate, deform, fracture and displace with velocities that change with time. Thus, as noted by Mujinza (2004), there are two aspects to this coupled problem:

- the evaluation of fluid pressure as the surface load for a solid,
- the deformability, fracture and fragmentation of a solid under fluid pressure.

From these two distinct aspects, full scale fluid flow models can be classified as follows:

- First, models based on tracing fluid flow through individual cracks. They require robust crack detection algorithms, which also incorporate procedures for the detection of connectivity between individual cracks and voids. These procedures
have proven much more difficult than the detection of contacts between solid particles. This is because the geometry of solid particles is readily available, while the geometry of voids is only implicitly defined and has to be deduced from the geometry of solid discrete elements. In these models, fluid penetration into the cracks and the spatial gradient of fluid pressure are taken into account through a set of problem parameters such as fluid penetration depth, see for example, Jing & Stephansson (2008). A combined finite-discrete element modeling has been proposed by Munjiza to solve this problem (Munjiza 2004).

\[
\sigma_{\text{horizontal}} / \sigma_{\text{vertical}} = 1, \quad b) \sigma_{\text{horizontal}} / \sigma_{\text{vertical}} = 3 \quad \text{and} \quad c) \sigma_{\text{horizontal}} / \sigma_{\text{vertical}} = 5
\]

(from Baghbanan and Jing 2008)

- Second, models based on porous media-based idealization of fractured solid. The fracturing solid is approximated by a porous medium requiring an estimation of the porosity. The errors arising from this process and the extent to which the final results are influenced by transient geometry of the fracturing solid are not easy to estimate (Munjiza 2004). Full scale fluid flow models are also coupled with considerable algorithmic complexities and extensive CPU requirements. To avoid these limitations when the fluid fraction amount remains low enough, a hybrid formulation for coupled pore fluid-solid deformation problems has been proposed by Sakagushi and Mühlhaus (2000) to tackle this problem (see for example Figure 21).
APPLICATION TO CONCRETE MATERIAL MECHANICS

Here again, the complex constitutive behavior of concrete, arising from extensive micro-cracking and macro-cracking, is difficult to characterize in terms of a continuum formulation. A numerical model of concrete should embody a suitable procedure to deal with the initiation and propagation of cracks and their effects on the overall behavior of concrete media. Discrete models, which take directly into consideration the physical mechanisms and the influence of the concrete aggregate structure, offer an interesting tool to model fracture in concrete. Extensive work has been done to develop lattice models to study fracturing process in concrete material in tensile mode, see for example, Van Mier et al. (2002). However, these models suffer from limitations when studying concrete in compressive mode, because no new local boundaries are generated during the deformation process. DEM models overcome this limitation and can be used in a more general manner.

Meso-scale description of concrete

It has been shown that the DEM can be used to model a granular material, when discrete elements represent a grain, see for example Thornton (2000); in this case, the characteristic size of the model is well defined. A quite complete approach using DEM should represent both, aggregates and cement paste, which is qualified as a meso-scale description. One possible strategy to set up such a model is to first generate the aggregate structure with high porosity, followed by the cement paste structure (Monteiro Azevedo et al. 2008), see Figure 22.
Figure 22: Particle assemblies – from the aggregate structure to the final compact assembly: (a) Circular aggregate, (b) Aggregate discretization and (c) Compact assembly (from Monteiro Azevedo et al. 2008).

According to this kind of model, the aggregate can be represented either as a rigid macro-element or as a deformable group of elements. It has been shown by Monteiro Azevedo et al. (2008) that aggregate deformability, together with the consideration of pure friction contacts working under compression, increases the fracture energy in compression. Whereas, the use of a softening interaction law, by adding a higher capability of load redistribution, led to a more ductile response under tension. This direct description of the mechanical interaction between aggregates and the cement matrix brings crucial insights in the understanding of local phenomenon, however, concrete fracture has a clear 3D effect and this approach, which deals with a fine description of the aggregate nature of concrete, remains too costly to be used in a three dimensional framework. Thus, the use of DEM to study concrete material in 3D requires some assumptions. Many authors have used the DEM to simulate granular materials at a higher scale (Cundall and Strack 1979; Potyondy and Cundall 1996; Donzé and Bernasconi 2004), i.e. the size of an element is higher than the real grain size, and for these cases, the discrete approach also gives interesting information on the local behavior (Meguro and Hakuno 1989).

