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On structural computations until fracture based on an anisotropic and unilateral damage theory

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Abstract

This paper describes the formulation and numerical implementation of a family of anisotropic and unilateral damage models for the prediction of damage and final rupture in engineering structures. The damage can be load-oriented, microstructure-oriented or (for the first time within this modeling framework) softening. The local equations are solved using a combination of fixed-point and Newton-Raphson algorithms, whose efficiencies are drastically improved through Aitken’s relaxation and BFGS approximation. A delay-effect method is used to control the localization of damage, which leads to an objective calculation of the final rupture of structures.

Keywords: Continuum damage mechanics; Anisotropic and unilateral damage; Structural computation; Rupture; Delay-effect localization control

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1. Introduction

Since continuum damage mechanics (CDM) first appeared [Kachanov, 1958, 1999], it has been studied and improved by many research groups worldwide [Leckie, 1978; Ladevèze, 1983; Murakami, 1983; Lemaître, 1985; Simo and Ju, 1987; Chaboche, 1988], taught in many universities [Kachanov, 1986; Lemaître, 1992; Krajinovic, 1996], and has become one of the classical tools of the structural mechanics community [Lemaître and Desmorat, 2005].

In practice, CDM consists in developing a model of the macroscopic behavior of a material in which microscopic damage is represented as a stiffness reduction. The form of the stiffness reduction is defined by the damage kinematics using damage variables, which are internal variables in thermodynamical terminology. The stiffness reduction, i.e. the magnitude of the damage variable, is defined as a function of the applied stress or strain using the damage kinetics. Damage models, and in particular their damage kinetics, usually involve several parameters (in addition to the classical Young and shear moduli and Poisson ratios) which must be identified experimentally through classical coupon tests. Then these models can be used to predict damage in engineering structures subjected to possibly complex loading and, for example, become part of a structural optimization process. Let us point out that homogenization techniques were recently used to derive damage kinematics and kinetics formally from an analysis on the damage scale, leading to generic models (i.e. models which are valid for a whole family of materials) for laminated composites [Ladevèze and Lubineau, 2002].

While early works concerned “only” unidirectional damage models, with applications to the creep rupture of metals [Kachanov, 1958, 1999; Leckie, 1978], CDM was rapidly extended to multidirectional models...
Involving damage anisotropy [Cordebois and Sidoroff, 1982; Ladevèze, 1983; Murakami, 1983; Chaboche, 1984; Chow and Wang, 1987b], with applications to the ductile [Lemaître, 1985; Chow and Wang, 1987a] and fatigue [Chow and Wei, 1991] rupture of metals. More recently, CDM was applied to laminated [Talreja, 1985, 1986; Voyiadjis and Kattan, 1993; Ladevèze and Lubineau, 2002], woven [Lesne and Saanouni, 1993; Aubard, 1995; Ladevèze, 1995] and braided [Gorbatikh et al., 2007] composites, to concrete [Peerlings et al., 1998; Pensée et al., 2002; Desmorat et al., 2007; Badel et al., 2007], etc. However, only a few published models are capable of reproducing all aspects of cracks, including anisotropy and unilaterality, especially when the orientation of damage is determined by the loading, i.e. when the damage kinematics is not known a priori. Indeed, in that case, anisotropy requires a tensor damage variable and the construction of a continuously differentiable potential involving tensors, and tension/compression partitioning is not straightforward [Ladevèze, 1983; Chaboche, 1992; Carol and Willam, 1996; Desmorat, 2000; Ladevèze and Letombe, 2000; Ladevèze, 2002]. This theoretical problem was solved by Ladevèze within the anisotropic and unilateral damage theory, first for second-order damage tensors [Ladevèze, 1983], then for more general representations of damage [Ladevèze and Letombe, 2000; Ladevèze, 2002]. Basically, the approach relies on a specific tension/compression partitioning of stress or strain which takes into account the damage state in order to ensure the continuity of the state law. Let us mention that another solution to this problem for fourth-order damage tensors was proposed in [Chaboche, 1995].

In this paper, we discuss several aspects of the formulation and nu-
numerical implementation of the family of models which belong to the sec-
ond version of the anisotropic and unilateral damage theory. This discus-
sion follows the classical Newton-Raphson/Finite Element framework. Al-
though other methods can be used to solve nonlinear partial differential
equations over a domain [Ladevèze, 1999; Passieux et al., 2010], this is the
most common method for dealing with material nonlinearities in science and
engineering. All the developments presented here were carried out within
Abaqus/Standard as C++ UMats based on the software development plat-
form of [Leclerc, 2010].

In the first part of the paper, we review the theory’s basis and present
several damage evolution laws which differ in the nature of the damage
mechanisms they represent. Regarding the modeling, the first fundamental
question concerning a crack network is whether its orientation is governed
by the loading (e.g. the inter-yarn cracking of woven ceramic matrix com-
posites (CMCs) [Ladevèze et al., 1994; Ladevèze, 1995; Lamon, 2001], the
cracking of concrete [Desmorat et al., 2007], etc.) or by the microstruc-
ture (e.g. the intra-yarn cracking of woven CMCs [Ladevèze et al., 1994;
Ladevèze, 1995; Lamon, 2001], the cracking of laminated composites [Tal-
reja, 1985, 1986; Lafarie-Frenot et al., 2001; Ladevèze and Lubineau, 2002],
etc.). The second question is whether the crack network becomes saturated
or reaches a critical value beyond which it localizes to form a macroscopic
crack [Needleman, 1988; Pijaudier-Cabot and Benallal, 1993; Peerlings et al.,
1998; Ladevèze et al., 2000]. Examples are presented for each situation. It
is worth mentioning that the softening case is addressed in this modeling
framework for the first time.

