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A critical comparison of nonlocal and gradient-enhanced softening continua

R.H.J. Peerlings ^{a,*}, M.G.D. Geers ^a, R. de Borst ^b, W.A.M. Brekelmans ^a

^a Department of Mechanical Engineering, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands

^b Koiter Institute Delft/Faculty of Aerospace Engineering, Delft University of Technology, P.O. Box 5058, 2600 GB Delft, The Netherlands

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Abstract

Continuous models of material degradation may cease to produce meaningful results in the presence of high strain gradients. These gradients may occur for instance in the propagation of waves with high wave numbers and at stress concentrators. Adding nonlocal or gradient terms to the constitutive modelling may enhance the ability of the models to describe such situations. The effect of adding nonlocal or gradient terms and the relation between these enhancements are examined in a continuum damage setting. A nonlocal damage model and two different gradient damage models are considered. In one of the gradient models higher order deformation gradients enter the equilibrium equations explicitly, while in the other model the gradient influence follows in a more implicit way from an additional partial differential equation. The latter, implicit gradient formulation can be rewritten in the integral format of the nonlocal model and can therefore be regarded as truly nonlocal. This is not true for the explicit formulation, in which the nonlocality is limited to an infinitesimal volume. This fundamental difference between the formulations results in quite different behaviour in wave propagation, localisation and at crack tips. This is shown for the propagation of waves in the models, their localisation properties and the behaviour at a crack tip. The responses of the nonlocal model and the implicit gradient model agree remarkably well in these situations, while the explicit gradient formulation shows an entirely different and sometimes nonphysical response. © 2001 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Classical continuum models cease to give a meaningful representation of the mechanical behaviour of materials when the scale of observation approaches that of the microstructure of the material. This is the case for instance for microparts and electronic components, which may typically be of the size of, or even smaller than, a grain. The material can no longer be considered homogeneous at this scale and descriptions in terms of the classical stresses and strains thus break down. In particular, the typical dimension of the

* Corresponding author. Tel.: +31-40-247-2788; fax: +31-40-244-7355.

E-mail address: r.h.j.peerlings@tue.nl (R.H.J. Peerlings).

microstructure (e.g., grain size, lattice distance, fibre length etc.) manifests itself in the mechanical response of the material, for instance in size effects. A similar situation arises in larger components when the scale of variation of the relevant variables becomes comparable to the microstructural scale. This may be the case for instance in wave propagation analyses and at stress concentrators such as notches and cracks.

The need to describe the microstructure-dominated behaviour in an averaged sense, without modelling the full detail of the microstructure and the deformation processes at the microscale, has led to the development of enriched continuum models. In these models, nonstandard deformation and/or stress quantities account for the influence of the microstructure on deformation processes. Taking into account long-range cohesive forces, which are neglected in the standard theory, has led to the classical Toupin–Mindlin gradient theory of elasticity (Toupin, 1962; Mindlin, 1965), see also Mindlin (1964) and Eringen (1966). In this theory first, second and possibly higher-order gradients of the strain and stress enter the constitutive model in order to describe the effect of the microstructure. More recently, some of these ideas have been extended to plasticity (Aifantis, 1984; Fleck and Hutchinson, 1993; Steinmann, 1996). Following arguments similar to those of Toupin and Mindlin, Kröner, Eringen, Edelen and others have arrived at nonlocal formulations of elasticity (Kröner, 1967; Eringen and Edelen, 1972). In the nonlocal theory long-range interactions are taken into account by weighted spatial averages of constitutive quantities. Both approaches introduce at least one length scale into the continuum modelling, which is related to the distance at which spatial interactions occur and thus to the scale of the microstructure of the material.

Starting from the mid-1980s, nonlocal and gradient continua have regained interest because of their potential as localisation limiters. When used to model degradation of the mechanical properties of a material, standard continuum models tend to predict a response in which the entire degradation process is concentrated in a vanishing volume. Apart from often being physically unrealistic, this localisation results in a perfectly brittle macroscopic fracture behaviour instead of the intended gradual loss of stiffness and/or strength. In numerical analyses, the volume contributing to the failure process is set by the spatial resolution of the discretisation. As a result, analyses become sensitive to the discretisation (mesh sensitivity) and converge to the nonphysical, perfectly brittle response in the limit of an infinite spatial resolution.

In reality, the microprocesses which are responsible for material damage usually extend over a band, the thickness of which is comparable to the characteristic microstructural length (e.g., the average grain size). This means that in a continuum mechanics description constitutive variables show strong variations at the scale of the microstructure. The pathological localisation of damage and deformation observed in standard continuum models is a direct consequence of the inability of these models to describe variations at the microstructural scale. This understanding has led to the use of nonlocal and gradient formulations to avoid pathological localisation. Both approaches have been successfully used to limit the localisation process to the microstructural scale. Since the influence of the microstructure becomes only noticeable upon localisation of the deformation and since this localisation results from the inelastic part of the constitutive modelling, the nonlocality or gradient terms often become active only in the inelastic domain in these models. For the elastic part, which does not generally lead to localisation, a standard, local continuum model is usually used.

Practical nonlocal models for localisation problems have first been developed by Pijaudier-Cabot and Bažant (1987) in a continuum damage setting and applied to creep problems by Saanouni et al. (1989). The concept has subsequently been translated to plasticity by, among others, Leblond et al. (1994) and Tvergaard and Needleman (1995). The development of nonlinear gradient models has taken place predominantly in plasticity (Aifantis, 1984; Coleman and Hodgdon, 1985; Lasry and Belytschko, 1988; Mühlhaus and Aifantis, 1991; de Borst and Mühlhaus, 1992) and has been transferred to damage mechanics only recently (Peerlings et al., 1995, 1996a; Frémond and Nedjar, 1996; Pijaudier-Cabot and Burlion, 1996; Comi and Driemeier, 1997; Comi, 1998; Geers et al., 1998).

It has been recognised at an early stage that both types of regularisation are closely related. In fact, gradient formulations can be derived as an approximation of nonlocal models by substituting a truncated

Taylor series for the averaged quantity (Kröner, 1967; Bažant et al., 1984). Despite this close connection, remarkable differences in behaviour have been reported between the two approaches. Indeed, even very similar gradient approaches have sometimes been found to show remarkably different responses (e.g., Pijaudier-Cabot et al., 1988; Peerlings et al., 1996b). The fact that the enhancements may have different effects in plasticity and damage complicates the comparison even further (de Borst et al., 1995).

The aim of this paper is to clarify some of the similarities and intrinsic differences of the nonlocal and gradient approaches. An elasticity-based continuum damage framework has been selected for this purpose because of the availability of reliable nonlocal and gradient continuum damage models and numerical schemes. A further advantage of taking elasticity-based damage as the framework is its conceptual simplicity, which allows for a clear focus on the respective enhancements. Although this study is limited to a damage context, it is believed that much of the understanding developed in it may also be relevant for enhanced plasticity formulations and coupled damage-plasticity models.

The models considered in this contribution are a nonlocal damage model based on that of Pijaudier-Cabot and Bažant (1987) and two different gradient damage formulations (Peerlings et al., 1995, 1996a; Peerlings, 1999). These models and the mathematical relationships between them are first introduced. Special attention is paid to the additional relations which must be provided to account for the influence of the boundary of the problem domain. The effect of each of the enhancements on the constitutive behaviour is then examined in detail by considering the propagation of loading waves, the localisation of damage and deformation and the behaviour at crack tips. Finally, the arguments gathered from these analyses are briefly discussed.

2. Constitutive modelling

The basis for our developments is formed by an isotropic, quasi-brittle damage model, in which a scalar damage variable D degrades the elastic stiffness. The classical stress–strain relation for this type of models reads (see for instance Lemaître and Chaboche, 1990):

$$\sigma_{ij} = (1 - D)C_{ijkl}\varepsilon_{kl}, \quad (1)$$

where Einstein's summation convention has been used and σ_{ij} ($i, j = 1, 2, 3$) denote the Cauchy stresses, C_{ijkl} the standard elastic constants and ε_{kl} ($k, l = 1, 2, 3$) the linear strains with respect to a stress-free reference configuration. The damage variable D satisfies $0 \leq D \leq 1$. A value of $D = 0$ represents the initial, undamaged material with the virgin stiffness; $D = 1$ represents a state of complete loss of stiffness, in which no stresses can be transferred.

The second law of thermodynamics requires that $\dot{D} \geq 0$, i.e., that the damage variable can only increase. This growth of damage is related to the development of the deformation. A scalar equivalent strain measure $\tilde{\varepsilon}$ is introduced for this purpose, which quantifies the local deformation state in the material in terms of its effect on damage. Here the von Mises equivalent strain

$$\tilde{\varepsilon} = \frac{1}{1 + v} \sqrt{-3J_2} \quad (2)$$

is used, where the second invariant of the deviatoric strain tensor, J_2 , is given by

$$I_1 = \varepsilon_{kk}, \quad J_2 = \frac{1}{6}J_1^2 - \frac{1}{2}\varepsilon_{ij}\varepsilon_{ij}. \quad (3)$$

The factor $1/(1 + v)$ in definition (2) scales the equivalent strain such that it equals the axial strain in the uniaxial tensile stress case.

In local damage models the damage growth can be related directly to the evolution of the equivalent strain $\tilde{\varepsilon}$. In the nonlocal and gradient damage formulations, however, a nonlocal equivalent strain $\bar{\varepsilon}$ enters

the relationship between deformation and damage. The way in which this nonlocal equivalent strain is connected to its local counterpart differs between the enhanced models and will be discussed below for each of them. Whether damage growth is possible is decided on the basis of a loading function in terms of $\bar{\varepsilon}$:

$$f(\bar{\varepsilon}, \kappa) = \bar{\varepsilon} - \kappa. \quad (4)$$

For $f < 0$ there can be no growth of damage and the response thus remains linear elastic. The magnitude of the loading function is governed by the Kuhn–Tucker relations

$$f\dot{\kappa} = 0, \quad f \leq 0, \quad \dot{\kappa} \geq 0 \quad (5)$$

such that always $f \leq 0$ (cf. elastoplasticity). An initial value κ_0 of κ sets the initial elastic domain.

