Combination of an adaptive remeshing technique with a coupled FEM-DEM approach for analysis of crack propagation problems

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Abstract This paper presents an enhanced coupled approach between the Finite Element Method (FEM) and the Discrete Element Method (DEM) in which an adaptative remeshing technique has been implemented. The remeshing technique is based on the computation of the Hessian of a selected nodal variable, i.e. the mesh is refined where the curvature of the variable field is greater. Once the Hessian is known, a metric tensor is defined node-wise that serves as input data for the remesher (MmgTools) that creates a new mesh. After remeshing, the mapping of the internal variables and the nodal values is performed and a regeneration of the discrete elements on the crack faces of the new mesh is carried out. Several examples of fracturing problems using the enhanced FEM-DEM formulation are presented. Accurate results in comparison with analytical and experimental solutions are obtained.

Keywords Remeshing technique · Coupled formulation · Fracture mechanics · FEM-DEM · Finite element method · Discrete element method

1 Introduction

The modelling and simulation of the mechanical process of fracturing of materials and structures is one of the most challenging topics in computational mechanics. The laboratory predictions of the ultimate strength of materials and the detection/propagation of fractures is also a complex research topic due to their typical prompt or abrupt behaviour of crack, which difficulties the experimental analysis.

In this paper a novel coupled FEM-DEM formulation is presented. The method is based on previous works of the authors in coupling the FEM and

DEM procedures [2][3]. The existing coupled FEM-DEM procedure is enhanced with an adaptive remeshing technique based on the Hessian of the distribution of a nodal variable of interest. Unlike in other fracture mechanics formulations [4][5][6][7][8][42][43], this methodology only uses the remeshing technique to improve the quality of the crack path. As shown in [2][3], the FEM-DEM formulation is capable of obtain accurate, consistent and mesh-independent results [2][3] due to the use of the super-convergent patch recovery technique [9], this avoids the need of stabilization of the stress field, as it is required in other alternatives [12][13][14].

The selection of a proper nodal variable whose Hessian is going to be computed is crucial in order to refine the mesh near the crack openings and not close to the Dirichlet or Newman boundaries.

The enhanced coupled FEM-DEM formulation here presented has been applied to a collection of benchmark problems. The numerical results presented in this paper prove the accuracy and correctness of the adaptive remeshing technique implemented.

2 State of the Art

2.1 State of the art in Fracture Mechanics

In the field of continuum mechanics, a fracture can be expressed mathematically as a discontinuity of the displacement field in a certain zone of the domain. In this way one must separate the body in two domains Ω^+ and Ω^- and define the boundaries between them. This approach is called *continuum strong discontinuity*. Another option is to regularize the strong discontinuity by imposing a finite zone in which the displacement field is continuous and the strains are discontinuous but not infinite [14]. This technique is usually called *continuum smeared approach* (Fig. 1).

If one moves on from the continuum to the discretized problem, i.e. to the FEM, the *discrete strong discontinuity* technique was introduced by Clough [15], Ngo and Scordelis [16], Nilson [17]. It consists in separating the elements that have achieved a certain stress threshold by duplicating the affected nodes (Fig. 2). This methodology has the drawback that is inherently mesh dependent due to the fact that the propagation directions are the element boundaries.

In order to solve the previous limitation, a *remeshed strong discontinuity procedure* was introduced by Shephard[4] and Wawrzynek and Ingraffea [15] and improved by Bittencourt et al. [16]. In this case the mesh is refined in zones near the crack tip so the affected elements are split into smaller ones. This methodology overcomes part of the problems of the *discrete strong discontinuity method* but it has an additional computational cost regarding the remeshing procedure. Moreover, the remeshing tool needs to know the propagation direction of the crack, which is difficult to predict using conventional displacement-based formulations.

Fig. 1: Discontinuities in a continuum (a) strong discontinuity (b) continuum smeared approach. Image from [18]

Fig. 2: Discontinuities in a discrete medium (a) strong discontinuity (b) discrete smeared approach. Image from [18]

After analysing those technical issues, the previous formulation lead to the Extended Finite Element Method (XFEM) [19][20][21][22][23], which uses an enriched set of shape functions to interpolate the displacement field in the elements crossed by the crack.

As for the remeshing techniques, the embedding of the crack path requires to know the directions of the evolution of the crack and this is not accurately predicted in displacement-based formulations. In the XFEM an additional set of integration quadratures are required to properly integrate the split elements that, in normal conditions, have a singular stiffness. Additionally, these techniques usually require tracking techniques in order to preselect the elements that are going to be enriched [26].

Anther option is the so-called *smeared crack approach*. This model was initially proposed by Rashid [27] and it describes the crack path by a band of elements whose displacements field is continuous and its strain field discontinuous but bounded. Fig. 2b shows the finite elements band affected by the

weak discontinuities. The *smeared crack approach* was very popular but after some years of its adoption Pietruszczak and Mroz [28] and Bazant and Oh [29] noticed that the fracture process is not only dependant on the fracture energy, but also on the characteristic length of the mesh analysed. This issue provokes that the finer the mesh is, the more brittle the behaviour is, which is an unacceptable inconsistency.

Despite the many different discrete weak discontinuities approaches, it was seen that the standard displacement-based formulations appeared to be inaccurate when dealing with the onset and propagation of fractures. This is due to the fact that on the crack tip the strains and stresses are not well predicted and, in general, the direction of the crack path is strongly dependant on the mesh orientation.

Regarding the enhanced or enriched finite element formulations, the multidimensional generalization of the displacement jump is not straight forward and it is usually accompanied by ill-conditioning problems. Additionally, since the mentioned enhancements are applied depending on the stress field of the previous time step and, taking into account that the standard displacement-based formulations do not guarantee the local convergence of the stress field, these methods often require the use of auxiliary crack tracking techniques.