In the second part, we discuss the resolution of the local behavior at
the integration point level. We use a fixed-point algorithm to solve the
local equations; we also present and evaluate several relaxation schemes, including Aitken’s. We also focus on the inversion of the state law. As will be seen later on, this law is nonlinear even if all the internal variables are fixed, and it requires a specific solver. Therefore, we use a Newton-Raphson algorithm; we also present and evaluate several optimization techniques, including BFGS operator updating and Aitken’s relaxation.

In the third part, we discuss the control of damage localization beyond the critical point of a softening model. We use a delay-effect method [Ladevèze et al., 2000] to overcome the loss of ellipticity [Pijaudier-Cabot and Benallal, 1993; Peerlings et al., 1998] and control the localization of damage in the form of a macroscopic crack, which eliminates any pathological mesh dependency. Again, let us mention that the simulation of localization in the context of this damage framework is presented here for the first time.

We end up with a relatively complete, efficient and robust computational environment for anisotropic and unilateral damage within the popular Abaqus/Standard finite element code.

2. The anisotropic and unilateral damage theory

2.1. State potential and state law

State potential. The damage framework introduced in [Ladevèze and Letombe, 2000; Ladevèze, 2002] is based on the following general form of the potential of elastic energy:

$$2\rho \phi \left( \sigma, S, Z \right) = \langle \sigma \rangle^S : S + \langle \sigma \rangle^S_+ : \left( S - S_0 \right) : \langle \sigma \rangle^S_0 + \sigma : Z : \sigma$$  \hspace{1cm} (1)

where $S_0$ is the compliance tensor of the undamaged material, which is always active in compression; $\frac{S}{\epsilon}$ is a damaged compliance, which is active
only in tension (initially, \( S(t = 0) = S_0 \)); and \( Z \) is an additional compliance, which is active both in tension and in compression (initially, \( Z(t = 0) = 0 \)).

Let us first observe that this potential gives maximum freedom in terms of damage modeling, which enables one to deal with load-oriented damage, \textit{i.e.} damage whose direction is not known \textit{a priori}: the damage kinematics is not set \textit{a priori}, but is defined completely by the damage evolution laws. Actually, there are no damage variables associated with specific damage mechanisms; the damage variables of the model are the whole compliance tensors \( S \) and \( Z \). Thus, any compliance can be reached from the initial compliance, which makes the model equivalent to an eighth-order damage tensor model \cite{Lemaître2009}.

Let us mention that we also considered strain-based formulations, but we had to abandon that idea because it could lead to cases in which the damaged stiffness tensor ceases to be positive definite before the actual stiffness in the loading direction gets to zero, which would make it impossible to model final rupture.

In order to deal with the crack closure effect, the model distinguishes clearly the tension state from the compression state: the stress tensor is divided into a positive part and a negative part, each associated with a different compliance operator. To ensure the continuous differentiability of the state potential, \textit{i.e.} the continuity of the state law, this partitioning is carried out in a specific way which takes into account the middle operator. It is well-known that the coupling between tensorial damage and tension/compression partitioning is not straightforward \cite{Ladevèze1983; Chaboche1992}. There-
fore, we use the following definitions of positive and negative stresses:

\[
\begin{align*}
\langle \sigma \rangle^S_S &= S^{-1/2} : \langle S^{1/2} : \sigma \rangle^+_S \\
\langle \sigma \rangle^{S_0} &= S_0^{-1/2} : \langle S_0^{1/2} : \sigma \rangle^-_S
\end{align*}
\] (2)

where \( \langle \quad \rangle^+_/- \) denotes the positive/negative decomposition of a second-order symmetric tensor (obtained by taking the positive/negative eigenvalues alone). It is important to note that unless both the positive part and the negative part are defined that way the state law is discontinuous.

With these definitions, the continuous differentiability of the potential can be clearly shown by introducing Equation (2) into Equation (1): 

\[
2\rho \phi \left( \sigma, S, Z \right) = \langle S^{1/2} : \sigma \rangle^+_S + \langle S^{1/2} : \sigma \rangle^-_S + \langle S_0^{1/2} : \sigma \rangle^-_S + \sigma : Z : \sigma
\] (3)

whose continuous differentiable property is trivial [Ladevèze and Letombe, 2000; Desmorat, 2000]. As a direct consequence of this property, the state law (which is the first derivative of the potential) will always be continuous, and the compliance operator (the second derivative) will always be symmetric.

Finally, our framework also enables us to distinguish between damage which is highly dependent on the tension/compression state (i.e., tension damage, added to \( S \)) and damage which is independent of the tension/compression state (i.e., shear damage, added to \( Z \)).

State law. The state law, derived from the elastic energy potential, is simply:

\[
\varepsilon = \frac{\partial \rho \phi}{\partial \sigma} = S : \langle \sigma \rangle^S + S_0 : \langle \sigma \rangle^{S_0} + Z : \sigma
\] (4)
2.2. Thermodynamic forces

First of all, let us define the following two thermodynamic forces, which are linked directly to the energy release rates associated with the evolutions of the damage variables:

\[
\begin{align*}
Y_S &= 2 \frac{\partial \rho \phi}{\partial S} = \langle \sigma \rangle^S \otimes \langle \sigma \rangle^S \\
Y_Z &= 2 \frac{\partial \rho \phi}{\partial Z} = \sigma \otimes \sigma
\end{align*}
\]  

(5)

These thermodynamic forces or the corresponding damage variables cannot be associated with specific damage mechanisms and, therefore, cannot be used as such to drive all damage mechanisms; several additional thermodynamic forces must be defined in order to drive any type of damage.