Damage growth becomes possible for $f = 0$. During this growth, the consistency condition $\dot{f} = 0$ must be satisfied. The growth of damage is governed by the evolution equation

$$\dot{D} = \begin{cases} \frac{\kappa_0 \kappa_c}{\kappa_c - \kappa_0} \frac{\dot{\kappa}}{\kappa^2} & \text{if } \kappa < \kappa_c, \\ 0 & \text{if } \kappa \geq \kappa_c. \end{cases} \quad (6)$$

Since both κ and D increase semi-monotonically, the damage variable D can be expressed directly in terms of the history variable κ by solving the differential Eq. (6):

$$D = \begin{cases} \frac{\kappa_c}{\kappa} \frac{\kappa - \kappa_0}{\kappa_c - \kappa_0} & \text{if } \kappa < \kappa_c, \\ 1 & \text{if } \kappa \geq \kappa_c. \end{cases} \quad (7)$$

The damage evolution given by Eqs. (6) or (7) results in linear softening followed by complete loss of stiffness at $\varepsilon = \kappa_c$ in a uniaxial tensile stress situation (see Fig. 1). It should be mentioned that the softening behaviour of real materials is usually nonlinear, although the linear relation following from Eq. (7) is sometimes used as an approximation. However, the analyses in this paper are by no means limited to the linear softening case and can be generalised to more complicated relations without difficulty (Peerlings, 1999).

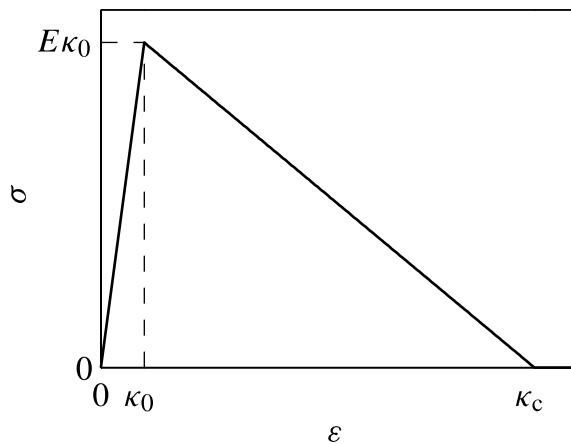


Fig. 1. Uniaxial stress–strain response following from damage growth relation (7).

2.1. Nonlocal model

In the nonlocal damage model the nonlocal equivalent strain $\bar{\varepsilon}$ in a point \mathbf{x} is defined as a weighted average of the local equivalent strain $\tilde{\varepsilon}$ in the entire problem domain Ω (cf. Pijaudier-Cabot and Bažant, 1987; Bažant and Pijaudier-Cabot, 1988):

$$\bar{\varepsilon}(\mathbf{x}) = \frac{1}{\Psi(\mathbf{x})} \int_{\Omega} \Psi(\mathbf{y}; \mathbf{x}) \tilde{\varepsilon}(\mathbf{y}) d\Omega, \quad (8)$$

where \mathbf{y} denotes the position of the infinitesimal volume $d\Omega$. The factor $1/\Psi(\mathbf{x})$, with $\Psi(\mathbf{x})$ defined by

$$\Psi(\mathbf{x}) = \int_{\Omega} \Psi(\mathbf{y}; \mathbf{x}) d\Omega, \quad (9)$$

scales $\bar{\varepsilon}$ such that it equals $\tilde{\varepsilon}$ for homogeneous strain states. The weight function $\Psi(\mathbf{y}; \mathbf{x})$ is assumed to be homogeneous and isotropic, i.e., it depends only on the distance $\rho = |\mathbf{x} - \mathbf{y}|$. It is usually defined as the Gauss distribution:

$$\psi(\rho) = \frac{1}{(2\pi)^{3/2} l^3} \exp \left[-\frac{\rho^2}{2l^2} \right]. \quad (10)$$

The factor $(2\pi)^{-3/2} l^{-3}$ in this expression normalises the weight function such that on \mathbb{R}^3

$$\int_{\mathbb{R}^3} \psi(\rho) d\Omega = 1. \quad (11)$$

The length parameter l in Eq. (10) determines the volume which contributes significantly to the nonlocal equivalent strain and must therefore be related to the scale of the microstructure. Indeed, when the microstructure of the material is known in full detail, this information can be used by applying the averaging on each microstructural element separately, cf. the cell-averaging method of Hall and Hayhurst (1991).

2.2. Explicit gradient formulation

For sufficiently smooth $\tilde{\varepsilon}$ -fields, the integral relation (8) can be rewritten in terms of gradients of $\tilde{\varepsilon}$ by expanding $\tilde{\varepsilon}(\mathbf{y})$ into a Taylor series (Bažant et al., 1984; Lasry and Belytschko, 1988; Peerlings et al., 1995, 1996a):

$$\begin{aligned} \tilde{\varepsilon}(\mathbf{y}) = \tilde{\varepsilon}(\mathbf{x}) &+ \frac{\partial \tilde{\varepsilon}}{\partial x_i} (y_i - x_i) + \frac{1}{2!} \frac{\partial^2 \tilde{\varepsilon}}{\partial x_i \partial x_j} (y_i - x_i)(y_j - x_j) + \frac{1}{3!} \frac{\partial^3 \tilde{\varepsilon}}{\partial x_i \partial x_j \partial x_k} (y_i - x_i)(y_j - x_j)(y_k - x_k) \\ &+ \frac{1}{4!} \frac{\partial^4 \tilde{\varepsilon}}{\partial x_i \partial x_j \partial x_k \partial x_l} (y_i - x_i)(y_j - x_j)(y_k - x_k)(y_l - x_l) + \dots \end{aligned} \quad (12)$$

Substitution of this relation and of Eq. (10) into Eq. (8) yields after some calculus for the problem on \mathbb{R}^3 :

$$\bar{\varepsilon}(\mathbf{x}) = \tilde{\varepsilon}(\mathbf{x}) + \bar{c}_2 \nabla^2 \tilde{\varepsilon}(\mathbf{x}) + \bar{c}_4 \nabla^4 \tilde{\varepsilon}(\mathbf{x}) + \dots \quad (13)$$

where the Laplacian ∇^n is defined by $\nabla^2 = \sum_i \partial^2 / \partial x_i^2$, $\nabla^{2n} = (\nabla^2)^n$ and the coefficients \bar{c}_2 , \bar{c}_4 are the given by $\bar{c}_2 = \frac{1}{2} l^2$ and $\bar{c}_4 = \frac{1}{8} l^4$. Odd derivative terms vanish in Eq. (13) as a result of the isotropy of the weight function. For the Gaussian weight function this is no longer true for finite domains $\Omega \subset \mathbb{R}^3$; in this case odd derivatives do not vanish and the coefficients \bar{c}_i change. However, the relevance of Eq. (13) lies not so much in its strict equivalence with Eq. (8), but in the fact that it provides the possibility to approximate the integral relation (8) by the differential relation

$$\bar{\varepsilon} = \tilde{\varepsilon} + \bar{c} \nabla^2 \tilde{\varepsilon}. \quad (14)$$

Eq. (14) is obtained by neglecting terms of order four and higher in Eq. (13). The dependence on the coordinates \mathbf{x} and the index of the second-order gradient coefficient \bar{c}_2 have been dropped for brevity. The parameter \bar{c} is of the dimension length squared, so that $(\bar{c})^{1/2}$ can be regarded as the characteristic length in the model. The Taylor expansion (12) is used here merely to establish a (well-known) link between the nonlocal and gradient models. It should be noted that convergence of Eq. (12) cannot be assured, particularly for highly localised deformations, and that this link is therefore not always rigorous (see also Huerta and Pijaudier-Cabot, 1994).

For a given deformation field, the nonlocal strain is given by Eq. (14) explicitly in terms of the local equivalent strain and its second-order derivatives. The gradient damage formulation based on this relation is therefore referred to as an explicit gradient formulation. As a result of the continuity of $\tilde{\varepsilon}$, the second-order derivative introduces a certain spatial interaction in the constitutive model. In contrast with the nonlocal model based on Eq. (8), however, the distance at which these interactions act is only infinitesimal, since variations of $\tilde{\varepsilon}(\mathbf{y})$ at a finite distance from \mathbf{x} have no effect on $\tilde{\varepsilon}(\mathbf{x})$ and $\nabla^2 \tilde{\varepsilon}(\mathbf{x})$, and thus on $\bar{\varepsilon}(\mathbf{x})$. Indeed, in a mathematical sense the second-order derivative is a local quantity and the explicit gradient model is therefore local. The truly nonlocal character can only be preserved in an explicit gradient format if the series (13) is not truncated.

The fact that damage growth depends on the second-order derivative of the equivalent strain also means that the order of the equations of motion increases. As a consequence, extra boundary conditions must be provided for the solution to be unique (see Section 3).