Using the DEM to tackle physical problems for real structures becomes a real challenge since billions of discrete elements would be needed to represent all grains, which would induce a totally prohibitive computational time. For this configuration, i.e. working at a higher scale model, the use of the DEM consists in considering, that a discrete element represents a large amount of real grains. By doing so, the local parameters must be chosen to predict the mechanical behavior of a granular material studied at a chosen macro scale.

Macro-scale description of concrete

When using the DEM to represent a concrete structure, the local constitutive parameters are assigned to each of the interaction force between the elements, such that the macroscopic behavior of the entire set of discrete elements is representative of the real material at the macro-scale. To assign the values of the local constitutive parameters, a calibration procedure can be used (Hentz et al. 2004a; Hentz et al. 2004b; Belheine et al. 2009). It is generally based on the simulation of quasi-static uniaxial and triaxial compression/traction tests. For example, a compression test model was developed (Shiu et al. 2008) in YADE (Kozicki & Donzé 2008) for a standard-sized specimen, with the following characteristics:

- a compact, polydisperse discrete element set is generated,
- an elastic compression test is run with local elastic parameters given by the "macro-micro" relations (Hentz et al. 2004b),
compressive rupture axial tests are simulated to deduce the plastic local parameters.

Figure 23 shows the results of the simple compression test. The numerical simulations fit well to the experimental ones. By performing these tests, the local parameters have been calibrated. However, simple uniaxial compression tests are not sufficient to obtain the full plastic response. Examples of triaxial tests are presented in the next paragraph.

![Figure 23: Strain-stress curves of the uniaxial compression test. The plain red curves correspond to the experimental test (from Vu et al. 2008) and the blue dashed curves to the DEM modeling (from Shiu et al. 2008)](image)

Note that to keep calculation costs as low as possible when dealing at the structure scale, spherical discrete elements are often used to represent the concrete material. In this case, the numerical implementation of the contact detection and resolution algorithms remain simple and fast. However, the major drawback of using spherical geometry is that excessive rolling occurs during shear displacement and such models underestimate the value of the friction angle as compared to real geomaterials. This is why a moment transfer needs to be added to the local constitutive law of spherical DEM in 3D (Iwashita and Oda 1998; Plassiard et al. 2008).

Working at the structure scale also imposes that the discretization, i.e. the size of the discrete elements, has little influence on the global response of the system. This property is particularly important in the present case, since the model is used at a macro-scale and it is of great concern that the results do not depend on the model resolution, which is often imposed by the computation capabilities; see for example Shiu et al., (2008) for an attempt at minimizing this discretization dependency.

**Concrete material at high confining pressure**

Using solely local elastic-brittle or even elastic-perfectly plastic constitutive laws is not sufficient to reproduce quantitatively the behavior of concrete for high confinement loadings, especially when compaction processes occur (Hentz et al. 2004a). An attempt has been made to develop a local elastic-bilinear hardening-damage constitutive law in order to capture the local compaction process which cannot be taken into account intrinsically, when using a dense packing
of non-deformable discrete elements (Shiu et al. 2008). This can be formulated as follows: if the normal interaction distance between two linked DE exceeds the elastic limit distance \( D_i \) in compression, then a hardening plastic behavior takes place (Section BC and CD on Figure 24), which is characterized by two successive stages. These two stages involve two different stiffness coefficients controlled by two ratios \( \zeta_1 \) and \( \zeta_2 \), representing the observed response of the concrete material at extreme loading conditions (Gabet et al. 2008). Note that, in section BC, the unloading path follows an irreversible behavior controlled by a softer coefficient \( K_{\text{unload}} \).

