Hybrid discrete element/finite element method for fracture analysis

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Received 12 February 2004; received in revised form 10 January 2005; accepted 7 October 2005

Abstract

The discrete element method DEM has been used in fracture mechanics studies of heterogeneous media, for example plain concrete. One of the current limitations of particle methods for fracture analysis is related with the high number of particles that are necessary in the discretization, which limits the use of particle systems in larger structures. In order to apply the particle method to the analysis of larger structures, a hybrid method is proposed which uses the DEM in the discretization of the fracture zone, and, uses for the surrounding areas a discretization based on the finite element method. Test results of the hybrid model and two applications to notched beam fracture experiments in mode I and in mixed mode are presented and discussed.

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Keywords: Particle methods; Discrete element; Meso-level analysis; Concrete fracture

1. Introduction

The discrete element method DEM was initially applied for the analysis of discontinuous media, e.g. rock mechanics and soil mechanics. Recently the DEM has been used in the fracture studies of continuous media, for example concrete. By simulating the concrete microstructure the DEM particle method prevents localization of damage into regions, not sufficiently large, when compared to the inhomogeneity size \cite{2}.

In \cite{3}, where an equivalent particle model to a DEM rigid circular particle scheme is used, the need of an interface method which connects the particle system used on the cracked zone to a finite element method FEM discretization applied on the remaining part is pointed out in order to reduce the number of particles used in 3D problems or in large 2D problems. In \cite{19} the lattice method is used only in the zone where the fracture process is expected to take place and a FEM element mesh is used to discretize the surrounding areas. As proposed in \cite{19} the bar finite elements are connected to the 4 node quadrilateral finite elements by imposing displacement compatibility between the bar element nodes and the finite elements edges to which they are found to belong.

In the context of the DEM several improvements have been adopted which have introduced FEM technology in the DEM formulation. The initial DEM which was based on rigid blocks now allows also the blocks to deform by discretizing each block with an internal FEM mesh. Simple elements are usually preferred, e.g. triangles in 2D and tetrahedra in 3D, which can be made to fit arbitrary geometries and also allow the block to retain the initial polygonal or polyhedral boundary after deformation, making contact definition simpler and more efficient \cite{6}.

Other algorithms have been proposed in the literature coupling the DEM with the FEM by replacing the rigid blocks with finite elements and adopting the original DEM procedures for the interaction of the several blocks. The incorporation
of the FEM technology increases the deformation capabilities of the previously rigid block mesh. Examples of these procedures can be found in [5] which uses single quadrilateral finite elements, in [15] for the study of impact-induced fragmentation of particles and in [11] for the fracture studies of solids.

In [4] is presented an algorithm which coupled quadrilateral finite elements with rigid blocks for the transient analysis of caverns in jointed media. Both the finite and the discrete element equilibrium equations are integrated explicitly by the centred difference method. At the FEM/DEM boundary, the FEM boundary nodes are assumed to be rigidly connected to the intersecting DEM rigid boundary block.

In [8] is presented a hybrid method for the analysis of arch dams on rock foundations. It combines deformable discrete elements which model the rock foundation with higher order hexahedral finite elements which are used to model the arch dam structure.

An example of DEM/FEM using rigid circular particles can be found in [14] where masonry arch bridges with granular back-fill are assessed. The granular back-fill is modelled with rigid circular discrete particles whereas for the masonry arch are adopted finite elements enhanced with DEM capabilities.

In the context of fracture studies rigid circular particles models, which take directly into consideration the meso-structure of concrete, have either been applied to experimental specimens with small dimensions or to a rather coarse particle assembly with consequences in terms of analysis [10]. Given computer restrictions, in order to be able to analyze large structures it is proposed a coupling algorithm which applies a DEM circular particle discretization only on the fracture zone and a FEM based discretization on the other zones where an elastic linear behaviour is acceptable. Each finite element is understood to be equivalent to a particle assembly which, on a given macro scale of observation, can be modeled as a linear elastic media. An interface element is defined that enables the coupling between circular rigid particle elements and plane quadrilateral finite elements.

The model is applied to the numerical study of a concrete beam in mode I fracture experiment in a notched beam of plain concrete tested by Petersson [13]. Also a mixed-mode concrete fracture experiment on a notched shear beam tested by Arrea et al. [1] is studied. It is shown that the hybrid model is able to model elasticity, the non-linear behaviour and the transition phase for different loading conditions in an emergent way, that is without including them directly in the constitutive model, a similar behaviour is found to occur in rock [16].

2. DEM–FEM coupling

2.1. Introduction

The coupling of the FEM using quadrilateral finite elements and the DEM using rigid circular finite elements can be accomplished by adopting special interface elements which enable the interaction of the circular particles with the edge of the quadrilateral finite elements that they are contacting.

In [7] a rigid wall element is defined in order to set boundary conditions: the wall is given by a line segment and the basis for a particle/line segment contact is defined. In this work, the same concept is used as the quadrilateral finite elements edges with only two nodes remain line segments after the element deformation. An equivalent procedure to the rigid wall algorithm is applied, the main issues that need to be defined are the edge motion in order to set the relative displacement at the contact and the distribution of forces from the contact interface to the adjacent edge nodes.

