# Simulating discontinuities in a gradient-enhanced continuum

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ABSTRACT: A continuum-discrete model for failure in quasi-brittle materials is presented. The continuum is regularised through the introduction of gradient terms into the constitutive model. At the transition to discrete failure, the problem fields are enhanced through the use of a discontinuous interpolation. The continuum model is able to simulate micro-cracking, while a traction-free discontinuity represents the macro crack. The discretisation procedure is described in detail.

## 1 INTRODUCTION

When introducing strain softening into a continuum material description, it is essential that some form of regularisation is introduced to maintain well-posed governing equations. However, the performance of many regularised continuum models deteriorates as inelastic deformations develop (Geers et al. 1998; Pamin and de Borst 1999). This stems from the inability of standard finite element models to represent the discrete material surfaces (macroscopic cracks) that develop. Where a discrete surface should develop, the local strain approaches infinity and interactions still occur across a zone where a physical stress-free crack should have develop.

A common regularisation techniques relies on nonlocal interactions (Bažant et al. 1984). One such model, which has been shown to be truly non-local, is the implicit gradient damage model proposed by Peerlings et al. (1996). In the work presented here, a framework for the development of discrete, tractionfree cracks in the implicit gradient damage model is proposed. At a fully damaged material point, a discontinuity in the problem fields is introduced. By introducing a discontinuity, non-local interactions across the crack cease. Discontinuities are introduced using the partition of unity concept (Melenk and Babuška 1996; Duarte and Oden 1996), which allows discontinuities in the problem fields to cross arbitrarily through a finite element mesh (Moës et al. 1999). The model is described in its essence and the finite element discretisation is presented in detail.

## 2 ENHANCED FIELDS

The inclusion of a discontinuity in a body requires the analysis and the characterisation of the problem fields. In the gradient-enhanced damage continuum model proposed by Peerlings et al. (1996), the problem involves the displacement field  $\mathbf{u}$  and the scalar non-local equivalent strain field e.

The body  $\overline{\Omega}$ , depicted in Figure 1, is bounded by  $\Gamma$ and it is crossed by a discontinuity surface  $\Gamma_d$ . Displacements  $\overline{\mathbf{u}}$  are prescribed on  $\Gamma_u$ , while tractions  $\overline{\mathbf{t}}$ are prescribed on  $\Gamma_t$ . The internal discontinuity surface  $\Gamma_d$  divides the body into two sub-domains,  $\Omega^+$ and  $\Omega^-$  ( $\Omega = \Omega^+ \cup \Omega^-$ ). The boundary surface of the body  $\overline{\Omega}$  consists of three mutually disjoint boundary surfaces,  $\Gamma_u$ ,  $\Gamma_t$  and  $\Gamma_d$  ( $\Gamma = \Gamma_u \cup \Gamma_t$ ).

In the body  $\overline{\Omega}$ , the displacement field can be decomposed as

$$\mathbf{u}(\mathbf{x},t) = \hat{\mathbf{u}}(\mathbf{x},t) + \mathscr{H}_{\Gamma_d}(\mathbf{x})\tilde{\mathbf{u}}(\mathbf{x},t), \quad (1)$$

where  $\mathscr{H}_{\Gamma_d}(\mathbf{x})$  is the Heaviside function centred at the discontinuity surface  $\Gamma_d$  ( $\mathscr{H}_{\Gamma_d} = 1$  if  $\mathbf{x} \in \Omega^+$ ,  $\mathscr{H}_{\Gamma_d} = 0$  if  $\mathbf{x} \in \Omega^-$ ) and  $\hat{\mathbf{u}}$  and  $\tilde{\mathbf{u}}$  are continuous functions on  $\overline{\Omega}$ . A similar decomposition holds for the non-local equivalent strain field:

$$e(\mathbf{x},t) = \hat{e}(\mathbf{x},t) + \mathscr{H}_{\Gamma_d}(\mathbf{x})\tilde{e}(\mathbf{x},t), \qquad (2)$$

where  $\hat{e}$  and  $\tilde{e}$  are continuous functions on  $\bar{\Omega}$ . For small displacements, the strain field is computed as the symmetric part of the gradient of the displacement field:

$$\boldsymbol{\varepsilon} = \boldsymbol{\nabla}^{s} \hat{\boldsymbol{u}} + \mathscr{H}_{\Gamma_{d}} \boldsymbol{\nabla}^{s} \tilde{\boldsymbol{u}} \quad \text{if } \boldsymbol{x} \notin \Gamma_{d}, \tag{3}$$

where  $(\cdot)^{s}$  refers to the symmetric part of  $(\cdot)$ .



