Using the finite cell method to predict crack initiation in ductile materials

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A B S T R A C T

In this paper, the Finite Cell Method (FCM) is used to predict the crack evolution in ductile materials under small strains and nonlinear isotropic hardening conditions. The FCM is the result of combining the p-version finite element and fictitious domain methods, and has been shown to be effective in solving problems with complicated geometries for which the meshing procedure can be quite expensive. The crack evolution is introduced to the constitutive equations by using the simplified Lemaitre ductile damage model. The performance of the method is verified by means of two numerical examples in both 2D and 3D problems.

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1. Introduction

To use an efficient numerical method is one of the most important steps in simulating engineering problems. Although the finite element method has been the most prevalent method used for several decades, some modified versions have proved their efficiency in special applications. For example, the generalized finite element method (GFEM) and extended finite element method (XFEM) can better resolve discontinuities and singularities [1]. The modifications may target the approximation space for special problems. For example, XFEM adds special functions to the polynomial Ansatz space to simulate the singularity near the crack tip [2].

As a combination of fictitious domain methods and high-order finite elements, the FCM is a promising choice for solving problems with complicated geometries. It replaces the mesh generation difficulties with efforts to integrate accurately and adaptively the stiffness matrix and load vector. Interesting to know is that mesh generation often takes longer than solving the equations in a general finite element set; for instance mesh generation takes about 14% of the whole engineering process while solving equations takes only 4% [3]. So, it is worth trying to reduce the mesh generation necessity. The FCM has been first introduced by Parvizian et al. [4] for two-dimensional problems and developed for three-dimensional problems by Düster et al. [5]. It was later successfully applied to shell elements and thin-walled structures [6]. The foci of the recent researches have been on both improving the numerical efficiency of the method, e.g. Abedian et al. [7], and on developing its applications in different problems of mechanical engineering, for instance geometrically nonlinear problems [8]. Düster et al. used this method for heterogeneous and cellular materials [9]. The method was developed for elastoplastic material behavior by Abedian et al. [10], and was used in topology optimization problems by Parvizian et al. [11]. The finite cell method can have great advantages in the field of biomechanics where geometries are very complex, for example in analyzing bones [12–14]. The hp-d adaptive finite cell method has been developed recently [15,16].

In this paper, the application of FCM in ductile crack initiation is investigated. The continuum damage mechanics (CDM) theory is used for this purpose. This theory is based on continuum mechanics, and aims to study the failure behavior of materials. Some internal state variables are introduced to the constitutive equations in order to model the crack bands of the material.

The damage analysis, which was already provided, converted to a continuum damage mechanics framework since about four decades ago [17]. It was first used by Hult [18], then by Gurson [19], Tvergaard and Needleman [20]. Lemaitre [21] developed the theory and introduced the continuum damage mechanics. The models have been presented up to now in the field of continuum damage mechanics can be categorized into four main classes: creep damage, ductile damage, quasi-brittle damage and fatigue damage. Creep failure of metals under uniaxial loads using a scalar internal variable was proposed by Kachanov [22]. In this model, damage does not have any direct physical meaning. Within the theory of...
elastoplasticity, Gursen [19] proposed a model for ductile damage where a damage variable is obtained from the consideration of microscopic spherical voids embedded in an elastoplastic matrix. A purely phenomenological model for ductile materials using a scalar damage variable was introduced by Lemaitre [21]. Murakami [23] proposed a model for anisotropic damage in brittle materials. Janson [24] developed a continuum theory to model fatigue crack propagation which was in good agreement with uniaxial experiments. Lemaitre [25] presented a general formulation considering low and high cycle fatigue as well as creep fatigue in an arbitrary stress state.

The research in the field of CDM continues either in developing different and suitable constitutive equations, or by developing the numerical methods for implementing the corresponding models. The constitutive equations sought for are either for special materials such as composites [26], glass, elastomers, piezoelectric or adhesive materials, or for special cases of loading such as fatigue [24], creep or impact [27]. Adaptive numerical methods for damage simulation have also been investigated in e.g. [28]. The numerical behavior of continuum damage models can be improved using nonlocal models; localization effect is intrinsically included in the local constitutive models of continuum damage mechanics. Although these models suffer from mesh sensitivity and localization problems, they are used widely in various mechanical applications to predict a good location of the crack initiation [29]. An extensive discussion about the reasons and remedies of localization can be found in the literature [30].