2.3. Implicit gradient formulation

An alternative gradient formulation can be derived from Eq. (13) by applying the Laplacian operator to it and multiplying by \bar{c} . If the result is subtracted from Eq. (13), the following relation is obtained:

$$\bar{\varepsilon} - \bar{c}_2 \nabla^2 \bar{\varepsilon} = \tilde{\varepsilon} + (\bar{c}_4 - \bar{c}_2^2) \nabla^4 \bar{\varepsilon} + \dots \quad (15)$$

Again neglecting terms of order four and higher in the right-hand side now gives a second approximation of the integral relation (8):

$$\bar{\varepsilon} - \bar{c} \nabla^2 \bar{\varepsilon} = \tilde{\varepsilon}, \quad (16)$$

where the index of \bar{c}_2 has again been dropped. In order to fix the solution of this Helmholtz equation, a boundary condition must be provided. Here we use the natural boundary condition

$$\frac{\partial \bar{\varepsilon}}{\partial n} \equiv n_i \frac{\partial \bar{\varepsilon}}{\partial x_i} = 0 \quad (17)$$

with \mathbf{n} the unit normal to Γ . With this boundary condition $\bar{\varepsilon}$ equals $\tilde{\varepsilon}$ for homogeneous deformations and the gradient approximation is thus consistent with the nonlocal relation (8) in this respect, see also the following section.

In contrast to definition (14), the nonlocal strain $\bar{\varepsilon}$ is now not given explicitly in terms of $\tilde{\varepsilon}$ and its derivatives, but in a more implicit fashion as the solution of the boundary value problem consisting of the partial differential equation (16) and boundary condition (17). The resulting gradient damage formulation will therefore be referred to as implicit. Notice that the coefficients of the higher-order terms which have been neglected in Eq. (16) are different from those in the explicit approximation. This means that an infinite series of higher-order derivatives of $\bar{\varepsilon}$ is still implicitly present in the gradient term in the left-hand side of Eq. (16). This in turn means that spatial interactions may act at a finite distance and thus that the implicit model has, in contrast to the explicit formulation, a truly nonlocal character. It will be shown in the re-

mainder that this subtle difference between the two gradient formulations has an important effect on their resulting behaviour.

The relation between the nonlocal and implicit gradient models can be further clarified by solving Eq. (16) analytically using the Green's function associated to the boundary value problem. Green's function $G(\mathbf{x}; \mathbf{y})$ is defined as the (weak) solution of the partial differential equation (16) with the source term replaced by a Dirac function $\delta(\mathbf{x} - \mathbf{y})$,

$$G(\mathbf{x}; \mathbf{y}) - \bar{c}\nabla^2 G(\mathbf{x}; \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}), \quad (18)$$

which satisfies the boundary condition (17). For the free-space problem (i.e., for $\Omega = \mathbb{R}^3$) this boundary condition is replaced by the requirement that $G(\mathbf{x}; \mathbf{y}) \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$. The corresponding free-space Green's function $G_f(\mathbf{x}; \mathbf{y})$ is given by (Zauderer, 1989):

$$G_f(\mathbf{x}; \mathbf{y}) = \frac{1}{4\pi\bar{c}\rho} \exp\left[-\frac{\rho}{\sqrt{\bar{c}}}\right], \quad (19)$$

where $\rho = |\mathbf{x} - \mathbf{y}|$. For problem domains $\Omega \subset \mathbb{R}^3$ this expression does not satisfy the boundary condition (17). Solutions of the homogeneous partial differential equation must then be added to G_f in order to obtain G .

The right-hand side of the original equation (16) is now considered as a superposition of Dirac functions:

$$\tilde{\varepsilon}(\mathbf{x}) = \int_{\Omega} \tilde{\varepsilon}(\mathbf{y})\delta(\mathbf{x} - \mathbf{y})d\Omega. \quad (20)$$

The solution of this problem is then obtained by the same superposition of the Green's functions $G(\mathbf{x}; \mathbf{y})$, which, since Green's functions for linear problems with constant coefficients are symmetric in their arguments, i.e., $G(\mathbf{x}; \mathbf{y}) = G(\mathbf{y}; \mathbf{x})$, can be rewritten as

$$\bar{\varepsilon}(\mathbf{x}) = \int_{\Omega} G(\mathbf{y}; \mathbf{x})\tilde{\varepsilon}(\mathbf{y})d\Omega. \quad (21)$$

This expression is of exactly the same form as Eq. (8) for the nonlocal model. Thus, the gradient damage model based on the differential equation (16) is nothing else than a special case of the class of nonlocal models, in which the weight function $\psi(\mathbf{y}; \mathbf{x})$ is defined as $\psi(\mathbf{y}; \mathbf{x}) = G(\mathbf{y}; \mathbf{x}) = G(\mathbf{x}; \mathbf{y})$ and $\Psi = 1$. Notice that the latter relation is always satisfied for the Green's function because of

$$\int_{\Omega} G(\mathbf{x}; \mathbf{y})d\Omega = \int_{\Omega} \delta(\mathbf{x} - \mathbf{y})d\Omega - \bar{c} \int_{\Omega} \nabla^2 G d\Omega = 1, \quad (22)$$

where the second step follows by use of the divergence theorem and Eq. (17).

For the free-space problem in three dimensions the weight function G_f associated to the implicit gradient formulation has been plotted versus ρ in Fig. 2(a). A value of $\sqrt{\bar{c}} = 1$ mm has been used for the internal length scale. The Gaussian weight function (10), with the corresponding internal length $l = \sqrt{2\bar{c}} = \sqrt{2}$ mm, is also shown for comparison. The most striking difference between the two functions is that the three-dimensional Green's function is singular at $\rho = 0$, while the Gaussian weight function remains finite. However, since the volume associated to small ρ is relatively small, the singularity of G_f has a limited effect on the value of the nonlocal equivalent strain. This is illustrated in Fig. 2(b), which shows the weight functions multiplied by the surface $4\pi\rho^2$ associated to the distance ρ . The diagram shows that the Green's function attributes more weight to the volume at a smaller distance compared to the Gauss distribution. One could therefore say that for the same internal length scale the average interaction distance is slightly smaller in the implicit gradient model than in the nonlocal model.

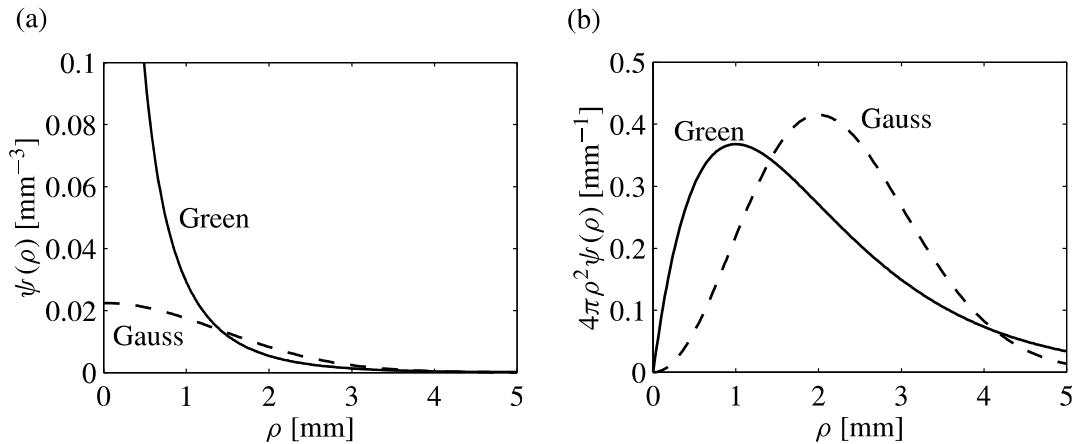


Fig. 2. Comparison of (a) the Green's function (19) and Gauss distribution (10) and (b) associated influence functions $4\pi\rho^2\psi(\rho)$ for an internal length $(\bar{c})^{1/2} = 1$ mm.

3. Boundary conditions

The need for additional boundary conditions in the gradient damage formulations has already been touched upon in the previous section. The treatment of boundaries may have an important effect on the behaviour of the models, since damage growth is often initiated at the surface of a component. The subject is therefore discussed here in detail for the two gradient formulations and for the nonlocal model.

In the explicit gradient approach, i.e., the model based on Eq. (14), stresses depend on second-order derivatives of the equivalent strain. Since these second-order derivatives of $\tilde{\varepsilon}$ are related to third-order derivatives of the displacements and since the equations of motion involve one more differentiation, fourth-order displacement derivatives enter the equations of motion. However, these fourth-order terms become active only in the process zone, i.e., in the region where damage grows. In the remaining part of the body the equations of motion are still of order 2. A similar situation thus arises as in the gradient plasticity model of de Borst and Mühlhaus (1992): additional conditions must be provided at the internal boundary between the process zone and the remaining material, or, where the process zone touches the boundary of the problem, at this external boundary. At the internal boundary these conditions can be provided by continuity requirements (cf. de Borst and Mühlhaus, 1992). At the external boundary, however, they must be explicitly defined in terms of higher-order derivatives of the displacements.

In the implicit gradient model spatial interactions enter the constitutive model by means of the partial differential equation (16) in terms of the nonlocal strain $\bar{\varepsilon}$. For a unique solution of this equation a boundary condition for $\bar{\varepsilon}$ must be given. Since Eq. (16) is valid in the entire problem domain Ω , this boundary condition must be applied at the boundary Γ of Ω instead of at the boundary of the process zone. Either the value of $\bar{\varepsilon}$, its normal derivative, or a linear combination of these quantities must be specified on Γ . Fixing $\bar{\varepsilon}$ itself seems to be difficult to motivate on physical grounds. For this reason the homogeneous natural boundary condition (17) is used here (cf. Mühlhaus and Aifantis, 1991; de Borst and Mühlhaus, 1992). With this condition the total deformation content is preserved in the nonlocal averaging, i.e.,

$$\int_{\Omega} \bar{\varepsilon} d\Omega = \int_{\Omega} \tilde{\varepsilon} d\Omega \quad (23)$$

and $\bar{\varepsilon}$ equals $\tilde{\varepsilon}$ for homogeneous deformations.

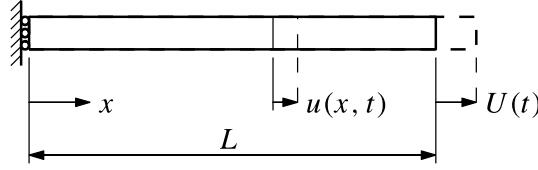


Fig. 3. One-dimensional bar problem.

