Aspects of the hybrid finite discrete element simulation technology in science and engineering

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SUMMARY

In this paper, the state of the art in the Combined Finite-Discrete Element Method (FDEM) has been summarized together with the fast emerging hybrid finite discrete element based simulation technology for multiphysics problems ranging from traditional engineering disciplines to biosciences and medical engineering. The key algorithmic aspects of FDEM have been summarized. The relationship between FDEM and virtual experimentation has been explained in more detail.

KEY WORDS: *FDEM; hybrid simulation; anisotropy; finite elements; combined finite discrete elements.*

1. INTRODUCTION

Since its inception the Finite-Discrete Element Method (FDEM) has become a tool of choice for diverse fields of practical engineering and scientific simulations [1-9]. The key idea of FDEM was integration of Discrete Element Methods (DEM) and Finite Element Methods (FEM) into a one powerful simulation tool that is able of simulating billions of deformable bodies that interact with each other. The initial idea of FDEM was first proposed in 1989 by Munjiza while working at Tohoku University in Japan. The idea was further developed at University of Swansea, Massachusetts Institute of Technology (MIT), and University of London in 1990s. Further developments took place in 2000s at Imperial College London, University of Toronto, Caltech, Berkeley, and National Laboratories in USA. In parallel, significant developments are taking place at some European Universities and centres of excellence in China, including Chinese Academy of Science.

In FDEM a large strain-large displacement formulation has been employed in its exact multiplicative decomposition (as opposed to co-rotational) formulation. In recent years this formulation has been generalized through the concept of the so called Munjiza material element, which enables a pragmatic engineering approach to anisotropic constitutive law formulation for both large displacements and large strains in the context of the exact decomposition-based format. This approach has been recently described in detail in the book entitled "Large Strain Finite Element Method: A Practical Course" by Munjiza, Rougier and Knight [4], where also some novel concepts of selective integration have been proposed and applied to a whole family of finite elements.

In the last ten years FDEM has been parallelized through the so called concept of virtual parallel engine, which enables parallelization that is independent of the hardware platform employed; as such, FDEM has been run on clusters comprising up to *3000* processors. Parallelization efficiencies of up to *90%* have been reported.

In its initial conception FDEM has included robust contact detection and contact interaction solutions. These have now matured through the so called NBS and MR (Munjiza-Rougier) search algorithms and associated contact detection algorithms. A research group at University of Toronto has made these applicable on a GPU processing unit achieving speed ups of up to 130 times as compared to a single processor serial code.

FDEM always had robust fracture and fragmentation solutions. Fracture and fragmentation solutions were one of the most important attributes of FDEM. However, FDEM could only deal with elastic pre-fracture materials. In the last few years this has changed completely and now FDEM has been developed to such a state that it naturally includes material libraries based on the latest hyperelastic and/or hypoelastic approaches with either co-rotational or multiplicative decomposition based plasticity and damage models.

On the application front FDEM has been extended in "all directions", including a notable extension to tissue engineering and medical applications for bone, soft tissue and artificial medical materials. As a result, FDEM has been integrated with the state of the art CFD solvers. One group of these addresses simulation of solids in fluid dominated problems, while the other part addresses simulation of fluid flow in solid dominated problems (such as flow through crack networks). In this paper, some of the above introduced aspects of FDEM have been described in more detail.

2. THE FEM SIDE OF FDEM

Integration of Discrete Elements (DEM) and Finite Elements (FEM) into FDEM, is not straight forward as it may appear. First of all, FEM has been traditionally built around the so called small displacements and small strains concepts, which in a nutshell means equilibrium for the un-deformed configuration and very little distortion of the material itself (small stretch). In contrast discrete elements have been originally devised to model motion of large number of discrete particles that are interacting with each other. The particles move so much that the special algorithms for detecting contacts between particles had to be devised (the so called contact detection algorithm).