For example, we will see that while tension damage can be driven correctly by \(Y_S\) (which is highly load-oriented, see Equation (5)) or its projections onto specific directions, this is not the case for shear damage. Because of the positive part of \(\sigma\), only the tension part \(i.e.\) the positive eigenvalue drives the evolution of damage. Besides, since \(Y_Z\) is active also in compression, we will not use it to drive any type of damage. Therefore, we must define another thermodynamic force to drive shear damage (see Sections 2.3.1 and 2.3.2). This additional force is simply a rotation of \(Y_S\) defined as:

\[
Y_{S'} = \left( R_{\pi/2} \langle \sigma \rangle^S \right)_{\text{sym}} \otimes \left( R_{\pi/2} \langle \sigma \rangle^S \right)_{\text{sym}}
\]

(6)

with

\[
R_{\pi/2} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}
\]

Since all the previous thermodynamic forces are proportional to stresses, they could not be used to model the localization of damage \(i.e.\) the soften-
ing phenomenon). Therefore, we will need to define an additional thermo-
dynamic force which is proportional to strains (see Section 2.3.3):

\[
X_S = S Y_S S
\]  

(7)

2.3. Damage evolution laws

Several damage evolution laws can be defined depending on the very
nature of the damage they represent: is this damage load-oriented or
microstructure-oriented? Does it reach saturation or does it localize into
a macroscopic crack? We present examples for each situation, including
(for the first time) localizing damage. The proposed formulation is closely
modeled after the associated classical framework with normality rule and
isotropic hardening [Lemaitre et al., 2009].

2.3.1. The case of load-oriented damage

For the sake of simplicity, from here on, we will use essentially the clas-
sical engineering notations \(^\wedge\) for second- and fourth-order tensors[Lemaitre
et al., 2009].

In the case of load-oriented damage, one can use the load-oriented ther-
modynamic forces directly to drive the evolution of damage. Thus, we define
the following effective thermodynamic force and its maximum over time:

\[
\begin{align*}
z &= \left( a \ \text{Tr} \left( \hat{Y}_S \right)^n + (1 - a) \ \text{Tr} \left( \hat{Y}^{n+1}_S \right) \right)^{1/n+1} \\
\bar{z}(t) &= \sup_{\tau \leq t} z(\tau)
\end{align*}
\]  

(8)

Then the corresponding evolution of the damage variables is:

\[
\begin{align*}
\dot{S} &= \dot{\alpha} \frac{\partial z}{\partial \hat{Y}_S} = \dot{\alpha} \frac{a \ \text{Tr} \left( \hat{Y}_S \right)^n \frac{1}{z^n} + (1 - a) \ \hat{Y}_S^n}{z^n} \\
\dot{Z} &= \dot{\alpha} \frac{b \ Y_S n}{z^n}
\end{align*}
\]  

(9)
where $\alpha$ is the “hardening variable”, a function of $\tilde{z}$ which must be calibrated experimentally. Usually, one assumes a shape depending on several parameters which must be identified. For example, the following shape was used in [Ladevèze and Letombe, 2000; Ladevèze, 2002; Genet et al., 2012]:

$$
\alpha = k\left(\frac{\sqrt{\tilde{z}} - \sigma_0}{\sigma_0}\right)^2_+
$$

(10)

where $\sigma_0$ characterizes the onset of cracking and $k$ its intensity. (In the case of a unidirectional load, $\sqrt{\tilde{z}}$ is simply the magnitude of the stress.) The corresponding responses of this and other laws are compared in Figure 3 of Section 2.3.3.

The dissipation associated with this evolution law is:

$$
\begin{align*}
\omega_S &= \frac{\partial \rho \phi}{\partial S} : \dot{S} = \frac{\dot{\alpha}}{2\tilde{z}^n} \left( a \text{ Tr} \left( \tilde{Y}_S \right)^{n+1} + (1 - a) \text{ Tr} \left( \tilde{Y}_S^{-n+1} \right) \right) \\
\omega_Z &= \frac{\partial \rho \phi}{\partial Z} : \dot{Z} = \frac{b\dot{\alpha}}{2\tilde{z}^n} \text{ Tr} \left( a \left( \frac{R_{\pi/2}}{\sigma} \langle \sigma \rangle^S_{+ sym} \right) \right)^2 \text{ Tr} \left( \tilde{Y}_S^{n-2} \right)
\end{align*}
$$

(11)

which is trivially positive.

As can be seen in Equation (9), the evolution of damage can be tuned using parameters $a$, $b$ and $n$ and can be made highly load-oriented. For example, if $a = 1$, the tension damage is fully isotropic; but if $a = 0$, the larger $n$, the more anisotropic the tension damage. Regarding shear damage, its magnitude is directly proportional to $b$. To illustrate the influence of $a$
and \(b\), let us define the relative angular tension and compression moduli:

\[
\begin{align*}
\tilde{E}_t (\theta) &= \frac{N (\theta) : S_0 : N (\theta)}{N (\theta) : (S + Z) : N (\theta)} \\
\tilde{E}_c (\theta) &= \frac{N (\theta) : (S_0 + Z) : N (\theta)}{N (\theta) : S_0 : N (\theta)}
\end{align*}
\]

(12)

with \(N (\theta) = n (\theta) ^t n (\theta)\)

and \(n (\theta) = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix}\)

These relative angular tension and compression moduli corresponding to a given amount of damage in different directions for an initially isotropic material are presented in Figure 1 for several values of \(a\) and \(b\). (In all cases, \(n = 2\); due to symmetry, only one quadrant was required for each set of parameters.) One can see that a rotation of the load leads simply to a rotation of the damage morphology.

