Numerical simulation of dynamical fracture in heterogeneous materials

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Abstract

A new numerical strategy, based on the coupling between the Cohesive Zone Model (CZM) concept and the Non-Smooth Contact Dynamic (NSCD) approach, for the simulation of the dynamical fracture of heterogeneous materials is presented. The associated software, composed of three libraries with Object Oriented Progamming, allows the simulation, in 3D and large deformation, of the dynamical fracture of non-linear and heterogeneous materials from fracture initiation to post-fracture. The ability of the software, developed by the French 'Institut de Radioprotection et de Sûreté Nucléaire' (IRSN) in the frame of its research program on nuclear reactor fuel safety, is illustrated on the fracture of an heterogeneous material – the hydrided Zircaloy-4 constituting standard nuclear cladding tubes – submitted to transient loading.

Keywords: Dynamical fracture; Heterogeneous media; Numerical simulation; Cohesive Zone Model

1. Introduction

An heterogeneous material comprises a multiphase material thus giving a non-uniform microstructure. To analyse the effects of this microstructure heterogeneity on material behavior, a micromechanical approach is needed.

One of the most recent approaches to dynamical fracture modeling is the use of the Cohesive Zone Model (CZM) which represents the mechanical processes in the fracture process zone in front of a crack tip. The CZM concept allows simulation of crack initiation (without any *ad hoc* criteria) and propagation (crack path is not known in advance) in brittle, ductile or heterogeneous materials at several scales. The material separation is described by a constitutive equation relating stress applied on the crack lips and the displacement jump (the difference of the displacements of the adjacent continuum elements). In this study, our attention focuses on the Frictional Cohesive Zone Model (FCZM) involving a standard CZM coupled with non-smooth surfacic behaviors such as unilateral contact and friction. The non-smooth behaviors are handled without regularization/penalization methods. This class of FCZM is larger than those of CZM and allows, in particular, consideration of post-fracture friction on the crack lips.

Since dynamical problems involving frictional contact are not regular and relative velocities can become discontinuous, the Non-Smooth Contact Dynamic (NSCD) method is used. The NSCD approach, initiated by Moreau [1] and Jean [2], consists in solving non-smooth equations of frictional contact without any regularization nor penalization. As proposed by Monerie and Acary [3], the NSCD framework is modified to take FCZM into account.

The numerical platform developed is composed of three independant libraries, each dealing with a part of the mechanical problem. The libraries LMGC90, MatLib and PELICANS respectively are dedicated to surfacic behaviors (FCZM), constitutive models of bulk material and Finite Element Method.

An example of the ability of this software is illustrated

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with the fracture of a hydrided Zircaloy-4 plate under transient loading.

2. Frictional cohesive zone model

The Frictional Cohesive Zone Model used is a model coupling unilateral contact and Coulomb friction with cohesion. Therefore, a cohesive force R^{coh}, is added on the Signorini–Coulomb complementary problem (Eqs. (1,2)).

Unilateral contact with cohesion:

$$0 \leq (R_N - R_N^{coh}) \perp u_N \geq 0 \tag{1}$$

Coulomb friction with cohesion:

$$\begin{cases} \|R_T - R_T^{coh}\| < \mu |R_N - R_N^{coh}| \Rightarrow \dot{u}_T = 0 \\ \|R_T - R_T^{coh}\| < \mu |R_N - R_N^{coh}| \Rightarrow \exists \lambda \geq 0 \text{ such as} \\ \qquad \dot{u}_T = \lambda (R_T - R_T^{coh}) \end{cases} \tag{2}$$

Subscripts N and T respectively denote the normal and the tangential component of the separation vector across the cohesive surface $[u]$, of the total contact-friction force R and of the cohesive force R^{coh}. In particular: $[u] = u_N n + u_T$ and $R^{coh} = R_N^{coh} n + R_T^{coh}$. The friction coefficient is denoted u.

At this stage, various CZM, giving R^{coh}, can be used. In this paper, in order to particularize the FCZM, we use the cohesive force introduced by Raous et al. [4] and Raous and Monerie [5] based on a variable β, introduced by Fremond [6] ($\beta = 1$: the cohesion is complete, $0 < \beta < 1$: the cohesion is partially broken and $\beta = 0$: there is no cohesion). This model is fully described by Eqs. (3,4).