In order to reconcile the two, the Finite Element Method side of FDEM had to be reformulated in terms of large strains and large displacements. This has been done by adopting modern continuum mechanics definition of deformation, where deformation is simply defined as a one

to one mapping that maps some initial configuration of the material points of solid body into what is usually termed current (or transient) configuration of the material points:

$$x = x(\xi, \eta, \zeta)$$
$$y = y(\xi, \eta, \zeta) \qquad \qquad (1)$$
$$z = z(\xi, \eta, \zeta)$$

Now, any such function (deformation) can be written as a composition of two or more functions (deformations), such that the right-most deformation occurs first:

$$f = f_3 \circ f_2 \circ f_1 \qquad \qquad (2)$$

In an infinitesimal vicinity of any material point P, deformation function can be represented exactly by a first order polynomial. The three constant terms of the polynomial represent translation. The nine linear terms of the polynomial represent deformation of the material relative to the point P, which then comprises of rotation and stretch. Rotation does not stretch material, i.e. it leaves for instance interatomic distances in a crystal unchanged. It is the stretch that changes these interatomic distances. Thus, one can calculate deformation gradient:

$$F = \nabla f = (\nabla f_3)(\nabla f_2)(\nabla f_1) = F_3 F_2 F_1 \qquad \qquad (3)$$

where F is deformation gradient. Deformation gradient is a second order tensor. In the infinitesimal vicinity of any material point P deformation gradient tensor can be considered constant and can be decomposed into a rotation followed by a stretch or a stretch followed by a rotation.

An interesting original engineering theory has been built on the above concept. The theory proposes pragmatic engineering approach to multiplicative decomposition of deformation into its successive components such as rotation, elastic stretch, plastic stretch, etc. The key ingredient of the theory is the usage of curved non-Cartesian coordinates in conjunction with material axes and the so called non-cubical infinitesimal material elements. These are all adopted for direct implementation into FDEM. The theory has been described in a topic specific book (monograph) published in 2015 [4]. It transpires that despite the deformation, rotation and stretches being represented exactly, the mathematical expressions involved become in actual fact as simple as the small strain elasticity, except that there is no longer any limitation to either displacements or stretches.

The new theory requires new terminology such as deformation vector, deformation gradient tensor, rotation tensor, and stretch tensor. In addition, stress tensor has been redefined in the light of the latest developments in continuum mechanics – the stress tensor is defined by the following equation:

$$q = \sigma a \qquad \qquad (4)$$

where q is the internal force "through" internal area a at the material point P, and both force and area are vectors – of course the force q is the sum of all electromagnetic forces between the atoms on the opposite side of the internal area a. The old definition of the stress:

$$\sigma = \frac{q}{a} \qquad \qquad (5)$$

is not valid in the above context and is only valid in special circumstances. It follows that stress tensor is a linear mapping from a space of internal surfaces through a given material point P onto a space of resultant interatomic forces through the same surface.

In order to deal with anisotropic materials, a separate local $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ material axes are introduced and the geometry of the material base is calculated from deformation kinematics. The initial position of the material axis:

$$\begin{bmatrix} \bar{\boldsymbol{\alpha}} & \bar{\boldsymbol{\beta}} \end{bmatrix} = \begin{bmatrix} \bar{\alpha}_i & \bar{\beta}_i \\ \bar{\alpha}_j & \bar{\beta}_j \end{bmatrix} \tag{6}$$

is provided as an input to FDEM simulation. From the above equation both hyperelastic and hypoelastic formulations have been derived with standard interfaces with material packages involving plasticity, damage, continuum fracture and similar permanent deformation issues. The volumetric part of the material law is treated separately through the so called equation of state, which may involve thermal and/or phase change aspects.

In traditional FEM the material law is defined in terms of a strain energy function [10], which is relatively difficult to generalize to anisotropic materials. In contrast, in FDEM the unified constitutive approach is employed: the stress due to the deformation kinematics are expressed in terms of the so called Munjiza stress components (also called Munjiza moments), which decompose stress contributions into orthogonal modes, for each of which any nonlinear function of a single variable can be employed; thus producing a large number of possible constitutive laws, all of which by definition have a strain energy function associated with them.

Full integration over the finite element may lead to locking, while reduced integration may lead to zero energy modes; which is the reason why selective integration is employed in FDEM, with different constitutive components being integrated at different integration points.