Both the FEM and the DEM equilibrium equations are integrated explicitly by the centred difference method. For both discretizations the same time increment is used, which is the smallest of the two. The influence of the interface element is also accounted before the application of the Gershgorin’s theorem [20] to the nodes and particles present in the simulation, in order to determine the time increment for numerical stability [10].

The equation for the translational and rotational motion for the global problem (DEM + FEM), with no damping, is given by

\[ \mathbf{F}_i^{(t)} = m(\ddot{x}_i - g), \]

\[ M_3^{(t)} = I\dot{\omega}_3 = (\beta mR^2)\dot{\omega}_3, \]

where \( \mathbf{F}_i^{(t)} \) is the total applied force at time \( t \), \( m \) is the total mass of the particle or the node, \( \ddot{x}_i \) is the particle translational acceleration, \( g \) is the body force acceleration, \( M_3^{(t)} \) is the total applied moment at time \( t \), \( I \) is the moment of inertia, \( \dot{\omega}_3 \) is the particle angular acceleration, and \( \beta \) is a coefficient reflecting the shape of the particle, 2/5 for a spherical shape and 1/2 for a disk shaped particle.

The total applied force at a given instant \( t \) for a given particle has to include the contribution of all contacts that the particle has, including the contacts with the edges of the quadrilateral finite elements and the exterior applied force. The total applied force at a given instant \( t \) for a given node has to include the internal forces resulting from the finite elements deformation that the node is part of, the contact forces of the particles which are interacting through common edges and the exterior forces applied at the nodes.
A DEM/FEM cycle as here proposed follows the principles defined for a DEM cycle, see Fig. 1. The main difference is that for the force displacement law the nodal internal forces and the interface contact forces for the DEM/FEM contact have to be added. Also in the law of motion, the motion of the quadrilateral finite element nodes has to be taken into consideration. The finite element nodes only have two degrees of freedom per node as no rotational degree of freedom is taken into consideration for the nodes.

2.2. Force displacement law

The boundary edges of the finite elements that are allowed to interact with the particle assembly are represented through wall/edge elements. The edges of the 4-node plane stress finite elements are equivalent to a truss finite element model with two degree of freedom per node with a given length $L$, for this reason the associated edge shape functions are linear, see Fig. 2.

The force displacement law for the interaction of a particle with a given edge of a plane finite element should be able to define the forces developed at the contact interface which are related to the incremental contact displacement at the interface and also the mechanism through which the forces are transferred to the edge nodal points and to the centre of gravity of the rigid circular particles.

At a given simulation instant the wall/edge length and the wall/edge axial direction are given in function of the nodal positions by

$$L = \sqrt{\left(x_{i,\text{node},j} - x_{i,\text{node},i}\right)\left(x_{j,\text{node},j} - x_{j,\text{node},i}\right)},$$

$$a_i = \frac{x_{i,\text{node},i} - x_{i,\text{node},j}}{L}. \tag{3}$$

The wall/edge transverse/normal direction, $n_i$, is defined based on the wall/edge axial direction through $n = (-a_2, a_1)$.

The contact between the wall/edge and the particle follows the principles defined in [7]. The main issues that need to be introduced are the definition of the wall/edge velocity at the contact point $\dot{x}_{i,[C]}$ and the mechanism through which the contact forces are related to the nodal forces.

$$X_{i,j} = \frac{X_i}{L} \quad N_j = \frac{1 - X_j}{L}.$$
In order to define the velocity of the wall/edge entity at the contact point, the nodal velocities are defined in a new set of local axes defined by the axial $a_i$ and transverse directions $n_i$, here called the wall/edge reference axes. For a given node $h$ the nodal velocities in the wall/edge reference axes are defined using:

\[ \dot{x}_{Eh} = \dot{x}_{h} a_i, \]  
\[ \dot{x}_{h} = \dot{x}_{Eh} n_i, \]

(5) (6)

where $\dot{x}_{Eh}$ and $\dot{x}_{h}$ are, respectively, the axial and the transverse velocity at node $h$ and $\dot{x}_{Eh}$ is the velocity vector of node $h$ relative to the global axes.

In order to define the wall/edge velocity at the contact point it is necessary to set the axial and the transverse velocity of the edge. Given the transverse velocity at the edge nodal locations and assuming a rigid body motion in the transversal direction, it is possible to define the velocity at the contact point given the transverse motion of the wall and the particle motion. As an approximation the axial velocity at the contact point is defined as being the axial velocity at the wall/edge contact point.

