Recent developments and future trends in distinct element methods – UDEC/3DEC and PFC codes

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ABSTRACT: The Distinct Element Method was proposed by Cundall in 1971 as a numerical technique to study rock mechanics problems, based on the representation of a rock mass as a system of blocks or particles. In recent years, the concepts underlying such 'discontinuum' approaches were adopted in numerous other fields, and a multitude of formulations and codes were developed by many researchers. In this paper, the characteristic features of the codes UDEC/3DEC and PFC, ultimately descending from Cundall's original ideas, are analyzed with reference to various recent applications, within the global context of discrete element modeling. Modeling needs and trends of development in this field are finally discussed.

1 INTRODUCTION

The designation 'Discrete Element Method' (DEM) applies today to a wide class of numerical methods aimed at the simulation of the physical behavior of systems of particles, grains or blocks. The multiplicity of techniques, formulations, terminology and codes which can be included in this class is mainly a consequence of the historical development of these methods, in marked contrast with the finite element method (FEM). The latter's derivation from continuum mechanics allowed it to be consistently formulated as a numerical approximation of well-established differential equations. The existing continuum theories provided, in addition, a set of closed form solutions for validation of the numerical results, and for benchmarking the various codes. DEM followed a very different path, from the outset attempting to address problems that the continuum codes could not handle adequately, and for which no accepted theory existed. The representation of the interactions of the blocks or particles was designed mostly in an empirical manner, without reference to theoretical concepts, and the solutions of the various problems encountered in the development of the codes were reached in a pragmatic way, in order to solve specific applications. As a result, we have today an array of different DE methods, still in many ways marked by their origins and field of application.

Rock mechanics was one the fields of early DE model development, the major motivation being the discontinuous nature of fractured rock masses. For example, rock slope stability depended essentially on the frictional interaction between the blocks, not continuum deformation analysis, either elastic or plastic. Blocks could be assumed rigid given the low stresses involved, but failure mechanisms involved large movements and changes in block contact locations which invalidated the small displacement assumptions common in early numerical models. Conceptual models beyond continuum mechanics existed, e.g. the "clastic mechanics" proposal of Trollope (1968), but the analytical solution procedures limited their practical application. Cundall (1971) devised a general numerical solution technique capable of materializing the block assemblage concept, based on the time integration of the equations of motion of each block. The modeling of mechanical contacts between the blocks, which could now be assumed perfectly rigid, and the methods to detect them, completed the novel features of the designated 'Distinct element method'. Large displacement analysis became manageable, with the system connectivity automatically updated during a simulation, as some contacts break and new ones are formed as a consequence of the evolving geometry (Figure 1).

Discrete element concepts and methods have expanded considerably in recent years to a multitude of fields in science and engineering, where many related numerical techniques were developed for specific purposes. Discontinuous Deformation Analysis (DDA), Manifold Method (NMM), Discrete-Finite Elements (DFEM), Non-Smooth Contact Dynamics (NCSD), Molecular Dynamics (MD) and others methods, to be found in the proceedings of this conference or in the technical literature, all share the common concept of a "discontinuum". Underneath the differences in terminology, and the variety of numerical formulations, there are many common approaches, for example, to the representation of the mechanical contact between particles, or to the internal discretization of blocks to obtain complex deformation patterns. More instructive than comparing different methods or computer packages globally is to inspect specific components, examining the physical and constitutive assumptions employed and the way they are implemented numerically. This type of study will contribute to the necessary consolidation of concepts in the DE community, and assist the sharing of knowledge gained in different research areas. It is also important to accompany the new developments achieved by those researchers that continue to work under the FEM umbrella, such as contact-impact formulations, joint elements and strong embedded discontinuities, lattice models, XFEM, particle finite elements, and many others techniques that relate to the analysis of discontinuous systems.

This paper focuses on the line of DE model development following Cundall's approach, which led to the UDEC, 3DEC and PFC codes (Itasca 2007, 2008a,b, 2011). While the 'distinct element method' may be regarded formally as a sub-set of the 'discrete element' class, the two designations are used as synonyms by many authors, and this practice will be followed in this paper. Selected recent applications in various fields are discussed, with an emphasis on geomechanics modeling. Trends of future development and outstanding issues are finally addressed, both in terms of the physical and engineering problems that need to be solved, and of the computational aspects and code user requirements.

