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CRACK PROPAGATION MODELLING USING XFEM, BUILDING MATERIALS APPLICATIONS

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Abstract. The paper shows some results of a computational modelling focused on the occurrence of damage in heterogeneous materials, mainly with brittle matrix, especially on the issue of modelling crack formation and propagation. The attention is paid to the application of the finite element method to the buildings materials in order to find critical parameters determining behaviour of materials at damage process with reference to the history of several approaches to solving this problem. The applications of damage mechanics and possible approaches to model the origin of a crack propagation through modifications in FEM systems are presented and some practical applications are tested. Main effort is devoted to cement fibre composites and the search for new methods for their more accurate modelling, especially ahead of the crack tip. Modified XFEM method and its suggested modifications as to proper modelling of the real stress distribution close to crack tip are shown.

Key words. Quasi-brittle materials, nonlocal approach, cohesive modelling, computational modelling, extended finite element method (XFEM).

AMS subject classifications. 74R10, 65M60

1. Introduction. The question of ensuring the safety of structural components and predicting their service life is increasingly associated with the development of new devices and components. In the case of constructions, it may be directly dependent on the occurrence of defects that may arise during the production stage or through their lifetime. One of the concepts used in construction and safety assessment is a set of theories and methods known in fracture mechanics. This scientific field, combining continuum mechanics with material engineering, describes the behaviour of defects in structures. It is a complex defect-stress-material relationship. To understand the relationships end extend lifetime, it is necessary to modernize construction practices and also use new numerical methods (at least new modifications).

The aim of fracture mechanics is to describe or predict the behaviour of bodies containing defects. In many cases, cracks can lead to total failure of the structure due to fracture. There are two basic approaches for deriving the conditions in the moment of initiation of unstable crack propagation. The first one uses the weakest link theory, the second model considers the accumulation of damage during loading. Failure of structural materials is understood as a continuous process in which the stages of plastic deformation, nucleation and initiation of cracks is intermingled. The final stage in the development of failure of bodies, which is the subject of investigation of fracture mechanics, is the propagation of cracks (unstable or stable). The goal of the presented works is how to find out the mutual relations between physical regularities and the physical laws themselves, often based on experiments such as the non-destructive identification of complex structures can be, see [47].

Currently, there are many ways how the problem of simulating crack propagation can be solved using FEM. Among the first and oldest are the modelling of stable crack growth using the node release method, where starting criterion is necessary to

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define. Modelling of crack propagation by the node release method is possible only in the case of a 2D problem, where effective plastic deformation is displayed, similar approach of [4] is based on the continuous remeshing. The second one old approach is the method of "disappearing" elements, within its framework are also included the various models using damage [25].

After this introductory *Section* 1, in *Section* 2 we shall continue with brief comments to mathematical and physical background, to obtain the basic orientation in various physical, mathematical and computational approaches. Then in *Section* 3 we will get to know the basic principles of extended finite element method, let's get a little familiar with the idea of cohesive modelling *Section* 4 and the idea of so-called smeared models will be presented in *Section* 5, whose nonlocal evaluation relies on [16], upgraded by [17].

However, this can cover only the initiation and propagation of microfractured zone, not the creation and development of particular macrocropic cracks and their systems. Coupling of both such processes will be sketched in *Section* 5, with the crucial reference to [28] and [29] based on the detailed description of cohesive interfaces. The application of these procedures is devoted to *Section* 6, emphasizing the similarity of such modelling to ceramic composites.

Section 5 will demonstrate how the potential removal of non-physical simplifications modifies all formulations of *Sections* 3, 4, 5, resulting in still unclosed mathematical and computational problems. Let us notice that the development of algorithms in [47] coming from [33], [40], [19], [8] and form a separate research area in two last decades; e. g. the review article [12] contains 317 relevant references. The concluding *Section* 7 contains the brief summary of presented results together with some research priorities for the near future.

2. Physical and Mathematical background. Complicated material structure of numerous materials for engineering applications, including cement-based composites, crucial in building practice, does not allow reliable prediction of their behaviour under mechanical, thermal, etc. loads using the conventional simplified methods of classical fracture mechanics, coming from [20] and precisely described in [6], [41], [43] and [44]. This was the strong motivation for the development of some more advanced approach, based on the cohesive zone modelling (CZM).