2.3.2. The case of microstructure-oriented damage

In this case, the load-oriented thermodynamic forces cannot be used directly, but must be projected onto the \textit{a priori} known damage directions. For example, for a crack network which is orthogonal to \(n\) and parallel to \(t\), we define the projectors:

\[
\begin{align*}
P_{nn} &= n ^t n, \quad P_{tt} = t ^t t, \quad P_{nt} = (n ^t t) _{\text{sym}} \\
P_{nnnn} &= \begin{bmatrix} P_{nn} & P_{nn} \\ P_{nn} & P_{nn} \end{bmatrix}, \quad P_{tttt} = \begin{bmatrix} P_{tt} & P_{tt} \\ P_{tt} & P_{tt} \end{bmatrix}, \quad P_{ntnt} = \begin{bmatrix} P_{nt} & P_{nt} \\ P_{nt} & P_{nt} \end{bmatrix}
\end{align*}
\]

(13)

and the effective thermodynamic force:

\[
\begin{align*}
z &= \left( a \ Tr \left( \hat{Y}_S \right) ^{n+1} + (1 - a) \ Tr \left( \hat{P}_{nmn} \hat{Y}_S ^{n+1} \hat{P}_{nmn} \right) \right) ^{1/(n+1)} \\
\bar{z} (t) &= \sup _{\tau \leq t} \bar{z} (\tau)
\end{align*}
\]

(14)
Figure 1: Damaged angular tension and compression moduli using a load-oriented damage evolution law and two load directions for several values of $a$ and $b$ (top: shear damage activated, $b = 4$; bottom: no shear damage, $b = 0$; left: anisotropic tension damage, $a = 0$; right: isotropic tension damage, $a = 1$)
The corresponding evolution of the damage variables is:

\[
\begin{align*}
\dot{\hat{S}} &= \dot{\alpha} \frac{\partial z}{\partial \hat{y}_S} = \dot{\alpha} a \text{Tr}(\hat{y}_S^n) \frac{1}{\hat{z}^n} + (1 - a) \hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn} \\
\dot{\hat{Z}} &= \dot{\alpha} \frac{b}{2^n \hat{z}^n} \text{Tr}(\hat{y}_S^n) \frac{\hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn}}{\hat{P}_{ntnt}}
\end{align*}
\]

(15)

where \(\alpha\) is again the “hardening variable” to be calibrated experimentally (see Section 2.3.1).

Let us note that in the case of a unidirectional tension load normal to the crack this evolution law is almost the same as the load-oriented law defined in Section 2.3.1. The only small difference is due to the positive stress, which is slightly different from the complete stress even for a unidirectional tension load and, therefore, slightly modifies the effect of projections. This difference is not significant, as can be seen in Figure 3 of Section 2.3.3 where the evolution laws are compared.

In this case, the dissipation is:

\[
\begin{align*}
\omega_S &= \frac{\partial \rho \phi}{\partial \hat{S}} : \dot{\hat{S}} = \dot{\alpha} a \text{Tr}(\hat{y}_S^n) \frac{1}{\hat{z}^n} + (1 - a) \hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn} \\
\omega_Z &= \frac{\partial \rho \phi}{\partial \hat{Z}} : \dot{\hat{Z}} = \dot{\alpha} \frac{b \hat{z}^n}{2^n \hat{z}^n} \text{Tr}(\hat{y}_S^n) \frac{\hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn} \hat{y}_S^n \hat{P}_{nn}}{\hat{P}_{ntnt}}
\end{align*}
\]

(16)

which is also positive.

Equation (15) clearly shows that in this case the evolution of damage is oriented by the microstructure. Relative angular tension and compression moduli corresponding to a given amount of damage in different directions are presented in Figure 2 for several values of \(a\) and \(b\) (in all cases, \(n = 2\)).

One can see that in this case a change in the load direction modifies the amount of damage, but not its morphology.
Figure 2: Damaged angular tension and compression moduli using a microstructure-oriented damage evolution law and two load directions for several values of $a$ and $b$ (top: shear damage activated, $b = 4$; bottom: no shear damage, $b = 0$; left: anisotropic tension damage, $a = 0$; right: isotropic tension damage, $a = 1$)
2.3.3. The case of softening damage

This is the first presentation of a softening damage evolution law in the proposed anisotropic and unilateral damage theory. In this case, formulations similar to those presented in Section 2.3.1 for load-oriented damage and in Section 2.3.2 for microstructure-oriented damage can be applied, but thermodynamic forces proportional to strains rather than stresses must be used (see Section 2.2). Indeed, beyond the critical point, the stress decreases and, thus, a thermodynamic force dependent on the stress alone could not cause the damage to increase. Therefore, one must consider a force based either on the effective stress or on the strain. We chose the latter. Thus, for a load-oriented mechanism, we use the effective thermodynamic force:

$$z = \left( a \text{ Tr} \left( \hat{X}_S \right)^{n+1} + (1-a) \text{ Tr} \left( \hat{X}_S^{-n+1} \right) \right)^{1/n+1}$$

$$\ddot{z} (t) = \sup_{\tau \leq t} z (\tau)$$

with the evolution of the damage variable:

$$\dot{\hat{S}} = \dot{\alpha} \frac{\partial z}{\partial \hat{X}_S} = \dot{\alpha} \frac{a \text{ Tr} \left( \hat{X}_S \right)^{n} \frac{1}{n} + (1-a) \hat{X}_S^{n}}{\dot{\bar{z}}^n}$$