Subsequently, other FEM formulations were developed in order to provide computational enhancements, such as mixed formulations. Mixed formulations are computationally more expensive than the standard ones since they require to solve multiple unknown fields. In addition, the finite elements have to satisfy the *Inf-Sup* condition [30][31] to ensure the stability of the solution. This condition is not easy to fulfil and several developments were introduced to mitigate this problem [32][33].

If one moves on from the methods based on the FEM to the DEM [36][37], the kind of problematic is intrinsically different. There are several approaches that discretize the continuum as a set of discrete elements (DE) (hereafter termed particles) attached by a bonding between them ruled by local or non-local constitutive laws [38][39]. However, the calibration of the local material parameters of the bonds between the particles is complex [40] and only under certain conditions behaves as a continuum. In addition, the large number of DE needed to solve practical problems discourages its use.

Bearing all this information in mind and trying to combine the best features of the FEM and the DEM, the FEM-DEM methodology was developed [2][3]. The continuum is initially represented with FE whose material behaviour is represented by an isotropic damage model. A smoothing procedure is used by computing the stresses at the element edges. When damage in a certain element achieves a maximum threshold, the element is removed from the mesh DE are placed at its nodes. The new DE avoid the indentation between the crack faces by the contact forces among them and these forces are transferred to the FE nodes as equivalent nodal forces.

2.2 State of the art in mesh refinement

2.2.1 Mesh generation

The early works of mesh generation by Zienkiewicz and Phillips[57] on the 1970s were based on the geometry boundary of the domain size and the required distribution of the element size. Since then many different technologies have been proposed, including mapping techniques and semi-automatic remeshing methods, where the domain has to be subdivided manually in a initial stage into simpler subdomains[49]. These methodologies depend on *know-how* from the user and are generally limited to *structured meshes* (quadrilaterals and hexahedra).

Alternatively to *structured meshing* algorithms, *unstructured meshing* techniques have been extensively developed for *simplex* element geometries: triangles in 2D and tetrahedra 3D. These techniques are based mainly in three algorithms[1]:

- *Delaunay* triangulation methods[50].
- The advancing front method[51].
- Tree methods: *quadtrees* for 2D and *octrees* for 3D cases[52].

2.2.2 Adaptive finite element refinement techniques

Mesh adaption is widely used in numerical simulations to improve the accuracy of the solutions, as well as to capture the behaviour of physical phenomena[60]. This technique allows to reduce considerably the computational cost, associated with a reduction of degrees of freedom (DoF from now on), while yielding an accurate solution[67].

Adaptive mesh refinement allows to compute complex problems with good results in 3D without requiring the initial remeshing during pre-processing step, which can be a time consuming and *error-prone*[1] task. Additionally, adapting the computation during the simulation, avoids the creation of an initial mesh that fits all the problem evolution, which can be *a priori* not known.

The mesh refinement process depends on the previous numerical results[1]. These methodologies were introduced originally by Babuka and Rheinboldt[53][54] in the late 1970s.

One of the most popular mesh remeshing strategies is based on the *recovery by equilibrium of patches* (REP) techniques. A widely used approach based on REP is the *Superconvergent Patch Recovery* (SPR) technique proposed by Zienkiewicz and Zhu [9]. The methodologies based on REP are not the only ones available to measure the error. Zienkiewicz and Zhu proposed other techniques by using different *recovery methods*[10]. Recently, techniques based on the *Hessian* of a solution field have been developed[66]. This requires that the variable to be used as error estimation has to be twice continuously differentiable. This methodology has the advantage of giving a proper measure in

Fig. 3: DE generation after removing a FE

order to create anisotropic meshes, which reduces the number of new elements necessary.

3 Coupled FEM-DEM Formulation

The coupled FEM-DEM formulation was developed by Zárate and Oñate[2] as an effective procedure for predicting the onset and propagation of cracks in concrete and rocks. Zárate, Cornejo and Oñate[3] extended the formulation to 3D problems.

Initially the continuum is modelled with simplex FE (3-noded triangles in 2D and 4-noded tetrahedra in 3D). The FE solution is obtained by reaching the dynamic equilibrium via an implicit transient dynamic solution scheme. An isotropic damage constitutive law is chosen in order to verify failure at the edges of the FE (using the SPR technique [9]). Once one of the failure modes of the FE is achieved, this FE is removed from the mesh and DE are placed at the nodes of the removed FE (see Fig. 3 and [2][3]).

Some important aspects inherent to the FEM-DEM formulation guarantee the good results obtained, such as a smoothed stress field, mass conservation and the use of a simple algorithm to ensure the post-fracture contact between the fractured edge and the adjacent FE and DE in the mesh[2][3].

3.1 FEM formulation

The predictive stress tensor $\bar{\sigma}$ on all the elements of the mesh is initially computed, as:

$$\bar{\sigma} = \mathbf{C}_0 : \varepsilon \quad (1)$$

where $\mathbf{C}_0$ is the elastic constitutive tensor and ε the strain tensor.

Once the predictive stresses at the integration points of all the elements of the mesh are computed, the smoothed stress field is evaluated at the edges of

the FE. The smoothing procedure is based on the average stress between the current element and the neighbour one sharing an edge, i.e.

$$\bar{\sigma}_{edge} = \frac{1}{2} (\bar{\sigma}_{current} + \bar{\sigma}_{neighbour}) \quad (2)$$

Next, the constitutive equation is integrated at the edges. An isotropic damage model is used if the stress state is outside the yield surface Φ , i.e.

$$\Phi := f(\bar{\sigma}) - \kappa > 0 \quad (3)$$

where $f(\bar{\sigma})$ is the uniaxial stress that is computed according to different yield surfaces and κ is the mechanical threshold that is related to the yield strength. In the examples performed in this work we have used the Rankine and Modified Mohr-Coulomb[41] yield surfaces. Once the initial threshold κ_0 is achieved it has to be updated according to the maximum historical stress state.

