Available online at www.sciencedirect.com

ScienceDirect

Procedia Structural Integrity 35 (2022) 173–180

Structural Integrity Procedia

www.elsevier.com/locate/procedia

2nd International Workshop on Plasticity, Damage and Fracture of Engineering Materials

Phase Field vs Gradient Enhanced Damage Models: A Comparative Study

Karthik S.[a,*], K. S. S. Reddy[a], A. Nasedkina[b], A. Nasedkin[b], A. Rajagopal[a]

[a]*Department of Civil Engineering, Indian Institute of Technology, Hyderabad, India*
[b]*Department of Mathematical Modeling, Southern Federal University, Rostov-On-Don, Russia*

Abstract

A comparison of the two different approaches for modelling damage in material in an infinitesimal strain setting is studied. The first approach is the nonlocal gradient enhanced damage model where the damage variable is taken as an independent variable which will be determined based on the local strain measure. Here, the nonlocal integral form is approximated to an implicit or explicit differential form using the Taylor's series expansion for simpler numerical implementation. The second approach is the phase field damage model where a Helmholtz free energy density function is considered that includes a new energy degradation function along with a phase field non-conserved order parameter. The first variational principle on this energy density functional with respect to the corresponding order parameter variable will reach a stationarity value resulting in the non-conserved Allen-Cahn equation. The relationship of the order parameter with the damage variable gives the Allen-Cahn evolution equation for damage. A 1D bar example is considered for commenting on the similarities and differences of the two approaches to damage based on the mesh convergence studies based on the results obtained for various meshing profiles, changing length scale parameter values and the obtained damage profiles.

Peer-review under responsibility of IWPDF 2021 Chair, Tuncay Yalçinkaya

Keywords: Phase field model; Gradient enhanced damage model; Damage mechanics.

1. Introduction

There is a need to understand the material behaviour at different loadings till the failure of material occurs. This is important for designing a structure made up of that material and ensure that the strength of the material is completely utilized till failure. Continuum Damage Mechanics (CDM) related stress-strain models are considered to define the damage in a material. CDM predicts the progressive degradation of the material from the micro scale to the macro scale by defining a damage variable (ϕ) at a continuum scale as discussed in Kachanov (1958). It is observed from the literature that when a CDM based model is used to predict damage in a strain softening type materials there are some

* Corresponding author. Tel.: +91-948-283-1340.
E-mail address: ce17resch01005@iith.ac.in

2452-3216
Peer-review under responsibility of IWPDF 2021 Chair, Tuncay Yalçinkaya
10.1016/j.prostr.2021.12.062

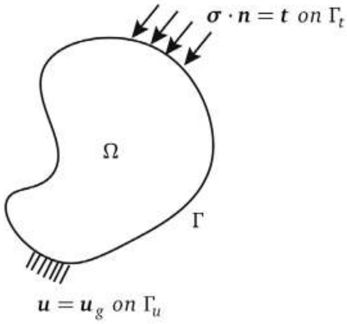


Fig. 1. 2D elastic domain

issues. The governing differential equations for such materials show loss of ellipticity and describes an ill-posedness to the problem giving uncharacteristic results as shown in Bazant et al. (1984). In a numerical implementation scheme, they give mesh dependent results as shown in Murakami and Liu (1995). The local continuum approach lacks a length scale in the formulation leading to an unspecified localization zone. Also there is no influence of the microstructure on the global behavior. The notion of generalized continuum theory accounts for size dependence arising due to the microstructure of the material. Hence there arises a need to regularize the localized model resulting in development of Nonlocal continuum theories [Bazant and Jirasek (2002)], Micromorphic continuum theories [Forest (2009)] and Gradient continuum theories [Peerlings et al. (1996)]. Recent advances in the nonlocal continuum models include a length scale parameter to regularize the solution, has a specific condition for onset of damage and gives a mesh independent solution from numerical implementations. This has lead to the development of popular approaches such as the phase field model [Raghu et al. (2019)][Kasirajan et al. (2020)][Karthik et al. (2021)][Pranavi et al. (2021)], peridynamics model [Ha and Bobaru (2010)] and the gradient enhanced damage model [Umesh and Rajagopal (2018)]. Numerical implementation has been done using an arc-length method as it captures both snap back and snap through which can be observed in the softening behaviour of the material. In section 2, the framework of a gradient enhanced damage model is presented from paper by Umesh and Rajagopal (2018). A short description of this model has been explained here showing the main governing equations considered. In section 3, the formulation of a phase field damage model is discussed and the framework of this approach along with the governing equations has been explained. In section 4, a 1D bar is considered to analyse and compare the results from the two approaches considered and brief remarks on the similarities, advantages and disadvantages of using these two approaches for solving a damage mechanics problem is presented.