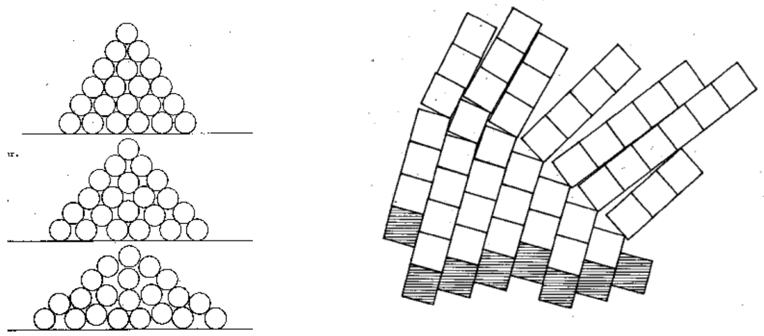

Figure 1. Two examples from Cundall's 1971 paper on the distinct element method: pile of disks and toppling failure mode of rock slope.

2 A REVIEW OF APPLICATIONS

2.1 *Fracture of geo-materials*

Rock mechanics is perhaps the field where a larger variety of DE models has been applied (e.g. Jing & Stephansson 2007). While the early efforts were intended to address engineering problems at the field scale, the potential of DE models to simulate the rock behavior at the scale of the lab test was soon recognized. The main motivation of the 2D circular particle code BALL presented by Cundall & Strack (1979) was to address the micro-mechanics of soils and other granular materials. However, by applying cohesive bonds between the particles, and letting them break in tension or shear, the same numerical formulation became the choice tool to study rock fracture, in the form of the bonded-particle models (BPM) (Potyondy & Cundall 2004). The random nature of the assemblies simulates the natural arrangement of grains in the rock matrix. Based on elementary constitutive laws governing the interaction between the rigid particles, complex forms of behavior develop, to be checked against experiments. In this active research field, developments on outstanding issues, such as the triaxial test behavior, are under way to improve the performance of bonded particle models (e.g. Cho et al. 2007, Potyondy 2010).

The fracture behavior of other geo-materials, such as concrete, may also be approached by these models, with different particles representing the aggregate and the cement paste (Azevedo & Lemos 2005). These authors introduced a general contact formulation for transmission of forces and moments between particles based on multiple contact points, as an alternative to the standard parallel bond model in PFC, which allows the progressive extension of the bond fracture between the two particles.

Analysis of the fundamental processes taking place during lab tests of rock joints have also been addressed. For example, Figure 2 (left) shows a very detailed particle model employed by Asadi & Rasouli (2011) to study the fracture patterns during shearing of a synthetic profile joint.

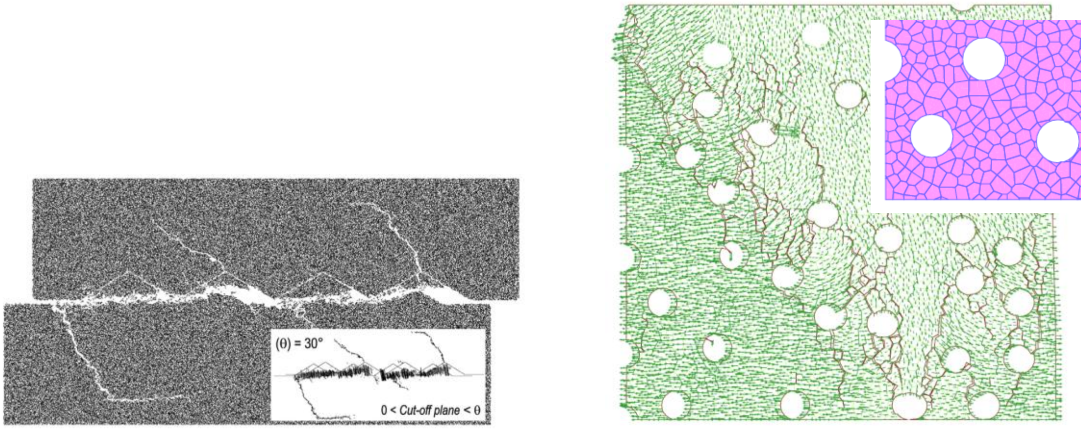

Figure 2. (left) Particle model of shear test of synthetic rock fracture profile (Asadi & Rasouli 2011); (right) UDEC model of uniaxial compression test on lithophysal tuff specimen (Damjanac et al. 2007).

Polygonal block models, while computationally more costly, are perhaps capable of a closer representation of the rock matrix structure. They are more demanding, mainly because the contact calculations between polygons involve many more operations than those in circular particle codes. Various authors have nevertheless obtained very interesting results of fracture analysis with UDEC models. Damjanac et al. (2007) studied the micro-mechanical behavior of lithophysal tuff specimens with both particle (PFC) and block (UDEC) models (Figure 2).