(18)

For a microstructure-oriented mechanism, we use the effective thermodynamic force:

$$z = \left( a \text{ Tr} \left( \hat{X}_S \right)^{n+1} + (1-a) \text{ Tr} \left( \hat{P}_{mmn} \hat{X}_S^{-n+1} \hat{P}_{mmn} \right) \right)^{1/n+1}$$

$$\ddot{z} (t) = \sup_{\tau \leq t} z (\tau)$$

with the evolution of the damage variable:

$$\dot{\hat{S}} = \dot{\alpha} \frac{\partial z}{\partial \hat{X}_S} = \dot{\alpha} \frac{a \text{ Tr} \left( \hat{X}_S \right)^{n} \frac{1}{n} + (1-a) \hat{X}_S^{n} \hat{P}_{mmn}}{\dot{\bar{z}}^n \hat{P}_{mmn}}$$

(20)
\( \alpha \) is still the “hardening variable” to be calibrated experimentally (see Section 2.3.1), but it must be redefined because the effective thermodynamic forces are now proportional to the strains. For example, one can use the following shape:

\[
\alpha = \begin{cases} 
0 & \text{if } \sqrt{\bar{z}} \leq \epsilon_0 \\
k \left( \frac{\sqrt{\bar{z}} - \epsilon_0}{\epsilon_1 - \sqrt{\bar{z}}} \right)^2 & \text{if } \epsilon_0 \leq \sqrt{\bar{z}} \leq \epsilon_1 \\
+\infty & \text{if } \sqrt{\bar{z}} \geq \epsilon_1
\end{cases}
\]  

(21)

where \( \epsilon_0 \) characterizes the onset of cracking, \( \epsilon_1 \) the final rupture, and \( k \) the amount of damage. (In the case of a unidirectional load, \( \sqrt{\bar{z}} \) is simply the longitudinal strain.) The responses of this and previous laws are compared in Figure 3.

In this case, the dissipation is:

\[
\omega = \frac{\partial \rho \phi}{\partial \bar{S}} : \dot{\bar{S}} = \frac{\dot{\alpha}}{2 \bar{z}^n} \left( a \, \text{Tr} \left( \dot{\bar{X}}_S \right)^n \text{Tr} \left( \dot{\bar{Y}}_S \right) + (1 - a) \, \text{Tr} \left( \dot{P}_{nnnn} \dot{\bar{X}}_S^n \dot{P}_{nnnn} \dot{\bar{Y}}_S \right) \right)
\]  

(22)

which is also positive.

Let us mention that only tension damage was considered here because the introduction of shear damage would lead to the same problem as strain-based formulations (see the remark in Section 2.1): sometimes the damaged stiffness tensor could cease to be positive definite before the actual stiffness in the loading direction gets to zero.

Another element must be added to this law in order to control the end of the damaging process. Since tension damage alone is being considered, the only internal variable is the tensor \( \bar{S} \) itself. (The case of shear damage with a softening law, which involves the second internal variable \( \bar{Z} \), has not yet been addressed.) Thus, the full damage criterion can be based directly
on the eigenvalues of $\hat{S}$:

$$\exists i \quad \frac{1}{M E_0} \leq \lambda_i \frac{\hat{S}}{\equiv} \leq \frac{M}{E_0} \implies \text{rupture} \quad (23)$$

where $\lambda_i$ are the eigenvalues of $\hat{S}$ and $M$ is a large number (in practice, we use $M = 10^3$). When this limit is reached, the corresponding integration point is considered to be broken and the damage ceases to evolve. It is worth mentioning that this criterion can be applied at no substantial additional cost because $\hat{S}$ must be diagonalized anyway in order to calculate $\sqrt{\hat{S}}$.

The responses of the model under unidirectional tension-compression loading using the damage evolution laws presented in Sections 2.3.1, 2.3.2 and 2.3.3 are compared in Figure 3. (In the case of the microstructure-oriented law, the load was orthogonal to the cracks.) One can see that every model recovers its stiffness in compression, that the load-oriented and microstructure-oriented non-softening models are nonseparable, and that the law presented in this section does have a softening character.

Figure 3: The responses of the model under unidirectional tension-compression loading ($k = 10^{-5}$, $\varepsilon_1/\varepsilon_0 = 10$) using different damage evolution laws
3. Calculation of the local behavior

Let us now present the key aspects of the numerical implementation of the family of models presented in Section 2 based on the anisotropic and unidirectional damage theory. In this section, only non-softening damage evolution laws are considered. The softening case will be discussed in Section 4.

3.1. The local loop

The local loop is run for each integration point and at each global iteration of each load increment. The input is $\epsilon^{l,i}$, the total strain tensor at load increment $l$ and global iteration $i$, and the output consists of the damage tensors $S^{l,i}$ and $Z^{l,i}$, the corresponding damage “hardening” variable $\alpha^{l,i}$, and the stress tensor $\sigma^{l,i}$. Starting here, in order to simplify the notation, the subscripts $l, i$ will be omitted.