Cohesive force:

$$\begin{Bmatrix} R_N^{coh} \\ R_T^{coh} \end{Bmatrix} = \beta^2 \begin{bmatrix} C_N & 0 \\ 0 & C_T \end{bmatrix} \begin{Bmatrix} u_N \\ u_T \end{Bmatrix} \tag{3}$$

Evolution of cohesion intensity:

$$b\dot{\beta} = -(w = (C_N u_N^2 + C_T \|u_T\|^2)\beta)^- \tag{4}$$

where $(x)^- = \max(0, -x)$ denote the negative part of x, C_N and C_T are the initial normal and tangent stiffness of the interface if cohesion is complete, b is the viscosity of the cohesion evolution and w is the limit of decohesion energy.

When the cohesion vanishes ($\beta = 0$ in this model), we obtain the classical Signorini problem for the normal behavior and the Coulomb friction problem for the tangential behavior.

3. Non-smooth contact dynamics

The dynamical problem is formed by the eqs. (1) and (2) and the discrete dynamical equation:

$$M\ddot{q} = F(q, \dot{q}, t) + r \tag{5}$$

where q, $\dot{q}$ and $\ddot{q}$ are discrete displacement, velocity and acceleration respectively, M is the mass matrix, $F(q,\dot{q}, t)$ represents internal and external forces and r is representative of local reaction forces. Since shocks are expected, the derivatives in the dynamical equation are to be understood in the sense of distributions.

The Non-Smooth Contact Dynamics (NSCD) method deals with solving dynamical frictional contact problems without any regularization nor penalization techniques. Monerie and Acary [3] have introduced cohesive force R^{coh} within the framework of NSCD method. For that, all contact points are considered as cohesive zones. The modified model allows to solve unilateral contact and Coulomb friction with cohesion (e.g. Eqs. (1) and (2)).

Dubois and Jean [7] have developed the NSCD method within a Fortran90 software LMGC90.

3.1. Time discretization

Denoting by a subscript i quantities at a time t_i and with $i + 1$ quantities at time t_{i+1}, the θ-method scheme writes:

$$\begin{cases} M_{i+1}(\dot{q}_{i+1} - \dot{q}_i) = h[(1-\theta)F_i + \theta F_{i+1}] + hr_{i+1} \\ q_{i+1} = q_i + h[(1-\theta)\dot{q}_i + \theta \dot{q}_{i+1}] \end{cases} \tag{6}$$

where h is the length of subinterval $[t_i, t_i + 1]$ and hr_{i+1} is the mean value impulse. The unknowns of the problem are the approximations of the velocity $\dot{q}_{i+1}$ and the impulse hr_{i+1}. The non-linear system (6) is solved using a Newton–Raphson method (superscript k stands for iterations).

$$\begin{cases} \dot{q}_{k+1}^{k+1} = \dot{q}_{i+1}^k + \Delta\dot{q}_{free} + hw^k r_{i+1}^{k+1} \\ \Delta\dot{q}_{free} = w_{i+1}^k(-M_{i+1}^k(\dot{q}_{i+1}^k - \dot{q}_i) + h[(1-\theta)F_i + \theta F_{i+1}^k] + hr_{i+1}^k \} \end{cases} \tag{7}$$

where w_{i+1}^k is the inverse of the iterations matrix.

3.2 NSCD and FCZM

Linking the global velocity (q) and reaction force (hr) with their relative values $\dot{u}$ and R with the help of linear mapping and using the change of variable $\tilde{R} = R - R^{coh}$ introduced by Monerie and Acary [3], we have to solve, for each contact α, the three-dimensional system (for more details see Jean [2] and Jean et al. [8]):

$$\begin{cases} \dot{U}^{\alpha} - \dot{U}^{\alpha}_{locfree} + W^{\alpha\alpha} h(R - R^{coh})^{\alpha} = 0 \\ R^{\alpha}_{N} - \text{proj}_{\mathbb{R}_{-}}(R^{\alpha}_{N} + \rho U^{\alpha}_{N}) = 0 \\ R^{\alpha}_{T} - \text{proj}_{D(u|R^{\alpha}_{N}|)}(R^{\alpha}_{N} + \rho U^{\alpha}_{T}) = 0 \end{cases} \tag{8}$$

where $\rho > 0$ and $D(\mu|R^{\alpha}_{N}|)$ is the section of Coulomb's cone for contact α, i.e. the disc with center 0 and radius $\mu|R^{\alpha}_{N}|$ and $\dot{U}^{\alpha}_{locfree}$ is the velocity at the contact α without any reaction coming from the FCZM.