2. Framework of gradient enhanced damage model

In this section we discuss an approach used in the framework of gradient enhanced damage model to predict the damage behavior of the material at various stages of loading. Here an isotropic damage variable is considered and it is quantified by a history parameter. A condition for evolution of damage is also proposed for this model.

2.1. Framework for isotropic damage

The Cauchy stress tensor ($\boldsymbol{\sigma}$) measures the response of the material. The damage variable (ϕ) measures the state of damage in the material. $\phi = 0$, represents material is undamaged and $\phi = 1$ represents that the material strength is completely lost. Lemaitre (1996) shows the concept of hypothesis of strain equivalence and the effective stress which is given as,

$$\boldsymbol{\sigma} = (1 - \phi)\, \boldsymbol{E} : \boldsymbol{\varepsilon} \tag{1}$$

where, $\boldsymbol{E}$ is the fourth order constitutive tensor in the undamaged state, where $\phi = 0$. The evolution of damage represents the damage variable ϕ expressed as a function of history parameter ($\mathcal{H}$), i.e. $\phi = \phi(\mathcal{H})$. Where, $\mathcal{H}$ shows the level of material deformation. A nonlocal formulation gives a well-posed result for the damage formulations Triantafyllidis and Aifantis (1986); Eringen (1983) shows that using a nonlocal approach for the damage mechanics problems results in well-posedness. The nonlocal equivalent strain ($\bar{s}$) is considered for obtaining the history parameter $\mathcal{H}$ which is defined from the following Khun-Tucker relations.

$$\dot{\mathcal{H}} \geq 0, \quad \mathcal{H} - \bar{s} \leq 0, \quad \dot{\mathcal{H}}\,(\mathcal{H} - \bar{s}) = 0 \tag{2}$$

A nonlocal approach accounts for the interaction between the material points and their neighbours at a micro level and hence the nonlocal equivalent strain ($\bar{s}$) can be calculated by the weighted integral of the local equivalent strain (s) given as,

$$\bar{s}(\boldsymbol{x}) = \int_{\mathrm{V}'} w(\boldsymbol{p})\, s(\boldsymbol{x} + \boldsymbol{p})\, d\mathrm{V}' \quad \text{with,} \quad \int_{\mathrm{V}'} w(\boldsymbol{p})\, d\mathrm{V}' = 1 \tag{3}$$

where, $\boldsymbol{x}$ denotes material point vector, $\boldsymbol{p}$ denotes material point vector in the surrounding volume V' and $w(\boldsymbol{p})$ denotes the weighting function which tells about the radius and intensity of the nonlocal area.

2.2. Gradient approach

The numerical implementation of this nonlocal integral formulation is very complex to solve in a numerical implementation as we will get two volume integrals when computing the stiffness matrix. Hence, a Taylor series formula about the point $\boldsymbol{x}$ is used to convert the integral form of the nonlocal equation to an equivalent explicit or implicit differential form. The explicit differential equation for an isotropic material is given as,

$$\bar{s}(\boldsymbol{x}) = s(\boldsymbol{x}) + a\,\boldsymbol{\nabla}^2 s(\boldsymbol{x}) + b\,\boldsymbol{\nabla}^4 s(\boldsymbol{x}) + ... \tag{4}$$

where, $a, b, ...$ are coefficients for the gradient terms. The material length scales are introduced from these coefficients. Here, the coefficient a can be equated to the square of the length scale variable. We can ignore the higher order terms and just write the above explicit equation as,

$$\bar{s} = s + a\,\boldsymbol{\nabla}^2 s \tag{5}$$

where, $\boldsymbol{\nabla}^2$ is the Laplacian operator. Eq.(5) leads to a strong C^1 continuity requirement for approximating the displacements for this explicit equation due to the Laplacian operator on s. Instead we can rewrite Eq.(5) by directly manipulating the explicit equation to obtain an implicit differntial equation that can be written as,

$$\bar{s} - a\,\boldsymbol{\nabla}^2 \bar{s} = s \tag{6}$$

This direct manipulation ensures that only C^0 continuity approximation is required for the displacement variable.