Lan et al. (2010) represented the microstructure of brittle rock by means of a deformable polygonal grain-like assembly, to study the effect of heterogeneous grain deformability. Kazerani & Zhao (2010) used both Voronoi and Delaunay block assemblies in order to match experimental results of triaxial and Brazilian tests of rock specimens (Figure 3). Expanding the model size from lab test to field scale, while still difficult, is becoming feasible. Alzo'ubi et al. (2011) have studied the buckling failure of rock slopes with inclined layers with a UDEC model.

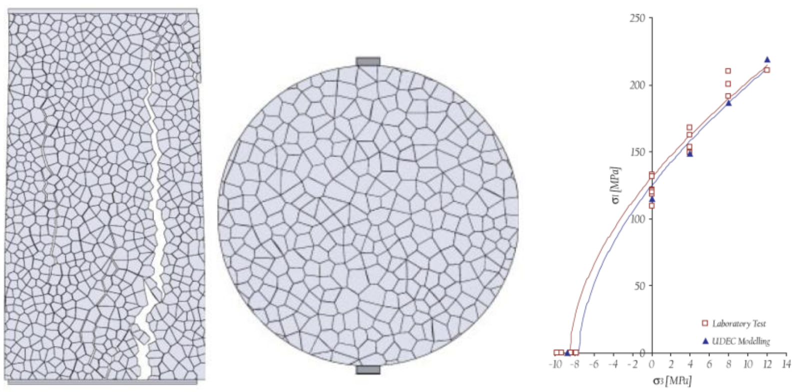

Figure 3. Rock specimens based on Voronoi polygons for simulation of uniaxial compression and Brazilian tensile tests and comparisons with experimental results (Kazerani & Zhao 2010).

Most numerical fracture studies of rock lab tests to date only attempted to replicate the quasi-static response. The interest in dynamic fracture, however, has grown significantly (e.g. Zhao et al. 2011). Contact constitutive models capable of addressing dynamic rock fracture were implemented by Kazerani (2011), and tested in UDEC models.

2.2 *The synthetic rock mass (SRM) concept*

When going from the lab test to the field scale, the influence of rock macroscopic discontinuities comes into play. The rock joint structure may be represented in particle models by means of the Synthetic Rock Mass concept (SRM). A discrete fracture network (DFN) is overlaid on a particle assembly, thus partitioning it into a system of grains or blocks formed by bonded circular particles (Figure 4) (Pierce at al. 2007). Different properties are assigned to the bonds of the contacts between particles belonging to the same block, representing the intact rock material, and to the contacts between adjacent blocks, representing the joint behavior. The key to this approach lies in Cundall's Smooth Joint Model (SJM), applied to the inter-block contacts. Even if the interface is not an exact straight line, the SJM logic forces these contacts to adopt a common normal, leading to a smooth sliding governed by a prescribed friction angle. Otherwise, the very irregular nature of the contact surfaces would lead to unrealistic friction and dilation values.

Figure 4. Synthetic rock mass (SRM) model (Pierce et al. 2007).

Mas Ivars et al. (2008) have created a SRM with PFC3D to study scale effects in jointed rock masses. The anisotropic response and the trends in tensile and compressive strength variation were investigated by performing a series of numerical tests on samples of various sizes (Figure 5). Starting with a model of a 80x40x40 m region, and then cutting it into smaller specimens, allowed a series of UCS tests, providing the trends in strength variation with sample size.

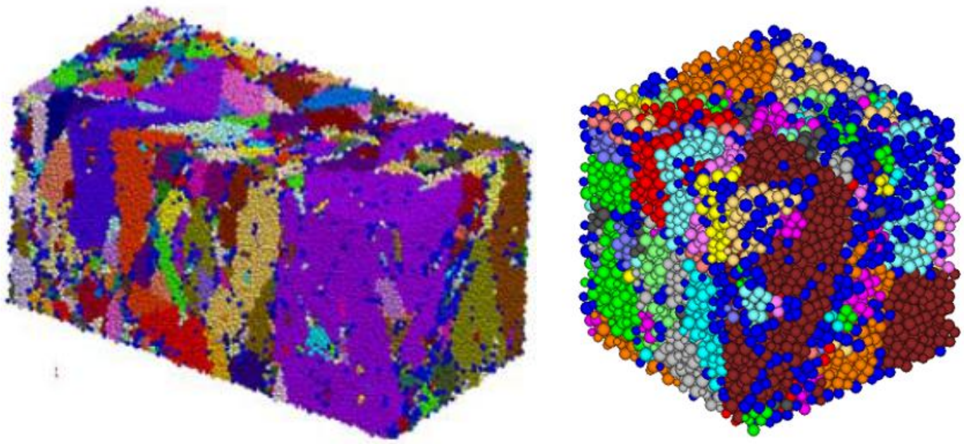

Figure 5. Three-dimensional SRM models: (left) view of the 80x40x40 m model; (right) detail view of DFN inserted on PFC brick (Mas Ivars et al. 2008).