The latest development on the plasticity and/or damage side have taken place on the above described lines of reasoning and are all based on the multiplicative decomposition of the stretch tensor into successive elastic and plastic components:

$$\boldsymbol{F} = \boldsymbol{V}_e \boldsymbol{V}_p \boldsymbol{R} \tag{7}$$

or:

$$\boldsymbol{F} = \boldsymbol{R} \boldsymbol{U}_e \boldsymbol{U}_p \tag{8}$$

as opposed to the traditional additive decomposition of small strain deformation theory with small displacements:

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p \tag{9}$$

where $\boldsymbol{U}$ and $\boldsymbol{V}$ are the right and the left stretch tensors respectively.

The rate theory is in FDEM done in a similar way, thus preserving energy and also being able to recover fully the deformation gradient, even if large deformation steps (time steps) are involved.

3. THE DISCRETE ELEMENT SIDE

The implementation of the unified material model together with associated plasticity and large strain large displacement deformation kinematics enables simulation of deformation of a single solid body. The applied theory is not any longer the linear theory (first order) or the second order theory – it is in actual fact the exact theory describing deformation kinematics of a solid body exactly regardless of the size of either displacements or stretches.

In other words, FDEM does not borrow the finite element theory; it develops its own generalized finite element theory. It then applies this to a large number of solid bodies simultaneously by discretizing each solid body into its own finite element mesh. Each solid body is called discrete element. These discrete elements interact with each other through mechanical or other interaction laws.

Interaction between large numbers of solid bodies is basically the discrete element side of FDEM, except that it had to be developed in a specific way to account for the fact that the solid bodies can be of any shape and can interact with any other body and also with itself.

In order to solve the contact interaction conundrum, the so called discretized penalty function method has been employed for normal interaction forces. This is done by defining contact potentials for each of the discrete elements using the existing finite element mesh. The latest generation of the algorithms involves smooth potentials regardless of the shape or the size of the finite element mesh.

The tangential interaction forces are superimposed onto the normal interaction forces and may involve friction, joints, viscosity, electrostatic forces and some other aspects of interaction associated with specific engineering application.

In order to accommodate interaction between billions of particles two issues had to be addressed:

1. Linear Complexity Contact Detection,
2. Efficient Parallel Processing.

Linear Complexity Contact Detection has been first achieved through the so called Munjiza-NBS contact detection algorithm. Later on the so called MR (Munjiza-Rougier) algorithm had been introduced together with its different modifications.

On the parallelization front, the so called generalized FDEM parallel virtual machine has been developed, enabling a speedy painless hardware independent parallelization on hardware ranging from clusters to desktop parallel architectures to grid computing. Processing efficiencies of up to *90%* have been achieved on clusters comprising up to *30000* cores.

4. HYBRID FDEM SOLUTIONS

Modern engineering and science involve multiphysics problems where different phases of matter may be present. Such problems for instance may involve biological tissue, red blood cells deforming and moving in blood plasma, fluid opening cracks in rock to enhance oil and gas recovery, high temperature processes with meteorite impacts, sedimentation and sediment transport processes, etc.

In order to address some of these, FDEM had to be integrated with the CFD solvers. Two approaches can be identified in the recent efforts to achieve FDEM-CFD integration:

1. Fluid dominated problems with deformable solid bodies (discrete elements) moving in the fluid – a typical problem of this nature is the flow of red blood cells in blood plasma.
2. Solid dominated problems with compressible fluid moving through solid voids, solid pores, cracks in solid, fissures in solid, joints in solid, etc.

The first group of problems has been addressed by taking existing CFD solvers and integrating them into FDEM packages through the so called immersed boundary method. The simulation

has been applied to sediment transport simulations, flow through flexible tubes, red blood cells aggregation.

The second group of problems has been addressed by developing a completely integrated FDEM specific fluid solver, which addresses seepage of fluid through porous solid, flow of fluid through solid voids and flow of fluid through cracks. In all cases the fluid is assumed to be compressible and transient stress wave propagation in the fluid is considered as well – thus one has a multiphase system comprising of a solid phase, fluid phase and interaction between the solid and fluid at a microstructural level such as pore and crack level.

5. SOME EXAMPLES OF THE LATEST FDEM CAPABILITIES

FDEM has become a tool of choice in many engineering and science applications ranging from mineral processing, mining, civil engineering, medical engineering, and oil and gas exploration to nanotechnology [10-15]. In many cases FDEM is the only simulation tool available that can produce reasonably accurate results. In this section some of the applications are illustrated using simulation results obtained from FDEM.