In this paper, we develop the FCM method for simulation of damage. The article is organized as follows: in Section 2 we briefly present the Lemaitre continuum damage theory and its numerical implementation procedure. Section 3 is to introduce the “Finite Cell Method” and its numerical implementation. Then, “Numerical Examples” are presented in Section 4 and followed finally by “Conclusions” in Section 5.

2. Damage theory

Due to the thermodynamically consistent formulation, the Lemaitre constitutive model is very appealing and has been frequently used in the literature. In this model, the damage internal state variable, $D$, is defined as a measure of degradation of the elastic modulus, which is a macroscopic mathematical representation of voids and micro-cracks growth. The extreme values of $D$ are 0 for the intact material and 1 for a unit volume element with a null load-carrying capacity and a complete local rupture. In the simplified Lemaitre damage model, kinematic hardening is excluded from the equations which can be used for all engineering applications without load reversal [31].

2.1. Thermodynamic framework

The specific free energy potential is given by [17]:

$$\psi = \psi^e(\varepsilon^e, D) + \psi^p(R),$$

(1)

where $\psi^e$ and $\psi^p$ are the elastic damage and plastic contributions to the free energy, respectively. In the present theory, the following forms are postulated:

$$\rho \psi^e(\varepsilon^e, D) = \frac{1}{2} \varepsilon^e : (1 - D)\mathbf{D} \cdot \varepsilon^e$$

$$\rho \psi^p(R) = \rho \psi^p(R)$$

(2)

in which $\mathbf{D}$ is the elasticity tensor and $\psi^p$ is an arbitrary function of the single argument $R$. The corresponding conjugate forces for $\varepsilon^e$, $D$ and $R$ are given respectively as:

$$\mathbf{f} = \rho \frac{\partial \psi^e}{\partial \varepsilon^e} = (1 - D)\mathbf{D} : \varepsilon^e$$

(3)

$$Y = \rho \frac{\partial \psi^p}{\partial R} = -\frac{1}{2} \varepsilon^p : \mathbf{D} : \varepsilon^p$$

(4)

$$\kappa = \rho \frac{\partial \psi^p}{\partial R} = \rho \frac{\partial \psi^p}{\partial R} = \kappa(R)$$

(5)

The yield function has a von Mises definition:

$$\varphi(\mathbf{\sigma}, \kappa, D) = \frac{\sqrt{2J_2(\mathbf{S})}}{1 - D} - \sigma_y(R)$$

(6)

in which $\mathbf{S}$ is the deviatoric stress tensor and $\sigma_y$ denotes the current yield stress of the material computed as:

$$\sigma_y = \sigma_{yo} + \kappa(R)$$

(7)

in which $\sigma_{yo}$ is the initial yield stress and $\kappa(R)$ is the isotropic hardening function. The dissipation potential $\Sigma$ is given as:

$$\Sigma = \varphi + \frac{r}{(1 - D)(s + 1)} \left( \frac{Y}{r} \right)^{s+1}$$

(8)

$r$ and $s$ are experimentally determined material parameters. The evolution laws are given by the normality rule of the plasticity theory:

$$\dot{\varepsilon}^p = \dot{\gamma} \frac{\partial \Sigma}{\partial \sigma}$$

(9)

$$\dot{D} = \dot{\gamma} \frac{\partial \Sigma}{\partial (\mathbf{\sigma})}$$

(10)

$$\dot{R} = -\dot{\gamma} \frac{\partial \Sigma}{\partial \kappa}$$

(11)

where $\dot{\gamma}$ denotes the plastic multiplier which meets the Kuhn–Tucker conditions:

$$\dot{\gamma} \geq 0, \quad \varphi \leq 0, \quad \dot{\gamma} \varphi = 0.$$  

(12)