The isotropic damage constitutive model is written as:

$$\sigma = (1 - d) \bar{\sigma} = (1 - d) \mathbf{C}_0 : \varepsilon \quad (4)$$

where d is the damage parameter that takes into account material degradation as well as the irreversibility of the constitutive model. As far as the computation of damage is concerned, we have used the exponential softening law[69]:

$$d(\bar{\sigma}) = 1 - \frac{\kappa_0}{f(\bar{\sigma})} \exp \left(A \left(1 - \frac{f(\bar{\sigma})}{\kappa_0} \right) \right) \quad (5)$$

where the A parameter is determined from the energy dissipated in an uniaxial tension test as[69]

$$A = \left(\frac{G_f E}{\hat{l} f_t^2} - \frac{1}{2} \right)^{-1} \quad (6)$$

where f_t is the tensile strength, G_f is the specific fracture energy per unit area (taken as a material property) and $\hat{l}$ is the characteristic length of the element. In this way one can compute the damage at the midpoint of the element edges. Next, the damage of the whole element is evaluated. By analysing all the fracture modes that can occur, the damage of the element corresponding to the mode with less energy is computed (Fig. 4). In 2D problem one can use average the two maximum values at the element edges, as:

$$d_{FE} = \frac{1}{2} (d_{edge,max} + d_{edge,max-1}) \quad (7)$$

Fig. 4: Different fracture modes in 2D and 3D element geometries

3.2 Tangent constitutive tensor approximations

The FEM solution is obtained via an implicit transient dynamic solution scheme. Thus, the tangent constitutive matrix is required at each iteration of the loading step. For this purpose, several numerical techniques have been developed and adapted to the FEM-DEM formulation.

The most robust but slower option is to use the secant constitutive tensor $\mathbf{C}_s$, computed as a function of the initial constitutive tensor $\mathbf{C}_0$ and the damage d :

$$\mathbf{C}_s = (1 - d)\mathbf{C}_0 \quad (8)$$

Another alternative is based on the derivatives approximation via finite differences, i.e. the tangent constitutive tensor relationship can be expressed as $\dot{\boldsymbol{\sigma}} = \mathbf{C}_T : \dot{\boldsymbol{\varepsilon}}$. A column of the tangent constitutive tensor $\mathbf{C}_T$ is defined as [34]:

$$\mathbf{C}_{T,j} = \frac{\delta^j \boldsymbol{\sigma}}{\delta \varepsilon_j} \quad (9)$$

An approximation of the tangent constitutive tensor can be obtained by defining n small perturbations of the strain tensor $\delta \varepsilon_j$ in order to obtain n stress tensor increments $\delta^j \boldsymbol{\sigma}$. This can be done in several ways, as stated below (depending on the finite difference scheme):

$$\mathbf{C}_{T,j} \simeq \frac{\boldsymbol{\sigma}(\boldsymbol{\varepsilon} + \delta \varepsilon_j) - \boldsymbol{\sigma}(\boldsymbol{\varepsilon})}{\delta \varepsilon_j} \quad ; \quad \mathbf{C}_{T,j} \simeq \frac{\boldsymbol{\sigma}(\boldsymbol{\varepsilon} + \delta \varepsilon_j) - \boldsymbol{\sigma}(\boldsymbol{\varepsilon} - \delta \varepsilon_j)}{2\delta \varepsilon_j} \quad (10)$$

where $\delta \varepsilon_j$ is a zero vector except for the j th component whose value is the strain perturbation $\delta \varepsilon_j$.

The most general option consists in perturbing the displacement field of the FEM solution [35]. This method is appropriate for small and large strain computations (the strain perturbation method is limited to small strains) and

for any kind of constitutive model. In this way, the approximation of the tangent stiffness matrix can be computed as:

$$\mathbf{K}_{T,j} \simeq \frac{\mathbf{F}_{int}(\mathbf{u}^{n,i} + \epsilon \Delta \mathbf{u}^n) - \mathbf{F}_{int}(\mathbf{u}^{n,i})}{\epsilon \Delta u^n} \quad (11)$$

Where $\mathbf{K}_{T,j}$ is the j th column of the tangent stiffness matrix, $\Delta \mathbf{u}^n$ is the displacement increment of that node in the previous time step, $\mathbf{F}_{int}$ is the internal force vector that depends of the displacement field and ϵ is a small constant computed as:

$$\epsilon = \sqrt{\varkappa} \left(1 + \frac{\|\mathbf{u}^{n,i-1}\|}{\|\Delta \mathbf{u}^{n,i-1}\|} \right) \quad (12)$$

being $\varkappa$ the computer precision. Note that the components of the vector $\Delta \mathbf{u}^n$ are null except for the j th component whose value is Δu^n .

3.3 DEM formulation

The DEM methodology used in the FEM-DEM formulation implemented in this work is based on the work of Casas et al [44], Oñate et al [38] and Thornton et al. [45].

The motion of the DE is computed by solving the dynamic equilibrium of forces at the center of each particle using an explicit dynamic solution scheme. A sub-stepping procedure has been implemented in order to combine the DEM explicit calculations with the implicit solution scheme[2][3] for the FEM.