3.1.1. The fixed-point solver

This set of nonlinear equations could be solved using a Newton-Raphson method, but the very different units and magnitudes of the unknowns would lead to very unbalanced problems. Besides, most of the derivatives in the equations are difficult to calculate or even to approximate. For these reasons,
we chose to use the following fixed-point algorithm instead:

\[
\begin{align*}
\text{initialization: } & j = 0 ; \, \alpha^j = \alpha^{l-1} ; \, S^j = S^{l-1} ; \, Z^j = Z^{l-1} \\
\text{loop: } & \\
\text{stress: } & \sigma^j / \varepsilon = S^j : (\sigma^j)_+ + S_0 : (\sigma^j)_- + Z^j : \sigma^j \\
\text{residual: } & R^j = \alpha (\sigma^j) - \alpha^j \\
\text{exit test: } & |R^j| / |\alpha^j - \alpha^{l-1}| < \text{tolerance} \implies \text{exit} \quad \text{(24)} \\
\text{damage: } & \\
& S^{j+1} = S \left( S^{l-1}, \alpha^{j+1} - \alpha^{l-1} \right) \\
& Z^{j+1} = Z \left( Z^{l-1}, \alpha^{j+1} - \alpha^{l-1} \right) \\
\text{end loop: } & j = j + 1
\end{align*}
\]

where \( \alpha \) is the function defined in Equations (10) or (21), and \( S \) and \( Z \) are the functions defined in Equations (9) or (15). Concerning the tolerance, in the absence of a reference value for the magnitude of the residual of the proposed algorithm, we used a stagnation criterion with a tolerance of \( 10^{-3} \).

3.1.2. Acceleration of the solver

The fixed-point method can be viewed as a Newton-Raphson method with a unit search direction and, therefore, can oscillate greatly. This is particularly true in our case because of the presence of unilateral conditions (damage can only increase, see Equations (8) and (14)) and because in practice Algorithm (24) has very poor convergence or no convergence at all. Therefore, we propose two relaxation methods which improve the algorithm convergence drastically. The only modification to Algorithm (24) concerns
the damage increase line, which becomes:

\[ \alpha^{j+1} = \alpha^j + s^j R^j \]  

(25)

where \( s^j \) is defined as follows:

**Basic relaxation.** One can consider that relaxation is required only if convergence fails to occur after a given number of iterations. This leads to the following very simple relaxation scheme:

\[ s^j = \frac{1}{1 + E(j/N)} \]  

(26)

where \( E \) is the classical integer part operator and \( N \) is the predefined number of iterations.

**Aitken’s relaxation.** Another acceleration scheme considered here is Aitken’s relaxation, whose excellent performance was demonstrated in recent works [Kassiotis et al., 2010]. This can be viewed as a search direction optimization based on previous iterations. Then, \( s^j \) is defined as:

\[
s^j = \begin{cases} 
1 & \text{if } j = 0 \\
-s^{j-1} \frac{R^{j-1}}{R^j - R^{j-1}} & \text{if } j > 0
\end{cases}
\]  

(27)

3.1.3. Performance

The performance of each of the options proposed for the resolution of the model’s equations was evaluated using a very simple problem involving no structural effect: a single linear quadrangular element with four integration points was subjected to pure unidirectional tension through symmetry conditions and prescribed displacements (see Figure 4). The damage law considered was that of Section 2.3.1, which leads to the most difficult local loop because damage is stress-driven (see Figure 3). Figure 5 shows how the
methods compare in terms of the number of iterations and time. Clearly, Aitken’s relaxation was found to be much more efficient than fixed-value relaxation, and it will be used from now on. For example, Figure 5(b) shows a 75% gain compared to the case where relaxation occurs after 10 unconverted iterations. Figure 5(c) also shows that this acceleration reduces the cost of the local loop to about 10% of that of the global loop, which is a very satisfactory ratio.

![Figure 4: The problem used for the evaluation of the performance of the solver (\(\epsilon^g_1\) denotes the applied strain)](image)

### 3.2. The behavior loop

In the previous discussion of the local loop (see Section 3.1), we never explained how to calculate \(\sigma\) when all the internal variables are fixed (see the second line of Algorithm (24)). While this step is straightforward for most existing models, it is not for ours. Because of the partitioning of \(\sigma\) into positive and negative parts, Equation (4) is nonlinear even with fixed operators, so the problem can be formulated as follows:

\[
\begin{cases}
\text{with } \epsilon, S, S_0 \text{ and } Z \text{ known, find } \sigma \text{ such that } \\
\epsilon = S : \langle \sigma \rangle_S + S_0 : \langle \sigma \rangle_{S_0} + Z : \sigma
\end{cases}
\]

(28)
Figure 5: Performances of the local loop acceleration methods
3.2.1. The Newton-Raphson solver

