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On the use of combined Finite/Discrete Element Method for impacted concrete structures

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Abstract. A combined finite/discrete element method is proposed for the prediction of reinforced concrete structure response under severe dynamic loads as impacts due to natural or anthropic hazards. A bridging subdomain is used, the Hamiltonian is chosen as a linear combination of discrete and continuum Hamiltonians. Discrete Element displacements and rotations are linking to Finite Element displacements by means of Lagrange multipliers. The discontinuities of discretization introduce spurious reflection ; numerical methods are proposed to attenuate it.

1. INTRODUCTION

The modeling of the whole structure under such impacts needs on one hand a model able to describe the occurrence of severe damage (fragmentation, spalling, tunneling) in the zone of impact, and on another hand a model able to capture the global response of the structure. The study aims at showing how the proposed combined finite/discrete element method satisfies both conditions. Locally, the discrete element model deals with nonlinear phenomena, far from impacted zone the finite element method allows the reduction of both times of modeling and computation. Using the combined method allows the prediction of projectile penetration, structural damage and global displacements.

The efficiency of DEM to study rocks, plain concrete and reinforced concrete has already been shown in 2D, Camborde [1], Potyondy [2] and in 3D, Hentz [3]. The applications of DEM to large scale structures were limited due to computing costs; the number of elements increase reduces drastically computational efficiency. To improve that point, the region without any assumed damage is modeled by means of the FEM. The same media is model with two different methods; the discretization size at the interface is discontinuous. In the vicinity of impact the DE discretization is fine, whereas FE size is adapted to the structural scale and is larger than DE. Discretization discontinuity induces spurious reflections.

Such a multi-scale analysis with a combined discrete/finite elements approach has already been proposed by different authors. Physicians first coupled FEM and molecular dynamics in order to look in details the interaction between particles, the crack propagation Broughton [4]. A large synthesis of these different approaches has been carried out by Xiao and Belytschko [5]. Suggested by these authors, the coupling between the FE and DE domains is carried out into a bridging domain where the Hamiltonian is taken as a linear combination of discrete and finite Hamiltonians. Kinematic conditions between FE and DE Degrees Of Freedom (DOF) allow the displacement continuities inside the bridging domain. These conditions are satisfied by means of Lagrange multipliers.

2. DISCRETE ELEMENTS METHOD

2.1 Modelling scale

Contrary to FEM, the DEM, Cundall [6] is convenient to describe discontinuous phenomena and large deformation into dynamical problems. Occurrence and propagation of fracture is naturally taken into account with a discrete model. DEM was originally developed for granular materials but seems well adapted to cohesive materials, like concrete. This discrete method allows to model heterogeneous materials at a micro level i.e. the millimetric heterogeneity scale. Another approach consists in modeling the material at a higher scale, where the whole assembly reproduces the macroscopic behavior, the fracturing process can be described and the response of large structures can be evaluated. Due to computational times in 3D problems, it is proposed to model concrete at a mesoscale.

2.2 Proposed discrete elements model

The model is constituted with spheres of different radius. Each sphere is a DE, those elements are in interaction. The overall behavior of a material can be reproduced by associating a simple constitutive law to each interaction.

Two elements *a* and *b* of radius R_a and R_b respectively, can interact without contact. It comes from the interaction range parameter, γ ($\gamma \geq 1$) . Elements *a* and *b* will interact if : $\gamma\left(R_a + R_b\right) \geq D_{a,b}$.
Where $D_{a,b}$ is the distance between the centroids of elements *a* and *b*. The interaction range parameter has a large influence for cohesive materials, it increase the number of interaction by element.

In order to analyze the response of concrete, the model has to be isotropic and homogeneous with a maximum compacity. The positions of elements are randomly distributed.

As DE are spherical, the interactions laws take into account, forces and momentum between two elements. They are calculating from normal and tangential stiffnesses, K_n and K_s and relative displacements. A modified Mohr-Coulomb model with softening is used.
More details about the constitutive equations of the DE model are presented in Hentz [3].

2.3 Discrete elements rotation characteristics

In comparison with FE node, a DE node has three more degrees of freedom, the three rotations. In order to couple the sub-domains, it is necessary to understand the signification of DE rotations at a macro-scale. The following results refer to static analysis of a 2D model. Loads are such that material remains elastic and all elements have the same radius. The central difference integration algorithm is used. The static response is obtained by means of a viscous damping.