Figure 1: Body  $\overline{\Omega}$  crossed by a discontinuity  $\Gamma_d$ .

## **3 PROBLEM STATEMENT**

The boundary value problem for the gradientenhanced continuum is expressed by two field equations, in terms of displacements **u** and non-local equivalent strains *e*, which are linked through the stress field (Peerlings et al. 1996). The equilibrium equations and boundary conditions for the body  $\overline{\Omega}$ without body forces can be summarised by

$$\nabla \cdot \boldsymbol{\sigma} = \boldsymbol{0} \qquad \text{in } \Omega \qquad (4)$$

$$\boldsymbol{\sigma}\mathbf{n} = \bar{\mathbf{t}} \qquad \text{on } \Gamma_t \qquad (5)$$

where  $\boldsymbol{\sigma}$  is the Cauchy stress tensor. The strong form is completed by the essential boundary condition

$$\mathbf{u} = \bar{\mathbf{u}} \qquad \text{on } \Gamma_u, \tag{6}$$

where  $\bar{\mathbf{u}}$  is a prescribed displacement, and by the constitutive relation for the isotropic description of continuum damage

$$\boldsymbol{\sigma} = (1 - \boldsymbol{\omega}) \mathbf{D} : \boldsymbol{\varepsilon} \qquad \text{in } \Omega \tag{7}$$

in which  $\omega$  is the isotropic damage parameter ( $0 \le \omega \le 1$ ), which is a function of the non-local equivalent strain *e*, **D** is the constitutive fourth order elasticity tensor and  $\varepsilon$  is the strain tensor.

The differential format of the non-local integral averaging of the local equivalent strain  $\varepsilon_{eq}$  (Pijaudier-Cabot and Bažant 1987) results in a modified Helmholtz equation (Peerlings et al. 1996) for *e*:

$$e - c \nabla^2 e = \varepsilon_{\text{eq}} \qquad \text{in } \Omega,$$
 (8)

where c is the gradient parameter, which, together with the homogeneous natural boundary condition

$$\nabla e \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma, \tag{9}$$

completes the coupled system of equations.

From the decomposition of the non-local equivalent strain e and using equation (9), the boundary conditions on the discontinuity surface (cf. Figure 1) can be written as:

$$\nabla \hat{e} \cdot \mathbf{v} = 0 \qquad \text{on } \Gamma_d^- \tag{10}$$

$$\nabla(\hat{e} + \tilde{e}) \cdot \mathbf{v} = 0 \qquad \text{on } \Gamma_d^+. \tag{11}$$

Since the function  $\hat{e}$  is a continuous function,  $\hat{e}^+ = \hat{e}^-$ , where  $\hat{e}^{+/-}$  indicates the value of  $\hat{e}$  on  $\Gamma_d^{+/-}$ . Therefore,

(

$$\boldsymbol{\nabla} \hat{\boldsymbol{e}} \cdot \boldsymbol{\nu} \right) \Big|_{\Gamma_d^+} = (\boldsymbol{\nabla} \hat{\boldsymbol{e}} \cdot \boldsymbol{\nu}) \Big|_{\Gamma_d^-} = 0.$$
(12)