This system may be written as a mapping ϕ:

$$\phi(U^{\alpha}, R^{\alpha}) = 0 \tag{9}$$

The non-linear equation (9) is solved using the generalized Newton method of Alart and Curnier [9].

4. Numerical platform

The numerical platform deals with three-dimensional thermomechanical problems with contact between finite elements. The architecture is composed of three libraries with Object-Oriented Programming (OOP). This design allows to modify the behavior of a module by writing extensions to the initial source code (which remains unchanged). So, the code is easy to maintain and extend. Moreover, each module has a clear meaning from a mechanical point of view. The three libraries are coupled with an encapsulated design LMGC90 > PELICANS > MatLib:

- LMGC90 is a software specially dedicated to contact problems. It is based on the NSCD method (see Section 3) and developed, in Fortran90, by Dubois and Jean [7].
- MatLib is a material constitutive models library written in C++. This library is developed by Stainier et al. [10]. It is based on a variational formalism of viscoplastic constitutive updates described in Ortiz and Stainier [11].
- PELICANS is a Finite Elements library writted in C++ developed by the French 'Institut de Radioprotection et de Sûreté Nucléaire' (IRSN) in the frame of its research program on nuclear safety [12,13].

Following the works of Xu and Needleman [14], the main idea used here is to embed cohesive surfaces along all finite element boundaries.

The finite element discretization is based on linear displacement triangular elements that are arranged in a 'crossed-triangle' quadrilateral pattern.

The developed software allows to simulate, in 3D and large deformation, the crack initiation (without initiation criteria) and propagation in heterogeneous materials.

5. Example: dynamic crack propagation in hydrided Zircaloy-4 plate

In a Pressurized Water Reactor (PWR), most of the structural parts of fuel cladding tubes consist of zirconium alloys such as Zircaloy-4. During nuclear reactor operation, hydride precipitation occurs. So microstructure of fuel cladding tubes appears as a bimaterial which is formed by hydride inclusions surrounded by a metallic matrix. Hydride content varies gradually in tube thickness.

In this example, we simulate an irradiated Zircaloy-4 plate with rectangular hydride inclusions which represent a part of a fuel cladding tube. Hydrides are distributed randomly (with a volumic fraction of 20%) and oriented horizontally. Two different levels of bonding strength values, weak ($w^i/w^h \simeq 10^5$) and strong ($w^i/w^h \simeq 10^{-4}$), between the two phases are considered. w^i and w^h denote the surface energy of interface Matrix/Hydride and Matrix/Matrix respectively. Matrix is assumed to be elastoplastic (J2 plasticity, hardening modulus 200 MPa) and hydrides elastic. The material properties and the cohesive coefficients, used in the present simulations, are given in Tables 1 and 2 respectively. We assume that there is no viscosity $b = 0$, small friction $\mu = 0.05$ and same compliance for the normal and tangential behaviors $c_N = c_T$. We impose velocity boundary conditions along horizontal faces: $V = 2\,\text{m/s}$ and $V = -2\,\text{m/s}$ on the right and left horizontal faces respectively.

Table 1
Material properties used in the finite element calculations. The material properties correspond to irradiated Zircaloy-4 matrix and δ-hydride

	Young modulus (GPa)	Poisson's ratio	Yield in tension (MPa)
Matrix	98	0.325	850
δ-hydride	135	0.32	–

Table 2
Constitutive parameters for cohesive surfaces

	$c_N = c_T$ (Pa/m)	w (J/m^2)
Matrix/Matrix	10^{13}	8.1×10^4
Matrix/Hydride (strong)	1.5×10^{13}	5.52×10^9
Matrix/Hydride (weak)	1.5×10^{13}	5.52
Hydride/Hydride	1.5×10^{13}	5.046×10^4