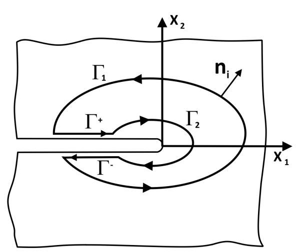

FIG. 2.1. *J integral representing the fracture energy.*

The aim of physical and mathematical analysis of [6] was i) the adequate prediction of strains and stresses in both cracked and uncracked structures, involving those with various notches, ii) the admissibility of a non-negligible size of fractured zones in comparison with other dimensions, iii) the incorporation of an initial crack in brittle materials, as needed for linear elastic fracture mechanics. CZM can be understood as the general framework for interfaces: it relies on the evaluation of cohesive forces occurring when particular material elements are being pulled apart. CZM guarantees the validity of formal mathematical continuity conditions, despite physical separation, which suppresses any stress singularity, limiting it to the cohesive strength of the material. However, the constitutive behaviour of a fracture must be characterized by certain traction-separation curve, whose experimental identification has to be performed for each material individually: namely the amount of fracture energy dissipated in the work region depends on the shape of the considered model, whereas the length of the fracture process zone decreases with the ratio between the maximum stress and the yield stress. As documented by [7] and [51], CZM is able to provide good predictions for some steels, for different notched samples of a glassy polymer and even for concrete, i.e. beyond the scope of purely brittle fracture [27].

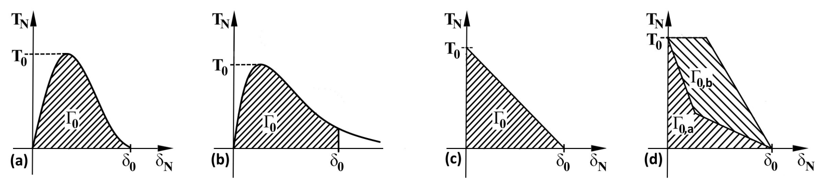

FIG. 2.2. *Traction–separation law for **(a)** plastic behaviour of materials, **(b)** modified plastic behaviour of materials, **(c)** elastic bilinear response, **(d)** composites with fibres. T_N here is the peak of (normal) stress, δ_N is the displacement in the direction of the crack growth, Γ_0 is the energy which can be represented by the fracture toughness, Γ_{0a} and Γ_{0b} are the mean energies for composites reinforced by fibres.*

Using the classical approach is necessary to pay attention to [24]. More general isotropic models need to respect bi-modularity, i. e. degradation in tension vs. compression, as analysed by [23] and [21], corresponding to principles of classical thermomechanics, more in [50] and [31], [13] and [38]. It should be noted that the origins of these ideas can be found in [32] and [4], [35], respectively in [51]. Partial existence, uniqueness, convergence, etc. results can be found in [22], [48] and [49], in contrast with the serious non-existence examples of and [14].

The area under the traction-separation curve, whether in the normal or tangential direction, gives us the energy J given by relevant integral [41, 42, 44] as in Fig. 2.1. A schematic overview of traction-separation models for some materials can be seen in Fig. 2.2.

From a mathematical point of view, the complete system of partial differential equations of evolution, both in its classical differential form and in its variational or weak integral form, relies on the conservation principles of classical thermomechanics, supplied by appropriate constitutive equations, as presented by [50]. Since such formulations work with function spaces of infinite dimension; thus, most computational approaches to real engineering problems need some discretisations both in the Euclidean space, 3-dimensional in general, and on certain time variables, even for a seemingly static, simplified evaluation of fracture development. The conservation principles contain both the total strain tensor ε and the stress tensor σ, both represented by symmetric square matrices of order 3. Since the values of components σ_{ij} of σ with $i, j \in \{1, 2, 3\}$ depend on the choice of a Cartesian coordinate system, for the following considerations, it is useful to introduce also three invariants of σ (independent of the choice of Cartesian coordinates) σ_I, σ_{II} and σ_{III}; the first (linear) one is $\sigma_I = \sigma_{11} + \sigma_{22} + \sigma_{33}$. Most computational tools ϵ are decomposed into four components, denoted as ϵ^e, ϵ^p, ϵ^c and ϵ^θ, referring to elastic, plastic, creep and thermal ones; moreover, an appropriate incorporation of the damage process is expected.

In particular, in the simplified small deformation theory for isotropic materials, using the standard Kronecker symbol $\delta_{ij} = 1 - \operatorname{sgn}|i-j|$, for purely elastic deformation, the following equation

$$\varepsilon_{ij} = \varepsilon_{ij}^{e} = \frac{1+\nu}{E}\,\sigma_{ij} - \frac{\nu}{E}\,\sigma_I\delta_{ij} \tag{2.1}$$

can be written for all $i, j \in \{1, 2, 3\}$; this relation is the famous empiric Hooke's law, containing a couple of material parameters (E, ν): E is the Young's modulus and ν is the Poisson's ratio. To derive ε for $\varepsilon \neq \varepsilon^e$, unlike (2.1), some appropriate decomposition of ε must be suggested: in most computational tools, ε is considered as a simple sum of ε^e, ε^p, ε^c and ε^θ.