2.3. Governing equation

The displacements are determined from the equilibrium equation which is given as:

$$\begin{aligned} \boldsymbol{\nabla} \cdot \boldsymbol{\sigma} + \boldsymbol{b} &= 0 \ \text{ in } \ \Omega \\ \text{given} \quad \boldsymbol{\sigma} \cdot \boldsymbol{n} &= \boldsymbol{t} \quad \text{on } \Gamma_t \\ \boldsymbol{u} &= \boldsymbol{u}_g \quad \text{on } \Gamma_u \end{aligned} \tag{7}$$

where $\boldsymbol{b}$ represents the body force, $\boldsymbol{t}$ represents the traction applied on Γ_t and $\boldsymbol{u}_g$ represents the displacements applied on Γ_u. This governing equilibrium equation has to be solved for displacements coupled with solution of the nonlocal equivalent strain from the implicit form of the differential equation given in Eq.(6).

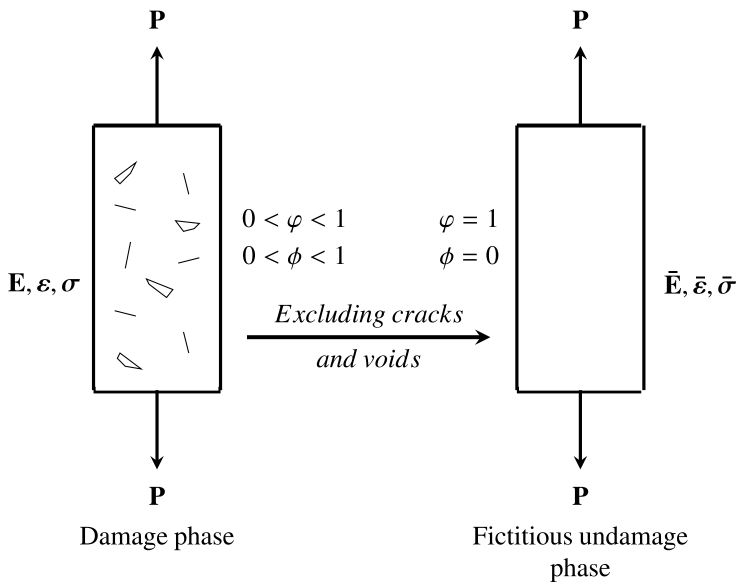


Fig. 2. Representation of variables in Damaged and Fictitious undamaged configurations

2.4. Damage Parameter

A linear damage evolution law is used to evaluate the damage variable ϕ as a function of the history variable $\mathcal{H}$ which is computed based on the level of the nonlocal equivalent strain $\bar{s}$.

$$\phi = \begin{Bmatrix} \frac{\mathcal{H}_c}{\mathcal{H}} \frac{(\mathcal{H}-\mathcal{H}_0)}{(\mathcal{H}_c-\mathcal{H}_0)} & \text{if } \mathcal{H}_c \leq \mathcal{H} > \mathcal{H}_0 \\ 1 & \text{if } \quad \mathcal{H} > \mathcal{H}_c \end{Bmatrix} \tag{8}$$

where, $\mathcal{H}_0$ and $\mathcal{H}_c$ are the initial and the critical history parameters.

3. Framework of Phase field model

In this section we discuss an approach in the framework of a phase field damage model to describe the damage behavior of the material at various stages of loading. Here an isotropic damage variable is considered and it is calculated from the Allen-Cahn evolution equation. A damage condition can also be used to improve the computational time for this model.