The run times for large 3D systems are still significant. Cundall (2011) proposed a faster alternative to PFC, the “lattice model”, in which the finite-sized particles are replaced by point masses, and the contacts between particles are replaced by breakable springs. Assuming small displacements, it achieves high computational efficiency because the interaction geometry (location and apparent stiffness of springs) can be pre-computed, eliminating contact detection as an overhead. A lattice SRM model was applied by Cundall & Damjanac (2009) to the analysis of slopes with discontinuous joint sets, to study the fracture of the intact rock bridges (Figure 6).

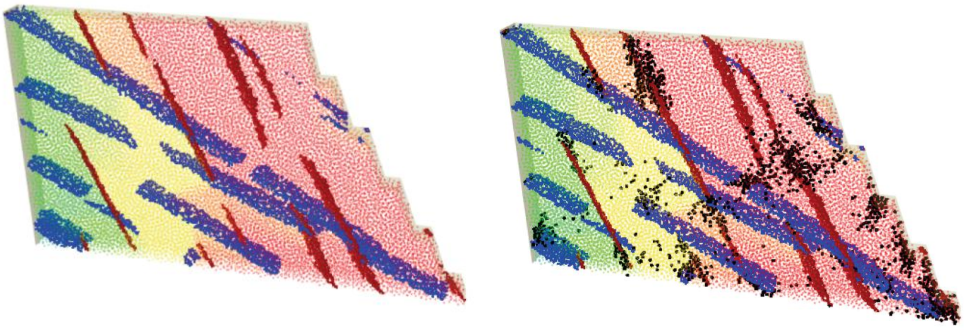

Figure 6. Cross-sectional slice through the upper part of a 1000-m slope modeled by SRM: (left) joint traces within the slice; (right) microcrack development (Cundall & Damjanac 2009).

2.3 *Concrete dam foundations*

The conceptual model of a rock mass as a blocky system has been employed for many years in the design of concrete dam foundations. A numerical DE model of an arch dam foundation may be viewed as an extension of classical block stability analysis. Instead of a single rock wedge, a block system is represented, and therefore, not just one, but multiple failure modes may be checked in a single run. Furthermore, block deformability can be considered, taking into account the dam-rock interaction, which could be relevant in valleys with marked heterogeneity. A key aspect in dam foundation problems is the effect of water pressures, which must be applied in the discontinuities (see section on coupled models below).

In the study of arch dams, the correct representation of the deformability and stresses in the concrete shell is important. For this purpose, 3DEC allows meshes of 20-node brick finite elements in the concrete structure, while the rock mass blocks are still discretized with tetrahedra. This combination was used in the model of the 110 m high Baixo Sabor dam (Figure 7) (Lemos & Antunes 2011). The model geometry was first established, including the surface topography (left figure). The concrete-rock interface and the contraction joints between the cantilevers are also model discontinuities with nonlinear behavior. The major rock mass discontinuities were placed at their known locations, and then a few joints of each of the 3 main sets were selected. Safety factors for foundation failure modes were evaluated by progressive reduction of the joint strength properties, leading to the development of mechanisms as the one depicted in Figure 8.

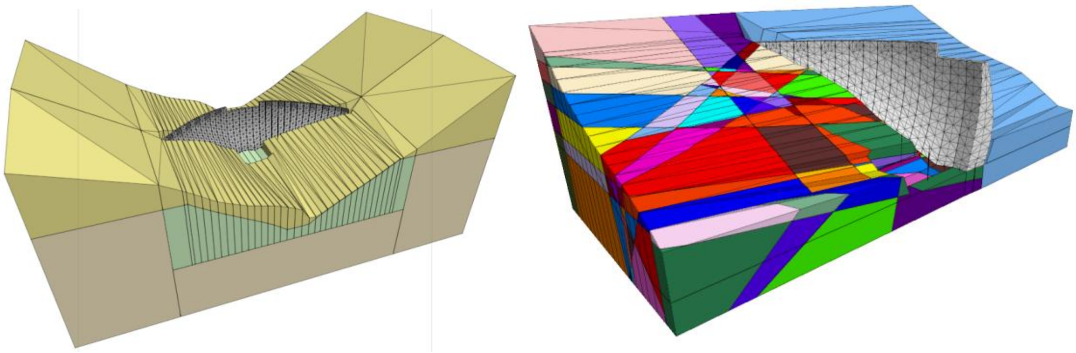

Figure 7. 3DEC model of Baixo Sabor dam: (left) global model geometry before discontinuities are inserted; (right) detail of half of the block model with rock discontinuities (Lemos & Antunes 2011).