2.2. Constitutive equations

The right hand side of the Eq. (3) can be expressed in terms of deviatoric and hydrostatic stresses. Therefore, the elasticity including damage reads as [31]:

$$\mathbf{s} = (1 - D)2G\varepsilon^e, \quad p = (1 - D)k\varepsilon^p$$

(13)

where $G$ is the shear modulus, $k$ is the bulk modulus, $\varepsilon^e$ and $\varepsilon^p$ are, respectively, the elastic strain deviator and elastic volumetric strain. Based on Eq. (4), the energy release rate $Y$ is computed as the following:

$$Y = \frac{q^2}{6G(1 - D)^2} - \frac{p^2}{2K(1 - D)^2}$$

(14)

where

$$q = \sqrt{2J_2(\mathbf{S})}$$

(15)

The evolution law of stress tensor is given by splitting the strain rate in small deformation theory,

$$\dot{\varepsilon} = \dot{\varepsilon}^e + \dot{\varepsilon}^p$$

(16)

The internal variables, $\varepsilon^p$, $D$ and $R$ are determined using Eqs. (9)–(11):


\[ \epsilon^p = \gamma \frac{\partial \varphi}{\partial \sigma} \]  

(17)

\[ D = \frac{1}{1-D} \left( - \frac{Y}{T} \right)^s \]  

(18)

\[ \bar{R} = \gamma \]  

(19)

### 3. Finite cell method

The departure point of the FCM from general finite element method is to extend the physical domain by a fictitious domain. It changes the real domain in such a way that only rectangular elements in two dimensional or hexahedral elements in three dimensional problems are necessary. The way of domain extension is shown in Fig. 1. The physical domain \( \Omega \) is embedded in the extended domain \( \Omega_b \). In Fig. 2 a mesh is shown for the prescribed heterogeneous material with pores and inclusions. Only rectangular elements cover the extended domain and no effort is necessary to fill the real domain with elements, which may cause some problems such as aspect ratio of the elements or distorted elements with small or even negative Jacobian. The non-conforming elements are called cells in the finite cell method.

As now some of the cells only partially intersect with the domain of computation, an adaptive integration procedure is needed to follow the boundary of physical domain. As shown in [7] the quadtree in 2D and the octree in 3D are efficient methods for adaptive integration in the FCM. In Fig. 3(a), the procedure of tracing the boundary using a quadtree integration method is shown. In this method, each parent cell intersected by the boundary is divided into four sub-cells with the same integration order. Each child again is divided to four sub-cells and this procedure continues until a certain accuracy is achieved in the geometry representation. The partitioning procedure can be stopped until the area of a subcell is smaller than a specific fraction of the main cell which is named integration threshold.

In the integration part, all Gauss points at each sub cells are considered. Each Gauss point is characterized by \( z \) which depends on its location. We define \( z = 1 \) if the Gauss point is in the physical domain, and \( z = 0 \) if not. A mapping to \( (\xi, \eta) \) which is the local coordinate system of the cell is also necessary for each Gauss point. The mapping procedure is shown in Fig. 3(b). In all numerical integrations, the integrant is multiplied by parameter \( z \) at the corresponding Gauss point. The stiffness matrix of a cell with \( n_{sc} \) sub-cells is then calculated by [7]:

\[ K_i = \sum_{k=1}^{n_{sc}} \int_B \int_r B_i^T(\xi(r))z(x(\xi(r)))CB(\xi(r)) \det J_f \det J_c^z d \varsigma d \tau \]  

(25)

in which \( C \) is the consistent tangent matrix and \( J \) denotes the determinant of the Jacobian matrix due to the change of variables [5].

### 4. Numerical examples

A subroutine is added to AdhoC [33] to compute stress and tangent stiffness matrices of a damaged material at a Gauss point. The direct solver “PARDISO” [34] is employed, being suitable for the FCM due to its numerical robustness.

#### 4.1. 2D example

This section illustrates, using a benchmark example, the use of FCM for crack initiation prediction in a cylindrical pre-notched bar subjected to a monotonic axial loading. The geometry is described in Fig. 4(a). This example has been reported in the literature quite frequently [31,35]. The material follows the hardening law given by [31] and [35]. The components of the material parameters and listed in Table 1 in conjunction with other elastic and damage parameters.