Numerical experiments show that in small perturbation hypothesis, the discrete rotation is the rigid rotation, i.e. the antisymmetric part of the displacement gradient. In the continuum model and with small strains, the displacement of point *N*, close to *M*, is given by:

$$\vec{U}(N) \cong \vec{U}(M) + \overline{\overline{\varepsilon}}(M)\overrightarrow{MN} + \overline{\overline{\omega}}\overrightarrow{MN} \qquad \overline{\overline{\omega}} = \frac{1}{2}\left(\overline{\overline{grad}}\ \vec{U} - \overline{\overline{grad}}^{T}\vec{U}\right)$$

We can also introduce the vector rotation : $\overline{\overline{\omega}}(M)\overrightarrow{MN} = \vec{\Omega}(M) \wedge \overrightarrow{MN}$

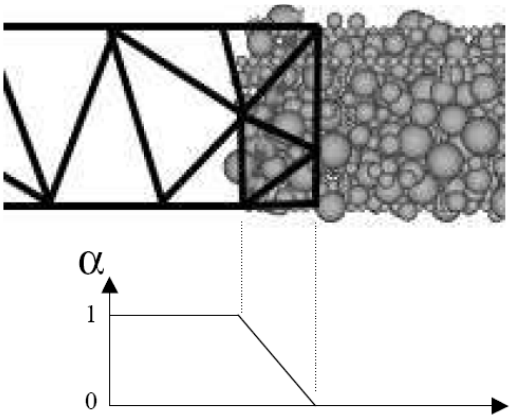
The displacement is written as the sum of a rigid body translation, a part due to strain and one due to rotation. The vector rotation is equal to vector **θ** corresponding to the rotation of DE.

3. COUPLING METHODS : the bridging domain method

3.1 Local equations

The start point of the method is based on a bridging sub-domain where the Hamiltonian is taken as a linear combination of discrete and continuum Hamiltonians. For that, a scaling parameter α is introduced in the overlapping domain. α is defined on FE by means of the element interpolation functions in order to ensure the continuity of α between elements.

In the following, we consider $\boldsymbol{u}$ for FE node displacement, n_f is the number of FE node and n_{fr}, the number of FE node in the bridging domain. u_i represent the i^{th} degree of freedom of FE. $\boldsymbol{d}$ represents the vector displacement of DE node. n_d is the number of DE node and n_{dr}, the number of DE node in the bridging domain. $\boldsymbol{\omega}$ represents the vector of DE node rotations.



In the overlapping subdomain, DE degree of freedom are linking to FE degree of freedom with the coupling relations, defined as :

$$d_j = \sum_{i=1}^{3.n_{fr}} k_{ij} u_i \qquad \omega_j = \sum_{i=1}^{3.n_{fr}} h_{ij} u_i$$

The solution minimize the Hamiltonian with the coupling constrains introduced by means of Lagrange multipliers defined with two vectors of size $3n_{dr}$. The function, Hg, to minimize is :

$$Hg\left(\vec{d},\vec{\omega},\vec{u},\vec{\lambda^d},\vec{\lambda^\omega}\right) = H\left(\vec{d},\vec{\omega},\vec{u}\right) + \vec{\lambda^d}\left(\vec{d} - \bar{\bar{k}}\vec{u}\right) + \vec{\lambda^\omega}\left(\vec{\omega} - \bar{\bar{h}}\vec{u}\right)$$

So local equations are :

- on FE and DE sub-domain, the local equation are written classical with mass lumping.
- on the bridging sub-domain, the local equations are defined by :

For discrete element :

$$m_j \ddot{d}_j = F_j + \lambda_j^d$$
$$J_j \ddot{\omega}_j = C_j + \lambda_j^\omega$$

For finite element

$$M_i \ddot{u}_i = F_i + \sum_{l=1}^{3ndr} \lambda_l^d k_{il} + \sum_{l=1}^{3ndr} \lambda_l^\omega h_{il}$$

3.2 Algorithm

The explicit central difference method is used to solve the local equations.
At first we compute the expression without Lagrange multipliers :

$\tilde{u}(t+\Delta t) = 2u(t) - u(t-\Delta t) + \frac{\Delta t^2}{M} F$. The verification of coupling relation at time step t+Δt allows the calculation of multipliers. Then displacement at time step t+Δt are update. The expressions of displacement and rotation are :