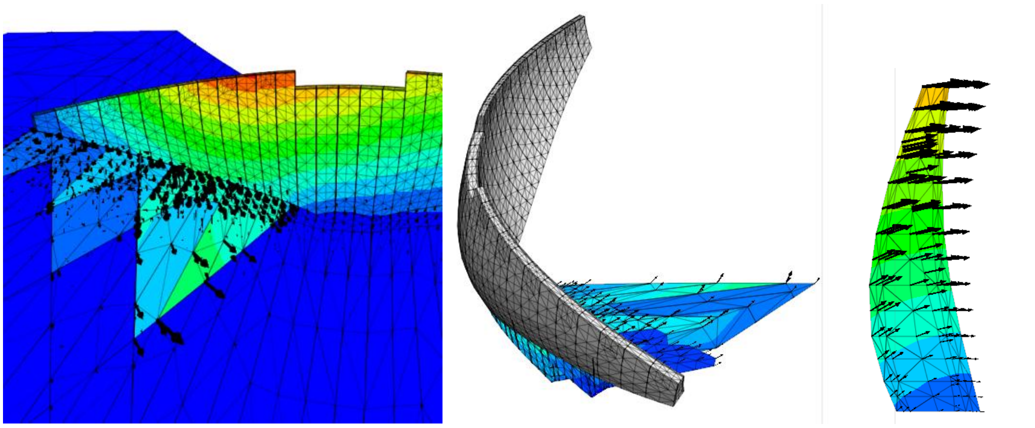

Figure 8. Nodal displacement vectors and contours denoting failure mechanism of arch dam foundation model obtained after progressive reduction of rock joint friction (Lemos & Antunes 2011).

2.4 *Underground excavations in rock*

A well-known early application of discontinuum models to underground works was the Gjovik cavern analysis by Barton et al. (1994), performed with a 2D UDEC model, in which the behavior of the discontinuities was represented by the Barton-Bandis joint model. The Tindaya cavern design was analyzed with 3DEC, involving a detailed representation of the rock mass discontinuities (Senís & Varona 2008). Figure 9 displays the unstable rock volumes in the roof and shaft sidewalls; an analysis with rock bolt support elements was subsequently performed.

Mining is a field where DE models have played an important role, as many problems involve conditions close to failure, whether in open pit or underground mining. The large displacement capabilities of these codes allow the simulations to proceed into the range of extensive material damage and breakage, for example, in cave mining problems (e.g. Sainsbury et al. 2011).

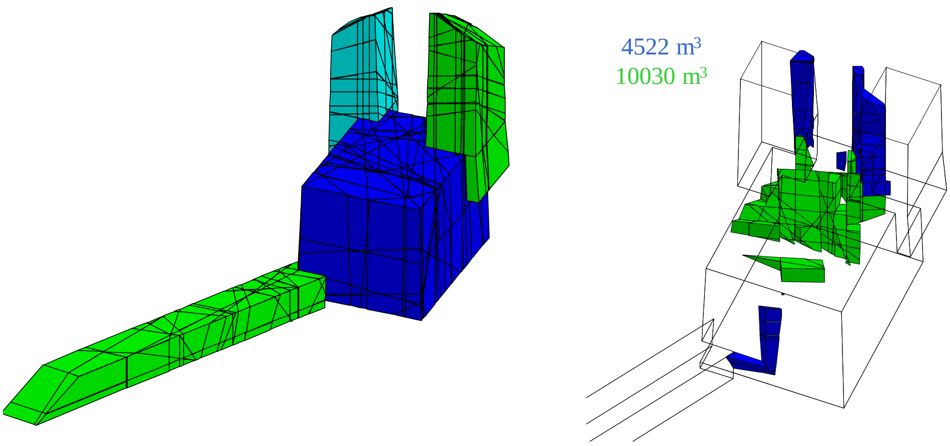

Figure 9. 3DEC model of Tindaya mountain project: (left) Excavation shapes; (right) Volumes of unstable rock in the unsupported case (Senís & Varona 2008).

2.5 *Coupled problems*

The study of fluid flow in rock masses was one of the early motivations for coupled DE formulations. For example, in dam foundation studies, water pressures along the joints play a key role in stability. In gravity dam studies, mostly done in 2D, coupled hydro-mechanical analyses pose no computational difficulties. The blocks are typically assumed impervious, with all fluid flow taking place along the discontinuities. The example of Albigna dam, performed by Gimenes & Fernandez (2006) with UDEC, allowed an interesting comparison with dam monitoring results. A fracture flow model for 3DEC was developed by Damjanac (1996).