In Figure 1 an example of granular flow comprising irregular deformable particles is shown. The results are obtained using dry FDEM, i.e. without presence of any fluid. In the latest FDEM applications, it is possible for the particles to move inside a fluid such as air or water. The interaction with fluid is achieved via the immersed boundary method. Finite volume techniques are used for fluid with incorporated turbulence models. Also, electromagnetic body forces have been added to take into account interaction of charged particles with electromagnetic fields in both fluid and solid domain. Interaction between dry particles can comprise complex physics including electrostatic forces. The particles can also break, deform (both elastically and permanently).
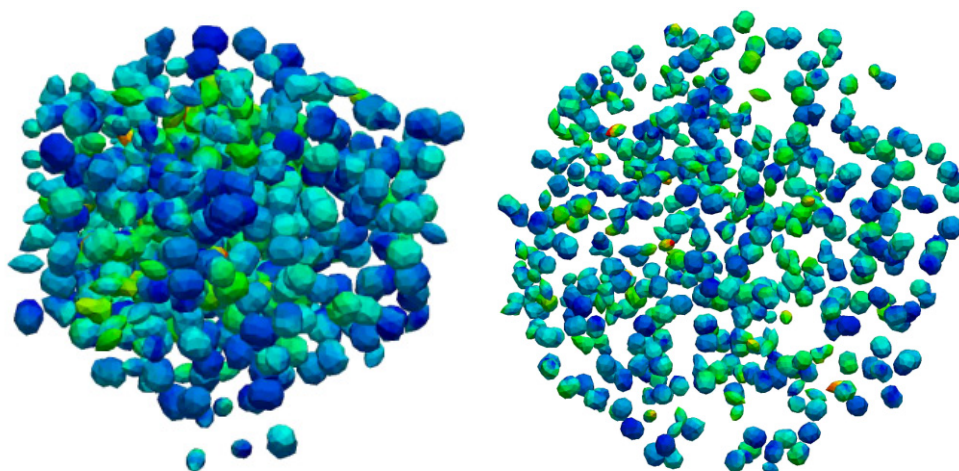

Fig. 1 *Granular flow comprising irregular deformable particles*

In Figure 2 an example of complex fracture patterns obtained using FDEM is shown. A rigid impactor impacts against laminated windscreen producing characteristic radial cracks, which are accompanied by circumferential cracks. The simulation was performed using shell elements specifically developed for FDEM.
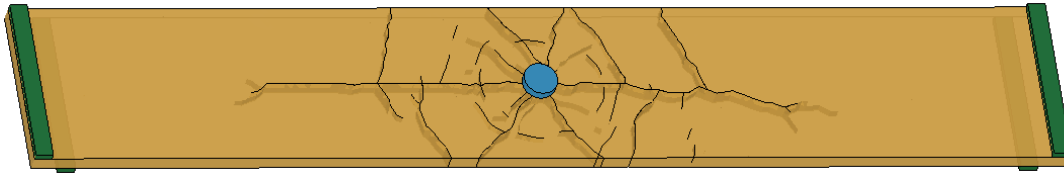
Fig. 2 *An example of a fracture pattern obtained using FDEM after an impact of a near rigid impactor against laminated car windscreen*