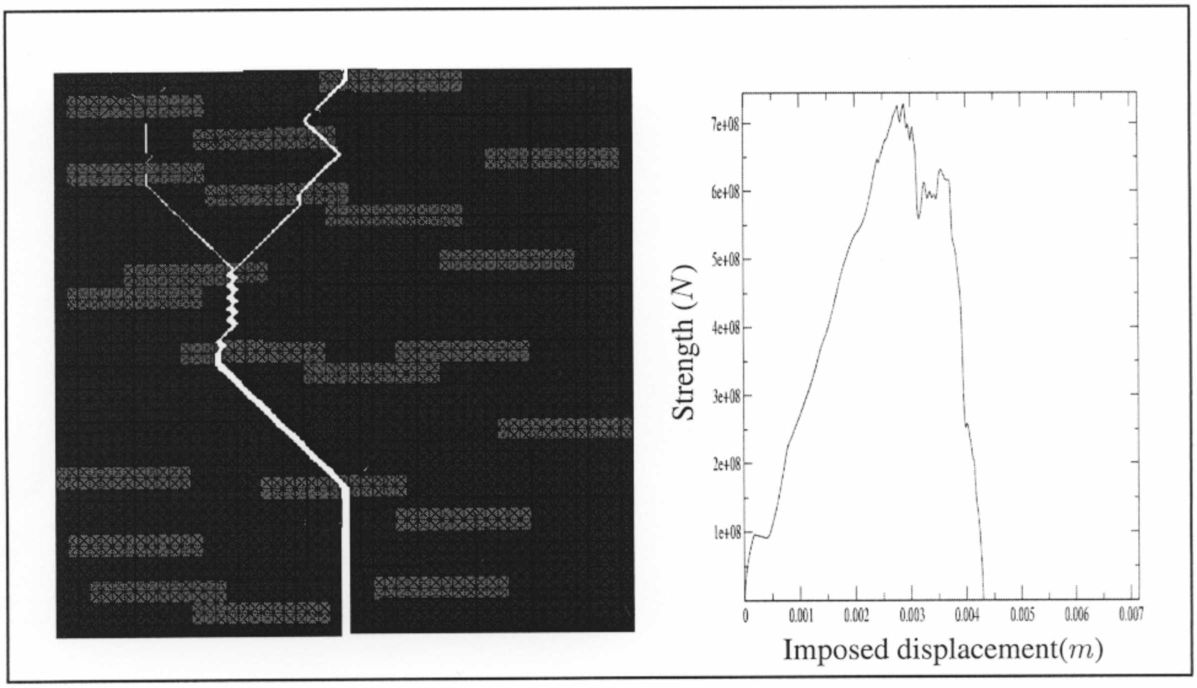

Fig. 1. Strong matrix/hydrides interface.

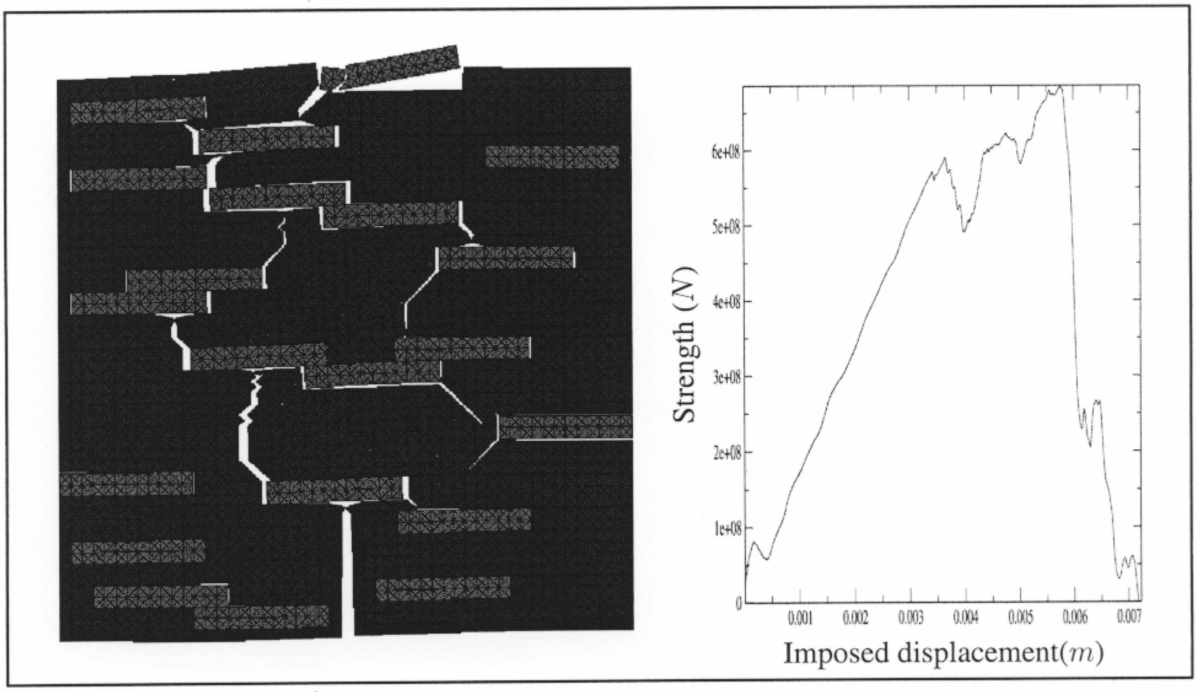

Fig. 2. Weak matrix/hydrides interface.