In the one-dimensional situation the effect of the natural boundary condition (17) on the spatial interactions modelled by the implicit gradient formulation can be determined analytically. It has been shown in the previous section that the nonlocal strain $\bar{\epsilon}$ can be written as a weighted average of the local strain if the Green's function associated to the boundary value problem is used as weight function (see relation (21)). For the case of a prismatic bar of length L (Fig. 3) this relation can be written as

$$\bar{\epsilon}(x) = \int_0^L \tilde{\psi}(y; x) \tilde{\epsilon}(y) dy \quad (24)$$

if the weight function $\tilde{\psi}$ is defined as $\tilde{\psi}(y; x) = G(x; y)$. The Green's function $G(x; y)$ is the solution of the problem given by the differential equation

$$G - \bar{c} \frac{d^2 G}{dx^2} = \delta(x - y) \quad (25)$$

and boundary conditions $dG/dx = 0$ at $x = 0$ and at $x = L$. In order to solve this problem, the singularity is first removed by subtracting the free-space problem, i.e., by setting $G(x; y) = G_f(x; y) + g(x; y)$, with $G_f(x; y)$ the free-space Green's function, which reads for the one-dimensional case (Zauderer, 1989)

$$G_f(x; y) = \frac{1}{2\sqrt{\bar{c}}} \exp \left[-\frac{|x - y|}{\sqrt{\bar{c}}} \right]. \quad (26)$$

The function $g(x; y)$ must then satisfy the homogeneous differential equation

$$g - \bar{c} \frac{d^2 g}{dx^2} = 0 \quad (27)$$

and boundary conditions

$$\begin{aligned} \frac{dg}{dx} \bigg|_{x=0} &= - \frac{dG_f}{dx} \bigg|_{x=0} = -\frac{1}{2\bar{c}} \exp \left[-\frac{y}{\sqrt{\bar{c}}} \right], \\ \frac{dg}{dx} \bigg|_{x=L} &= - \frac{dG_f}{dx} \bigg|_{x=L} = \frac{1}{2\bar{c}} \exp \left[-\frac{L-y}{\sqrt{\bar{c}}} \right]. \end{aligned} \quad (28)$$

It can easily be verified that the solution of this problem reads

$$g(x, y) = \frac{A(y)}{2\sqrt{\bar{c}}} \exp \left[\frac{x}{\sqrt{\bar{c}}} \right] + \frac{B(y)}{2\sqrt{\bar{c}}} \exp \left[\frac{L-x}{\sqrt{\bar{c}}} \right] \quad (29)$$

with

$$A(y) = \frac{\exp[\frac{y}{\sqrt{c}}] + \exp[-\frac{y}{\sqrt{c}}]}{\exp\left[\frac{2L}{\sqrt{c}}\right] - 1}, \quad B(y) = \frac{\exp[\frac{L-y}{\sqrt{c}}] + \exp[-\frac{L-y}{\sqrt{c}}]}{\exp\left[\frac{2L}{\sqrt{c}}\right] - 1}. \quad (30)$$

Combination of Eqs. (26) and (29) yields Green's function for the finite bar as

$$G(x; y) = \frac{1}{2\sqrt{c}} \exp\left[-\frac{|x-y|}{\sqrt{c}}\right] + A(y) \exp\left[\frac{x}{\sqrt{c}}\right] + B(y) \exp\left[\frac{L-x}{\sqrt{c}}\right]. \quad (31)$$

The function $\tilde{\psi}(y; x) = G(x; y)$ has been plotted in Fig. 4(a) at several positions x along the length of the bar for an internal length $\sqrt{c} = 1$ mm. The length of the bar has been set to $L = 100$ mm, but only the first 10 mm have been plotted. Note that, in contrast with the two- and three-dimensional cases, the Green's function does not contain a singularity. The diagram clearly shows that the weight function associated to the implicit gradient model becomes increasingly nonsymmetric when x approaches the boundary $x = 0$ in order to satisfy the natural boundary condition. As a result, material points close to the boundary have a greater influence on the nonlocal strain than points at the same distance, but in the opposite direction. This increased influence of the material at the surface can be further manipulated by imposing an inhomogeneous Neumann boundary condition. It corresponds qualitatively to the strong influence of surface effects on the development of damage and cracks. However, a rigorous, quantitative connection between the mathematical boundary condition and the underlying physics is not yet available.

In the nonlocal model, the normalisation of $\bar{\varepsilon}$ by Ψ ensures that $\bar{\varepsilon}$ does not become unrealistically small when part of the support of the weight function lies outside the problem domain. This normalisation can therefore be regarded as the nonlocal counterpart of the additional boundary conditions in the gradient models. In the one-dimensional case the nonlocal strain can be written in the format (24) by setting

$$\bar{\psi}(y; x) = \frac{\psi(y; x)}{\Psi(x)}, \quad (32)$$

where

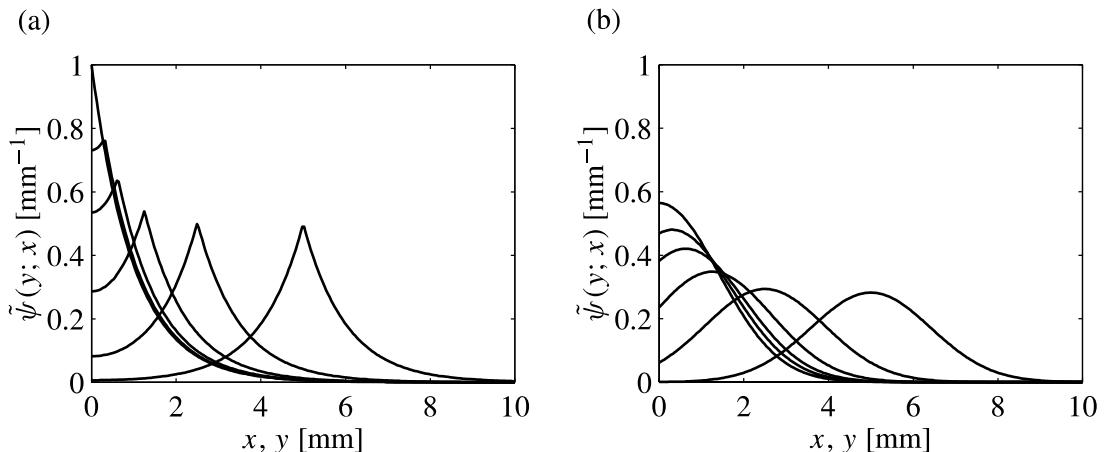


Fig. 4. Effective weight functions $\tilde{\psi}$ near the left end of the bar for an internal length $(\bar{c})^{1/2} = 1$ mm: (a) Green's function (implicit gradient model) and (b) Gauss distribution (nonlocal model).

$$\Psi(x) = \int_0^L \psi(y; x) dy. \quad (33)$$

For the one-dimensional Gauss distribution

$$\psi(y; x) = \frac{1}{\sqrt{2\pi}l} \exp \left[-\frac{(y-x)^2}{2l^2} \right] \quad (34)$$

the normalisation factor Ψ satisfies

$$\Psi(x) = \frac{1}{2} \left(\text{err} \left[\frac{x}{\sqrt{2}l} \right] + \text{err} \left[\frac{L-x}{\sqrt{2}l} \right] \right) \quad (35)$$

with $\text{err}[x]$ the error function, defined by

$$\text{err}[x] = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt. \quad (36)$$

The effective weight function $\tilde{\psi}$ then reads

$$\tilde{\psi}(y; x) = \frac{\sqrt{2}}{\sqrt{\pi}l} \frac{\exp \left[-\frac{(y-x)^2}{2l^2} \right]}{\text{err} \left[\frac{x}{\sqrt{2}l} \right] + \text{err} \left[\frac{L-x}{\sqrt{2}l} \right]}. \quad (37)$$

The development of this weight function as x approaches the boundary at $x = 0$ is shown in Fig. 4(b). The internal length parameter has been set to $l = \sqrt{2}$ mm; this value corresponds to the value of the gradient parameter used for the implicit gradient model. Closer to the boundary the amplitude of the weight function becomes larger to compensate for the part of its support which falls outside the problem domain. In contrast with the implicit gradient model, however, the presence of a boundary does not affect the symmetry of the effective weighting and the influence of the boundary is thus less pronounced.

In more general, two- or three-dimensional cases the spatial interactions modelled by the standard nonlocal approach may become questionable for strongly concave geometries. Consider for instance the sharp notch of Fig. 5. In the standard nonlocal model the influence of the strain in a point \mathbf{y} across the notch has the same effect on the nonlocal strain in \mathbf{x} as the strain in a point \mathbf{y}' at the same distance, but on

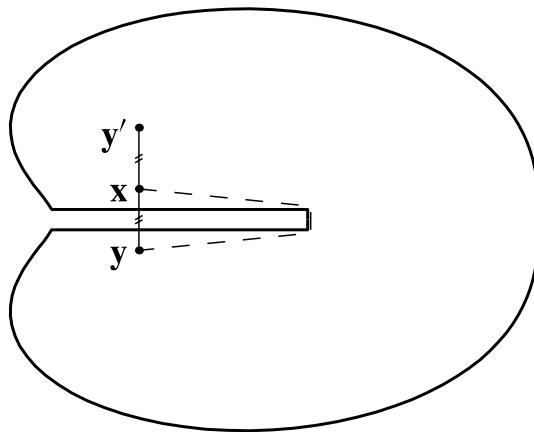


Fig. 5. Nonlocality at a sharp notch.

the same side of the notch. This example may seem academic, since the domain of influence around \mathbf{x} , which is related to the intrinsic length scale l , will often be small compared with the width of the notch. However, the same situation arises at cracks, which have a thickness which is of the same order as l or even smaller. The problem could be avoided by reformulating the weight function in Eq. (8) in terms of the smallest distance within the domain Ω , i.e., by considering the shortest path along which the two points can physically interact (see the dashed line in Fig. 5). However, this modification is difficult to implement in a numerical algorithm. Notice that direct interactions across a notch or crack are impossible in the gradient models because the differential equations in which the gradient terms appear are cut off at the boundary, either a priori for pre-existing cracks or by the introduction of an internal boundary if the crack is the result of damage growth, see Peerlings (1999) and Peerlings et al. (2001).