A *spring-dashpot type soft-sphere* approach for the contact between spheres has been selected. Considering two contacting spheres, whose centres are $\mathbf{r}_1$ and $\mathbf{r}_2$, the normal vector that connects the centers of the spheres can be computed as follows:

$$\mathbf{n}_{21} = \frac{\mathbf{r}_2 - \mathbf{r}_1}{\|\mathbf{r}_2 - \mathbf{r}_1\|}, \quad \mathbf{n}_{21} = -\mathbf{n}_{12} \quad (13)$$

The normal indentation δ_n between the discrete particles is computed as:

$$\delta_n = R_1 + R_2 - \|\mathbf{r}_{21}\| \quad (14)$$

where R_i are the radii of the particles. The total contact force between two particles is defined as the sum of a normal and a tangential force:

$$\mathbf{F} = F_n \mathbf{n} + F_t \mathbf{t} \quad (15)$$

The normal contact force F_n is obtained as a combination of an elastic and a viscous contribution:

$$F_n = F_{n,el} + F_{n,damp} \quad (16)$$

Where the elastic part can be computed as:

$$F_{n,el} = \frac{4}{3} \tilde{R}^{\frac{1}{2}} \tilde{E} \delta_n^{\frac{3}{2}} \quad (17)$$

where $\tilde{R} := (1/R_1 + 1/R_2)^{-1}$, $\tilde{E}_i := E_i/(1 - \nu^2)$, $\tilde{E} = (1/\tilde{E}_1 + 1/\tilde{E}_2)^{-1}$. The corresponding viscous damping contribution is modelled as:

$$F_{n,damp} = c_n \delta_n^{1/4} \dot{\delta}_n \quad (18)$$

For particle-particle contact the constant c_n can be expressed as:

$$c_n = \gamma \sqrt{8 \tilde{E} \tilde{M} \sqrt{\tilde{R}}} \quad (19)$$

being $\tilde{M} := (1/m_1 + 1/m_2)^{-1}$ and γ a viscous damping coefficient.

On the other hand, the tangential force is computed as:

$$\mathbf{F}_t = F_{t,el} \mathbf{t}_d + F_{t,damp} \mathbf{t}_\nu \quad (20)$$

where the directions $\mathbf{t}_d$ and $\mathbf{t}_\nu$ are based on the kinematics during tangential deformation [40].

The elastic tangential contribution is obtained by:

$$F_{t,el} = \delta_n^{1/2} \int a(t) dt \quad (21)$$

and the tangential viscous contribution as

$$F_{t,damp} = c_t \delta_n^{1/4} \dot{\delta}_t \quad (22)$$

with

$$c_t = 2 \gamma \sqrt{8 \tilde{G} \tilde{M} \sqrt{\tilde{R}}} \quad (23)$$

where $\tilde{G} = G/(4 - 2\nu)$ and $G = E/(2 + 2\nu)$.

3.4 Coupling between the FEM and the DEM

Once the damage parameter for an individual element computed by Eq. (7) reaches a maximum threshold, the damaged element is removed from the FE mesh and a set of DE are placed at the nodes of the removed element (Fig. 3, [2][3]). Following this, the displacements and velocities of the element nodes are transferred to the DE. The next step is the integration of the dynamic equations of motion of the DE using an explicit scheme using a substepping procedure.

After performing a contact search among all the DE, the contact forces at each DE (as defined in Section 3.3) are computed. Once these contact forces are known, this information is transferred to the FEM mesh as an equivalent nodal force (Fig. 3) whose objective is to prevent indentation between the crack faces. More information about the time integration of the dynamic equations for the DEM and the FEM is given in [2].

4 Hessian Based Remeshing Technique

In this section we analyse on detail the techniques considered for remeshing. We introduce first the concepts of metrics (Section 4.1) and general *Hessian* based error measures (Section 4.2). Then we present the transfer operators for the damage parameter.

4.1 Metric based remeshing

In order to understand the concept involving the *Hessian* metric[58], we first introduce the concept of metric. Then, we will show the intersection operations needed in case than more that one metric is taken into consideration.

Fig. 5: Metric analogies. Images from [58]

4.1.1 Concept of metric

The notion of length in a metric space is related to the notion of metric[67] and therefore to an adequate definition of the scalar product in the vector space considered. We define a metric tensor at a point P , respect an element K from a mesh $\mathcal{T}_h$, represented by a matrix $\mathcal{M}$ ($d \times d$) defined symmetric positive and not degenerated. In 3D, the following definition of $\mathcal{M}$ (24) is used, which can be assimilated to the analogy of an ellipsoid (Fig. 5a).

$$\mathcal{M} = \begin{bmatrix} a & b & c \\ b & d & e \\ c & e & f \end{bmatrix} \text{ such that } a > 0, d > 0, f > 0 \quad (24)$$

and $\det(\mathcal{M}) > 0$, considering $a, b, c, d, e \in \mathbb{R}$

Tensor $\mathcal{M}$ can be diagonalized because it is symmetrical. Then, $\mathcal{M}$ can be written as $\mathcal{M} = \mathcal{R}\mathcal{A}\mathcal{R}^{-1}$, where $\mathcal{R}$ and $\mathcal{A}$ are the matrix of the eigenvectors and eigenvalues of $\mathcal{M}$, respectively.

Fig. 6 illustrates the effect of the metric on the mesh. The tetrahedra presented gets sketched accordingly to the metric computed at each node, represented with ellipsoids (Figure 5a).

Fig. 6: Effects of the metric on a tetrahedra

4.1.2 Metric intersection

In the case that several metrics are specified at the same point of the mesh (for example if we want to use various nodal variables whose Hessians return different metrics) one have to define a procedure of intersection of all these metrics into one.

To define the intersection of two metrics, we use the fact that a metric tensor is represented geometrically by an ellipse (in 2D) or an ellipsoid (in 3D). The metric intersection consists then in keeping the most restrictive size constraint in all the directions imposed by this set of metrics[58] (Fig. 5b).