5.1. Crack path

Figures 1 and 2 show that the crack path is significantly influenced by the interface Matrix/Hydride bonding strength. For the strong interfaces, cracks propagate through hydride inclusions due to its high cohesive strength with the matrix. In case of weak interfaces, cracks propagate inside the matrix and along the inclusions boundaries due to the formation of microcracks along weak interfaces.

5.2. Energy release

Curves in Figs. 1 and 2 show the evolution of strength during cracking process for weak and strong interfaces. Energy release decreases with increasing interfacial bonding strength due to formation of microcracks and their coalescence in case of weak interfaces. The energy release for weak interfaces is approximately 50% lower than for strong interfaces.

6. Conclusions

This paper has presented a procedure for analyzing dynamical fracture in heterogeneous materials with a Frictional Cohesive Zone Model (FCZM). This model allows to simulate crack initiation and propagation without any fracture criteria. The non-linear behavior and the discontinuities of the relative velocities during dynamical fracture are dealt with the Non-Smooth Contact Dynamic (NSCD) method. A new software based on FCZM with NSCD is developed by coupling libraries with the Object Oriented Method. An example of the ability of this software has been illustrated on the dynamical crack propagation of an hydrided Zircaloy-4 plate. This example shows the importance of the multiphase material interfaces.

References

[1] Moreau J-J. Unilateral contact and dry friction in finite freedom dynamics. In: J-J Moreau and PD Panagiotopoulos, editors, Non Smooth Mechanics and Applications, volume 302 of CISM – Courses and Lectures, 1–82. Vienna: Springer, 1988.
[2] Jean M. The non-smooth contact dynamics method. Computer Methods in App Mech and Eng 1999;177:235–257.
[3] Monerie Y, Acary V. Formulation dynamique d'un modèle de zone cohésive tridimensionnel couplant endommagement et frottement. Revue Européenne des Elements Finis 2001;10:489–503.
[4] Raous M, Cangémi L, Cocu M. A consistent model coupling adhesion, friction and unilateral contact. Computer Methods in App Mech and Eng 1999;177(3–4):383–399.
[5] Raous M, Monerie Y. Unilateral contact, friction and adhesion: 3D crack in composite material. In: JAC Martins and MDP Monteiro Marques, editors, 3D contact mechanics international symposium, Collection Solid Mechanics and its Applications. Peniche (Portugal), 17–21 June 2002. Kluwer, pp. 333–346.
[6] Fremond M. Adhérence des solides. Journal de Mécanique Théorique et Appliquée 1987;6(3):383–407.
[7] Dubois F, Jean M. Une plateforme de développement dédiée la modélisation des problèmes d'intéraction. In: Actes du sixième colloque national en calcul de structures – CSMA-AFM-LMS, volume 1, 111–118, Giens, 2003.
[8] Jean M, Acary V, Monerie Y. Non smooth contact dynamics approach of cohesive materials. Phil Trans R Soc Lond 2001;A359:2497–2518.
[9] Alart P, Curnier A. A generalized Newton method for contact problems with friction. Journal de Mécanique Théorique et Appliquée 1988;7:67–82.
[10] Stainier L, Dubois F, Peyroux R. MatLib, une bibliothèque portable de modèles constitutifs pour la mécanique non-linéaire des solides: concepts et implémentation. In: 6ème Colloque National en Calcul des Structures, M. Potier-Ferry, M Bonnet, A Bignonnet, editors. Vol. 3, Giens, France, 2003, pp. 25–32.
[11] Ortiz M, Stainier L. The variational formulation of viscoplastic constitutive updates. Computer Methods in Applied Mechanics and Engineering 1999;171:419–444.
[12] Piar B. PELICANS: a component framework for scientific computing application to the solution of some moving boundary problems. In: Journées de travail sur la modélisation de problèmes à interfaces avec couplage, PPF Mécanique Numérique Hautes Performances. ESM2, 2002.
[13] Piar B, Chailan L, Vola D. Scientific software architectures designed to survive change. In: Trend in Physical and Numerical of Multiphase Industrial Flows. Cargse, 2003.
[14] Xu X-P. Needleman A. Numerical simulations of fast crack growth in brittle solids. Journal of Mech and Phys of Solids 1994;42(9):1397–1434.