4. Wave propagation

Wave propagation in nonlocal and gradient models is usually dispersive. In fact, the need to describe the dispersive behaviour of waves at small wavelengths has been an important motive for the development of the first generation of enhanced continua (Mindlin, 1964; Eringen and Edelen, 1972). Predictions by these models of the dispersive propagation of elastic waves in crystalline materials as the wavelength approaches the lattice spacing are consistent with experimental observations. In the enhanced models which are discussed here, the nonlocality or gradient terms do not come into play in the elastic regime. As a result, the elastic behaviour is nondispersive and scale effects in the elastic regime cannot be modelled. However, if it is accompanied by damage growth, the propagation of waves is affected by the nonlocal and gradient terms and the wave velocity will thus become dispersive.

The dispersive character of wave propagation plays an important role in preventing pathological localisation of damage in dynamic problems. In conventional continua, the governing partial differential equations may lose hyperbolicity at a certain stage of the damage process. This means that loading waves can no longer propagate and the deformation is trapped in an infinitely narrow band in which the strain can grow unboundedly (Read and Hegemier, 1984; Bažant and Belytschko, 1985). The hyperbolicity of the initial-boundary value problem is lost when the acoustic tensor becomes singular in some direction (Hill, 1962; Pijaudier-Cabot and Benallal, 1993). Enhanced continuum descriptions ensure that hyperbolicity of the problem is preserved and waves can also be propagated in a softening zone. Instead of localising in a vanishing volume, the deformation is concentrated in a finite band, the width of which is related to the length parameter of the model (Sluys, 1992; Sluys and de Borst, 1994; Peerlings et al., 1996b).

The effect of the respective enhancements on wave propagation is demonstrated here for the one-dimensional bar problem of Fig. 3. The axial strain ε in the bar is assumed to be positive at all times; the equivalent strain $\tilde{\varepsilon}$ can then be set equal to ε . The relevant equation of motion reads

$$\frac{\partial \sigma}{\partial x} = \rho \frac{\partial^2 u}{\partial t^2} \quad (38)$$

with ρ the density of the material, σ the axial stress in the bar and u the axial displacement. The one-dimensional stress-strain relation

$$\sigma = (1 - D)E\varepsilon \quad (39)$$

(cf. Eq. (1)) renders Eq. (38) nonlinear in terms of the deformation. However, the problem can be linearised by considering the associated rate problem

$$\frac{\partial \dot{\sigma}}{\partial x} = \rho \frac{\partial^2 v}{\partial t^2} \quad (40)$$

with $v(x, t)$ the axial velocity in the bar, and assuming damage growth everywhere in the bar. Notice that this linearisation is equivalent with the classical assumption of a linear comparison solid (Hill, 1958; Lasry and Belytschko, 1988; Huerta and Pijaudier-Cabot, 1994).

For the local damage model, i.e., for $\bar{\varepsilon} = \varepsilon$, differentiation of Eq. (39) with respect to time and using the consistency condition $f = 0$ gives the stress rate as

$$\dot{\sigma} = \bar{E}\dot{\varepsilon}, \quad (41)$$

where the tangential stiffness \bar{E} is defined as

$$\bar{E}(D, \varepsilon) = (1 - D)E - \frac{\partial D}{\partial \kappa}E\varepsilon. \quad (42)$$

Substitution of Eq. (41) and the kinematical relation $\dot{\varepsilon} = \partial v / \partial x$ into Eq. (40) results in a linear partial differential equation in terms of v :

$$\bar{E}(D, \varepsilon) \frac{\partial^2 v}{\partial x^2} + \frac{\partial \bar{E}}{\partial x} \frac{\partial v}{\partial x} = \rho \frac{\partial^2 v}{\partial t^2}. \quad (43)$$

If a reference solution with homogeneous strain ε_0 and damage D_0 is now assumed, the second left-hand side term in Eq. (43) vanishes and the coefficient of the second derivative of v is constant:

$$\bar{E}(D_0, \varepsilon_0) \frac{\partial^2 v}{\partial x^2} = \rho \frac{\partial^2 v}{\partial t^2}. \quad (44)$$

A solution of this equation is the single harmonic wave

$$v(x, t) = \hat{v}e^{ik(x-ct)} \quad (45)$$

with wave number k and corresponding velocity c . Substitution of Eq. (45) into Eq. (44) shows that solutions of the form (45) must satisfy the dispersion relation

$$k^2(\rho c^2 - \bar{E}(D_0, \varepsilon_0)) = 0, \quad (46)$$

which, apart from the trivial solution $k = 0$, yields a phase velocity

$$c = \sqrt{\frac{\bar{E}(D_0, \varepsilon_0)}{\rho}} = c_e \sqrt{1 - D_0 - \varepsilon_0 \frac{\partial D}{\partial \kappa}} \quad (47)$$

with c_e the elastic wave velocity $c_e = \sqrt{E/\rho}$. As long as the tangential stiffness \bar{E} is positive the wave velocity c according to Eq. (47) is real. But when the reference state ε_0, D_0 is such that $\bar{E} < 0$, i.e., in case of strain softening, the wave velocity is imaginary for all wave numbers k , so that loading waves cannot propagate. Substitution of Eq. (47) into Eq. (45) shows that the velocity amplitude then increases unboundedly.

In the nonlocal and gradient models the rate equation of motion (40) reduces for the homogeneous situation to

$$(1 - D_0)E \frac{\partial^2 v}{\partial x^2} - E\varepsilon_0 \frac{\partial D}{\partial \kappa} \frac{\partial \dot{\varepsilon}}{\partial x} = \rho \frac{\partial^2 v}{\partial t^2}, \quad (48)$$

where use has been made of the fact that the nonlocal strain $\bar{\varepsilon}_0$ equals ε_0 . For the explicit gradient model the nonlocal strain rate $\dot{\varepsilon}$ can be written in terms of the velocity by differentiation of the one-dimensional equivalent of Eq. (14) with respect to time and substitution of $\dot{\varepsilon} = \dot{\varepsilon} = \partial v / \partial x$:

$$\dot{\varepsilon} = \frac{\partial v}{\partial x} + \bar{c} \frac{\partial^3 v}{\partial x^3}. \quad (49)$$

Using this relation, Eq. (48) can be rewritten as the fourth-order partial differential equation

$$\bar{E}(D_0, \varepsilon_0) \frac{\partial^2 v}{\partial x^2} - \bar{c} E \varepsilon_0 \frac{\partial D}{\partial \kappa} \frac{\partial^4 v}{\partial x^4} = \rho \frac{\partial^2 v}{\partial t^2}, \quad (50)$$

where \bar{E} denotes the tangential stiffness of the local model as defined by Eq. (42). Substitution of Eq. (45) results in the dispersion relation

$$k^2 \left(\rho c^2 - \bar{E}(D_0, \varepsilon_0) - k^2 \bar{c} E \varepsilon_0 \frac{\partial D}{\partial k} \right) = 0 \quad (51)$$

and a nontrivial wave velocity equal to

$$c = \sqrt{\frac{\bar{E}(D_0, \varepsilon_0) + k^2 \bar{c} E \varepsilon_0 \frac{\partial D}{\partial k}}{\rho}} = c_c \sqrt{1 - D_0 - \varepsilon_0 \frac{\partial D}{\partial \kappa} (1 - k^2 \bar{c})}. \quad (52)$$

This wave velocity depends on the wave number k and is therefore dispersive. Since the term $k^2 \bar{c} E \varepsilon_0$ is always positive, c does not become imaginary when the tangential stiffness changes sign. However, at a certain level of damage the velocity of waves with a small wave number may still be imaginary. The critical wave number above which the wave velocity is real is given by

$$k_c = \sqrt{\frac{1}{\bar{c}} \left(1 - \frac{1 - D_0}{\varepsilon_0 \frac{\partial D}{\partial \kappa}} \right)}. \quad (53)$$

For wave numbers $k < k_c$ the perturbation of the linearised system is still unbounded. In a ‘real’ softening solid however, damage can only be progressive in a zone of width π/k_c , while it remains constant in the surrounding material. The large wavelengths associated to wave numbers smaller than k_c cannot exist in such a softening zone, so that the response remains bounded (Lasry and Belytschko, 1988; Sluys and de Borst, 1994).

