Damage smoothing effects in a delocalized rate sensitivity model for metals

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Abstract It has been long time established that application of damage delocalization method to softening constitutive models yields numerical results that are independent of the size of the finite element. However, the prediction of real-world large and small scale problems using the delocalization method remains in its infancy. One of the drawbacks encountered is that the predicted load versus displacement curve suddenly drops, as a result of excessive smoothing of the damage. The present paper studies this unwanted effect for a delocalized plasticity/damage model for metallic materials. We use some theoretical arguments to explain the failure of the delocalized model considered, following which a simple remedy is proposed to deal with it. Future works involve the numerical implementation of the new version of the delocalized model in order to assess its ability to reproduce real-world problems.

Keywords Bammann-Chiesa-Johnson model, damage smoothing, Fourier transform, softening

The introduction of characteristic length scales to constitutive models involving softening through damage delocalization method is very well known to remove the pathological mesh size effects in the finite element (FE) solution of problems involving these constitutive models. Another closely related technique which consists of incorporating gradient terms in the evolution equation of the parameter(s) governing softening yields the same conclusions, although its numerical implementation into FE codes is not an easy task compared to that of the delocalization technique. A complete review of this technique and its associated numerical implementation can be found in Ref. 5. Despite these successes, nonlocal or gradient models have not yet reached a situation where they are applicable to small or large scale structure problems. For example, Enakoutsa et al.1 have demonstrated that the use of nonlocal Gurson model does eliminate spurious mesh size effects in FE simulations of ductile rupture of typical pre-cracked T specimens, but fails to reproduce the experimental load versus displacement curve, i.e., the predicted load-displacement curve remains quasi-stationary for some time and decreases abruptly. According to these authors, this undesirable feature is due to excessive smoothing of the damage distribution in the ligament ahead of the crack tip of the specimen. They provided a theoretical explanation of this phenomenon based on such as crude assumptions as unboundness of the body considered and homogeneity of the mechanical fields. Namely, they showed that the nonlocal evolution equation for the damage is qualitatively similar to some diffusion equations which result in an excessive smoothing of the damage. Following this theoretical analysis, they proposed a simple remedy to deal with the excessive smoothing of the damage. It consists of adopting the nonlocal concept for the logarithm of the damage instead of the damage itself; this has the advantage to eliminate the analogy between the nonlocal evolution equation and a diffusion equation. Good agreements between experimental and numerical results were then obtained.

The objective of the present paper is to follow up the study of the applicability of the delocalization method in numerical simulations of material behavior. The motivation is to predict accurately the post-bifurcation regime of metals as the design of metal structures requires to understand more and more physics of metals in this particular regime. The model considered will be that proposed by Bammann-Chiesa-Johnson (BCJ)7–10 but with a modified, delocalized evolution equation for the damage following an earlier suggestion of Bijaudier-Cabot and Bazant.11 The introduction of the convolution integral of the evolution equation of the damage in the BCJ model incorporates a diffusive effect in the constitutive model, which prevents the nonlocal damage variable to spurious localize into vanishing bands. However, the diffusive effect unavoidably leads to an unwanted excessive smoothing of the damage. Just like that in Ref. 1, we provide a theoretical explanation of this shortcoming, following which a simple remedy is proposed to deal with it. The rest of the paper provides the constitutive relations of the BCJ model and its nonlocal extension, then it is devoted to a theoretical explanation of the unwanted excessive smoothing of the damage. Finally, it presents a simple solution to overcome the excessive damage smoothing shortcoming.

The BCJ model is a physically-based plasticity/damage model which incorporates load path, strain rate, temperature, and history effects through the use of internal state variables (ISVs); it also accounts for both deviatoric deformation resulting from the presence

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of dislocations and dilatational deformation and failure from void growth.

The kinematics assumes a multiplicative decomposition of the deformation gradient into elastic, deviatoric plastic, dilatational plastic and thermal parts. The constitutive equations of the model are written with respect to the natural configuration defined by the plastic deformation such that the current configuration variables are co-rotated with the elastic spin. The pertinent equations of the BCJ model are expressed as the rate of change of the observable and internal state variables and consist of the following elements.