The angular velocity of the wall/edge entity $\omega^{[CG,E]}_3$ is defined as

\[ \omega^{[CG,E]}_3 = \frac{\dot{x}_{Eh} - \dot{x}_{th}}{CG}. \]

(10)

In order to completely define the motion in the transversal direction it is necessary to further define the equation of motion in the simulation reference axes:

\[ \dot{x}_{th} = \dot{x}_{Eh} n_i. \]

(11)

The centre of gravity of the wall given the new geometry, the equivalent wall angular velocity and the wall translational velocity:

\[ CG = \frac{\int (\dot{x}_{Eh} n_i + CG_0 n_i) \, dA}{\int n_i \, dA}. \]

(8)

The nodal velocities in the local coordinates are then given by

\[ \dot{x}_{i}^{CG,E} = \frac{\dot{x}_{Ei}^{CG,E} + \dot{x}_{th}^{CG,E}}{2}. \]

(7)

where \( \dot{x}_{Ei}^{CG,E} \) is the edge shape function associated with node $h$.

The contact velocity is defined as the relative velocity of the two entities, discrete particle/edge plane finite element, in contact at the contact point. The relative velocity of entity $\Phi^2$ relative to entity $\Phi^1$ at the contact point is given by

\[ \dot{x}_{i}^{[CG,E]} = \left( \dot{x}_{i}^{[CG,E]} \right)_{\Phi^1} - \left( \dot{x}_{i}^{[CG,E]} \right)_{\Phi^2}. \]

(13)

The velocity of the discrete particle $\Phi^1$ at the contact point is given by

\[ \left( \dot{x}_i^{[CG,E]} \right)_{\Phi^1} = \dot{x}_i^{[CG,E]} + \epsilon_{3 \Phi^1} \omega^{[CG,E]}_3 \left( x_i^{[CG,E]} - x_i^{[CG,E]} \right), \]

(14)

where $x_i^{[CG,E]}$ is the translation velocity of the entity $\Phi^1$.

The velocity of the wall/edge $\Phi^2 = E$ at the contact point taken in consideration both the transverse and the axial wall/edge velocity is given by

\[ \left( \dot{x}_i^{[CG,E]} \right)_{\Phi^2} = \left( \dot{x}_i^{[CG,E]} + \epsilon_{3 \Phi^2} \omega^{[CG,E]}_3 \left( x_i^{[CG,E]} - x_i^{[CG,E]} \right) \right) + \dot{x}_i^{[CG,E]} a_i. \]

(15)
The increment of the contact displacement \( \Delta x_i^c \) for a time increment of \( \Delta t \) is given by
\[
\Delta x_i^c = x_i^c \Delta t.
\] (16)

The displacement increment at the contact point can be decomposed into its shear \( \Delta x_i^s \) and normal \( \Delta x_i^n \) components:
\[
\Delta x_i^s = \Delta x_i^c n_i,
\] (17)
\[
\Delta x_i^n = \Delta x_i^c - \Delta x_i^s n_i.
\] (18)

As Eqs. (17) and (18) indicate, the normal component is stored as a scalar and the shear component is stored as a vector in global coordinates. Both the normal and shear components are given as the reaction forces to, respectively, the relative normal and shear displacements at the contact. The normal component has a positive value if the interface is under compression. The contact force increments are obtained by using the following linear incremental law:
\[
\Delta F_{n}^i = -k_n \Delta x_{n i}^c,
\] (19)
\[
\Delta F_{s i}^c = -k_s \Delta x_{s i}^c,
\] (20)

where \( \Delta F_{n}^i \) is the normal contact force increment given as a scalar, \( k_n \) is the normal contact stiffness, relating normal displacements increments with normal contact forces increments, \( \Delta F_{s i}^c \) is the shear contact force increment given as a vector in global coordinates and \( k_s \) is the shear contact stiffness.

Due to the fact that the shear contact force is stored as a vector in global coordinates it is necessary to define the old shear contact force referred to the old contact plane in the new contact plane. Assuming that between each time increment the contact entities rotations are infinitesimal, the corrected shear force is given by
\[
F_{s i}^{c, \text{corrected}} = F_{s i}^{c, \text{old}} - \epsilon_{ijklm} F_{j}^{c, \text{old}} n_{m i} n_l.
\] (21)

The predicted normal and shear forces acting at the contact are then updated by applying the following equations:
\[
F_{n}^i = F_{n}^{c, \text{old}} + \Delta F_{n}^i,
\] (22)
\[
F_{s i}^{c} = F_{s i}^{c, \text{old}} + \Delta F_{s i}^c,
\] (23)

where \( F_{n}^{c, \text{old}} \) is the previous normal contact force (scalar storage) and \( F_{s i}^{c, \text{corrected}} \) is the corrected previous shear contact force (vector storage).

The contact forces are then tested against a given constitutive contact model. Given the corrected normal and shear component, the real contact force acting at the contact point is defined by
\[
F_{i}^c = F_{n}^{c} n_i + F_{s i}^{c}.
\] (24)

The contribution of the contact force to the resulting force of the particle in contact \( \phi_1 \) is obtained by applying the following expressions:
\[
F_{i}^{(\phi_1)} = F_{i}^{(\phi_1)} - F_{i}^{c},
\] (25)
\[
M_{3}^{(\phi_1)} = M_{3}^{(\phi_1)} - \epsilon_{ijklm} (x_{i}^{c} - x_{j}^{(\phi_1)}) F_{k}^{c},
\] (26)

where \( F_{i}^{(\phi_1)} \), \( M_{3}^{(\phi_1)} \) is the applied force and moment sums for entity \( \phi_1 \) particle B, Fig. 3.