An important field of application of FDEM is structural stability and structural integrity under seismic loading. An example of the response of a dome (Duomo of the Cathedral of Santa Maria del Fiore, located in Florence, Italy) to a horizontal (shaking) seismic load is shown in Figure 3.
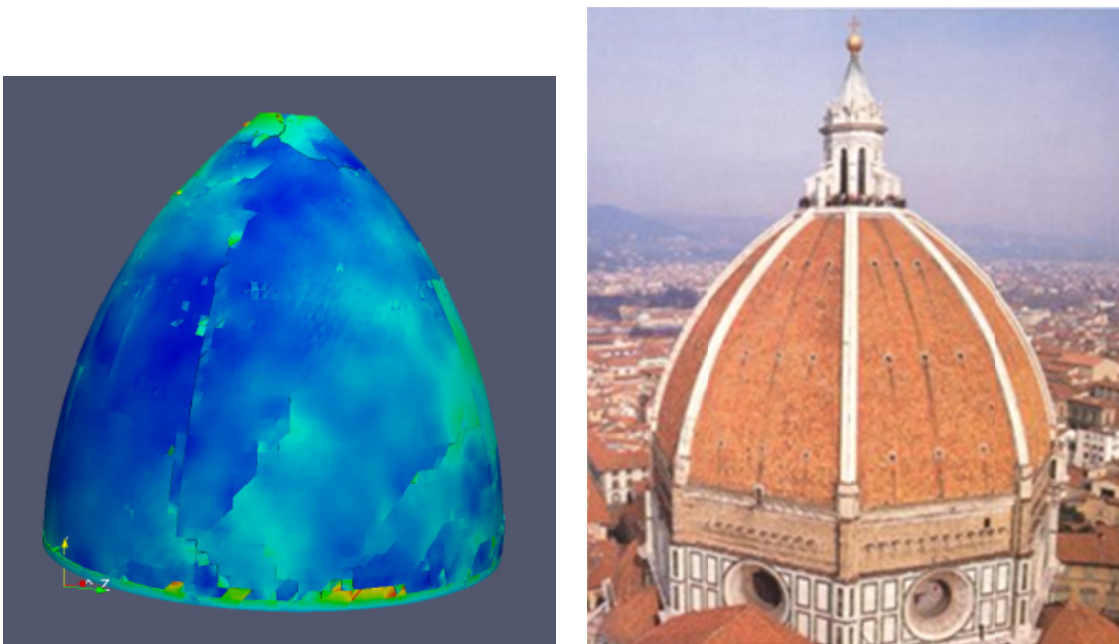
Fig. 3 *Dome cracking under seismic loading (Duomo of the Cathedral of Santa Maria del Fiore, located in Florence, Italy) (Courtesy of Rougier at all)*

In Figure 4 shear flow of red blood cells in plasma is performed experimentally and reproduced using FDEM. In both cases red blood cells move within the plasma under shear stress in plasma – they also deform and coalesce together forming distinct coalescence patterns. Experimental and simulation patterns look very similar, which is yet another example of FDEM simulations being able to reproduce actual experiment to the point that the emergent properties are reproduced as well. In this context, FDEM has moved from being a sophisticated simulation tool into being a virtual experimentation tool - since first being proposed by Munjiza in 2001. Virtual experimentation has become one of the three legs of the three legged stool on which modern science sits (experimental observation, theoretical reasoning and virtual experimentation).
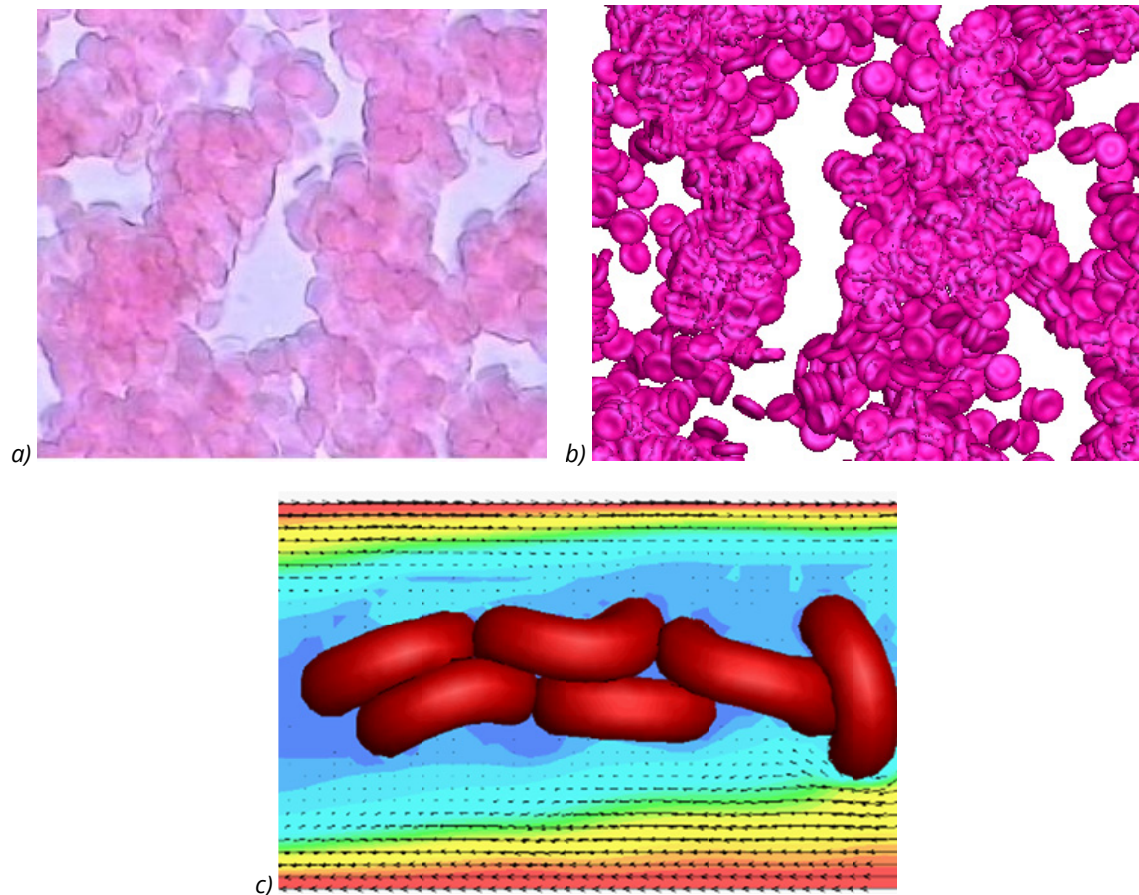
Fig. 4 *a) A microscope snapshot of experimentally observed coalescence pattern of red blood cells in a plasma shear flow; b) The same coalescence pattern produced using FDEM; c) An example of deformation of red blood cells in a shear flow [17]*