A hyper-elastic law: The hyper-elastic law connects the elastic strain rate to an objective time-derivative Cauchy stress tensor and is given by the equation

$$ \tilde{\sigma} = \lambda (1 - \phi) \text{tr}(D^e) I + 2\mu (1 - \phi) D^e - \frac{\dot{\phi}}{1 - \phi} \sigma + (1 - \phi) \hat{\theta} [(\lambda, \c) \text{tr}(D^e) I + 2(\mu, \c) D^e], \quad (1) $$

where $\lambda$ represents the Lamé constant, $\mu$ is the shear modulus, $\theta$ is the temperature, $\lambda, \c$ is the partial derivative of the Lamé coefficient with respect to $\theta$, and $\phi$ is the partial derivative of the shear modulus with respect to $\theta$. The Cauchy stress $\sigma$ is convected with the elastic spin $\mathbf{W}^e$ through the formulae

$$ \tilde{\sigma} = \dot{\sigma} - \mathbf{W}^e \sigma + \sigma \mathbf{W}^e, $$

where, in general, for any arbitrary second-rank tensor $\mathbf{X}$, $\tilde{\mathbf{X}}$ represents the convective derivative.

Note that the rigid body rotation is included in the elastic spin; therefore, the constitutive model is expressed with respect to a set of directors whose direction are defined by the plastic deformation. Also, the partition of Eq. (1) into its hydrostatic and deviatoric components leads to the governing equations for the pressure (which is useful to calculate the damage) and the Jaumann rate of the deviatoric stress

$$ \dot{p} = (K + \hat{\theta} K, \c) (1 - \phi) \text{tr}(D^e) - \frac{\dot{\phi}}{1 - \phi} p, $$

$$ \tilde{\sigma}' = 2(1 - \phi) (\mu + \hat{\theta} \mu, \c) d^e - \frac{\dot{\phi}}{1 - \phi} \sigma', \quad (2) $$

where $K$ is the bulk modulus, and $d^e$ is the elastic part of the deviatoric deformation rate defined by

$$ d^e = D - \frac{1}{3} \text{tr}(D) I. \quad (3) $$

The decomposition of both the skew-symmetric and symmetric parts of the velocity gradient into elastic and inelastic parts for the elastic stretching rate $D^e$ and the elastic spin $\mathbf{W}^e$ in the absence of elastic-plastic couplings yields

$$ D^e = D - D^p - D^d - D^{th}, $$

$$ \mathbf{W}^e = \mathbf{W} - \mathbf{W}^p. \quad (4) $$

Note that for problems in the shock regime, only the deviatoric elastic strain rate part is linearized, enabling prediction of large elastic volume changes.

Flow rules: The flow rules for $D^p$ and $D^d$, and the stretching rate due to the unconstrained thermal expansion $D^{th}$, are introduced in addition to the equation for the plastic spin $\mathbf{W}^p$. From the kinematics, the dilatational plastic part $D^d$ is given by

$$ D^d = \frac{\dot{\phi}}{1 - \phi} I. $$

Assuming isotropic thermal expansion, the unconstrained thermal stretching rate $D^{th}$ can be given by the relation

$$ D^{th} = A \dot{\theta} I, $$

where $A$ is a linearized expansion parameter.

For the plastic flow rule, a deviatoric flow rule, consulting Bammann,11 is assumed and defined by the equations

$$ D^p = \sqrt{\frac{3}{2}} f(\theta) \sinh \left\{ \left( \frac{||| \mathbf{X} ||| - (1 - \phi)|\kappa + Y(\theta)|}{(1 - \phi) V(\theta)} \right) \right\} \zeta, $$

$$ \xi = \sigma' - \frac{2}{3} \alpha, \quad \zeta = \frac{\xi}{||| \zeta |||}. \quad (5) $$

where $\theta$ represents the temperature, $\kappa$ is the scalar hardening variable, $\sigma'$ is the deviatoric Cauchy stress, and $||| \mathbf{X} |||$ is the magnitude of any arbitrary second-rank tensor $\mathbf{X}$.

There are several choices for the form of $\mathbf{W}^p$. The assumption that $\mathbf{W}^p = 0$ allows to recover the Jaumann stress rate. Alternatively, this function can be described by the Green-Naghdy rate of Cauchy stress.

Evolution equations for the isotropic and kinematic ISVs: The evolution equations for the isotropic and kinematic hardening ISVs are given in a hardening minus recovery format

$$ \dot{\kappa} = H(\theta)||D^p|| - \left[ \sqrt{\frac{3}{2}} R_d(\theta)||D^p|| + R_s(\theta) \right] \kappa^2, $$

$$ \dot{\tilde{\alpha}} = h(\theta) D^p - \left[ \sqrt{\frac{3}{2}} r_d(\theta)||D^p|| + r_s(\theta) \right] ||| \alpha ||| \alpha, \quad (6) $$

where $h$ and $H$ are the hardening moduli, $r_s$ and $R_s$ are scalar functions of $\theta$ describing the diffusion-controlled “static” or “thermal” recovery, and $r_d$ and $R_d$ are the functions of $\theta$ describing the dynamic recovery, $\dot{\alpha}$ is the objective rate of change of $\alpha$, the tensor hardening variable.