3. Extended finite element method - XFEM. There is no doubt that the FEM is widely used mainly in the area of solving differential equations. However, the FEM mesh may not always be ideal for modelling crack propagation. And this is one of the most significant interest in solid mechanics problems. First models were based on the weak (strain) discontinuity that could pass through finite element mesh using variational principle, [36]. Other authors and investigators considered strong (displacement) discontinuity by modifying the principle of virtual work statement (which is also the case for models with the traction separation law), [2], [26], including stability and convergence of such problems and improvement of the precision of numerical procedure, [45].

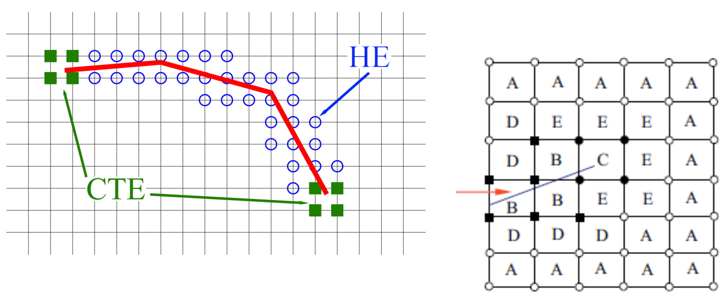

Fig. 3.1. *The path through FEM mesh using XFEM, CTE - crack tip enrichment, HE - heaviside.*

In the strong discontinuity approach, the displacement consist of regular and enhanced components, where the enhanced components yield via jump across discontinuity surface, [2]. A modification of the basic equation is needed, for the relationship between displacements $u^e(x)$ on particular points x of the e-th element (3-dimensional vectors of functions in general) and displacements at selected element nodes u^i, utilizing some standard shape functions $N_i(x)$, i. e.

$$u^e(x) = \sum_{i\in E_A} N_i(x)u^i\,; \tag{3.1}$$

where E_A denotes the set of nodes corresponding to the standard e-th element.

For the extended finite element method (XFEM), some more terms must be added to slightly modified displacements inside element end displacements at element nodes of (3.1). The second term realizes the technique of penetration into the element and the movement of the crack, the third criterion the failure (decohesion) and the possible direction of movement according to the preferred criteria. So the previous equation for the case of crack growth for 2-dimensional modelling (not limited to one element) is modified into the form

$$u^h(x) = \sum_{i \in E_A} N_i(x)u^i + \sum_{j \in C_B} N_j(x)H_j(x)a_j + \sum_{k \in C_C} N_k(x) \sum_{m=1}^{4} \Phi_k^m(x)c_k^m \qquad (3.2)$$

including certain specialized shape functions $N_i(x)$, $N_j(x)$ and $N_k(x)$ for intrinsic version of XFEM, same shape function for extrinsic version, where E_A, C_B, C_C are the sets of points corresponding to Fig. 3.1 and $H(x)$ is the Heaviside function realised by discontinuous function with values 0 and 1. The setting with m = 4 is used for two-dimensional crack propagation, function Φ_k represents the initiation criterion.

4. XFEM - strategy for enrichment function. The standard FEM is based on the approximation properties of polynomials. If the solution shows a pronounced non-polynomial behaviour, such as weak or strong discontinuities, the standard FEM approximation may represent very poor performance. In fact, the standard FEM is not able to adequately represent the discontinuity or singularity in a suitable way, for example, at the crack tip area. A number of methods have been developed to overcome these difficulties; however, the enrichment of approximation space is one of the most efficient techniques that can be used to capture the weak or strong discontinuities. The enrichment can be attributed to the degree of consistency of the approximation, or to the capability of approximation to reproduce a given complex field of interest. The principal of enrichment is basically equivalent to the principal of increasing the order of completeness that can be achieved intrinsically or extrinsically. However, the enrichment aims to increase the accuracy of the approximation by including information of the analytical solution. There are basically two ways of enriching an approximation space; enriching the basic vector known as the "intrinsic enrichment" and enriching the approximation known as the "extrinsic enrichment". Intrinsic enrichment is an idea to enhance the approximation space $u(x)$ by including the new basis functions in order to capture a certain condition of a complex field, such as discontinuity or singularity. The partition of unity, see [3], is a concept for enriching the approximation extrinsically by adding the enrichment functions to the standard approximation.