Only a quarter of the bar is modeled due to axial symmetric properties along the \( xz \) plane. The geometry and mesh of the model can be seen in Fig. 4(b). We are using the \( p \)-version of finite elements in two dimensional or hexahedral elements in three dimensional problems are necessary.
element method to compute a reference solution. The mesh has been refined to: (a) minimize the localization effect, (b) reach acceptable convergence in the values of damage parameter and von Mises equivalent stress and (c) reduce the computational costs. Based on these requirements we have chosen the element size and polynomial degree accordingly. A coarse mesh is selected with 90 axisymmetric quadrilaterals while the polynomial degree is 6. The mesh is refined near the root and center of the specimen, due to strain softening in this region. The global element size is of the order of 2 mm while in the softening zone it is reduced to a typical size of 1 mm. A displacement of $u = 0.576$ mm has been applied in 86 steps. The way how the load is applied is very important in presence of softening since the problem will not remain elliptic as soon as the damage variable begins to evolve. Considering Eqs. (6) and (8), a non-associated flow rule is used in the Lemaitre damage model because the dissipation potential is not the same as the yield function. Therefore, an unsymmetrical solver is necessary to solve the finite element equations.

Fig. 5 represents damage parameter contours when the edge displacement reaches about 0.24 mm. The maximum damage parameter is verified by numerical results available in the literature [31] and a good agreement is observed.

Now, let us move towards the FCM implementation. The simple 2D coarse mesh together with the adaptive subcell refinement introduced for the integration is shown in Fig. 6. To avoid mesh dependency problem and have a fair comparison of the results the mean mesh sizes in both $p$-FEM and FCM are almost equal. The fictitious domain is penalized by factor $x = 10^{-12}$ to avoid the ill-conditioning of the stiffness matrix and polynomial degree is set to 6. The threshold for adaptive integration, defined in Section 3, is $10^{-5}$.

In the FCM algorithm, the stress and consistent tangent matrices are calculated first, and then, in the numerical integration process, will be multiplied by $x$. A Hooke elastic material is used for the points within the fictitious domain to avoid expensive computational costs of the return mapping algorithm for the Gauss points which are beyond the yield surface. Actually, the material behavior in this region is not important due to the null contribution of the corresponding Gauss points in the stiffness matrix composition.

The damage variable contour plot is shown in Fig. 7. It can be seen that the maximum damage parameter appears near the root during the early stages of loading. As the specimen is stretched more, the maximum damage variable moves toward the center and gradually localizes in a very small zone, which is in agreement with Neto [31]. If the damage behavior is ignored and only plastic behavior is considered, the softening point appears near the root, while experimental observations show that fracture initiation happens at the center [36]. The reason of occurring maximum damage variable in the center is the stress triaxiality ratio which is the highest at the center of the specimen. Ductility decreases as the triaxiality ratio increases. This phenomenon is captured by the Lemaitre ductile damage model. To show the accuracy of FCM results more precisely, in Table 2 the damage parameter in the center of the specimen is compared with the $p$-FEM results in different steps of loading. Softening behavior of the material due to plastic strain accumulation is captured in Fig. 8 which is in a good agreement with $p$-FEM.
4.2. 3D example

A flat rectangular notched bar specimen is considered using both finite element and finite cell methods, Fig. 9. The thickness of the specimen is 8 mm. Due to symmetry conditions only one eighth of the specimen is modeled using eight-node, hexahedral, high-order elements with polynomial degree 4. The mesh density in both FEM and FCM models is equal near the notch root to justify a fair comparison of the results. More than 600 hexahedral elements are used in both p-FEM and FCM. A monotonic load is applied to the specimen under displacement control on the top surface of the specimen equal to 1.2 mm and the load step size is equal to 0.02 mm. The threshold for adaptive integration is $10^{-4}$. The material properties of the specimen are listed in Table 3.