3.1. Order parameter for the phase field model

The phase field model introduces a variable named the order parameter which describes the transition between different material configurations. From this we can define all the phases of the microstructure by describing the order parameter value for each of them. For a two phase system the order parameter takes the value $\varphi = 1$ for the ordered phase and $\varphi = 0$ for the disordered phase. In the context of CDM, this order parameter is related to measure the cracks and voids content in a representative volume element (RVE) of the domain considered. Hence we can relate the damage variable and order parameter as $\phi = 1 - \varphi$ such that $\phi = 0$ denotes the undamaged phase and $\phi = 1$ denotes the damaged phase and the interface region of the two phases is denoted by a smooth diffuse function represented by $0 < \phi < 1$. These phase field representations are shown in Figure.2.

3.2. Energy density functional

The energy density functional consists of phase field variable and its gradients terms. The terms involving gradients of damage variable are also included to define the nonlocal nature of damage in the material. The Helmholtz free energy is thus defined as

$$F = \int_V \left[G_0(\varphi) + \frac{\kappa^2}{2} (\nabla\varphi)^2 \right] dV \tag{9}$$

where, G_0 is the strain energy density and κ is the energy coefficient for the gradient term. G_0 is known for homogeneous phases but not for the interface region where it has to be extrapolated. The expression of G_0 over the entire domain $(0 \leq \varphi \leq 1)$ reduces to the free energy of a homogeneous phase, if only that phase is present.

Hence, the total strain energy density G_o consists of

$$G_0(\varphi) = h(\varphi) G_0^{und}(\varphi) + [1 - h(\varphi)]\, G_0^{fud}(\varphi) + W G_1(\varphi) \tag{10}$$

where, G_o^{fud} is the strain energy density in a damaged phase and G_0^{und} is the strain energy density in an undamaged phase which can be defined as,

$$G_0^{fud}(\varphi) = 0, \quad G_0^{und}(\varphi) = \frac{1}{2} \bar{\boldsymbol{\varepsilon}} : \bar{\mathbf{E}} : \bar{\boldsymbol{\varepsilon}} \tag{11}$$

where $\bar{\mathbf{E}}$ is the constitutive fourth order tensor and $\bar{\boldsymbol{\varepsilon}}$ is the second order strain tensor. The bar on the symbol denotes them as the quantities in the undamaged phase. W is the interfacial energy coefficient. $h(\varphi)$ is the interpolation function for the two phases. $G_1(\varphi)$ is a double well potential function such that,

$$G_1(\varphi) = \varphi^2 (1 - \varphi)^2 \tag{12}$$

Substituting all the above equations in the energy density functional given in Eq.(9) we get,

$$F = \int_V \left[(10\varphi^3 - 15\varphi^4 + 6\varphi^5) \frac{1}{2} \bar{\boldsymbol{\varepsilon}} : \bar{\mathbf{E}} : \bar{\boldsymbol{\varepsilon}} + W\varphi^2 (1 - \varphi)^2 + \frac{Wl^2}{2} (\nabla\varphi)^2 \right] dV \tag{13}$$

We have established a relation that $\phi = 1 - \varphi$, hence substituting this we can rewrite the energy density functional in terms of the damage variable ϕ as,

$$F = \int_V \left[(1 - 10\phi^3 + 15\phi^4 - 6\phi^5) \frac{1}{2} \bar{\boldsymbol{\varepsilon}} : \bar{\mathbf{E}} : \bar{\boldsymbol{\varepsilon}} + W\phi^2 (1 - \phi)^2 + \frac{Wl^2}{2} (\nabla\phi)^2 \right] dV \tag{14}$$

3.3. Governing equations

We apply the first variational principle on the energy density functional given in Eq.(14) with respect to the displacements to obtain the equilibrium equation which is given as

$$\boldsymbol{\nabla} \cdot \left[\left(1 - 10\phi^3 + 15\phi^4 - 6\phi^5 \right) \bar{\mathbf{E}} : \bar{\boldsymbol{\varepsilon}} \right] = 0 \tag{15}$$

Allen-Cahn evolution equation relates the change of order parameter with respect to time with the change of energy density with respect to the order parameter. Therefore, the evolution equation cab be represented as

$$\frac{\partial\varphi}{\partial t} = -M \left(\frac{\delta F}{\delta\varphi} \right) \tag{16}$$