Fig. 3. Wall driven by force—contact geometry.
For the interface of a DEM/FEM contact it is further required to define how the contact forces are transmitted to the nodes. The shear and the normal contact forces are distributed to the edge nodes according to the nodal edge shape functions. It is possible to show that by applying the shape functions in the edge transverse direction the same distribution of forces as that assuming a rigid body motion is obtained. Given this, the nodal force vector can be updated given the total contact force and the assumed axial shape function for the wall element:

\[
\begin{align*}
F^{[E_1]}_i &= F^{[C_1]}_i N_i(x = l), \\
F^{[E_2]}_i &= F^{[C_2]}_i N_j(x = l).
\end{align*}
\]

(27)

(28)

The moment \( M = |F_{ii}| \frac{L_s}{2} \) caused by the shear contact force is not taken into consideration. It is assumed that for the problems to which the formulation is going to be applied the overlaps are small so that this contribution to the wall/edge nodal forces can be disregarded.

The force displacement law is applied to all the DEM/FEM contacts present in the simulation. At end of this procedure the total applied forces at each of the entities, discrete particles/plane stress finite elements are known. The applied forces are then used to define the new particle positions and also to calculate energy terms.

2.3. Global stiffness contribution

In order to implement the discrete element/finite element contact interface in an explicit algorithm it is necessary to define the global stiffness contribution of the contact interface to each node and to each particle in order to obtain the critical time increment or the scaled mass.

An expression for the node translational stiffness can be defined using the stiffness matrix of the discrete particle/edge plane finite element contact which can be obtained through equilibrium considerations. Based on the conventions of Fig. 4 the local element stiffness matrix can be defined by

\[
[k^e] = 
\begin{bmatrix}
k_a N_i^2 & 0 & k_a N_i N_j & 0 & -k_a N_i & 0 & 0 \\
0 & k_a N_j^2 & 0 & k_a N_j N_i & 0 & -k_a N_j & 0 & 0 \\
k_a N_i N_j & 0 & k_a N_j^2 & 0 & -k_a N_j & 0 & 0 \\
0 & k_a N_j N_i & 0 & k_a N_j^2 & 0 & -k_a N_j & 0 & 0 \\
-k_a N_i & 0 & -k_a N_j & 0 & k_s & 0 & 0 \\
0 & -k_a N_i & 0 & -k_a N_j & 0 & k_s & 0 & 0 \\
-k_a N_j & 0 & -k_a N_i & 0 & -k_a N_j & 0 & k_s & -d_{BC} k_s \\
0 & d_{BC} k_s N_i & 0 & d_{BC} k_s N_j & 0 & -d_{BC} k_s & d_{BC} k_s & 0
\end{bmatrix}.
\]

(29)

By applying Gershgorin’s theorem to the stiffness matrix transformed to the global axes, the maximum translational and the maximum rotational stiffness contributions for the nodes and particle involved can be obtained [10]. The maximum particle rotational stiffness and an upper bound for the translation stiffness which does not take into consideration the contact orientation of the nodes and particle can be defined by

\[
\begin{align*}
k_{\text{rot,particle}} &= k_s d_{BC}^2, \\
k_{\text{trans, node}} &= 2.0 k_a N_{\text{Node}} + 2.0 k_s N_{\text{Node}}, \\
k_{\text{trans, particle}} &= 2.0 k_a + 2.0 k_s.
\end{align*}
\]

(30)

(31)

(32)

In order to check the energy balance it is necessary to define the energy terms related to the nodes and particles, e.g. strain energy, kinetic energy, exterior forces, damping forces [14].

Fig. 4. Forces and deformations for discrete particle/plane finite element contact.
3. Examples

3.1. Tensioned column

In order to investigate the versatility of the hybrid method presented to model the interaction between a FEM domain discretization and a DEM domain discretization a column loaded in tension is analyzed. The column was first modeled with a quadrilateral mesh of finite elements with three elements over its height and six plane finite elements over its length with a unit thickness, Fig. 5. The finite elements at the outer layers have an height of 0.33 m while the finite elements at the inner layer have an height of 0.34 m. The column has the following mechanical and geometric properties: length of 4.80 m, depth of 1.0 m, width of 1.0 m, Young's modulus of 20 GPa and Poisson's ratio of 0.20.

The same column was modeled using a hybrid discretization adopting both plane quadrilateral finite elements and circular rigid particles. On the first hybrid discretization, Hexagonal—H1, the finite elements 3, 9 and 15 were replaced by an hexagonal assembly of particles with 0.02 m radius generating 595 particles. The same finite elements were also replaced by a random assembly of particles defined based on the principles defined in [6], 1258 particles were generated with a radius varying uniformly between 0.01 m and 0.02 m, Random—H1.