The tensile part (section AE on Figure 24) uses the same tangent module \( K_n \) as the compressive section AB. After the tensile force has reached its maximum value, \( F_{\text{max}} \), which is calculated by

\[
F_{\text{max}} = F_{c1} \gamma_t
\]

where \( F_{c1} \) is the maximum elastic compressive force and \( \gamma_t \) is an amplified factor to control the value of \( F_{\text{max}} \), a softening behavior will occur with a modified tangent stiffness \( \frac{K_n}{\zeta} \), where \( \zeta \) is the softening coefficient (See Figure 24).

If the interaction distance exceeds the rupture distance \( D_{\text{rupture}} \), then the interaction force is equal to zero: the cohesive link breaks.

![Figure 24: Local normal interaction force for discrete elements representing concrete for high confining pressure.](image)

The constitutive parameter values were set using a series of compressive experiment tests on concrete, which were carried out with a high confinement triaxial cell (Gabet et al. 2008). The maximum confining pressure was about 1 GPa which is close to the maximum pressure which can be expected in the impacted area.

It is thus necessary to calibrate the plasticity stiffness ratios \( \zeta_1 \) and \( \zeta_2 \), with a hydro-static test at a high confining pressure. The 650 MPa test was used as comparison. The result is shown in
Figure 25. Using the same elastic parameter as in the uniaxial compression test, the numerical result agrees well with the experimental test.

**Figure 25**: Hydro-static test with a confinement of 650MPa (left) to set up \( \zeta_1 \) and \( \zeta_2 \) values; \( \varepsilon \) corresponds to the axial loading. Triaxial test after a 500 MPa hydro-static confinement (right); \( \varepsilon_1 \) and \( \varepsilon_2 \) correspond to the axial and the lateral deformations respectively. For both graphics, the plain red curves correspond to the experimental test (From Gabet et al. 2008) and the blue dashed curves to the DEM modeling (from Shiu et al. 2008).

### Concrete loaded at high strain rate

One of the main features of concrete dynamic behavior, that a model must reproduce, is the significant increase of the apparent concrete strength with the strain rate. The understanding of this rate effect has been the subject of a number of experiments, as well as of numerous models. The ratio dynamic strength over static strength seems to be rather more rate-sensitive in tension than in compression. On the other hand, it now seems clear that the strain rate effect at least when \( \dot{\varepsilon} \leq 10 \text{s}^{-1} \) is explained by the presence of free water in concrete, inducing an effect similar to the Stefan effect (Rossi et al., 1994). For higher strain rates, the situation is not as clear: in tension, some new insight was gained recently (Hild et al. 2003) and in compression, Janach (1976) proposed the hypothesis that the effect of bulking combined with inertia was responsible for the increase of load-carrying capacity of the specimen, making it a structural effect. The aid of the DEM was used to confirm this last hypothesis. Split Hopkinson Pressure Bar tests were simulated (Donzé et al. 1999), at strain rates ranging from 350 to 700 \text{s}^{-1} (see Figure 26).

**Figure 26**: On the right, setup for a Split Hopkinson Pressure Bar experiment and on the left, the recorded data on both sizes of the sample (from Donzé et al. 1999)

The concrete apparent strain rate sensitivity is well represented, and this, without requiring the use of any viscosity or characteristic time in the model (see Figure 27). With the discrete
element method the transient phenomena (stresses, damage) in the specimen during and after impact can be investigated.

**Figure 27:** Stress-strain curves for different loading rates: plot (a) is for 350 s\(^{-1}\), plot (b) is for 500 s\(^{-1}\) and plot (c) is for 700 s\(^{-1}\). The dotted lines are the experimental curves and the solid lines are the numerical curves (from Donzé et al. 1999)

This confirmed the inertia-based hypothesis: In this range of strain rates, the increase of load-carrying capacity of concrete comes from the transition from a state of uniaxial strain to a state of uniaxial stress, associated with bulking; it is a structural effect (Figure 28).