By applying the first variational principle on the energy density functional given in Eq.(13) with respect to the order parameter and writing it in terms of the damage vaiable and substituting in Eq.(16) results in

$$\frac{\partial\phi}{\partial t} = M \left[-30\phi(\phi - 2\phi^2 + \phi^3) \frac{1}{2} \bar{\boldsymbol{\varepsilon}} : \bar{\mathbf{E}} : \bar{\boldsymbol{\varepsilon}} + 2W\phi(1 + 2\phi^2 - 3\phi) - Wl^2 \left(\nabla^2\phi \right) \right] \tag{17}$$

where, M is the moblity. Eq.(15) and Eq.(17) are solved in a staggered approach.

4. Comparison of Gradient Enhanced Damage formulation with Phase Field formulation

A 1D bar whose dimensional length is 100mm, area of c/s 10mm^2 and modulus of elasticity 200000 MPa is considered for the comparison of the two models is as shown in Fig.3. The left end of the bar is fixed and force is applied at the right end. The cross section of the bar is reduced by 10% at the center to trigger the localization.

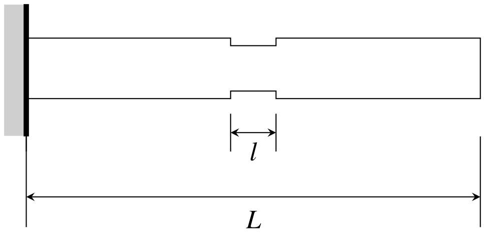


Fig. 3. One dimensional bar

Comparing the gradient enhanced damage (GED) approach with the phase field (PF) approach, the following remarks are made

- The phase field evolution equation and the nonlocal equivalent strain equation derived in the two models, i.e. Eq.(17) and Eq.(6), are having the length scale term which relates the microstructure dimension and thus useful to study size effects. Both are non local approaches as they are having the gradient terms.
- The GED includes a fourth order differential equation, due to the laplacian operator on the strain, for the considered 1D model problem whereas the phase field method includes a second order differential equation for the same 1D model problem. The PF results in (because of better regularities) more accurate results especially in post peak behavior compared to GED as seen in Fig.5, however they are achieved with slightly more computational effort.
- From the stress-strain relations, the energy degradation function is identified from Eq.(1) for GED model and from Eq.(14) for PFM model. PF2 indicates the standard degradation function $(1-\phi)^2$ for phase field models as seen in Miehe et al. (2010). A comparison of the three is shown in Fig.4. We can observe that the degradation function considered for the PF1 model is better as it does not show a significant reduction in stiffness untill higher values of damage variable.