For the second hybrid model only the plane quadrilateral element 9 of the initial finite element mesh was replaced by particle assemblies. An hexagonal particle assembly with 357 particles of 0.015 radius, Hexagonal—H2, and an uniform particle distribution based on the principles defined in [6], 773 particles were generated with a radius varying uniformly between 0.0075 m and 0.015 m, Random—H2. On the second hybrid model, the particle assembly interacts with the finite element mesh over all the particle boundaries. The hybrid discretizations are presented in Fig. 6.

The column has its axial motion restrained on one end and an applied axial load of 10.0 kN/m on the other end. In order to model the adopted motion boundary conditions, nodes 1, 8, 15 and 22 are assumed to have their motion restrained in the axial direction. The applied load is modelled through nodal forces at the end tip, nodes 7 and 28 have an applied nodal force of 1.67 kN and nodes 14 and 21 have an applied load of 3.33 kN.

An elastic constitutive model is adopted for the quadrilateral plane frame finite elements, for the inter-particle contacts and for the FEM/DEM interface contacts. The normal $k_n$ and the shear $k_s$ contact stiffness for the random assemblies are defined using:

$$k_n = \frac{E' H}{L} t, \quad k_s = \frac{E'' H}{L} t,$$

where $L$ is the inter-particle distance, $t$ is the thickness of the particle assembly, $H$ is defined as the contact height being equal to the smaller diameter of the particles involved, and for plane stress $E' = \frac{E}{1-\nu}$ and $E'' = \frac{E}{2(1+\nu)}$, where $E$ and $\nu$ are the Young's modulus and the Poisson's ratio of the continuum material.

![Fig. 5. FEM discretization.](image)

![Fig. 6. Hybrid discretizations tested. (a) Hexagonal—H1, (b) Random—H1, (c) Hexagonal—H2 and (d) Random—H2.](image)
For the hexagonal particle assemblies the contact stiffness expressions are derived by assuming that the particle model and the equivalent continuum should produce the same strain energy [9,12]. For hexagonal arrangements the following formulas for the contact stiffnesses can be defined:

\[ k_n = \frac{\sqrt{3}}{3(1-v)} E, \quad k_s = \frac{\sqrt{3}(1-3v)}{3(1-v^2)} E. \]  

(34)

The contact stiffness of the FEM/DEM interface elements are defined using the same formulas as previously given for the interparticle contacts. For the interface elements the distance \( L \) is defined as the distance of the particle centre of gravity to the edge of the plane quadrilateral finite element. In order to simplify the generation process an initial particle overlap is adopted. A mass scaling algorithm is adopted in order to reduce the number of steps necessary to reach the desired steady-state solution [20].

In Table 1(a) are presented the Young’s modulus \( E_c \) and Poisson’s coefficient \( \nu_c \) used to define the interparticle contact stiffnesses and also the macroscopic values of the Young’s modulus and the Poisson’s coefficient for each global direction, obtained using a numerical procedure where the particle assemblies are loaded on each direction and the deformations and the applied stress are defined, plane stress constitutive equations are assumed.

Table 2(a) and (b) present, respectively, the nodal displacements at the loaded boundary for the global \( X \) and the reactions at the restrained boundary for all the discretizations analyzed. For all the hybrid discretizations a good agreement is found with the FEM case in both the global displacements at the loaded tip and the reactions forces. As the random assemblies are not fully isotropic the problem symmetry is lost.

Table 1(b) presents the number of time steps necessary for the dynamic relaxation algorithm to reach convergence and the total execution time for each discretization. It can be verified that by introducing the particle assembly the number of time increments to reach convergence increases. This is related to the fact that the particle system decreases the critical time step and greatly increases the number of degrees of freedom.

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Properties and solution time</th>
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<tbody>
<tr>
<td></td>
<td>( E_c ) [GPa]</td>
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<tr>
<td>(a) Micro/macro particle assembly properties</td>
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<tr>
<td>Hexagonal—H1</td>
<td>20.00</td>
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<tr>
<td>Random—H1</td>
<td>15.00</td>
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<tr>
<td>Hexagonal—H2</td>
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<tr>
<td>Random—H2</td>
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<table>
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<tr>
<th>(b) Solution time</th>
<th>Time steps</th>
<th>Execution time [s]</th>
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<tr>
<td>FEM</td>
<td>160</td>
<td>( \approx 0.0 )</td>
</tr>
<tr>
<td>Hexagonal—H1</td>
<td>816</td>
<td>7.0</td>
</tr>
<tr>
<td>Random—H1</td>
<td>1123</td>
<td>26.0</td>
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<tr>
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<tr>
<td>Random—H2</td>
<td>1032</td>
<td>13.0</td>
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<table>
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<tr>
<th>Table 2</th>
<th>Global ( X ) numerical values</th>
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<tr>
<td></td>
<td>Node 7 [( \mu m )]</td>
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<td>(a) Displacements at the loaded boundary</td>
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<tr>
<td>Hexagonal—H1</td>
<td>2.406</td>
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<tr>
<td>Random—H1</td>
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<tr>
<td>Hexagonal—H2</td>
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<td>Random—H2</td>
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<table>
<thead>
<tr>
<th>(b) Reactions at the restrained boundary</th>
<th>Node 1 [kN]</th>
<th>Node 8 [kN]</th>
<th>Node 15 [kN]</th>
<th>Node 22 [kN]</th>
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<tbody>
<tr>
<td>FEM</td>
<td>-1.650</td>
<td>-3.350</td>
<td>-3.350</td>
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<tr>
<td>Hexagonal—H1</td>
<td>-1.651</td>
<td>-3.348</td>
<td>-3.348</td>
<td>-1.651</td>
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<tr>
<td>Random—H1</td>
<td>-1.652</td>
<td>-3.350</td>
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<tr>
<td>Hexagonal—H2</td>
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<td>-3.350</td>
<td>-3.350</td>
<td>-1.650</td>
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</table>
For the case study Random—$H1$ is presented in Fig. 7 the energy terms history. The energy terms involved for the undamped case are the kinetic energy, the strain energy and the body work at the nodes where the exterior force is applied. The sum of the kinetic and strain energy term agrees well with the body work with a 1% maximum error which shows that the hybrid solutions with the contact interfaces is conserving the total system energy.