Nuclear waste isolation studies and petroleum engineering are two of the fields that drive the research on modeling of coupled processes in rock, and considerable recent literature exists on these subjects. For example, solute transport in networks of rock fractures was approached with UDEC models by Zhao et al. (2011), highlighting the importance of the stress effects on these processes. Hydraulic fracturing with a Synthetic Rock Mass model was addressed by Damjanac et al. (2010). In this particle model, fluid flow analysis was performed, allowing the fluid effects on propagation of fractures to be assessed.

2.6 *Masonry structures*

Stone masonry structures are one of the applications in which the assumptions of DE models are more closely reproduced. In fact, these structures are often made of regularly shaped blocks, and their exact geometry can be introduced in the numerical representation. In the case of dry joints, simple frictional models are fairly accurate. For competent stone materials, the assumption of block rigidity is also adequate. Therefore, DE models are now extensively used in this field, in particular for the seismic analysis of monuments and structures that are considered a valuable part of the architectural heritage. Figure 10 shows a 3DEC model of a section of the Parthenon Pronaos, in Athens (Psycharis et al. 2003). The rocking behavior of the drum columns is complex, and requires the consideration of large displacements and rotations. Arched structures and traditional constructions have also been studied (Figure 10).

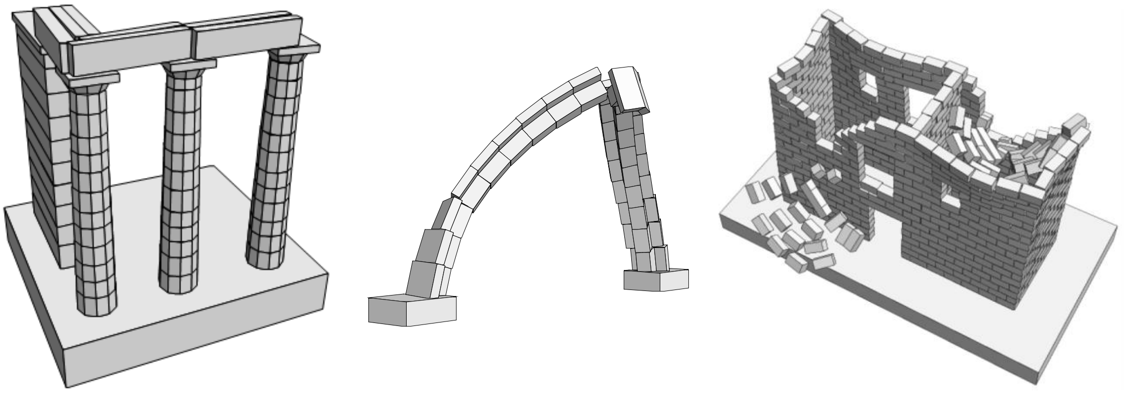

Figure 10. Rigid block models for seismic analysis of stone masonry. (left) Parthenon Pronaos (Psycharis et al. 2003); (center) free-standing arch (Lemos 2007); (right) traditional house (Alexandris et al. 2004).

2.7 *Rockfill and ballast models*

There are many systems that may be addressed by DE models, such as rockfill dams, railway ballast, or handling of bulk materials (e.g. Shimizu & Cundall 2001). Aikawa (2011) presents a three-dimensional dynamic numerical model for studies of a ballasted railway track using 3DEC (Figure 11). A discontinuous model of the ballasted track was created, comprising an assemblage of ballast polyhedrons, rail pads, sleepers, and a roadbed. The dynamic responses of track structure members in response to dynamic traffic loading of the train passing were simulated.

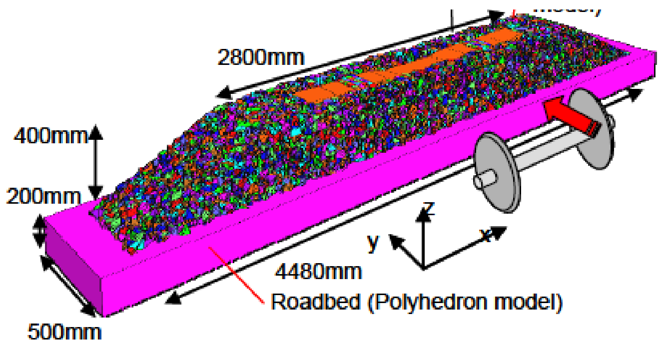

Figure 11. 3DEC model of ballasted railway track (Aikawa 2011).