**Figure 28:** On the left axial cut of the numerical sample. The darker the discrete elements get, the more cohesive links they have lost (damage indicator). On the right, a simplified unloading process proposed for cylindrical specimen which fails by brittle fracture in SHPB compressional tests (from Donzé et al. 1999)

Then simulations of tensile SHPB tests were run, at strain rates ranging from 36 to 70 s\(^{-1}\). Unchanged, the model did not show any strain rate dependency, but an increase of the local tensile strength is enough to fit the experimental results. This finding tends to show firstly that inertia alone cannot explain the increase of strength in this range of strain rates, and secondly that in tension, the rate sensitivity is more a material intrinsic effect. This could justify the introduction of a local discrete rate dependence law. The pattern, the number and the positions of the ruptures are accurately simulated, as well as the increase of strength (Hentz et al. 2004).
CONCLUSION

The purpose of this article is to provide a brief overview of DEM applied to the study of geomaterials. The main discrete elements methods, i.e., the molecular dynamics based approach and the contact dynamics approach, were first presented before addressing the extensions and the applications of these methods for soil, rock and concrete materials. Note that only non deformable discrete element methods were considered, since they do not need any continuum assumptions to describe the material (as opposition of the DDA method, which consider the deformation if the discrete elements using a continuous formulation).

It has been seen that the use of DEM for complex responses of geomaterials could bring new ways to study the behavior of these highly heterogeneous media, however, some important issues remain. Some of them are outlined below:

- DEM can be used to describe a mechanical problem at the grain scale but it can also be used at the structure scale because of its capability to describe, in a very natural and simple way, the nucleation and growing process of discontinuities. In this latter case, it has been seen that the discrete element represents a volume of matter and not a grain anymore and to limit the characteristic size dependency, the formulation of the local constitutive laws can be chosen to be dependent on the discrete element size. However, the contribution of these assumptions on the localization of the deformation needs to be examined in more details. Moreover, there remains the question of what the limits are of such an approach when dealing with highly dynamical events, since inertial effects of the discrete elements play a major role on the system response.

- What are the limits of representing soil, rock and concrete materials with spherical discrete elements? For example, an artifact introduced with this spherical geometry, is a resulting numerical porosity, which differs from the real porosity. This combines with the fact that the elements are non deformable and have a different size scale than real grains which leads to cross effects with the local constitutive law on the macroscopic behavior. It is a challenging difficulty because with this very simple geometry the calculation cost remains low and large systems can then be simulated.

- Related to the previous remark, there is a need for relationships between the local/macroscopic constitutive laws, depending on the numerical porosity and the shapes of the discrete elements. Presently, only a calibration procedure can be done to propose local constitutive parameters to ensure a “roughly” correct macroscopic response. However, building these relationships using only data obtained from classical geomechanical tests (like triaxial tests) seems hopeless to assign a single solution set. New investigation tools such as tomography (Landis 2006) would provide additional information to improve the model formulation.
As pointed out by Jing and Stephansson (2008), the effects of fluid flow in DEM models are not commonly considered, due to the complexity in numerical processing of fluid–solid interactions. Considering fluid effects demands intrinsic coupling, at the pore scale, between the pore fluid and the skeletal structure represented as solid particles in the particle models with challenging requirements for detailed characterizations of structure and connectivity of the pores and deformability of the skeletons. This development is just starting and there is a need to take into account fluids in geomaterials since their presence have a major effect on geomaterial responses.

Despite the outstanding issues as highlighted above, DEM for modeling mechanical behavior of geomaterials is growing fast, not only in research but also in geotechnical engineering. This is because it naturally exhibits localization, a phenomenon which is difficult to represent in a continuum model that uses a mesh. The last advances have shown that DEM reproduces the results expected from well established theory, like fracture mechanics, for example, but also bringing new explanations for the geomaterials’ behavior.

REFERENCES