3.2. Mode I fracture in notched beam

A mode I fracture experiment on an notched beam of plain concrete tested in [13] was analyzed using the hybrid method here proposed. The beam geometry is shown in Fig. 8(a). The concrete had an a Young’s modulus of 30 GPa, a Poisson’s ratio of 0.20 and a tensile stress $f_{ct} = 3.33$ MPa.

The concrete beam was discretized using circular rigid particles on the notched area and 4 node plane quadrilateral finite elements on the remaining part, see Fig. 8(b). The circular rigid particle zone has a width of 0.20 m being approximately 17 times higher than the maximum rigid particle used which is equal to the maximum aggregate used, 12.0 mm diameter. For the finite elements a linear elastic constitutive model is adopted using a Young’s modulus of 30 GPa and a Poisson’s ratio of 0.20.

The circular particle assemblies were generated according to the aggregate content defined in Table 3. A given threshold for the minimum particle diameter has been adopted. All the particles with a diameter smaller than 2.0 mm are not taken into consideration. All the particle content above the threshold value was inserted followed by a void elimination procedure [10] using a fixed particle diameter of 2.00 mm.

![Energy terms history—5000 steps.](image)

![Notched beam: (a) geometry and (b) hybrid model discretization.](image)

<table>
<thead>
<tr>
<th>Aggregate [mm]</th>
<th>0.00–1.00</th>
<th>1.00–2.00</th>
<th>2.00–4.00</th>
<th>4.00–8.00</th>
<th>8.00–12.00</th>
</tr>
</thead>
<tbody>
<tr>
<td>1879 kg/m³</td>
<td>32%</td>
<td>10%</td>
<td>14%</td>
<td>20%</td>
<td>24%</td>
</tr>
</tbody>
</table>
The several random assemblies were created according to the principles defined in [10] taking advantage of the discrete element method capabilities for discontinuous media. In order to simplify the generation process an initial particle overlap is adopted.

One of the particle assemblies used over the notched area is shown in Fig. 9 in terms of particle discretization and in terms of the particle/particle and particle/wall active contacts. The particle assembly shown in Fig. 9 has 3038 particles, 8795 particle to particle contacts and 121 particle to finite element edge contacts.

The particle method requires a previous calibration of the microscopic parameters in order to obtain the desired macroscopic parameters. For this reason uniaxial tensile and compression tests were carried out. The numerical tensile tests were performed on specimens of $200 \times 100 \times 100$ mm and the compression numerical tests on specimens of $200 \times 200 \times 200$ mm. Both tests were conducted by applying displacement increments to the upper boundary; a zero friction condition is adopted for the contact between the rigid walls and the particles.

The calibration of the micro-parameters through tensile and compression tests enables the DEM particle model to be predictable. The same Young's modulus, Poisson's coefficient, tensile strength and cohesion are adopted for all the particles. Table 4(a) lists the adopted Young's modulus $E_c$ and Poisson's ratio $\nu_c$ for the interparticle contacts. The macroscopic values of the Young's modulus $E$ and the Poisson's coefficient $\nu$ are numerically determined for both the uniaxial tensile and compression tests adopting plane stress constitutive equations, Table 4(a).

The microscopic strength parameters also need to be calibrated. A Mohr–Coulomb failure criterion is adopted, after failure is reached, a one-fourth bilinear tension/shear softening model proposed by Rokugo [17] is adopted. A given softening fracture energy is adopted for the tensile, $G_{ft}$, and for the shear, $G_{fc}$, direction, Table 4(b).

Table 4(b) presents the microscopic strength values adopted for the contacts which give the best fit for the numerical models in terms of tensile uniaxial strength and compression uniaxial strength. In Table 4(b) are also presented the macroscopic uniaxial tensile stress $\sigma_t$, the macroscopic uniaxial compression stress $\sigma_c$ and the fracture energy value $G_f$ obtained given the area of the stress/deformation diagram for the tensile tests.