Another example of FDEM being able to produce complex emergent properties in the context of virtual experimentation is the fracture of an egg-like shell shown in Figure 5. The complex fracture pattern produced by FDEM simulation stands to the scrutiny of the eye and one could say reproduces even some of the natural beauty of similar experimental patterns; it is now well known that natural beauty in deterministic systems comes from the natural phenomena called deterministic chaos. Deterministic chaos gives eye pleasing look to the clouds, mountain tops, sea shores and as such is an important aspect of the universe. FDEM is able to reproduce beauty as an emergent property, once again confirming that FDEM has crossed the boundary from pure simulation into virtual experimentation, where real world is reproduced together with its emergent properties. Some civil engineering related FDEM simulations like slope collapse [10-12], dry stone structure of the ancient monument Protiron in the heart of the Diocletian's Palace in the City of Split, Croatia, under seismic load [15] what was later demonstrated by shaking table testing of the appropriate model [16], and particle entrainment in water flow [4] are shown in Figure 6.
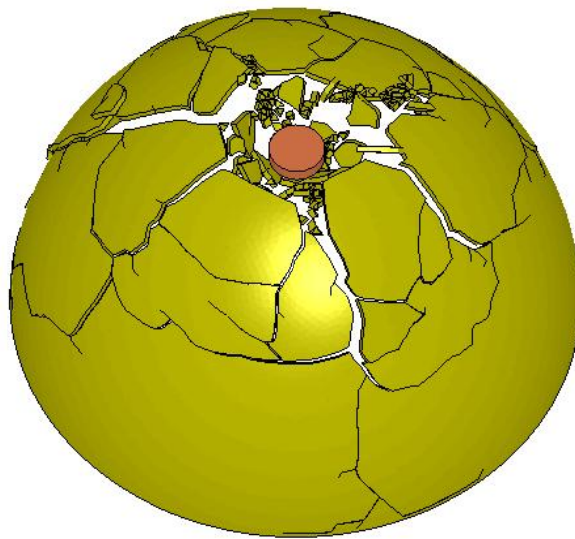
Fig. 5 *A virtual experiment in which a spherical shell has been cracked using velocity projectile [18]*
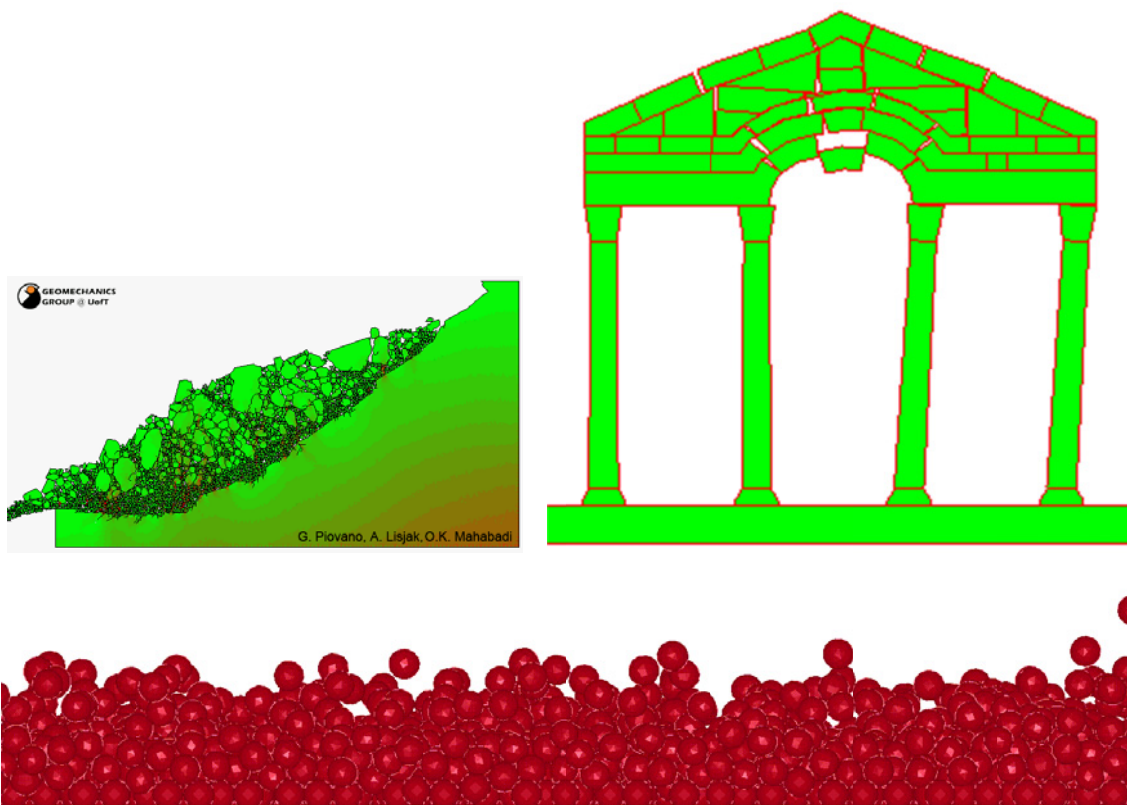
Fig. 6 *Some civil engineering related FDEM simulations: Slope collapse [11]; Stone structure under seismic load [15]; Particle entrainment in water flow [4]*