The simultaneous reduction enables us to find a common basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ such that $\mathcal{M}_1$ and $\mathcal{M}_2$ are congruent to a diagonal matrix. In this basis we can define a new tensor $\mathcal{N}$, whose expresion is:

$$\mathcal{N} = \mathcal{M}_1^{-1} \mathcal{M}_2 \quad (25a)$$

$\mathcal{N}$ can be diagonalized in $\mathbb{R}$ because it is symmetrical in the metric $\mathcal{M}_1$. The base in question is given by the normalized eigenvectors of $\mathcal{N}$ that we denote $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$ (they form a base because $\mathcal{N}$ is diagonalisable) . The eigenvalues of $\mathcal{M}_1$ and $\mathcal{M}_2$ are found in this base using the *Rayleigh* quotient:

$$\lambda_i = \mathbf{e}_i^t \mathcal{M}_1 \mathbf{e}_i \text{ and } \mu_i = \mathbf{e}_i^t \mathcal{M}_2 \mathbf{e}_i \quad (25b)$$

Considering $\mathcal{P} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$ be the matrix the columns of which are the eigenvectors of $\mathcal{N}$ (common basis) one can obtain

$$\mathcal{M}_1 = \mathcal{P}^{-t} \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \mathcal{P}^{-1} \text{ and } \mathcal{M}_2 = \mathcal{P}^{-t} \begin{bmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{bmatrix} \mathcal{P}^{-1} \quad (25c)$$

The metric intersection can be computed as:

$$\mathcal{M}_{1 \cap 2} = \mathcal{M}_1 \cap \mathcal{M}_2 = \mathcal{P}^{-t} \begin{bmatrix} \max(\lambda_1, \mu_1) & 0 & 0 \\ 0 & \max(\lambda_2, \mu_2) & 0 \\ 0 & 0 & \max(\lambda_3, \mu_3) \end{bmatrix} \mathcal{P}^{-1} \quad (25d)$$

4.2 Hessian based error measure

Before introducing the theory involving the *Hessian* based metric, we summarize the following properties[67]:

- The analysis and results obtained by this methodology are not asymptotic. This means that the size of the mesh h does not tend to zero, avoiding potential errors, like the collapse of the mesh at certain points.
- The metric is based in the *Hessian* of the solution.
- The metric is anisotropic.
- It is independent of the nature of the operator, so it can be used with any type of equation.

4.2.1 Theory

We compute the *Hessian*[66] matrix $\mathbf{H}$ of a scalar variable f as

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \quad \text{or just: } H_{i,j} = \frac{\partial^2 f}{\partial x_i \partial x_j} \quad (26)$$

Once the *Hessian* matrix has been computed we compute the corresponding anisotropic metric by [58].

$$\mathcal{M} = \mathcal{R}^t \tilde{\mathcal{A}}^t \mathcal{R} \quad \text{where } \tilde{\mathcal{A}} = \text{diag}(\tilde{\lambda}_i) \quad \text{being} \quad (27a)$$

$$\tilde{\lambda}_i = \min \left(\max \left(\frac{c_d |\lambda_i|}{\epsilon}, \frac{1}{h_{max}^2} \right), \frac{1}{h_{min}^2} \right)$$

Being λ_i the eigenvalues of $\mathbf{H}$ and ϵ the error threshold and c_d a constant ratio of a mesh constant. The interpolation ratio ϵ has been taken as 10^{-6} . On the other hand c_d can be taken as $\frac{2}{9}$ and $\frac{9}{32}$ for 2D and 3D cases, respectively. For an isotropic mesh the metric will be,

$$\mathcal{M}_{iso} = \text{diag}(\max(\tilde{\lambda}_i)) = \begin{bmatrix} \max(\tilde{\lambda}_i) & 0 & 0 \\ 0 & \max(\tilde{\lambda}_i) & 0 \\ 0 & 0 & \max(\tilde{\lambda}_i) \end{bmatrix} \quad (27b)$$

For an anisotropic mesh we have

$$\begin{aligned}\mathcal{M}_{aniso} &= \mathcal{R}^t \tilde{\Lambda}_{aniso} \mathcal{R} \text{ with} \\ \tilde{\Lambda}_{aniso} &= \text{diag}(\max(\min(\tilde{\lambda}_i, \tilde{\lambda}_{max}), R_{\lambda rel})) \text{ being} \\ R_{\lambda rel} &= |\tilde{\lambda}_{max} - R_\lambda| \text{ where } R_\lambda = (1 - \rho)|\tilde{\lambda}_{max} - \tilde{\lambda}_{min}|\end{aligned}\quad (27c)$$

4.2.2 Example

Fig. 7: Initial mesh

The objective is to remesh the structured mesh of Fig. 7 according to the Hessian of the nodal variable (objective function) defined in Eq. (28). The original mesh has 40000 structured elements. Our objective is to obtain an unstructured mesh where the smaller elements will be in the vicinity of the objective function.

The nodal variable values are computed according to:

$$\begin{aligned}f(x, y) &= \tanh(-100(y - 0.5 - 0.25 \sin(2\pi x))) \\ &\quad + \tanh(100(y - x))\end{aligned}\quad (28)$$

The results obtained are depicted in Fig. 8b, using a mesh of 15000 elements. The smaller elements are placed around the χ shape displayed in Fig. 8a showing also the nodal value of the function defined in Eq. (28).