For the mode I notched tests the micro properties calibrated for the uniaxial tests were adopted. The FEM/DEM interface contacts properties are defined using the microparameters adopted for the particle to particle contacts. The load is applied to the notched beam by imposing displacement to a platen which is simulated with a rigid wall. The loading platen has a width of 16.5 mm that is close to 0.10 of the beam height, 200 mm.

Fig. 10 presents the notched beam load deflection response for 4 random assemblies. It is seen that the coupling model DEM/FEM shows a good agreement with the experimental before the peak load which shows that the microscopic stiffness scale well with the problem. For a rigid particle system with a tensile stress around 3.3 MPa, Table 4(b), it is shown that the peak load is lower than the experimental result of plain concrete with similar tensile stress. Also the response is less ductile, a rigid circular particle 2D system shows higher brittleness when compared to the equivalent concrete material [10].

Table 4

<table>
<thead>
<tr>
<th>Micro/macro properties</th>
<th>$E_c$ [GPa]</th>
<th>$\nu_c$</th>
<th>$E$ [GPa]</th>
<th>$\nu$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a) Elastic properties</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>21.90</td>
<td>0.25</td>
<td>30</td>
<td>0.19</td>
</tr>
<tr>
<td>$\sigma_t$ [MPa]</td>
<td>$C$ [MPa]</td>
<td>$\mu$</td>
<td>$G_{ft}$ [N/m]</td>
<td>$G_{fc}$ [N/m]</td>
</tr>
<tr>
<td>(b) Strength properties</td>
<td>1.80</td>
<td>6.50</td>
<td>0.2</td>
<td>10.0</td>
</tr>
</tbody>
</table>

Fig. 9. Notched beam random particle assemblies: (a) particles and (b) contacts.
Fig. 11 shows the final crack patterns obtained for random particle assemblies 1 and 4. They agree well with the experimental data on plain concrete, the cracking process starts at the notch tip and then it grows towards the loaded zone around the rigid particles in a mode I type originating some tortuosity of the crack pattern.

Given that the particle assemblies have a different spatial discretization, the crack initiation and further crack growing do not coincide as the crack in the particle system is only allowed to grow around the rigid particles. Different particle arrangements at the crack tip lead to different cracks, but the global load deflection response are relatively similar.

3.3. Mixed mode fracture in shear notched beam

A mixed-mode concrete fracture experiment on a notched shear beam tested by Arrea et al. [1] was analyzed using the hybrid method. The same experiment was analyzed by Rots et al. [18] using a smeared crack finite element approach. The beam geometry is shown in Fig. 12, in the same figure it is shown the experimental crack surface. The load was applied via a steel beam which distributed the load to the concrete beam, the experimental steel beam had a height of 155 mm and a width of 51 mm. The concrete had a Young\'s modulus of 24.8 GPa, a Poisson\'s ratio of 0.18 and a tensile strength \( f_{ct} = 2.80 \) MPa.

The concrete beam was discretized using circular rigid particles on the notched area and 4 node plane quadrilateral finite elements on the remaining part, see Fig. 13. The circular rigid particle zone has a width of 0.30 m being approximately 25 times higher than the maximum rigid particle used which is equal to the maximum aggregate used, 12.0 mm diameter. For the quadrilateral finite elements a linear elastic constitutive model is adopted using a Young\'s modulus of 24.8 GPa and a Poisson\'s ratio of 0.18. For the loading steel beam, a beam finite element model is used.

The circular particle assemblies were generated according to the aggregate content defined in Table 3 and followed the principles previously defined in Section 3.2. One of the particle assemblies used over the notched area is defined in Fig. 14 in terms of particle discretization and in terms of the particle/particle and particle/wall active contacts. The particle assemblies adopted had in average 6908 particles, 20,212 particle to particle contacts and 195 particle to finite element edge contacts.
As mentioned in Section 3.2 the particle method requires a previous calibration of the microscopic parameters in order to obtain the desired macroscopic parameters. The same Young’s modulus, Poisson’s coefficient, tensile strength and cohesion are adopted for all the particles. Table 5(a) presents the adopted Young’s modulus and Poisson’s coefficient for the interparticle contacts, $E_c$ and $v_c$. Table 5(a) also shows the macroscopic values of the Young’s modulus $E$ and the Poisson’s coefficient $v$ are numerically determined for both the uniaxial tensile and compression tests adopting plane stress constitutive equations.

The microscopic strength parameters also need to be calibrated as mentioned in Section 3.2. Table 5(b) presents the microscopic adopted strength properties and the macroscopic strength properties obtained through tension and compression numerical tests in particle assemblies. A Mohr–Coulomb failure criterion is adopted, after failure is reached, a one-fourth bilinear tension/shear softening model proposed by Rokugo [17] is adopted. The FEM/DEM interface contacts properties are defined using the microparameters adopted for the particle to particle contacts. The load is applied to
the mixed notched beam by imposing displacement at the node of the beam finite element at the notch location that is modelling the steel beam. The loading platens, see Fig. 13 have a width of 30.0 mm and are represented through flexible walls driven by force, see [10] for implementation details.