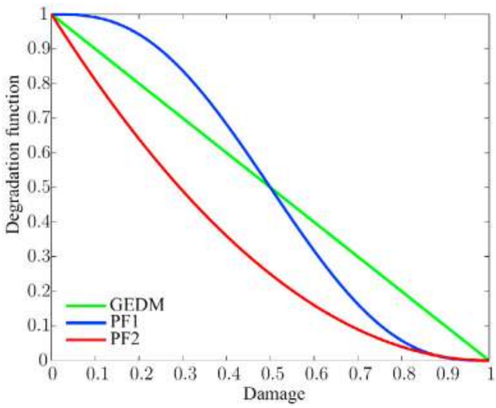
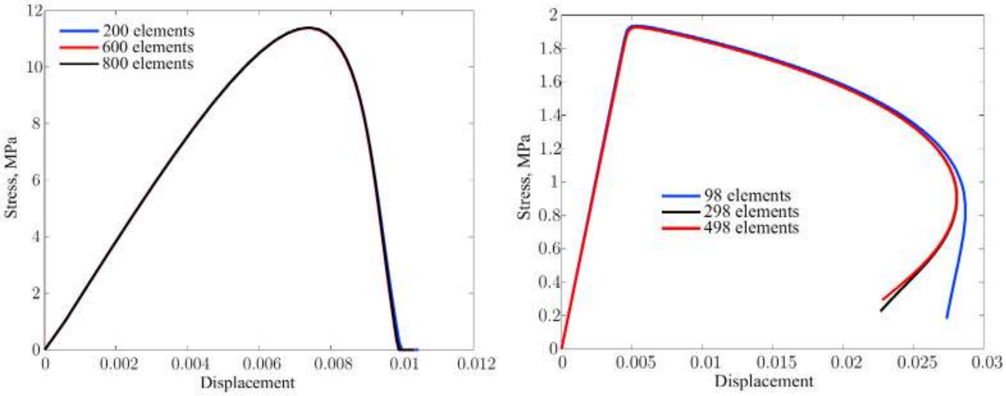
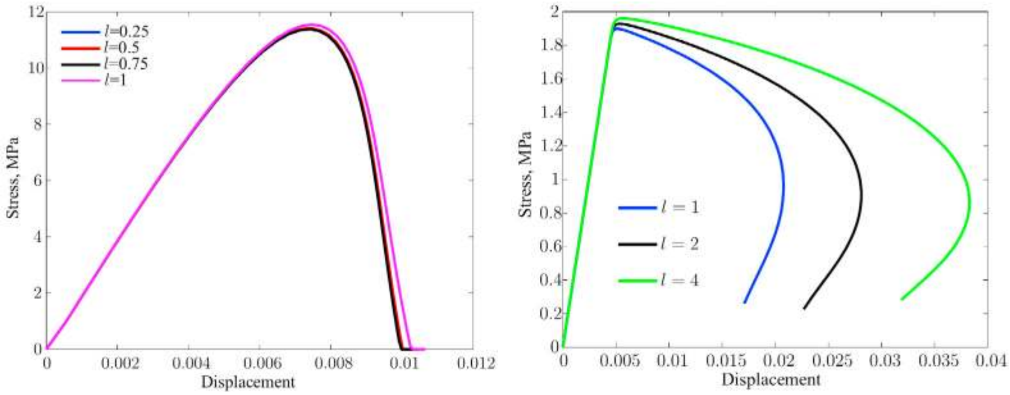


Fig. 4. Energy degradation functions for various models



(a) (b)

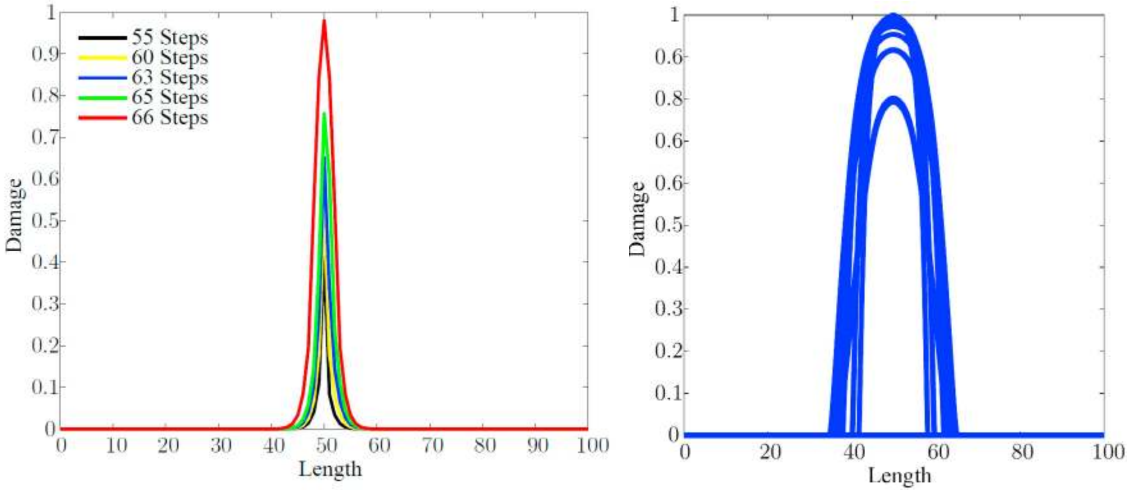
Fig. 5. h-refinement studies: (a) PFM; (b) GED.



(a) (b)

Fig. 6. Effect of length scale parameter: (a) PFM; (b) GED.