4.3 Hessian nodal indicator

In order to optimize the remeshing technique and refine the elements close to the crack opening we define a proper nodal variable Υ whose *Hessian* is

Fig. 8: Nodal values of the remeshed mesh for the error function from Eq. (28)

computed. Initially, the nodal extrapolation of the predictive Cauchy's stress tensor was selected but the meshes generated with this indicator were suboptimal, as it refines the zones near the boundary conditions where, in general, there is no interest. In the end, a normalized energetic nodal variable indicator was selected. The expression of the mesh refinement indicator is:

$$\gamma = \frac{1}{2\rho} \left(\varepsilon : \mathbf{C}_0 : \varepsilon (1 - d) \left(\frac{r}{g_t} + \frac{1 - r}{g_c} \right) \right) \quad (29)$$

where ρ is the material density, d is the damage internal variable, g_t and g_c are the regularized fracture energies in tension and compression, respectively and r is a tension indicator computed as:

$$r = \frac{\sum_{i=1}^3 \langle \sigma_i \rangle}{\sum_{i=1}^3 |\sigma_i|}, \quad \langle \sigma_i \rangle = \frac{1}{2} (\sigma_i + |\sigma_i|) \quad (30)$$

being σ_i the principal components of the stress tensor. The mesh refinement indicator can be interpreted as the energy dissipated, normalized with the total energy available.

4.4 Internal variables interpolation

The internal variables information has to be recovered in the refined mesh in order to work with constitutive models that depend on historical values, such as the damage model used in this work. Fig. 9 shows graphically how each one of the *transfer operators* work[56] (all of them are available in *Kratos*[48]).

Fig. 9: Transfer operators: a) Closest Point Transfer b) Shape Function Projection Transfer c) Least-Square Projection Transfer . Image from [56]

- **CPT**: *Closest Point Transfer*. **(a)**. It takes the value from the closest point. It provides acceptable results at low cost.
- **SFT**: *Shape Function Projection transfer*. **(b)**. It interpolates the values using the standard FEM shape functions. It leads to an artificial damage diffusion, but preserves the original shape of the damage profile.
- **LST**: **Least-Square Projection transfer**. **(c)**. It considers a *least-square* transfer across the closest points. Probably it is the most accurate technique but also the most expensive from a computational point of view.

In our simulations we have used the **CPT** technique.

5 Implemented Algorithm

The FEM-DEM formulation presented can be summarized in the algorithm below.

Initialization of the implicit transient dynamic scheme for the FEM:

$t_i = t_i + \Delta t_i$, $k = 0$ being t_i the current time of the implicit scheme.

Apply the DE contact forces from the previous time step as equivalent nodal force for the FEM

if *It is time to remesh* **then**

 Compute nodal indicator $\Upsilon = \frac{1}{2\rho} \left(\varepsilon : \mathbf{C}_0 : \varepsilon (1 - d) \left(\frac{r}{g_t} + \frac{1-r}{g_c} \right) \right)$

 Evaluate the *Hessian* matrix $\mathbf{H}$

 Calculate the metric tensor $\mathcal{M}$

 Perform the remeshing

 Mapping of the internal variables and nodal values

end

while $\Delta F = |\mathbf{F}^{int} - \mathbf{F}^{ext}| < tol$ **do**

for *Elements* **do**

 Compute the effective stresses $\bar{\sigma} = \mathbf{C}_0 : \varepsilon$

 Smoothing of the effective stress field at the FE edges

 Compute the damage d at the edges by Eq. (5)

 Obtain the elemental damage by Eq. (7)

 Calculate the tangent stiffness matrix $\mathbf{K}_e^T$ and the updated internal forces vector $\mathbf{F}_e^{int}$

end

 Assemble the global expression of $\mathbf{K}^T$ and $\mathbf{F}^{int}$

 Calculate the displacement increments $\Delta \mathbf{u}_k^t = \mathbf{K}^{-1} \Delta \mathbf{F}$

 Check convergence $\Delta F < tol$

$k = k + 1$

end

for *Elements* **do**

if *Damage* > 0.98 **then**

 ERASE the FE

 Generate the Discrete Elements (DE) at the nodes of the damaged FE

end

end

Initialization of the explicit transient dynamic scheme for the DEM

Import the kinematic information (displacements and velocities) from the FEM nodes to the DE as an initial condition

while $t_e = t_e + \Delta t_e < t_i$ **do**

 Compute the contact forces between the DE

 Integrate the equations of motion

 Compute the displacements, velocities and accelerations at the DE

end

Transfer the contact forces as equivalent nodal forces to the FE

Algorithm 1: Enhanced FEM-DEM algorithm

6 Numerical Examples

Several examples are presented in order to show the accurate results and good representation of the fracture paths obtained with the enhanced FEM-DEM formulation developed in this work. The first example is the well-known four point bending test whose fracture path is theoretically known and the force-displacement evolution has been compared with the results from [46]. The second example is a tensile test whose analytical solution is trivial, so it is very useful in order to validate the formulation. Finally, a three-point bending test on skew notched beam has been performed. The FEM-DEM results have been compared with those obtained by Cervera et al. [47]. For the 2D examples (Section 6.1) we have used 3-noded triangles. The 3D problems have been solved using 4-noded linear tetraedra.

6.1 Four-Point Bending Beam

This example is a plane stress four point supported beam with a double notch. In the two central supports a vertical displacement is imposed whereas in the exterior supports only the vertical displacement is enforced to be zero (one of them must be clamped, as depicted in Fig. 10). The dimensions of the beam are $134 \times 30.6 \times 30$ cm. The yield surface used is the Modified Mohr-Coulomb[41]. The material properties used are: $E = 30$ GPa, $\nu = 0.2$, $t = 0.3$ m, $f_t = 2$ MPa, $G_f = 100$ J/m² and the friction angle $\phi = 32^\circ$. The initial FE mesh is displayed in Fig. 11. Fig. 12 shows that the remeshing technique and the Hessian variable indicator defined in the Section 4.2 are performing excellently as far as capturing the crack path is concerned. Another interesting feature is that the number of FE does not increase indefinitely. Fig. 12 shows that the number of FE in the mesh increases with respect to the initial coarse mesh but during the calculation is bounded up to a reasonable value (even decreasing at the end of the simulation) so the computational cost is balanced.