Fig. 15(a) and (b) show the final crack patterns obtained for two different random particle assemblies. At maximum load only a very few contacts are cracked, only after the peak load is reached the progressive cracking occurs. The crack predicted with the hybrid contact model takes a large swing to the right and then it vertically grows towards the top of the beam to the right side of the load. An equivalent crack process was experimentally identified by Arrea et al. [1], see Fig. 12(b). It is also noted that even if the model includes cracks to occur by shear only tensile cracks occur in the particle assemblies.

Fig. 15(c) show the damaged contacts distributions in the notched area. It gives an indication of the fracture process area which occurs between the loaded and the fixed supports on the top and on the bottom of the beam. As shown in Fig. 15(a) and (b), the particle model coupled with a FEM model gives a clear picture of the final localized crack and also of the fracture process zone related with the micro-cracking zone. It is also shown that the crack process is localized within the notched area discretized with DEM rigid particles, which agrees with the fact that an elastic behaviour was adopted for the remaining part of the beam.

Fig. 16 presents the average load crack mouth sliding displacement, CMSD, behaviour obtained in the four random particle assemblies tested. In Fig. 16 the numerical values are compared with the experimental curves obtained by Arrea et al. [1] and with the numerical results obtained in Rots et al. [18]. As shown, the maximum load and the pre-peak load are well captured by the numerical model given the calibration procedure.

---

Table 5

| Micro/macro properties | | | | |
|---|---|---|---|
| $E_c$ [GPa] | $v_c$ | $E$ [GPa] | $v$
| (a) Elastic properties | 18.80 | 0.22 | 25 | 0.18 |
| $\sigma_t$ [MPa] | $C$ [MPa] | $\mu$ | $G_{lt}$ [N/m] | $G_{lt}$ [N/m] | $\sigma_t$ [MPa] | $\sigma_c$ [MPa]
| (b) Strength properties | 1.85 | 5.00 | 0.2 | 10.0 | 500 | 2.74 | 30.40 |

Fig. 15. Final crack patterns and contact damage: (a) Assembly A—crack pattern, (b) Assembly B—crack pattern, (c) Assembly A—contact damage and (d) Assembly D—contact damage.
Fig. 16 also shows that the post-peak behaviour of the numerical model differs from the experimental behaviour, this can be partially explained by the fact that the experimental test was performed under CMSD-control. The CMSD was the feedback for the hydraulic actuator on top of the steel beam, whereas the computation was carried under the displacement control of the loading point on top of the steel beam. Also during the experiment, cycle loading was applied and holding stages were introduced so that the load could decrease while the CMSD was kept constant. Rots et al. [18], using a smeared crack finite element approach, also adopted a displacement control of the loading point on the steel beam and also obtained a ductile post-peak response.

The width of the area with contact damage which is directly related to the fracture process width is close to the one obtained in [18]. The particle model with a Mohr–Coulomb failure criterion with bilinear tension/shear softening model allows both discrete cracks both and smeared damage throughout the assembly, Fig. 15.

4. Conclusion

A DEM/FEM coupling algorithm has been presented which enables the use of rigid circular particles only on the fracture processes, being the remaining part of the structure modelled with finite elements. The coupling between the two different discretizations is done by introducing interface elements with shear and normal springs in the boundaries between the two different discretizations.

The rigid particle assemblies in 2D behave like an assembly of rods. In order to assume plane strain or plane stress for the rod assembly it is necessary to calibrate the contact stiffnesses in order to a obtain a given macroscopic Young’s modulus and Poisson’s coefficient. The macroscopic coefficients are found using the plane stress or plane strain equations for the stress/strain relationships. In order to have a displacement compatibility between the two different discretizations it is required to have on both discretizations an equal macroscopic Young’s modulus and Poisson’s ratio.

The hybrid model after a pre-calibration procedure using uniaxial tension and compression tests is shown to give good results in terms of crack patterns, crack localization process and pre-peak load displacement relationship for both mode I and mixed mode fracture beam experiments. Further research is still required in order for the particle model to display a more ductile post-peak response in mode I.

Assemblies of discrete circular rigid particles connected through simple interaction laws are shown to be able to capture the global behaviour of quasi-brittle macro-material, like concrete. When compared to continuum formulations particle methods are conceptually simpler and the creation of cracks and rupture surfaces appear naturally as part of the simulation process given its discrete nature.

The hybrid model is shown to allow significant computer savings, both in processing velocity and memory requirements, when compared to a pure DEM model. Finally, the hybrid model here proposed increases the domain of application of the particle models allowing new possibilities of calibration/development of the DEM.

Through the application of the hybrid model to concrete beams it is shown that the DEM rigid particle model is able to predict the behaviour of concrete beams under mode I and also under the more complex mixed mode state of stress. Finally, the coupling model here proposed for 2D fracture simulations can be easily extended to 3D, but instead of a contact edge one may have for example a triangular contact surface with three nodes and with the equivalent shape functions.
Acknowledgments

Partially supported by the Foundation for Science and Technology of Portugal (Praxis XXI-BD-18018-98).

References