In the implicit gradient formulation the nonlocal strain is defined by Eq. (16). Differentiation of this relation with respect to time gives for the one-dimensional case

$$\dot{\hat{\varepsilon}} - \bar{c} \frac{\partial^2 \dot{\hat{\varepsilon}}}{\partial x^2} = \frac{\partial v}{\partial x}. \quad (54)$$

Substitution of Eq. (45) and

$$\dot{\hat{\varepsilon}}(x, t) = \hat{\varepsilon} e^{ik(x-ct)} \quad (55)$$

into relations (48) and (54) gives the set of equations

$$k^2 (\rho c^2 - (1 - D_0) E) \hat{v} - ik E \varepsilon_0 \frac{\partial D}{\partial \kappa} \hat{\varepsilon} = 0, \quad (56)$$

$$-ik \hat{v} + (1 + k^2 \bar{c}) \hat{\varepsilon} = 0. \quad (57)$$

For a nontrivial solution the coefficient determinant of these equations must be equal to zero, i.e.,

$$k^2 \left((\rho c^2 - (1 - D_0) E)(1 + k^2 \bar{c}) + E \varepsilon_0 \frac{\partial D}{\partial \kappa} \right) = 0, \quad (58)$$

which gives the nontrivial wave velocity

$$c = c_c \sqrt{1 - D_0 - \frac{\varepsilon_0 \frac{\partial D}{\partial \kappa}}{1 + k^2 \bar{c}}}. \quad (59)$$

This wave velocity is real for wave numbers $k \geq k_c$ with

$$k_c = \sqrt{\frac{1}{c} \left(\frac{\varepsilon_0 \frac{\partial D}{\partial \kappa}}{1 - D_0} - 1 \right)}. \quad (60)$$

For the nonlocal model a similar analysis can be carried out if it is assumed that the bar has an infinite length (Pijaudier-Cabot and Benallal, 1993; Huerta and Pijaudier-Cabot, 1994). If it is furthermore assumed that the weight function ψ has been normalised such that the scaling factor $\Psi = 1$, the nonlocal strain rate can be written as (cf. Eq. (8))

$$\dot{\varepsilon}(x) = \int_{-\infty}^{\infty} \psi(|y - x|) \frac{\partial v}{\partial x} dy. \quad (61)$$

Substitution of relations (61) and (45) into Eq. (48) results in

$$k^2((1 - D_0)E - \frac{\partial D}{\partial \kappa}E\varepsilon_0\hat{\Psi}(k) - \rho c^2)\hat{v}e^{ikx} = 0 \quad (62)$$

with $\hat{\Psi}(k)$ the Fourier transform of the weight function ψ . Nontrivial solutions of this equation satisfy

$$c = c_e \sqrt{1 - D_0 - \varepsilon_0 \frac{\partial D}{\partial \kappa} \hat{\Psi}(k)}. \quad (63)$$

It can be verified that the scaling factor Ψ is indeed equal to one for the Gauss distribution (34) on the domain $(-\infty, \infty)$. Its Fourier transform reads

$$\hat{\Psi}(k) = \exp \left[\frac{1}{2} k^2 l^2 \right], \quad (64)$$

so that for the Gaussian weight function equation (63) can be rewritten as

$$c = c_e \sqrt{1 - D_0 - \varepsilon_0 \frac{\partial D}{\partial \kappa} \exp \left[\frac{1}{2} k^2 l^2 \right]}. \quad (65)$$

This velocity is real for wave numbers larger than the critical wave number

$$k_c = \frac{1}{l} \sqrt{2 \ln \left(\frac{1 - D_0}{\varepsilon_0 \frac{\partial D}{\partial \kappa}} \right)}. \quad (66)$$

The wave velocities according to Eqs. (52), (59) and (65) have been plotted in Fig. 6 at the initiation of damage ($\varepsilon_0 = \kappa_0$). Young's modulus has been set to $E = 20,000$ MPa and the density has been chosen such that a value of $c_e = 1000$ m/s is obtained for the elastic wave velocity. The damage model parameters have been set to $\kappa_0 = 0.0001$ and $\kappa_c = 0.0125$, while a value of $\sqrt{c} = 1$ mm has been used for the internal length scale. In the nonlocal model the corresponding value $l = \sqrt{2}$ mm of the length parameter has been used. For small wave numbers, the three regularisation methods have almost identical propagation properties. Below the critical wave number k_c , which at the peak stress is virtually equal for all three models, the wave speed is imaginary. For higher wave numbers, the approximations which are made in deriving the gradient models from the nonlocal formulation become apparent. The difference between the curves is larger for larger wave numbers because the Taylor approximation becomes increasingly inaccurate for the strong variations associated to large wave numbers. A striking discrepancy is observed between the two gradient models. While the implicit formulation (16) and the nonlocal model exhibit a horizontal asymptote equal to the elastic wave speed $c_e = 1000$ m/s, the formulation based on the explicit relation (14) is not bounded. As a consequence, waves with an infinitely short wavelength can propagate with an infinite speed in the explicit model, which is questionable from a physical point of view.

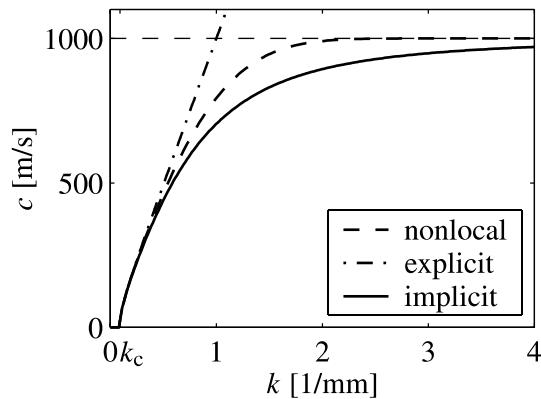


Fig. 6. Wave velocities in the nonlocal and gradient models.

The dispersion diagram depends on the strain level ε_0 for the damage models. Since damage evolution can be regarded as a stiffness degrading mechanism, wave propagation becomes slower for a higher damage level. Indeed, for the nonlocal and the implicit gradient model the wave velocity is bounded by the elastic wave speed in the damaged material, given by $c_e(1 - D_0)^{1/2}$. At the same time the critical wave number, below which the phase velocity is imaginary and waves cannot propagate, increases for an increasing damage level. Thus, the critical wavelength, which sets the width of the localisation band (Sluys, 1992; Sluys and de Borst, 1994), decreases during the material degradation process. This observation is consistent with the narrowing of the damage evolution zone in a static analysis (Peerlings et al., 1995, 1996a, see also the next section). Fig. 7 shows the critical wavelength $\lambda_c = 2\pi/k_c$, with k_c according to Eqs. (53), (60) and (66), as a function of the uniform strain ε_0 for all three localisation limiters. For relatively small strains the deviations between the curves are negligible, but at higher strain levels considerable differences are observed. These must be attributed to the contribution of higher-order terms in the nonlocal model, which have been at least partly neglected in constructing the gradient formulations. The nonlocal and the implicit gradient damage models predict a narrowing of the damage zone, until its width becomes zero at $D_0 = 1$. In contrast, the explicit gradient formulation results in a finite width of the damage process zone, equal to $(\pi/2)\sqrt{2}l$, also for complete loss of coherence.

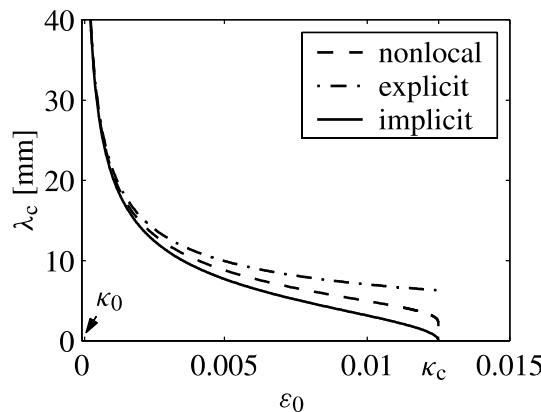


Fig. 7. Critical wavelength of inhomogeneous response versus reference strain level for the nonlocal and gradient models.

5. Localisation behaviour in statics

Pathological localisation of deformation due to softening is observed not only in dynamics, but also in quasi-static problems. Indeed, the phenomena which are responsible for localisation and the conditions under which it may occur are very similar for the two situations. In quasi-static analyses, softening may lead to loss of ellipticity of the rate equilibrium problem. This means that real characteristics appear in the partial differential system, across which the displacement solution may become discontinuous (Hill, 1962; Rice, 1976; Ottosen and Runesson, 1991; Peerlings, 1999; Peerlings et al., 2001). The condition for loss of ellipticity in the local continuum under quasi-static loading coincides with that for loss of hyperbolicity of the dynamic problem, i.e., singularity of the acoustic tensor.

In the one-dimensional case of Fig. 3 the localisation condition reduces to $\bar{E} = 0$. When this condition is met simultaneously in the entire bar, the problem becomes ill-posed in the sense that it is undefined in which parts of the bar the damage process continues and where it stops. This indefiniteness no longer exists if it is assumed that the deformation in the bar is slightly inhomogeneous, for instance as a result of small variations in the thickness of the bar. The limit point $\bar{E} = 0$ is then first reached in only one cross-section of the bar, say at $x = x_c$. Since the peak in the stress–strain response has not yet been reached in the remainder of the bar, each cross-section $x \neq x_c$ must unload. This means that the deformation and the damage growth localise in the critical cross-section $x = x_c$. Since the volume involved in the damage development thus vanishes, no work is dissipated in the remainder of the damage process, even if the specific energy dissipation is positive. The energy which is released as a result of the elastic unloading of the rest of the bar therefore cannot be dissipated and the static response becomes unstable.

In the nonlocal and gradient models the spatial interactions prohibit the localisation of deformation and damage in a vanishing volume, so that the softening response remains stable. Analytical solutions are difficult to obtain for these models, even in the one-dimensional case. A semi-analytical solution has been derived by Peerlings et al. (1996a) for the damage equivalent of perfect plasticity, i.e., a damage growth law which results in a constant stress level. For the linear softening law (7) the one-dimensional nonlinear bar problem (Fig. 3) has been solved numerically using the nonlocal model and the implicit gradient model (Peerlings et al., 1996a,b). The stronger continuity requirements of the explicit gradient model render this model more difficult to implement in a finite element code; numerical solutions for this model have been obtained by Askes et al. (2000) using an element-free Galerkin approach. The same parameter set has been used here as in the analyses of boundary conditions and wave propagation, but the cross-section has been reduced by 10% in the centre of the bar in order to trigger a localised response.