The equivalent von Mises stress for both FEM and FCM is presented in Fig. 10 which shows a good agreement between FEM and FCM results. As soon as damage parameter begins to evolve,
a discrepancy is observed between FEM and FCM results. This can be due to several sources of error such as: (a) FCM geometry approximation; this can be reduced by increasing the integration

**Table 2**
Damage parameter at the center of the notch in FEM and FCM methods.

<table>
<thead>
<tr>
<th>Top edge displacement (mm)</th>
<th>Damage value in FEM</th>
<th>Damage value in FCM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.124</td>
<td>0.00296</td>
<td>0.00296</td>
</tr>
<tr>
<td>0.499</td>
<td>0.361</td>
<td>0.360</td>
</tr>
<tr>
<td>0.517</td>
<td>0.392</td>
<td>0.391</td>
</tr>
<tr>
<td>0.569</td>
<td>0.538</td>
<td>0.540</td>
</tr>
<tr>
<td>0.576</td>
<td>0.574</td>
<td>0.577</td>
</tr>
</tbody>
</table>

**Fig. 7.** Damage variable contour plots in FCM presentation of the notched bar.

**Fig. 8.** Softening behavior of the material in the center of the specimen.

**Fig. 9.** (a) Flat rectangular notched bar specimen geometry and dimensions, (b) finite element model of 1/8 specimen using symmetry condition, (c) FCM representation of the geometry.

**Table 3**
Material parameters for the flat rectangular notched bar specimen.

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>200 GPa</td>
</tr>
<tr>
<td>(\nu)</td>
<td>0.3</td>
</tr>
<tr>
<td>(\sigma_0)</td>
<td>430 MPa</td>
</tr>
<tr>
<td>Power-law work hardening</td>
<td>(\sigma_y = 998)(^{0.18}) MPa</td>
</tr>
<tr>
<td>(s)</td>
<td>1.0</td>
</tr>
<tr>
<td>(r)</td>
<td>2.8 MPa</td>
</tr>
</tbody>
</table>

a discrepancy is observed between FEM and FCM results. This can be due to several sources of error such as: (a) FCM geometry approximation; this can be reduced by increasing the integration
tolerance, (b) mesh-dependency of the employed local damage model; this is more serious especially in 3D problems when the damage parameter evolves, and (c) the density of the integration points is increasing within the damaged region in FCM compared to the p-FEM. A combination of such errors causes the discrepancy of the two methods in the softening area. However the error is negligible within the engineering disciplines.

Table 4 shows a comparison of damage value in different steps of loading; the higher the plastic strain, the higher the error in the damage parameter. This phenomenon is due to the localization effect which will be more serious by approaching the fracture time.

The damage contours for both p-FEM and FCM are shown in Fig. 11. The elements cut by the notch boundary are removed to better observe the damage parameter distribution in the critical zone. The damage parameter reaches to its maximum value near the notch which follows the experimental results [37]. For similar mesh densities as presented here, p-FEM with conforming mesh and FCM with non-conforming mesh yield in similar damage contours.

5. Conclusions

Employing the FCM, this research predicts the location of the crack initiation in 2D and 3D problems using the Lemaitre damage constitutive law in some benchmark problems. The achievements are advantageous in industrial applications with a complex geometry, while FCM provides a solution without relying on a conforming mesh. The damage results of the FCM representation of 2D and 3D numerical examples are in good agreement with the p-FEM and the point of crack initiation is confirmed by experimental results. Finally, an extension of the model to a nonlocal damage constitutive equation to reduce the localization effects is under investigation.

Acknowledgement

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References


Fig. 10. Equivalent von Mises stress in the middle of xz symmetric plane of the flat bar at the apex of the notch.

<table>
<thead>
<tr>
<th>Top surface displacement (mm)</th>
<th>Damage value in FEM</th>
<th>Damage value in FCM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>0.0080</td>
<td>0.0082</td>
</tr>
<tr>
<td>0.2</td>
<td>0.033</td>
<td>0.034</td>
</tr>
<tr>
<td>0.4</td>
<td>0.071</td>
<td>0.075</td>
</tr>
<tr>
<td>0.8</td>
<td>0.129</td>
<td>0.136</td>
</tr>
<tr>
<td>1.2</td>
<td>0.207</td>
<td>0.219</td>
</tr>
</tbody>
</table>

Fig. 11. Damage contour plots in the flat rectangular notched bar using (a) FEM, (b) FCM.