- In GED, damage is indirectly calculated based on the history of the nonlocal equivalent strain and hence behaviour is linear until peak stress. In PFM, the displacements and damage variable are coupled and solved simultaneously, hence behaviour is nonlinear before the peak stress is reached as seen in Fig.5.
- The damage variable is bounded by the range of $0 \leq \phi \leq 1$ in GED but in PF model the solution of the evolution equation may result in the damage variable value going beyond 1.
- From the length scale studies shown in Fig.6 we can observe that the results are same at all length scales in PF model but there is a wide gap in the results for various length scales in GED model indicating better regularization is obtained from PF models.
- The damage pattern is cusp shaped for the PF model and is bell shaped for the GED model as seen in Fig.7. It can also be observed that the width of damage region gradually increases in case of PF model while the width of damage region arbitrarily charges as damage evolves.
- In PF model, the damage and displacement are at the same level in the equation but in GED model, the damage is based on the strains which is the derivative of the displacement. So in GED, we require a linear interpolation for the non-local equivalent strain and a quadratic interpolation for displacement whereas in PFM, the same basis functions can be used for interpolating both damage and displacement.
- The boundary conditions are determined from the variational derivatives in PF model but it is taken Ad hoc in GED models.



(a) (b)

Fig. 7. Damage parameter evolution: (a) PFM; (b) GED.

- The damage process in GED model is static type and the damage process in PF model can be static or quasi static type depending on the formulation.
- GED model is suitable for large scale engineering problems and PF model is suitable for small scale problems due to its expense of computation.

References

Bazant, Z., Belytschko, T., Chang, T., 1984. Continuum model for strain softening. Journal of Engineering Mechanics ASCE 110, 1666–1692.

Bazant, Z.P., Jirasek, M., 2002. Nonlocal integral formulations of plasticity and damage: Survey of progress. Journal of Engineering Mechanics ASCE 128, 1119–1149.

Eringen, A.C., 1983. On differential equations of nonlocal Elasticity and solutions of screw dislocation and surface waves. Journal of Applied Physics 54, 1703–1710.

Forest, S., 2009. Micromorphic approach for gradient elasticity, viscoplasticity, and damage. Journal of Engineering Mechanics 135, 117–131.

Ha, Y.D., Bobaru, F., 2010. Studies of dynamic crack propagation and crack branching with peridynamics. International Journal of Fracture 162, 229–244.

Kachanov, L.M., 1958. On the creep fracture time. Izv Akad. Nauk USSR Otd Tekh. 8, 26–31.

Karthik, S., Rajagopal, A., Reddy, J., 2021. Nonlocal phase field approach for modeling damage in brittle materials. Mechanics of Materials 157, 103797.

Kasirajan, P., Bhattacharya, S., Rajagopal, A., Reddy, J., 2020. Phase field modeling of fracture in quasi-brittle materials using natural neighbor galerkin method. Computer Methods in Applied Mechanics and Engineering 366, 113019.

Lemaitre, J., 1996. A course on damage mechanics. Springer-Verlag, Berlin, Heidelberg.

Miehe, C., Hofacker, M., Welschinger, F., 2010. A phase field model for rate-independent crack propagation: robust algorithmic implementation based on operator splits. Computer Methods in Applied Mechanics and Engineering 199, 2765–2778.

Murakami, S., Liu, Y., 1995. Mesh-dependence in local approach to creep fracture. International Journal of Damage Mechanics 4, 230–250.

Peerlings, R.H., De Borst, R., Brekelmans, W.A., De Vree, J.H., 1996. Gradient enhanced damage for quasi-brittle materials. International Journal for Numerical Methods in Engineering 39, 3391–3403.

Pranavi, D., Rajagopal, A., Reddy, J., 2021. Interaction of anisotropic crack phase field with interface cohesive zone model for fiber reinforced composites. Composite Structures 270, 114038.

Raghu, P., Rajagopal, A., Reddy, J.N., 2019. Thermodynamically consistent variational approach for modeling brittle fracture in thick plates by a hybrid phase field model. Journal of Applied Mechanics 87, 021002.

Triantafyllidis, N., Aifantis, E.C., 1986. A gradient approach to localization of deformation: I. Hyperelastic materials. Journal of Elasticity 16, 225–237.

Umesh, B., Rajagopal, A., 2018. Higher order continuous approximation for the assessment of nonlocal-gradient based damage model. Mechanics of Advanced Materials and Structures 26, 1671–1682.