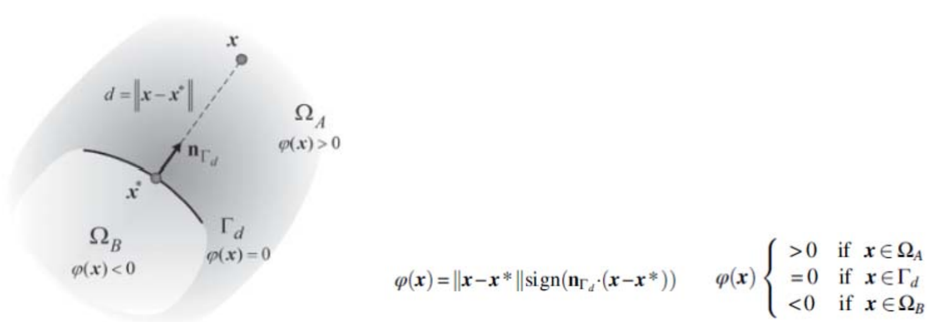

FIG. 4.1. *The enrichment function realization, Heaviside function is created using $\phi(\boldsymbol{x})$. Where $\boldsymbol{x}^*$ is the closest point projection of $\boldsymbol{x}$ onto the discontinuity Γ_d, $\boldsymbol{n}_{\Gamma_d}$ is the normal vector to the interface at point $\boldsymbol{x}^*$, $\|\boldsymbol{x}-\boldsymbol{x}^*\|$ specifies the distance of point $\boldsymbol{x}$ to the discontinuity Γ_d.*

A numerical technique for tracking of moving interfaces is called the level set method, where interfaces are modelled using functions allowing for a natural treatment of merging interfaces, intersection with boundaries, and so on. Consider a domain Ω_A and Ω_B. The interface between these domains is denoted by Γ_d. The most common level set function is in our description the signed distance function, which is defined in Fig. 4.1.

5. Some problems as to correct application of XFEM. When applying the extended method to a specific problem in the field of solid mechanics, we solve a number of sub-problems. These can be characterized by the following scheme:

- Using the correct crack initiation criterion:
  (a) maximum tangential stress (Erdogan), [18], resp. [20],
  (b) minimum strain energy density criterion (Sih) [43]
  (c) crack opening criterion (Li) [30],
  (d) for small stress intensity factor K interpolation methods.
- Realization of microscopic behaviour of composite with fibres (e.g. bridging effect), [1, 5, 54].
- The fundamental question is the determination of the real stress in front of the crack. These are some stress averaging (e.g. Eringen non-local approach) [16, 14, 15], smeared models (e.g. Jirásek) [23], [52], spatial crack solution (e.g. Bažant microplane model) [7].

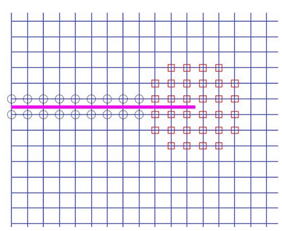

Fig. 5.1. *Non-local approaches.*

Initiation and development of visible cracks of macroscopic size, described as internal interfaces with possible discontinuities in u, v and a, do not agree with the smeared damage approach (as non-local access can be classified in the smeared group), but the incorporation of this process may be necessary, due to certain values of non-local strain or stress invariants: such criteria as strange energy density, crack driving force, special nonlocal integrals, related to the stress and strain at possible crack tip. The development of such models is connected e. g. with [39], [28] and [30].

6. Buildings and ceramics materials. A sample with a cement matrix and steel fibres was selected for computational modelling, see Fig. 6.1 and Fig. 6.2. Numerical results show the surface propagation of cracks in the damaged body depending on the location fibre and material properties. The reinforcing effect of the fibres plays a significant role in the direction of crack propagation. The attention is paid in particular to Eringen's model for generating the multiplicative damage factor, related quasi-static analysis, the existence of weak solution of the corresponding boundary value and initial value problem with a parabolic partial system differential equations.

The proposed procedure thus combines the possibilities of several approaches for modelling crack propagation in fibre composites. The XFEM method is primary, the stress in front of the crack is recalculated according to the non-local approach, in the entire body according to the exponential or power law of violation, [9, 10, 11, 39] which implies some degree of averaging (especially as to stress) ahead of the crack.

Two dimensional relatively simple body with an a priori crack of a circular shape (fulfilling the plane strain condition) has been chosen as a illustrative example. A uniform load was applied to the surface of this a priori crack, and thus the formation of the following cracks emanating from this stress concentrator is assumed using modified XFEM. The basic calculation system was the commercial software Abaqus 2018, into which a user subroutine in the Fortran 90 language was implemented, realizing the modelling of matrix damage using exponential law, based on the planar element CPE4. The following basic input data corresponding to reinforced cement paste were used for this task: the Young's modulus $E = 3.2$ GPa, the Poisson's constant $\nu = 0.3$ and the tensile strength 10 MPa. For approximately 20 mm long and 3 mm thick circular steel fibres, the Young's modulus $E = 190$ GPa and the same Poisson's constant $\nu = 0.3$ were used. The results of modelling are described in the following Fig. 6.3 due to the well-tried so-called Mazars' model, [31]. The Fig. 6.4 can serve as an example of a pure Eringen model.