This nonlinear problem is solved using a Newton-Raphson algorithm:

\[
\begin{align*}
\text{initialization: } & k = 0 ; \sigma^k = \sigma^{l-1} \\
\text{loop:} & \\
\text{residual: } & R^k = \epsilon - S : \langle \sigma^k \rangle_S - S_0 : \langle \sigma^k \rangle_Z \sigma^k + Z : \sigma^k \\
\text{exit test: } & ||R^k|| < \text{tolerance} \implies \text{exit} \\
\text{stress: } & \sigma^{k+1} = \sigma^k + D^k : R^k \\
\text{end loop: } & k = k + 1
\end{align*}
\]

for which several search directions \( D^k \) can be used. The actual tangent direction is not an option because one cannot derive the state law (4) with respect to \( \sigma \) in the general case where \( \langle \sigma \rangle^S \neq 0 \) and \( \langle \sigma \rangle^S_0 \neq 0 \). One can choose, for example, the initial operator \( H_0 = S_0^{-1} \), which is not a good direction, especially when the damage is significant, but which is fast because the calculation of the operator is very inexpensive. Another option is to use the quasi-secant operator, defined as:

\[
D^k = \begin{cases} 
(S^l + Z^l)^{-1} \text{ if } \text{Tr}(\sigma^k) > 0 \\
(S_0 + Z^l)^{-1} \text{ if } \text{Tr}(\sigma^k) < 0 
\end{cases}
\]

which is a much better search direction, but also a more expensive one because these operators are usually not saved and must be recalculated at each iteration. Other means of drastically improving the performance of the solver will be presented in Section 3.2.2.

Regarding tolerance, in practice, since the residual of the proposed algorithm is a strain, we use \( 10^{-9} \).
3.2.2. Acceleration of the solver

In practice, the initial operator converges very slowly, or even does not converge at all if the damage is significant. The secant operator defined in Equation (30) generally converges very poorly, too. Therefore, we propose two acceleration methods in order to improve the convergence of the algorithm drastically.

BFGS search direction. The first acceleration scheme one can consider is the BFGS method [Matthies and Strang, 1979], whose ability to provide a very good compromise between cost and quality for the search direction is well-known: a quasi-tangent direction is generated at the cost of $4k$ additional scalar products compared to the initial direction [Matthies and Strang, 1979]. The algorithm for the calculation of $D^k$ is well-known and will not be recalled here; the only specificity is that the secant operator defined in Equation (30) is used for the central operator because the tangent operator cannot be derived formally.

Aitken’s relaxation. Another acceleration considered here is Aitken’s relaxation, which was already used in Section 3.1.2 and which can also be viewed as a search direction optimization based on previous iterations. The only modification to Algorithm (29) is the last line, which becomes:

$$a^{k+1} = a^k + s^k D^k : R^k$$

(31)

with

$$s^k = \begin{cases} 
1 & \text{if } k = 0 \\
-s^{k-1} \frac{R^{k-1} : (R^k - R^{k-1})}{(R^k - R^{k-1}) : (R^k - R^{k-1})} & \text{if } k > 0 
\end{cases}$$

For the same reason as for the BFGS acceleration, we use the secant operator defined in Equation (30) for $D^k$. 
3.2.3. Performance

Let us now evaluate the performances of the different methods proposed for the inversion of the state law of the model. We used the same test case as in Section 3.1.3 (see Figure 4), but the damage law considered was that of section 2.3.3, which is the most difficult behavior loop because damage increases until it reaches the criterion defined in (23) (see Figure 3). The methods are compared in terms of the number of iterations and time in Figure 6. Clearly, the secant operator performs very poorly and should not be used. The Aitken and BFGS operators have comparable performance in terms of both the number of iterations and time. Figure 6(b) shows that they lead to a gain by a factor 2 to 200 compared to the secant operator and reduce the cost of the inversion of the state law to approximately 50% of that of the local loop (see Figure 6(c)) even when damage approaches saturation. The BFGS operator, which is slightly more efficient than Aitken’s, will be used from now on. In order to appreciate the importance of this gain, one should bear in mind that this loop is run at each local iteration of each global iteration of each time increment, which makes it the key factor in the performance of the implementation.

4. Control of the damage localization

The calculation of softening models such as those defined in Section 2.3.3 over a domain goes through a critical point where a loss of ellipticity, i.e. a loss of uniqueness of the solution [Needleman, 1988; Piaudier-Cabot and Benallal, 1993; Peerlings et al., 1998], occurs and leads to pathological mesh dependencies [Ladevèze et al., 2000; Desmorat et al., 2010]. Several remedies exist for damage models, including nonlocal formulations [Piaudier-Cabot
Figure 6: Performance of the state law inversion methods
and Benallal, 1993; Peerlings et al., 1998; Voyiadjis et al., 2004; Desmorat et al., 2010] and delay-effect approaches [Ladevèze et al., 2000; Kerfriden et al., 2009; Desmorat et al., 2010]. The latter was chosen for our work because it is a local method, which is easy to implement in FE codes such as Abaqus/Standard.

4.1. The delay-effect method

First, in order to have a damage variable with an order of magnitude of 1, let us rewrite Equation (21) as follows:

\[
\begin{align*}
    d &= \begin{cases}
        0 & \text{if } \sqrt{\bar{z}} \leq \epsilon_0 \\
        \frac{(\sqrt{\bar{z}} - \epsilon_0)}{\epsilon_1 - \epsilon_0} & \text{if } \epsilon_0 \leq \sqrt{\bar{z}} \leq \epsilon_1 \\
        1 & \text{if } \sqrt{\bar{z}} \geq \epsilon_1
    \end{cases} \\
    \alpha &= k \frac{d}{1 - d}
\end{align*}
\]

(32)

Now, the delay-effect method for controlling the localization of damage consists in replacing the evolution of this damage variable by an evolution with a bounded rate:

\[
\dot{d} = \frac{1}{\tau_c} \left( 1 - e^{-(d_{\text{static}} - d)^+} \right)
\]

(33)

where \(d_{\text{static}}\) is the static function defined in Equation (32) and \(\tau_c\) a fictitious time parameter which must be chosen in order to avoid uncontrolled localization [Ladevèze et al., 2000; Kerfriden et al., 2009]. The numerical resolution of such a simple nonlinear, but scalar, equation is straightforward and will not be discussed here.