- for finite element : $u_i(t+\Delta t) = \tilde{u}_i(t+\Delta t) + \frac{\Delta t^2}{M_i}\sum_{l=1}^{3ndr}\left(\lambda_l^d k_{il} + \lambda_l^\omega h_{il}\right)$

$$d_j(t+\Delta t) = \tilde{d}_j(t+\Delta t) + \frac{\Delta t^2}{m_j}\lambda_j^d$$

- for discrete element :

$$\omega_j(t+\Delta t) = \tilde{\omega}_j(t+\Delta t) + \frac{\Delta t^2}{J_j}\lambda_j^\omega$$

With the coupling relation :

$$g_j^d = \tilde{d}_j(t+\Delta t) - \sum_{i=1}^{3nfr} k_{ij}\tilde{u}_i(t+\Delta t) = \Delta t^2\left(-\frac{\lambda_j^d}{mj} - \sum_{i=1}^{3nfr} k_{ij}\left(\sum_{l=1}^{3ndr}\frac{\lambda_l^d k_{il} + \lambda_l^\omega h_{il}}{Mi}\right)\right)$$

$$g_j^\omega = \tilde{\omega}_j(t+\Delta t) - \sum_{i=1}^{3nfr} h_{ij}\tilde{u}_i(t+\Delta t) = \Delta t^2\left(-\frac{\lambda_j^\omega}{J_j} - \sum_{i=1}^{3nfr} h_{ij}\left(\sum_{l=1}^{3ndr}\frac{\lambda_l^d k_{il} + \lambda_l^\omega h_{il}}{Mi}\right)\right)$$

Those expressions can be summarized in matrix systems :

$$\vec{g}^{\,d} = \overline{\overline{A}}\vec{\lambda}^d + \overline{\overline{B}}\vec{\lambda}^\omega$$
$$\vec{g}^{\,\omega} = \overline{\overline{C}}\vec{\lambda}^d + \overline{\overline{D}}\vec{\lambda}^\omega$$

$$A_{jl} = -\frac{\Delta t^2}{m_j}\delta_{jl} - \Delta t^2\sum_{p=1}^{3nfr}\frac{k_{jp}k_{pl}}{M_p} \qquad B_{jl} = -\Delta t^2\sum_{p=1}^{3nfr}\frac{k_{jp}h_{pl}}{M_p}$$

$$C_{jl} = -\Delta t^2\sum_{p=1}^{3nfr}\frac{h_{jp}k_{pl}}{M_p} \qquad D_{jl} = -\frac{\Delta t^2}{J_j}\delta_{jl} - \Delta t^2\sum_{p=1}^{3nfr}\frac{h_{jp}h_{pl}}{M_p}$$

With known Lagrange multipliers, we obtain the corrected finite and discrete displacements and discrete rotations.

A, ***B***, ***C***, ***D*** are scare matrix of size 3 n_{dr}. The determination of Lagrange multipliers needs at each time step the resolution of a linear system of size $6n_{dr}$. With a linear behavior in the mixed domain, we need only to compute the matrix inversion at the first step. Xiao proposed to replace this matrix by a diagonalized matrix. They sum each line of the matrix on the diagonal term. This method is less time consuming and we will see in an example, its effect on the spurious wave reflection.

3.3 Relaxed Lagrange multipliers

To reduce spurious reflections due to discretization discontinuity on FE/DE interface, we proposed to attenuate Lagrange multipliers by a parameter *r* before to compute displacements and rotations at t+Δt $\lambda^d = \frac{\lambda^d}{r}$ and $\lambda^\omega = \frac{\lambda^\omega}{r}$.

As Lagrange multipliers can be considered as forces between a DE and a FE node, the method relaxes forces applied to the DE. This relaxation reduces the spurious wave. We have also demonstrated that using diagonal matrix and relaxation is very efficient for applications, this approach is equivalent to penality method where displacement in penality terms are compute with $\tilde{u}(t+\Delta t)$. The penality coefficient is adapted to each dof, or if we want constant penality parameters we choose the minimum.

4. APPLICATIONS

4.1 Wave propagation

Due to discontinuity of discretization size in the media, a reflection wave occurs when the wave frequency is too high to be defined by FE. Spurious waves may affect the damage prediction in the impacted zone, the method must attenuate this phenomenon.