Mazars damage model is based on a strain formulation and generally is used for the physically nonlinear analysis of concrete structures. The main objective is modification of damage model, in which both tension and compression damage evolution laws are regularized using a classical fracture energy methodology. Its hypothesis is founded on the base of an elastic damage isotropic behaviour. This model assumes the premises that damage occurs only due to positive strains in the principal directions, which indirectly promotes "smeared crack grow"; only one scalar damage variable is defined, this is due to the damage model being isotropic; represents the material as totally damaged, and it is limited in the interval; no permanent strains are admitted, and the unloading path is linear, therefore no hysteresis loops are presented.

FIG. 6.1. *Fibres in cement pasta.*

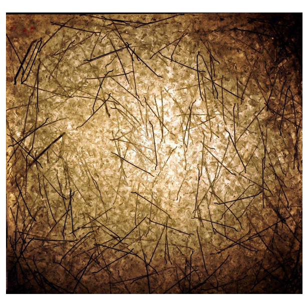

FIG. 6.2. *Xray image, fibres in matrix.*

Moreover, regardless of [51], some particular theoretical results as to dynamic response are available, as an estimation technique via crack tip velocity by [10, 52, 53, 38, 45], or the proof of local well-possessedness for a model problem by referring to again.

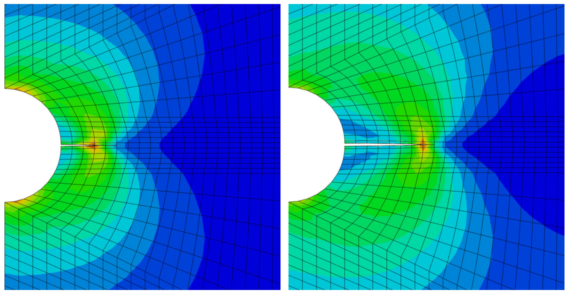

FIG. 6.3. *Maximum principal stress for Mazars' exponential model. Coloured maps represents the scale from* 8.2×10^6 *to* 8.0×10^5 *MPa.*

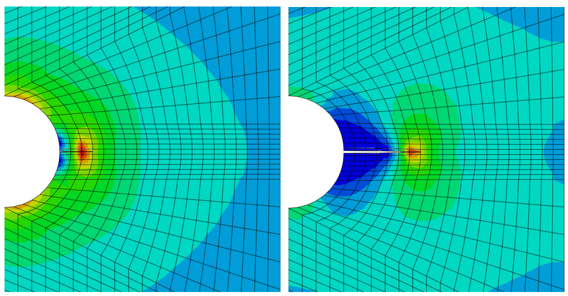

FIG. 6.4. *Maximum principal stress for Erinden's non-local approach. Coloured maps represents the same scale as previous Figure 6.3.*

7. Conclusion. A cement matrix reinforced with metal fibres was chosen for the following numerical tests. In practice, the most important case is cement composite containing short and intentionally or quasi-randomly oriented steel fibres, sometimes ceramic or polymer fibres with primary suppression of some stress components, while a more detailed mathematical formulation is expected. We have sketched several types of approaches to the evaluation of damage in these composite materials and structures, but the influence of averaged stress distribution ahead the crack tip is presented. New trends in numerical modelling and simulation reflecting the development of advanced materials, structures and technologies and the long-time experience of their designers, based on standard laboratory experiments and observations, is needed.

The article contains a link to the theoretical foundations of the issue presented in [50], the reader can find them in the same 22nd *Algoritmy* Proceedings. However, in several parts of this paper still unclosed problems are mentioned, especially on modelling based on thermodynamic principles. Its numerical approach relies on a modified XFEM where one can use as a criterion for the formation of a crack, the cohesive traction separation. The results in the case of implementation of the nonlocal constitutive stress-strain relation of the integral type are very perspective. Then attention is paid in particular to Eringen's model for generating the multiplicative damage factor, related quasi-static analysis. In the first step the XFEM is used, then the stress in front of the crack tip is recalculated according to the non-local approach, in the entire body according to the exponential law of violation. As already mentioned, the algorithm is ready for the case of dynamic response, but financially demanding experiments must be carried out in advance.

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