Fig. 8 shows the development of the strain and damage along the bar for the two enhanced models. Notice that the damage process affects a finite band in both models. The width of this band depends on the length scale parameter (Peerlings et al., 1996a). For relatively small deformations, the strain distributions of the nonlocal and the gradient-dependent model match almost perfectly. At a certain stage the deformation and damage growth start to localise in an ever smaller region. For the gradient model this localisation is slightly stronger than for the nonlocal model. This trend is consistent with the wave propagation analysis, which predicts a decreasing wavelength for increasing deformation and a smaller wavelength for the implicit gradient formulation than for the nonlocal model. The latter is also consistent with the fact that the implicit gradient model has a smaller average interaction distance than the nonlocal model (cf. Fig. 2(b)).

The stress in the bar has been plotted versus the displacement of its right end, U , in Fig. 9 for the nonlocal and implicit gradient models. Both enhanced formulations predict a finite energy dissipation instead of the perfectly brittle response of the local model. Although the linear softening law has been used, the softening branches of the load–displacement curves are nonlinear as a result of the progressive localisation of deformation. The strongly localised deformations at the end of the process result in snap-back behaviour. The responses of the two models agree quite well in a qualitative sense. The predicted tensile strengths are practically equal, but the gradient-enhanced formulation exhibits a somewhat more brittle

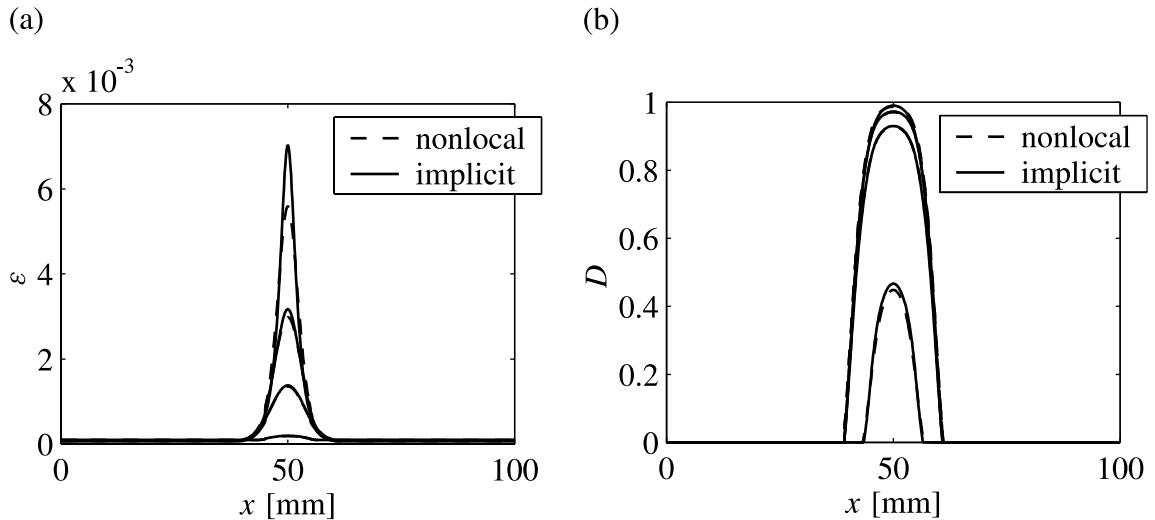


Fig. 8. Comparison of the development of (a) strain and (b) damage in the nonlocal and implicit gradient formulations.

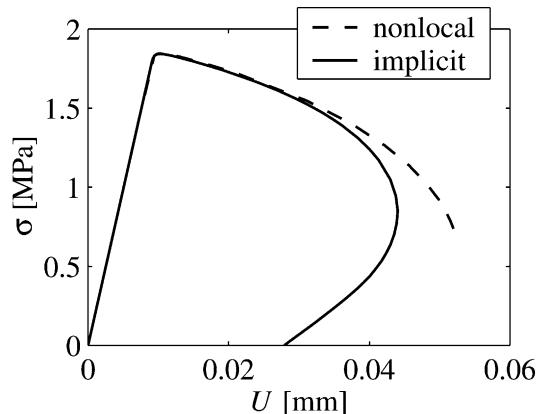


Fig. 9. Comparison of the stress–displacement responses of the nonlocal and implicit gradient formulations.

post-peak behaviour than the nonlocal model as a result of the slightly more localised damage growth (Fig. 8).

6. Crack tip fields

An important application of continuum damage models consists of modelling fracture processes by the so-called local approach to fracture (e.g., Lemaître, 1986; Chaboche, 1988a,b). In this approach, a crack is represented by a region of the problem domain in which the damage variable has become critical ($D = 1$) and the stiffness has thus vanished. The deformation and damage growth are concentrated in a relatively small region in front of the tip of the crack. The crack grows (i.e., the contour of the completely damaged zone changes) when the damage variable becomes critical in this process zone. Thus, crack growth is

governed by the constitutive behaviour of the material instead of separate fracture criteria. The fact that the fracture process is governed by the coupled effect of deformation and damage means that it is essential that the deformation and damage processes at the crack tip are described realistically and in a mathematically consistent way. Standard, local damage models are often found to fail in this respect. In particular, the local damage model of Section 2 theoretically results in crack growth at an infinite growth rate and without any energy consumption (Peerlings, 1999; Peerlings et al., 2001). In numerical analyses the growth rate and energy consumption remain finite, but depend on the spatial discretisation of the problem. For increasingly finer discretisation grids the numerical results converge to the nonphysical, perfectly brittle behaviour. This apparent mesh sensitivity is encountered not only in elasticity-based damage, but also in other damage and softening plasticity formulations (e.g., Saanouni et al., 1989; Liu et al., 1994; Needleman and Tvergaard, 1998).

The nonphysical crack growth predictions of standard continuum models are related to – but are not a direct consequence of – the emergence of discontinuous solutions and the associated localisation of damage growth. The key problem is that the local model predicts instantaneous failure of the material when the strain becomes singular. Here the strain singularity may be the result of loss of ellipticity, but it may also follow from the geometry of the component. In either case the singularity of the strain means that the softening curve of Fig. 1 is traversed instantaneously and therefore that the damage variable instantaneously reaches its critical value $D = 1$. This in turn means that all stiffness is locally lost and a crack is created. Since the material adjacent to the crack must unload elastically in order to follow the resulting stress drop, the width of the crack remains zero. This implies that the strain at the crack tip remains singular as the crack grows and consequently that the crack grows at an infinite rate, since each new critical point in front of the momentary crack tip fails immediately. No work is needed in this instantaneous fracture process, since it involves damage growth in a vanishing volume. Finite element solutions are limited by their spatial resolution in capturing the singularity at the crack tip. As a result, the crack tip strain is finite in the numerical analyses, but approaches infinity as the spatial discretisation is refined.

The above reasoning shows that solely avoiding loss of ellipticity is not necessarily sufficient to obtain mesh objective and physically realistic fracture analyses. Even if discontinuous solutions are avoided, the development of a crack by stable damage growth may still introduce a singularity in the problem. In order to avoid the perfectly brittle response of the local damage model, the damage variable then should not immediately become critical, so that the softening process is not completed instantaneously. This is achieved if the field variable which governs the damage growth remains finite even at a crack tip. In the enhanced damage formulations discussed here, damage growth depends on the nonlocal equivalent strain $\bar{\varepsilon}$. It is therefore important to examine the behaviour of this nonlocal quantity in the three enhanced models.

Closed form solutions are difficult to obtain for the (highly nonlinear) fully coupled crack problem, i.e., where the crack growth follows from the growth of damage. We will therefore limit ourselves to a crack in an infinite, linearly elastic medium. One should realise that this situation is not necessarily representative for crack growth in a damaging material, since the development of damage in front of the crack may have an important effect on the strain singularity at the crack tip (see e.g., Liu and Murakami, 1998). The present analysis, which assumes the $r^{-1/2}$ singularity predicted by linear fracture mechanics, can therefore only give an indication of the real crack growth behaviour. It is also relevant for situations where a singularity is a priori present as a consequence of the problem geometry, e.g., at sharp notches. The conventional, local damage theory then predicts immediate, complete fracture for each positive loading level. In order to avoid this nonphysical behaviour, $\bar{\varepsilon}$ must also remain finite for such geometrical singularities.

A two-dimensional, plane stress configuration is considered here (see Fig. 10). Cartesian coordinates x_1 , x_2 and polar coordinates r , ϑ will be used as convenient; the origin of both coordinate systems coincides with the crack tip. The crack is assumed to be loaded in mode I. Using the asymptotic strains at the crack tip given by linear elastic fracture mechanics (e.g., Kanninen and Popelar, 1985), the von Mises equivalent strain (2) can be elaborated

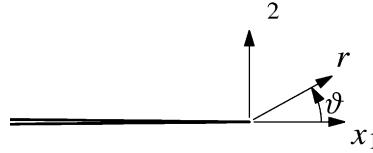


Fig. 10. Linear elastic crack problem.

$$\tilde{\varepsilon} = \frac{K_I}{2E\sqrt{2\pi r}} \sqrt{(1 - \cos \vartheta)(5 - 3 \cos \vartheta)} \quad (67)$$

with K_I the stress intensity factor. For the nonlocal damage model, the nonlocal equivalent strain at the crack tip, $\bar{\varepsilon}(\mathbf{0})$, is given by

$$\bar{\varepsilon}(\mathbf{0}) = \int_{\Omega} \psi(r) \tilde{\varepsilon}(r, \vartheta) d\Omega, \quad (68)$$

where the integration domain Ω is defined as $\Omega = \{\mathbf{x} \in \mathbb{R}^2 | r > 0, -\pi < \vartheta < \pi\}$ and it has been assumed that $\Psi = 1$. Substitution of the normalised Gaussian weight function in \mathbb{R}^2 ,

$$\psi(\rho) = \frac{1}{2\pi l^2} \exp\left[-\frac{\rho^2}{2l^2}\right] \quad (69)$$

and the equivalent strain according to Eq. (67) into relation (68) results in

$$\bar{\varepsilon}(\mathbf{0}) = \frac{K_I}{4\pi\sqrt{2\pi El^2}} \int_0^{\infty} \sqrt{r} \exp\left[-\frac{r^2}{2l^2}\right] dr \int_{-\pi}^{\pi} \sqrt{(1 - \cos \vartheta)(5 - 3 \cos \vartheta)} d\vartheta. \quad (70)$$