Quantitatively, the force-displacement evolution in one of the central supports is depicted in Fig. 14. In this figure the results from [46] and the ones from the FEM-DEM formulation, with or without remeshing, are compared, showing a good agreement between them.

Additionally, the comparison between the crack paths using the remeshing technique and the standard FEM-DEM formulation is depicted in Fig. 15. As one can see, the quality of the crack path is improved with the inclusion of the remeshing technique but, as the non-remeshed solution uses a coarser mesh, the CPU is about 14 min whereas the remeshed solution increases the CPU time up to 45 min. The main advantage of this methodology lies in obtaining great quality crack paths without the requirement of a very fine original mesh.

Fig. 10: Geometry and boundary conditions of the four point bending test (units in cm)

Fig. 11: Initial FE mesh used in the calculation (2912 3-noded triangles elements and 1573 nodes)

6.2 Tensile Test

In this example a conventional 3D tensile test has been reproduced. The geometry of the sample is depicted in Fig. 16 with a thickness equal to 0.2 m. The left end is clamped and the right one has a monotonic imposed displacement. The Modified Mohr-Coulomb yield surface has been used. The material parameters are: $E = 35$ GPa, $\nu = 0.2$, $f_t = 1.5$ MPa, $G_f = 30$ J/m² and the friction angle $\phi = 32^\circ$.

Fig. 17 shows that the mesh refinement is concentrated at the center zone, where all the energy dissipation is taking place due to the damage in the necking zone. The force-displacement evolution at one of the ends of the sample is depicted in Fig. 18. The results are in good agreement with the analytical expected solution ($R_{max} = Area * f_t$).

In Fig. 19 the final fracture of the sample is depicted. As expected, fracture occurs at the center of the necking. It is important to notice that the remeshing technique improves the quality of the cracking path (see the comparison in Fig. 20) but quantitatively is always consistent (Fig. 18), even when using coarse meshes.

Fig. 12: FE meshes during calculation (a) 5388 FE, b) 6276 FE, c) 8985 FE, d) 8188 FE, e) 6252 FE and f) Final result without remeshing technique

6.3 Three-Point Bending Skew Notched Beam

In this section, a skew notched beam subjected to three-point bending is analysed. The same problem was studied by Cervera et al. [47]. The original experiment was performed by Buchholz et al. [68] using Plexiglass in order to identify the fracture path along the sample. The geometry of the sample is

Fig. 13: Zoom of the refined FEM mesh in Fig. 12b

Fig. 14: Force-displacement evolution in the four point bending test at one of the inner supports

shown in Fig. 21 in which the deviation of the notch can be seen. The Rankine yield surface was used in this test as in [47]. The material parameters are: $E = 28 \text{ GPa}$, $\nu = 0.38$, $f_t = 40 \text{ MPa}$ and $G_f = 3000 \text{ J/m}^2$. The analysed problem is symmetric with respect to the notch and it fractures under a mixed Mode I and Mode III. Initially the crack path twists around the vertical axis until it is oriented perpendicular to the longitudinal direction of the beam. The initial mesh is depicted in Fig. 22. The FE meshes generated during the calculation using the remeshing technique can be analysed in Fig. 23. As it can be seen, the remeshing technique refines the elements near the notch due to

Fig. 15: Crack paths comparison between the remeshed and non-remeshed solutions

Fig. 16: Tensile test geometry (units in m)

the high dissipation that takes place in these zones. As the crack propagates, the remeshing follows the expected path by refining the front of the fracture at each remeshing step.

If one compares the results obtained with the simulation (Fig. 24) with the experimental results (Fig. 25) it is clear that the crack path follows the pattern obtained by the experiment accurately. As stated before, the solution obtained is skew-symmetrical. Also, the crack surface is perpendicular to the longitudinal axis at the end of the propagation as expected. The force-displacement evolution can be seen in Fig. 26. No numerical results regarding the force-displacement evolution was provided by the authors of this experiment.

7 Conclusions

In this work a coupled FEM-DEM formulation enhanced with a novel adaptive remeshing technique has been presented. The proposed methodology has demonstrated a good performance: quantitatively, when comparing the force displacement curves obtained with the analytical ones, and qualitatively when analysing the crack paths obtained versus the expected or experimental results.

Fig. 17: Tensile test FE meshes during the remeshed FEM-DEM calculation using 4-noded tetrahedra (a) 12000 FE, b) 8248 FE, c) 14092 FE and d) 70749 FE

Fig. 18: Force-displacement evolution for the tensile test at one of the ends of the sample

Fig. 19: Tensile test fracture in the sample at the end of the calculation

Fig. 20: Tensile test comparison of the crack pattern between the solution with (a) or without (b) the remeshing technique

Fig. 21: Three point bending skew notched beam geometry (units in m)

Fig. 22: Three point bending skew notched beam initial FE mesh (15546 4-noded tetrahedra)

The standard FEM-DEM is an accurate numerical procedure due to its intrinsic mesh-independence and consistency features[2][3]. However, the adaptive remeshing technique here presented improves considerably the crack path geometry obtained and optimizes the calculation cost, because it only refines the zones of interest, where the non-linear dissipation takes place.

Regarding the remeshing technique, the *Hessian* based methodology combined with the nodal variable indicator developed (normalized free energy) has behaved very well in all the examples performed, capturing the zones of interest where the mesh needs to be refined.