Plastic response functions: To describe the plastic response, the BCJ model introduces nine functions that can be separated into three groups. The first three are the initial yield, the hardening and the recovery
functions, defined as

\[ V(\theta) = C_1 \exp(-C_2/\theta), \]
\[ Y(\theta) = C_2 \exp(-C_4/\theta), \]
\[ f(\theta) = C_3 \exp(-C_6/\theta). \]

The second group is related to the kinematic hardening process and consists of the following functions

\[ r_d(\theta) = C_7 \exp(-C_8/\theta), \]
\[ h(\theta) = C_9 \exp(-C_{10}/\theta), \]
\[ r_s(\theta) = C_{11} \exp(-C_{12}/\theta). \]

The last group is related to the isotropic hardening process and consists of

\[ R_d(\theta) = C_{13} \exp(-C_{14}/\theta), \]
\[ H(\theta) = C_{15} \exp(-C_{16}/\theta), \]
\[ R_s(\theta) = C_{17} \exp(-C_{18}/\theta). \]

In the Eqs. (7)–(9), \( C_i \) represents a parameter of the model which needs to be determined.

**Evolution equation for the damage ISV**: The evolution equation for damage, credited to Cocks and Ashby, is given by

\[ \dot{\varepsilon} = \frac{1}{(1 - \phi)^n} \left( 1 - \phi \right) \cdot \sinh \left( \frac{(1 - n) \mathbf{p}}{(1 + n) \mathbf{\sigma}} \right) ||D^p||, \]

where \( \mathbf{p} \) and \( \mathbf{\sigma} \) denote the pressure (governed by Eq. (2)) and the effective stress, respectively. Note that Eq. (10) displays a “\( \sinh \)”-dependence upon the triaxiality factor \( \frac{\mathbf{p}}{\mathbf{\sigma}} \), as well as an additional parameter “\( n \)” along with the initial value of the damage \( \phi_0 \) required to calculate damage growth.

**Adiabatic temperature change**: The last equation to complete the description of the model is the one that computes the temperature change during high strain rate deformation, such as those encountered in high rate impact loadings problems. For these problems, a non-conducting (adiabatic) temperature change, following the assumption that 90% of the plastic work is dissipated as heat, is assumed. Therefore, the rate of the change of the temperature is assumed to follow the equation

\[ \dot{T} = \frac{0.9}{\rho C_v} \mathbf{\sigma} : D^p, \]

where \( \rho \) and \( C_v \) represent the material density and a specific heat coefficient, respectively. The empirical assumption in Eq. (11) has permitted a non-isothermal solution by FE that is not fully coupled with the energy balance equation, consulting Bammann et al. We follow the suggestion of Pijaudier-Cabot and Bazant to introduce the nonlocal concept into the BCJ model. In this model, softening arises from two mechanisms: a gradual increase of the damage (under isothermal conditions) and/or a temperature rise (in adiabatic conditions) followed by an increase of damage. In fact, review of the model’s constitutive equations provided previously reveals that temperature and damage parameters are indeed related toward their sequential governing equations in adiabatic conditions. We propose to introduce the nonlocal concept into the damage evolution equation, which appears quite appealing from a physical point of view because, as is the case in heterogeneous materials, the damage can only be defined by considering “elementary” volumes of size greater than the voids spacing and is therefore a nonlocal quantity.

The evolution equation for this variable is given by a convolution integral, including a bell-weighting function the width of which introduces a mathematical length scale. This equation is given by

\[ \dot{\phi}(x) = \frac{1}{B(x)} \int_{\Omega} \delta(x - y) A(x - y) d\Omega_y. \]

In this expression, \( \Omega \) denotes the volume of the body studied, \( x \) and \( y \) denote the vector coordinates, and \( A \) is the bell-weighting function defined as

\[ A(x) = \exp(-\|x\|^2/l^2), \]

where \( l \) is the mathematical length scale and \( \|x\| \) represents the magnitude of the vector \( x \). The factor \( B(x) \) and the “local damage rate \( \delta_{loc} \)” are given by

\[ B(x) = \int_{\Omega} A(x - y) d\Omega_y. \]

and Eq. (10), respectively. The function \( A \) is indefinitely differentiable and does not involve any Dirac’s \( \delta \)-distribution at the point zero. This means that the function \( \phi \) is not partially local but entirely nonlocal. The function \( A \) is also isotropic and normalized. Notably, then, \( \phi \) must be equal to \( \phi_{loc} \) if the latter variable is spatially uniform. This would not be the case near the boundary of \( \Omega \) in the absence of the normalization factor \( 1/B \). The presence of this term allows for the coincidence everywhere.