The first integral in this expression can be rewritten as

$$\int_0^{\infty} \sqrt{r} \exp\left[-\frac{r^2}{2l^2}\right] dr = \frac{l^{3/2}}{\sqrt[4]{2}} \Gamma\left(\frac{3}{4}\right), \quad (71)$$

where $\Gamma(\alpha)$ denotes the gamma function

$$\Gamma(\alpha) = \int_0^{\infty} e^{-t} t^{\alpha-1} dt. \quad (72)$$

The second integral in Eq. (70) yields after some manipulation

$$\int_{-\pi}^{\pi} \sqrt{(1 - \cos \vartheta)(5 - 3 \cos \vartheta)} d\vartheta = 8 + \frac{4}{\sqrt{3}} \operatorname{arctanh}\left(\frac{1}{2}\sqrt{3}\right). \quad (73)$$

Substitution of these two results into Eq. (70) finally results in

$$\bar{\varepsilon}(\mathbf{0}) = \frac{\sqrt[4]{2} K_I \Gamma(\frac{3}{4})}{\pi^{3/2} E \sqrt{l}} \left(1 + \frac{1}{2\sqrt{3}} \operatorname{arctanh}\left(\frac{1}{2}\sqrt{3}\right)\right). \quad (74)$$

This expression is indeed finite for $l > 0$, so that the damage variable at the crack tip does not immediately become critical in the nonlocal model.

For the implicit gradient formulation, the partial differential equation (16) must be solved to obtain $\bar{\varepsilon}$. Because of the symmetry of the problem with respect to the x_1 -axis, the equation need only be solved for the half-plane $\Omega^+ : x_2 > 0$. Assuming $\bar{\varepsilon}$ to be differentiable, a Neumann boundary condition $\partial \bar{\varepsilon} / \partial x_2 = 0$ is imposed at $x_2 = 0$. For $x_1 \leq 0$ this condition represents the free boundary of the crack surface and for $x_1 > 0$ it

follows from the symmetry of the problem. The boundary value problem is solved using Green's function. The free-space Green's function for Eq. (16) in \mathbb{R}^2 reads (Zauderer, 1989):

$$G_f(\mathbf{x}; \mathbf{y}) = \frac{1}{2\pi\bar{c}} K_0\left(\frac{\rho}{\sqrt{\bar{c}}}\right) \quad (75)$$

with $\rho = |\mathbf{x} - \mathbf{y}|$ and $K_0(z)$ the modified zero-order Bessel function of the second kind. It can easily be verified that Green's function for the half-space problem with the homogeneous Neumann boundary condition is then given by

$$G(\mathbf{x}; \mathbf{y}) = G_f(\mathbf{x}; \mathbf{y}) + G_f(\mathbf{x}; \mathbf{y}') \quad (76)$$

with $\mathbf{x}, \mathbf{y} \in \Omega^+$ and $\mathbf{y}' = [y_1, -y_2]^T$ the mirror point of \mathbf{y} in the line $x_2 = 0$. The solution of the half-space problem can now be written as

$$\bar{\varepsilon}(\mathbf{x}) = \int_{\Omega^+} \tilde{\varepsilon}(\mathbf{y}) G(\mathbf{x}; \mathbf{y}) d\Omega, \quad (77)$$

or, using Eq. (76) and the symmetry $\tilde{\varepsilon}(\mathbf{y}') = \tilde{\varepsilon}(\mathbf{y})$ of the equivalent strain, as

$$\bar{\varepsilon}(\mathbf{x}) = \int_{\Omega} \tilde{\varepsilon}(\mathbf{y}) G_f(\mathbf{x}; \mathbf{y}) d\Omega. \quad (78)$$

In the limit $r \rightarrow 0$ the nonlocal strain approaches

$$\bar{\varepsilon}(\mathbf{0}) = \int_{\Omega} \tilde{\varepsilon}(\mathbf{y}) G_f(\mathbf{0}; \mathbf{y}) d\Omega, \quad (79)$$

which, using Eqs. (67) and (75), can be written as

$$\bar{\varepsilon}(\mathbf{0}) = \frac{K_1}{4\pi\sqrt{2\pi E\bar{c}}} \int_0^\infty \sqrt{r} K_0\left(\frac{r}{\sqrt{\bar{c}}}\right) dr \int_{-\pi}^{\pi} \sqrt{(1 - \cos \vartheta)(5 - 3 \cos \vartheta)} d\vartheta. \quad (80)$$

The second integral in the right-hand side is identical with that in Eq. (70) and is thus given by Eq. (73). The first integral can be written as (Gradshteyn and Ryzhik, 1994)

$$\int_0^\infty \sqrt{r} K_0\left(\frac{r}{\sqrt{\bar{c}}}\right) dr = \frac{1}{\sqrt{2}} e^{-3/4} \Gamma^2\left(\frac{3}{4}\right). \quad (81)$$

Combination of these results yields

$$\bar{\varepsilon}(\mathbf{0}) = \frac{K_1 \Gamma^2\left(\frac{3}{4}\right)}{\pi^{3/2} E \sqrt[4]{\bar{c}}} \left(1 + \frac{1}{2\sqrt{3}} \operatorname{arctanh}\left(\frac{1}{2}\sqrt{3}\right)\right), \quad (82)$$

which is again finite. This result can be compared with expression (74) for the nonlocal model by setting $\bar{c} = \frac{1}{2} l^2$. The two expressions then differ exactly by a factor $\Gamma\left(\frac{3}{4}\right) \approx 1.23$, i.e., the nonlocal equivalent strain is approximately 23% higher in the implicit gradient model than in the nonlocal model. Note that this trend is consistent with the observation in Section 2.3 that the effective interaction length is slightly smaller in the gradient model than in the nonlocal model. As a result, more weight is attributed to the region close to the crack tip in which (local) strains are high.

The nonlocal equivalent strain (14) according to the explicit gradient model follows by differentiation of Eq. (67). It can be seen directly that the $r^{-1/2}$ singularity of $\tilde{\varepsilon}$ then results in a $r^{-5/2}$ singularity of $\bar{\varepsilon}$, which means that the $\bar{\varepsilon}$ -field has a stronger singularity than the local strain field. Indeed, $\bar{\varepsilon}$ may become singular at

the crack tip even if the local strain is nonsingular. This result seems to indicate that the explicit gradient model cannot realistically describe crack growth.

7. Discussion and concluding remarks

The crack tip fields derived in the previous section as well as the wave propagation behaviour (Section 4) show substantial differences between the two gradient approaches. Whereas the implicit gradient model based on Eq. (16) follows the nonlocal model at least in a qualitative sense, the explicit model shows a response which is entirely different and which is even nonphysical in several aspects. In particular, the wave velocity is unbounded and the predicted crack growth may be instantaneous. In the implicit gradient formulation the wave velocity and crack growth rate remain finite, as in the nonlocal model. This difference between the two gradient formulations is quite remarkable since both methods introduce the same degree of approximation with respect to the nonlocal model. However, two fundamental differences exist between the two approaches, which are responsible for their different behaviour.

Firstly, gradient terms of orders higher than two have been rigorously neglected in the explicit model, whereas these terms have indirectly been preserved in the implicit formulation. As a result, spatial interactions span the entire domain in the implicit model, similarly to the nonlocal model. Indeed, it has been shown that the implicit gradient formulation can be written in the integral format of the nonlocal approach by using the appropriate Green's function as weight function. This means that the implicit gradient model is truly nonlocal. The explicit formulation, on the other hand, is local in a mathematical sense, because the nonlocal strain in a point depends only on the local strain and its gradients in that same point. Spatial interactions are therefore limited to an infinitesimal neighbourhood in this model.

Secondly, the explicit gradient formulation imposes stronger continuity requirements on the displacements than the implicit and nonlocal approaches, since it introduces fourth-order displacement derivatives in the equilibrium equations. These requirements may be difficult to meet in the strongly localised or singular deformation fields considered here and may therefore have an important effect on the predicted response.

The wave propagation behaviour and asymptotic crack tip fields obtained for the explicit formulation show that this formulation cannot realistically describe dynamic problems and fracture problems. The method may give valid results in static problems in which the deformation is only weakly localised and no cracks are formed. However, the special continuity requirements and boundary conditions then still render it computationally less attractive than the nonlocal and implicit gradient formulations, for which reliable and efficient algorithms are available.

The nonlocal and implicit gradient formulations have been found to be largely equivalent. Qualitatively, the responses of both models in wave propagation, localisation and at cracks agree remarkably well. In the rare situation where well-defined spatial interactions exist in a material, the nonlocal approach may be preferred because it models the nonlocality in a more transparent way. This requires, however, that questionable interactions near notches and cracks are somehow removed. This issue is not present for the gradient approach, where the treatment of boundaries is much better defined from a mathematical viewpoint. Since in most practical cases the nonlocality is introduced on a phenomenological basis, this seems to be a strong argument in favour of using the implicit gradient formulation rather than the integral model.

The fact that the subtle difference between the two gradient approaches has far-reaching consequences for the behaviour of the resulting enhanced damage models indicates that one should be careful in generalising arguments made for a particular formulation to entire classes of models. Based on such generalisations, the differences between nonlocal and gradient-enhanced models have sometimes been exaggerated. For the very same reason, the extrapolation of the understanding obtained in damage mechanics to a plasticity framework is not trivial. Although some work has already been done in this direction

(de Borst et al., 1995; Engelen et al., 1999, 2001), it is believed that further integration of the knowledge on enhanced plasticity and damage models will be of benefit to both fields.

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