In conclusion the FEM-DEM formulation, enhanced with the adaptive remeshing technique presented, is suitable for simulating complex fracture mechanics problems at an affordable computational cost. For instance, the four

Fig. 23: Adaptive FE meshes of 4-noded tetrahedra during calculation a) 15546 FE, b) 14436 FE, c) 16707 FE, d) 25811 FE, e) 27478 FE and f) 29738 FE

point bending test was run in 50 min, the tensile test in 9 hours and the three point bending test in 4 hours. All the tests were carried out in a personal computer (CPU: Intel Core i7-8700, RAM: 16 GB DDR4) using 12 threads.

8 Appendix

8.1 Kratos multiphysics

The FEM-DEM formulation presented has been implemented in the *Kratos* multi-physics framework [48] that has been specially designed for helping the development of multi-disciplinary finite element programs. We can summarize the following features:

- **Kernel:** The kernel and application approach is used to reduce the possible conflicts arising between developers of different fields.
- **Object oriented:** The modular design, hierarchy and abstraction of these approaches fits to the generality, flexibility and re-usability required for the current and future challenges in numerical methods. The main code is developed in *C++* and the *Python* language is used for scripting

Fig. 24: 3-Point bending beam test skew fracture path obtained with the simulation

- **Open source:** The *BSD (Berkeley Software Distribution)* licence allows to use and distribute the existing code without any restriction, but with the possibility to develop new parts of the code on an open or close basis depending on the developers. Additionally *Kratos* can be freely used.

8.2 Mmg library

8.2.1 What is Mmg and how does it work?

Mmg is an open source software for anisotropic automatic *remeshing* for *unstructured meshes* based on *Delaunay* triangulations. It is licenced under a **LGPL** license and it has been integrated in *Kratos*[48] via the `mmg_process.h` in the `MeshingApplication`. It provides three applications and four libraries:

Fig. 25: 3-Point bending skew beam experimental results with Plexiglass [68]

Fig. 26: 3-Point bending skew beam force-displacement evolution at the center of the beam

Fig. 27: *Kratos* Multiphysics logo. <https://github.com/KratosMultiphysics/Kratos>

Fig. 28: Mmg logo. Image from Mmg web

- The `mmg2d` application and the `libmmg2d` library: adaptation and optimization of a two-dimensional triangulation and generation of a triangulation from a set of points or from given boundary edges.
- The `mmgs` application and the `libmmgs` library: adaptation and optimization of a surface triangulation and isovalue discretization.
- The `mmg3d` application and the `libmmg3d` library: adaptation and optimization of a tetrahedral mesh and implicit domain meshing.
- The `libmmg` library gathering the `libmmg2d`, `libmmgs` and `libmmg3d` libraries.

The *Mmg* remeshing process modifies the mesh[63][64] iteratively until it is in agreement with the prescribed sizes on the idealized (Fig. 29) contour (and directions in case of anisotropic mesh). The software reads the mesh and the metric, then the mesh is modified using local mesh modifications of which an intersection procedure based on anisotropic *Delaunay* kernel.

We can resume the remeshing algorithm in the following steps:

1. *Mmg* tries to have a good approximation of the surface (with respect to the *Hausdorff* parameter).
2. It remeshes according to a geometric criterion. *Mmg* scans the surface tetrahedra and splits the tetrahedra using predefined patterns if the *Hausdorff* distance[65] between the surface triangle of the tetrahedra and its curve representation does not respect the *Hausdorff* parameter.
3. The library scans again the surface tetrahedra and collapse all the edges at a *Hausdorff* distance smaller than a threshold defined in terms of the *Hausdorff* parameter.
4. Next it intersects the provided metric and a surface metric computed at each point from the *Hausdorff* parameter and the curvature tensor at the point.

Fig. 29: *Mmg* idealized geometry. Image from [64]

5. Then *Mmg* smooths the metric to respect the gradation parameter. The metrics are iteratively propagated until the respect of the gradation everywhere.
6. Next it remeshes the surface tetrahedra in order to respect the new metric.
7. Finally it remeshes both the volume and surface to have edges between 0.6 and 1.3 (in the metric). The long edges are cutted and short ones are deleted (collapsed).

8.2.2 Integration between *Mmg* and *Kratos*

In order to understand the integration between *Kratos* and *Mmg* is important to understand the data structure of *Kratos*. On Fig. 30 an example of the data structure of the `Model` can be analysed. The `Model` stores the whole model to be analyzed, and manages the different `ModelPart` used on the simulation. The `ModelPart` holds all data related to an arbitrary part of model. It stores all existing components and data like `Nodes`, `Properties`, `Elements`, `Conditions` and solution data related to a part of the `Model`.

Fig. 30: Model data structure

The entities stored on the `ModelPart` are:

- **Node** It is a point with additional facilities. Stores the nodal data, historical nodal data, and list of *DoF*.

- **Condition** encapsulates data and operations necessary for calculating the local contributions of **Condition** to the global system of equations.
- **Element** encapsulates the elemental formulation in one object and provides an interface for calculating the local matrices and vectors necessary for assembling the global system of equations. It holds its geometry that meanwhile is its array of **Nodes**.
- **Properties** encapsulates data shared by different **Elements** or **Conditions**. It can store any type of data.

In our implementations we used a process to set the **BC** (both *Neumann* or *Dirichlet*). In order to preserve that information after remeshing we need to create an identification system, so we are able to create a unique ID that will allow us to reconstruct the submodelpart structure after remeshing, this methodologies are commonly called *colour identification*. Fig. 31 shows the concept of this idea.

Fig. 31: Concept of colours

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9 Compliance with Ethical Standards

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