3 CURRENT ISSUES, MODELING NEEDS AND FUTURE TRENDS

3.1 *Modeling methodologies*

There are many available options for representing a given physical system by means of a numerical model, ranging from simplified continuous medium idealizations to very detailed DE simulations of its micro-structure. All of these have their role in science and engineering and the purpose of the analysis is a major factor in the choice of the most appropriate and effective. In engineering practice, models are often tools to answer a given question, regarding, for example, the suitability of a design aspect. Only the features that impact on the particular behavior under scrutiny need to be included in the model, so many details are better omitted. Starfield & Cundall (1988) addressed these and other methodological questions, namely how data limitations constrain the building of a model. The potential of the model as a numerical laboratory, to gain knowledge on the problem at hand, was also stressed.

The evolution of engineering modeling methodologies will progressively shape the manner in which DE codes are employed. The need for reliable tools capable of providing answers in a cost-effective manner will drive the design of general-purpose codes and their user interfaces. The importance of user interfaces is likely to grow, assuming a higher weight in development costs, as they tend to become a decisive factor in code selection.

3.2 *Interaction of multiple DE components*

As a consequence of the applications of flexible and adaptive modeling approaches, there is a tendency to employ various types of representations, even within the same project. Thus, it is becoming more important the transparent interchange of data between different models and codes. In the future, engineers will demand easier ways to build DE systems capable of mixing different types of elemental components, e.g., from spherical particles to macro-particles and polyhedral blocks, and interfacing them with FE meshes, always ensuring consistent physical interaction assumptions.

3.3 *Model building*

The tendency towards larger and more complex models implies that the tasks of model building take a larger percentage of the engineer's time. Improved procedures to create models are essential. This involves physical representation issues, as well as numerical aspects. For example, in rock mechanics, improved ways to describe and generate DFNs (discrete fracture networks), which better represent the natural rock mass state, are needed. In addition, efficient numerical procedures must be devised to materialize these DFNs in a particular DE code, offering the user simple and controllable means of model generation and verification.

The generation of large random particle assemblies in 3D is still a time consuming task. For large assemblies, setting initial stress states and driving strains according to prescribed paths have to be adequately thought. Furthermore, the procedures used to pack and load the particles may affect the mechanical response of the system, as discussed by Potyondy & Cundall (2004). In particular, for system geometries characterized by random parameters, it is essential to have automated ways to create many different samples with reduced user effort.

3.4 *Sound representation of physics*

The most distinctive feature of DE models is the contact formulation that governs the mechanical interaction between blocks or grains. The physical assumptions implied in the numerical implementation need to have solid foundations, and to be properly documented so that the user is aware of them, and may interpret the results accordingly. For example, whether the normal stiffness concept or a non-interpenetration assumption are employed, the numerical limitations and tolerances built into the contact detection and update procedures have to be consistent, robust and transparent to the user.

This requirement applies obviously to all the code essential components, from the use of FE meshes in deformable blocks, to fracturing and block splitting criteria. Continued validation of each specific feature against experimental data is mandatory to build confidence in the codes and their predictive capabilities.

3.5 *Coupled processes*

The importance of representing coupled physics processes will necessarily grow as more comprehensive treatment of phenomena is envisaged. Thermal-hydro-mechanical coupled models are currently used in various fields, with chemical parameters starting to be inserted into the common framework. With many interdependent variables, experimental validation becomes lengthy and more difficult, and a sound judgment is even more important in the assessment of numerical results.

3.6 *Access to data structures*

Many DE codes have been developed in research environments and are used mostly by their developers or other people within a relatively restricted environment. As these codes become available to wider audiences, the potential for erroneous use also increases. Large open-source projects have many merits, but also their own management difficulties. Commercial software invokes higher reliability, but drastically restricts the user autonomy, without the option to inspect the source or to modify it.

Granting the user access to the internal data structure, without the need to know the source details, delivers a much better degree of autonomy to the user, and also the ability to test and verify completely the code performance, and the manual's accuracy. The FISH language, developed by Cundall and implemented in UDEC/3DEC and PFC, is extremely useful in all modeling stages, namely in parameterized model generation, execution control or treatment of numerical or graphical output. For any code with a wide community of users, it is important to provide means to use the codes consistently, accessing all internal data structures without dependence on coding details or version changes.

3.7 *User-programmed constitutive models*

One of the critical factors in the choice of codes is the wealth of constitutive models offered. In DE codes, joint or contact constitutive models generally govern the system response. Giving the user the ability to program its own material models has greatly enhanced the software range of application. In particular, it extends the range of commercial codes in innovative research projects, to which they may bring all of their facilities for model generation and graphical user interfaces that special purpose codes often lack. User-defined constitutive models in UDEC/3DEC were initially written in the internal FISH language, but currently C++ is preferred, providing a standard programing framework. This also permits libraries of tested models to be built and made available to the user community.