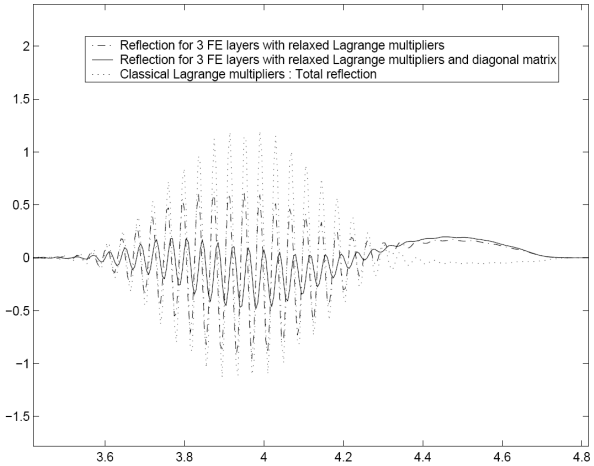


Figure 1 comparison of spurious reflections

Table 1. Percentage of attenuation of the total reflective energy.

Nb. FE layers	0	3	6	9
Usual Lag. Multipliers	0 %	0 %	0 %	0 %
With diag. matrix	0 %	16 %	20 %	23 %
Relax. Lag. multipliers	0 %	56 %	82 %	84 %
Relax. And diag. matrix	0 %	94 %	96 %	98 %

When considering classical Lagrange multipliers without simplification or relaxation, high frequency waves see the bridging domain as a rigid body. DE degrees of freedom are strongly linked to FE ones, so discretization size in the bridging domain is similar to the FE discretization size.

Using matrix simplification or relaxed Lagrange multipliers introduce freedom on DE and reduce the spurious reflection.

Concerning relaxed Lagrange multipliers, numerical simulations demonstrate that the best parameter for relaxation is the number of DE layers in the overlapping domain. Table 1 gives a comparison between the percentage of attenuation of the total energy in the spurious wave, for classical Lagrange multipliers and the relaxed Lagrange multipliers when matrix are taking without simplification, or when matrix are diagonalized.
Best results are obtained with a diagonal matrix and relaxed Lagrange multipliers. The impact of the method on low frequencies is small (less than 0.1 % of total energy, but it depends of application).

4.2 Impact on a concrete slab

In this part, the behavior of a concrete slab under a rocky impact is studied. This slab is the upper part of a rock shed used to protect roads. The proposed method is compared with an equivalent DE method without coupling. Figure 3 compares the displacement of DE node between the pure DEM and the coupled method, the node is not exactly at the same point.

Complete comparison and results on the slab will be presented.

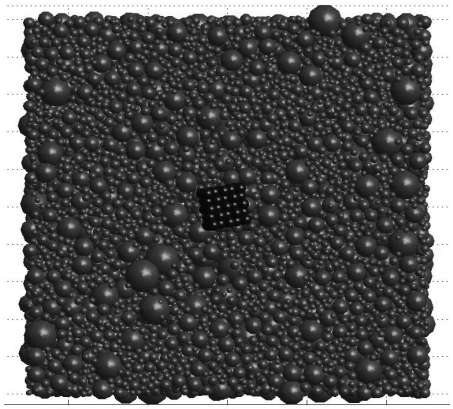


Figure 2 : Discrete model

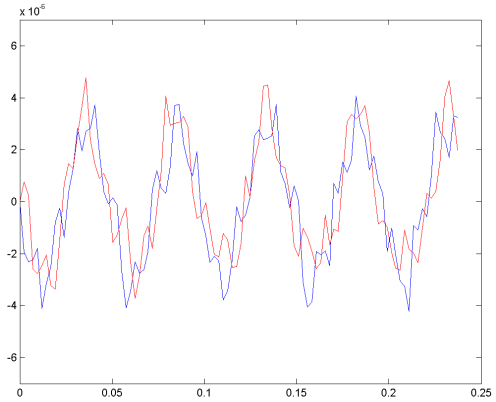


Figure 3 : Comparison of displacement between DE (red) method and coupled method (blue)

The combined method is more than 10 times faster than the DE method. Moreover we did not use a multi-time step algorithm for this application.

5. CONCLUSION

The presented method reduce drastically computational time, this method introduce spurious reflexion which become negligible with specific numerical methods. Two more aspects have not been presented: the attenuation of spurious reflexion with damping, and the behavior of the method with reinforcements. The general aspect of this method can be applied on different material, preferably for large models.

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