The first version of the nonlocal BCJ model consists of all the equations presented previously, except the evolution equation for the damage Eq. (10), which is replaced by Eq. (12). The integral nonlocal evolution equation of the damage introduces in the model a diffusive term which allows to understand why damage or deformation can not localize into vanishing width zones in FE computations. However, such a diffusive term can lead to excessive smoothing of damage, resulting in undesirable consequences such as delay of crack initiation, spurious homogeneous reparation of the damage in regions located in the vicinity of the crack tip, leading to sharp drop of the predicted load-displacement curve. We rigorously explain the diffusive nature of Eq. (12) next.
A theoretical explanation of the excessive smoothing of the damage which results from the nonlocal evolution equation Eq. (12) is given as follows. The explanation is based on a previous argument used by Enakoutsa et al.\(^1\) to analyze the excessive damage smoothing observed in the numerical results of a pre-cracked tensile specimen test using an integral-type nonlocal Gurson model. As in the work of Enakoutsa et al.,\(^1\) the explanation will be based on crude approximations such as infinity of the body considered and unboundness of the mechanical fields.

The local evolution equation for the damage Eq. (10) can be replaced, after development, by the relation

\[
\dot{\phi} = \phi g ||D^p||, \quad g = \sum_{k=1}^{n} \left( \frac{(-1)^{k+1}}{(1 - \phi)^n} |\phi|^n \right)^{k-1} \left( \frac{1 - n}{(1 + n)} \right)^p \sinh \left( \frac{(1 - n)}{(1 + n)} \sigma \right). \tag{14}
\]

Therefore, replacing the local evolution equation of the damage Eq. (10) by the nonlocal one, Eq. (12) is equivalent to replace the equation Eq. (14) by the relation

\[
\hat{\phi}(x, \tau) = \frac{1}{B(x)} \left[ A \ast (\phi g ||D^p||) \right](x, \tau), \tag{15}
\]

where the symbol \(*\) denotes the convolution product; the dependence upon the variables \((x, \tau)\) is specified here only for the sake of clarity. In the following, we shall assume that the body considered in the problem is infinite and the quantities \(g\) and ||\(D^p||\) in Eq. (15) are independent of the spatial variable \(x\), but not with respect to the time variable \(t\). Hence, the factor \(A(x)\) in Eq. (15) is uniform and can be incorporated into the smoothing function; also, the quantities \(g\) and ||\(D^p||\) can be easily extracted from the convolution product.

Taking the Fourier transform (with respect to the spatial variable) of Eq. (15) we get the equation

\[
\frac{\partial \hat{\phi}}{\partial \tau}(p, t) = g(t)||D^p(t)|| \hat{A}(p) \hat{\phi}(p, t), \tag{16}
\]

or equivalently the expression

\[
\frac{\partial \hat{\phi}}{\partial \epsilon_{eq}}(p, \epsilon_{eq}) = g(\epsilon_{eq}) \hat{A}(p) \hat{\phi}(p, \epsilon_{eq}), \tag{17}
\]

where \(\epsilon_{eq}\) denotes the cumulative equivalent plastic strain \(\int_0^t ||D^p(\tau)||d\tau\). The growth rate \(\hat{\phi}(p, \epsilon_{eq})\) in Eq. (17) is governed by the factor \(g(\epsilon_{eq}) \hat{A}(p)\). Now, the Fourier transform of the Gaussian function Eq. (13), \(\hat{A}(p)\), is another Gaussian function which is positive and reaches its maximal value for \(p = 0\). As a result, the growth rate \(\hat{\phi}(p, \epsilon_{eq})\) is maximum for \(p = 0\), that is, when the wavelength is infinite. This shows that the spatial components of Fourier transform with large wavelengths develop more quickly than the components with short wavelengths, which means that the damage distribution smoothed out.