6. CONCLUSIONS

Recently published generalized large strain large displacements deformation kinematics (Munjiza et al. [4]) has opened a whole range of possibilities for FDEM developments - instead of using traditional approaches to defining material laws such as energy functions, a pragmatic engineering approach for calculating stress from stretches has been introduced together with its natural extensions into plasticity and damage.

On the fluid front, different research groups have achieved good progress in coupling and/or integrating fluid into FDEM. When combined with important developments on the permanent deformation front and the most recent fracture solution, these have enabled hybrid multiphysics simulation of nonlinear behaviour of both solid and fluid phases. As a result, the field of application of FDEM has been extended considerably to the point that it is now routinely applied in both industrial engineering applications, and fundamental and applied scientific research and developments.

FDEM has become one of the key virtual experimentation tools for hybrid and multyphysics problems. An open source Y-code [2] has been available free of charge and has been used and further developed by different groups at various centres of excellence in Japan, China, USA, Canada, India, and Europe. In parallel proprietary FDEM packages have been developed under different names such as CDEM (Continuum DEM). In addition different companies have introduced FDEM into their portfolio. A good example is ELFEN commercial package, but LS-Dyna and ABAQUS [5] have also integrated FDEM concepts into their software packages.

At the same time, fundamental developments in FDEM core technology are taking place all over the world. Some of these developments concentrate on multiphysics aspects of FDEM, while others concentrate on the computational aspects of FDEM, such as GPU computing, cluster computing, learning machines and even cognitive computing.

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