The behavior law is modified with the introduction of this viscous-like parameter. Figure 7 shows the stress-strain curves obtained with different values of \(\tau_c\).
4.2. Illustrative examples

CT specimen. The effectiveness of the delay-effect method in controlling the localization of damage was evaluated using a simple CT-like test, i.e. a pre-cracked specimen subjected to tension (see Figure 8). The model consisted of an initially isotropic material (with $E_0 = 250$ MPa and $\nu_0 = 0.3$) whose state evolution was modeled using a microstructure-oriented softening damage law (see Equations (19) and (20) of Section 2.3.3, with $a = 0$, $n = 2$ and $\mathbf{n}$ orthogonal to the initial crack) and the limited-rate kinetics of the delay-effect method (see Equations (32) and (33) of Section 4.1, with $\epsilon_0 = 1 \times 10^{-3}$, $\epsilon_1 = 3 \times 10^{-3}$, $k = 10^{-5}$ and $\tau_c = 3 \times 10^{-2}$ s). The response and the damage fields for different meshes (generated with GMSH [Geuzaine and Remacle, 2009]) are shown in Figure 9. One can clearly observe that the solution is objective, i.e. mesh-independent, in terms of both the mechanical response and the damage fields. Indeed, while the response of the coarse mesh is slightly different, the responses of the medium and fine meshes are very
Figure 8: The problem used for the evaluation of localization control based on delay-effect damage ($u$ is the applied displacement, $F$ is the calculated force, and $\dot{u} = 0.2$ mm/s)

Plate with an open hole. Now let us consider a first structural example which consists in a plate with an open hole (see Figure 10). The model was the same as for the CT specimen, except for $\tau_c = 1 \times 10^{-2}$ s. Figure 11 shows the response of the model using different meshes (again generated with GMSH [Geuzaine and Remacle, 2009]). Once again, the response of the coarse mesh is slightly different, but the responses of the medium and fine meshes are very similar, which attests to the fact that the method can be used to make an objective prediction of the structure’s final rupture.

5. Conclusion

This paper examined several key aspects of the formulation and numerical implementation of a family of models belonging to the anisotropic and unilateral damage theory. This modeling framework is based on a general expression of the damaged elastic energy potential which enables one to distinguish between tension behavior and compression behavior throughout
Figure 9: The response and the damage field for the CT specimen at $t = 0.75$ s (dark grey: no damage; light gray: full damage criterion reached, see Equation (23) of Section 2.3.3): objectivity of the mesh and prediction of the crack’s propagation.
the evolution of the damage, even when the orientation of the damage is not known \textit{a priori} (see Section 2.1).

Several damage evolution laws were presented in order to deal with all types of damage: load-oriented or microstructure-oriented; reaching saturation or localizing into a macroscopic crack (see Section 2.3). The formulation of the microstructure-oriented damage law was modified slightly compared to the previous formulation [Ladevèze, 2002] in order to make it equivalent to the load-oriented laws when the load is normal to the crack (see Section 2.3.2). In addition, softening laws were presented in this framework for the first time (see Section 2.3.3). Let us note that even though this paper discusses only models with a single damage evolution law, it is possible to define models with several laws, each associated with a different damage mechanism. For example, in the model proposed for CMCs in [Ladevèze, 2002; Genet et al., 2012], three damage evolution laws were defined: one load-oriented law for inter-yarn cracking and two microstructure-oriented laws for intra-yarn cracking of the longitudinal and transversal yarns.

Then we presented our current implementation of the whole family of models in Abaqus/Standard. The local equations are solved using a fixed-point method. Among several relaxation schemes which were considered,
Figure 11: The response and the damage field for the open hole specimen at $t = 1$ s (dark grey: undamaged; light gray: full damage criterion reached, see Equation (23) of Section 2.3.3): objectivity of the mesh and prediction of the final rupture.
Aitken’s appears to be the most efficient and reduces the cost of the local
resolutions to approximately 10% of that of the global iterations (see Section
3.1). Since the model’s state law is nonlinear even when all the internal
variables are fixed, its inversion is carried out using a Newton-Raphson
method. Once again, several acceleration schemes were considered, among
which the BFGS quasi-tangent method appears to be the most efficient.
This reduces the cost of inverting the state law to approximately 50% of
that of the local iterations, even with significant damage (see Section 3.2).

Finally, a delay-effect method was used to control damage localization
in the case of softening evolution laws. This enabled us to simulate the
propagation of a macroscopic crack and the final rupture of a structure
with no mesh dependency (see Section 4).

Regarding perspectives, since this framework has already been applied to
the case of CMCs [Ladevèze, 2002; Genet et al., 2012], the new capabilities
of simulating the creation and propagation of macroscopic cracks will replace
the simple criterion used until now (see [Cluzel et al., 2009; Genet et al.,
2012]). In addition, microanalyses of cracked media will be carried out in
order to derive in a generic way some of the model parameters, such as those
which define the damage anisotropy (see Sections 2.3.1 and 2.3.2) or the
projectors (see Section 2.3.2). This has already been done for the kinematics
of a macroscopic damage model for concrete [Delaplace and Desmorat, 2007]
and for both the kinematics and the kinetics of a mesoscopic damage model
for laminated composites [Ladevèze and Lubineau, 2002].
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