Allowing the user to implement new constitutive assumptions without requiring knowledge of the internal code structure or changes in the source is an essential advantage for research-oriented projects. It also helps to clarify the relation between the assumptions about physical behavior and the strictly numerical issues.

3.8 *User interfaces*

As models become more elaborate, and codes offer a wider diversity of options, the design of user interfaces assumes a major role. Engineers demand robust and validated software packages capable of exploiting the available resources in an effective manner. It is particularly important that the codes are versatile, adaptable to the various levels of use, from the quick solution of fairly standard problems to the more elaborate types of analysis arising in research projects (Russell 2011).

Different users have their own preferences and requirements for the way they interact with the code. A novice user may prefer a well-designed menu interface, which simplifies the learning process and permits elementary problems to be set up without effort. An experienced user prefers more advanced procedures, possibly based on scripts or intelligible command files, which permit reuse of previous problem data, or the expedite creation of many related models. Of course, these procedures require learning time, and are only productive if frequent use of the code is intended. Ideally, a code interface should be flexible enough to allow both of these approaches. In particular, it is useful to be able to record interactive model building and execution, automatically creating command scripts that may be edited and reutilized.

For any type of user, high quality graphics are essential. The question of model verification, involving the checking of assigned properties, boundary or load conditions, and all critical input data items, is immensely aided by a good graphical interface.

3.9 *Analysis of results*

Analysis and interpretation of the results of a numerical simulation becomes increasingly difficult and time-consuming when advanced material behavior models are employed. Often, the output of many parametric studies needs to be compared and synthesized. Internal programming languages, such as FISH, with access to the complete data structure of the problem, provide an excellent tool to treat the output of many runs, and create suggestive graphical representations.

Code output has evolved from large amounts of raw numbers to realistic graphical results. A further step is imperative to make the analyst's time more effective, by lending the codes better facilities to produce higher level indicators of performance, suited to the user needs.

Soft-computing techniques are now increasingly applied to assist in building knowledge from the results of numerical simulations. For example, DeGagné et al. (2011) used neural networks to develop behavior prediction tools for tunnels in squeezing ground, based on an extensive series of FLAC analysis.

3.10 *Computational aspects*

Run times remain the critical limit to analysis feasibility, as users continue to increase the size and complexity of their representations to take advantage of every advance in processor speed. There are clear trends to apply 3D models routinely to more problems, and to resort more frequently to dynamic, transient and coupled physics problems. Faster analyses are thus indispensable. Parallel processing techniques appear to be critical to achieve such goal. The availability of multiple core processors at reduced costs has already produced significant performance improvements, with multithreading techniques sometimes not involving substantial code redesign. However, various issues need to be addressed, for example, memory access management, as bandwidth limitations seriously affect performance (e.g. Williams et al. 2010, Russell 2011).

It should be noted that, in many research projects, large series of runs need to be undertaken. The time constraints depend not only on the run time of each analysis, but also on effective methods to treat and interpret output, as understanding of these results is indispensable to plan the runs ahead.

4 CONCLUSIONS

Over the years, advances in computer power have always been matched by the increase in both size and complexity of numerical models. The pursuit of faster analyses, whether by means of parallel processing techniques or improved algorithms, remains a challenge for code developers. Nevertheless, it must be recognized that fairly intricate three-dimensional DE models are now routinely applied in engineering practice with very reasonable computational costs.

In DE modeling, finer representations or extended domain problems weigh substantially on the computational effort. Cundall (2001) argued that the future trend for numerical modeling in soil and rock may consist of the replacement of continuum methods by particle methods, as assemblies of discrete particles capture the complicated material behavior with simple assumptions and few parameters at the micro level. The research of the fundamental behavior of materials seems indeed to steer us from meso-scale to micro-scale, or even nano-scale analysis. In parallel with more elaborate models, engineering practice will continue to apply simplified continuous or coarse-grained block models, as long as these solve the problems at hand in a satisfactory and cost-effective manner. The articulation of a variety of models, tailored to different user needs, will certainly become easier to achieve and more prevalent.

The development of constitutive laws that better simulate the experimentally observed behavior and the focus on multi-physics coupled processes will continue to expand. However, as follows the discussion in the previous section, perhaps the most significant change in the future will be the way in which we use the codes. Advances in graphical user interfaces will improve substantially our ability to build large and complex representations, to automate the execution of extended series of parametric studies, and to extract from the output more elaborate and meaningful indicators of physical behavior or design performance, in order to advance our knowledge of the world and our engineering capabilities.

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