To be more specific, let us assume that the quantity \(g\) is time-independent in addition to be independent of the spatial variable. Hence, we get the relation

\[
\hat{\phi}(p, \epsilon_{eq}) = \hat{\phi}(p, 0) \exp \left[ g \hat{A}(p) \epsilon_{eq} \right] \quad \tag{18}
\]

by solving Eq. (17). The development of \(\hat{\phi}(p, \epsilon_{eq})\) as a function of the time is governed by the growth factor \(\exp(g \hat{A}(p) \epsilon_{eq})\). The ratio of the growth factors corresponding to \(p = 0\) and \(p \neq 0\) is given by the relation

\[
\frac{\hat{\phi}(0, \epsilon_{eq})/\hat{\phi}(0, 0)}{\hat{\phi}(p, \epsilon_{eq})/\hat{\phi}(p, 0)} = \exp \left\{ g \left[ \hat{A}(0) - \hat{A}(p) \right] \epsilon_{eq} \right\}, \tag{19}
\]

the function \(\hat{A}(p)\) being maximum for \(p = 0\), the term \{\cdots\} is positive. The ratio considered is greater than the unity and becomes very large in the limit \(t\) tending to +\(\infty\) (in fact for large value of \(\epsilon_{eq}\)) due to the rapid growth property of the exponential function. This confirms the previous conclusion that between the Fourier components of \(\phi\) with short and large wavelengths, the latter ones develop more quickly than the former ones.

The evolution equation (17) presents some similarity with a diffusion equation. Indeed, let us consider a fictitious diffusion equation of the damage (the cumulative equivalent plastic strain \(\epsilon_{eq}\) replacing the time)

\[
\frac{\partial \phi}{\partial \epsilon_{eq}}(x, \epsilon_{eq}) = D \Delta \phi(x, \epsilon_{eq}), \tag{20}
\]

where \(D\) is a constant and the symbol \(\Delta\) represents the Laplacian. Taking the Fourier transform of Eq. (20), we get the equation

\[
\frac{\partial \hat{\phi}}{\partial \epsilon_{eq}}(p, \epsilon_{eq}) = -D ||p||^2 \hat{\phi}(p, \epsilon_{eq}), \tag{21}
\]

which gives after integration the relation

\[
\hat{\phi}(p, \epsilon_{eq}) = \hat{\phi}(p, 0) \exp(-D ||p||^2 \epsilon_{eq}). \tag{22}
\]

Therefore, the ratio of the growth rates corresponding to \(p = 0\) and \(p \neq 0\) is given by the expression

\[
\frac{\hat{\phi}(0, \epsilon_{eq})/\hat{\phi}(0, 0)}{\hat{\phi}(p, \epsilon_{eq})/\hat{\phi}(p, 0)} = \exp(D ||p||^2 \epsilon_{eq}). \tag{23}
\]

This result is exactly what we get by developing to the second order with respect to \(p\) in the term \{\cdots\} in the right-hand side of Eq. (19).

A new version of the nonlocal BCJ model which is capable to avoid the excessive damage smoothing shortcoming is proposed. The new model introduces a nonlocal evolution equation of the damage originated from the analogy between Eq. (18) and a diffusion equation.
such as Eq. (20) found in the previous theoretical analysis of the excessive smoothing of the damage. Indeed, the diffusive nature of Eq. (20) is connected to the presence of the Laplacian of $\phi$ in the right-hand side. If $\Delta \phi$ were absent from the right-hand side, Eq. (20) should not be a diffusion equation and the excessive smoothing of the damage would not take place. The solution to avoid such a shortcoming is to eliminate the damage of the right hand side of the local evolution equation of the damage Eq. (10) by dividing the two sides of the equation by $\phi$, that is

$$\frac{d(\ln \phi)}{dt} = \frac{1}{\phi} \left( \frac{1}{(1-\phi)^n} - (1-\phi) \right),$$

$$\left(1-n\right) \frac{p}{(1+n) \sigma} \|D^p\|,$$

(24)

The presence of $\phi$ at the denominator of the right hand side is only apparent, since the term $\cdots$ is proportional to $\phi$. This local equation can be changed into a nonlocal equation exactly as Eq. (10) was changed into Eq. (12), and the result is not the same, although the local equations (10) and (24) are equivalent. Hence, we can postulate that

$$\frac{d(\ln \phi)}{dt}(x) = \frac{1}{B(x)} \int_{\Omega} A(x-y) \cdot \left(\frac{d(\ln \phi)}{dt}\right)^{\text{loc}}(y) dV_{\phi},$$

(25)

With the new evolution equation of the nonlocal damage equation (25), the analogy with a diffusion equation breaks down. Indeed, using the convolution product framework, Eq. (25) gives the relation

$$\frac{\partial}{\partial t} \left(\ln \phi\right)(p,t) = g(t) \|D^p(t)\| \hat{A}(p),$$

(27)

which demonstrates that in the evolution equation of the Fourier transform of the damage, the right-hand side does no longer contain $\hat{\phi}(x,t)$, that is, Eq. (25) does not present any similarity with a diffusion equation.

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