From equation (12) and the above boundary conditions on  $\Gamma_d^+$ , it follows that  $\nabla \tilde{e} \cdot \boldsymbol{v} = 0$  on  $\Gamma_d^+$ . In summary, the boundary conditions for *e* at the discontinuity surface can be written as:

$$\nabla \hat{e} \cdot \mathbf{v} = 0$$
 on  $\Gamma_d^{+/-}$  (13)

$$\nabla \tilde{e} \cdot \mathbf{v} = 0 \qquad \text{on } \Gamma_d^+. \tag{14}$$

### 4 VARIATIONAL FORMULATION AND DIS-CRETISATION

The governing system of coupled partial differential equations can be cast in a weak form. To this end, equation (4) is multiplied by a weight function  $\mathbf{w}_u$ , which is decomposed considering the displacement decomposition in equation (1), and integrated over the domain  $\Omega$ :

$$\int_{\Omega} \left( \hat{\mathbf{w}}_{u} + \mathscr{H}_{\Gamma_{d}} \tilde{\mathbf{w}}_{u} \right) \cdot \left( \nabla \cdot \boldsymbol{\sigma} \right) \ d\Omega = 0.$$
(15)

Following standard procedures and using the additional condition

$$\tilde{\mathbf{u}} = \mathbf{0} \qquad \text{on } \Gamma_u \tag{16}$$

for the magnitude of the displacement jump (Wells and Sluys 2001), the above weak equilibrium equation leads to two variational statements:

$$\int_{\Omega} \nabla^{\mathbf{s}} \hat{\mathbf{w}}_{u} : \boldsymbol{\sigma} \ d\Omega = \int_{\Gamma_{t}} \hat{\mathbf{w}}_{u} \cdot \bar{\mathbf{t}} \ d\Gamma$$
(17a)

$$\int_{\Omega^+} \nabla^{\mathsf{s}} \tilde{\mathbf{w}}_u : \boldsymbol{\sigma} \ d\Omega = \int_{\Gamma_t^+} \tilde{\mathbf{w}}_u \cdot \bar{\mathbf{t}} \ d\Gamma.$$
(17b)

In a similar fashion, equation (8) can be recast in a variational form by multiplying it by a scalar weight

function  $w_e$  and by integrating over the domain  $\Omega$ :

$$\int_{\Omega} \left( \hat{w}_{e} + \mathscr{H}_{\Gamma_{d}} \tilde{w}_{e} \right) \left( \hat{e} + \mathscr{H}_{\Gamma_{d}} \tilde{e} \right) d\Omega$$
$$- c \int_{\Omega} \left( \hat{w}_{e} + \mathscr{H}_{\Gamma_{d}} \tilde{w}_{e} \right) \nabla^{2} \left( \hat{e} + \mathscr{H}_{\Gamma_{d}} \tilde{e} \right) d\Omega$$
$$= \int_{\Omega} \left( \hat{w}_{e} + \mathscr{H}_{\Gamma_{d}} \tilde{w}_{e} \right) \varepsilon_{eq} d\Omega. \quad (18)$$

Using the product rule for the Laplacian of a discontinuous scalar field, the term  $\nabla^2 \left( \mathscr{H}_{\Gamma_d} \phi \right)$  in the previous equation is equal to:

$$\nabla^{2} \left( \mathscr{H}_{\Gamma_{d}} \phi \right) = \mathscr{H}_{\Gamma_{d}} \nabla^{2} \phi + \phi \nabla \delta_{\Gamma_{d}} \cdot \boldsymbol{\nu} + 2 \delta_{\Gamma_{d}} \nabla \phi \cdot \boldsymbol{\nu}.$$
(19)

Substitution of the above relation into equation (18) leads to the term  $\int_{\Omega} \phi \nabla \delta_{\Gamma_d} \cdot \mathbf{v} \ d\Omega$  which can be expanded using the directional derivative of a function  $\phi$  in the direction of a generic unit vector  $\mathbf{v} \ (D_{\mathbf{v}}\phi = \nabla \phi \cdot \mathbf{v})$ :

$$\int_{\Omega} \left( \boldsymbol{\nabla} \delta_{\Gamma_{d}} \cdot \mathbf{v} \right) \phi \ d\Omega = \int_{\Omega} D_{\mathbf{v}} \delta_{\Gamma_{d}} \phi \ d\Omega$$
$$= -\int_{\Gamma_{d}} D_{\mathbf{v}} \phi \ d\Gamma = -\int_{\Gamma_{d}} \boldsymbol{\nabla} \phi \cdot \mathbf{v} \ d\Gamma. \quad (20)$$

Equation (20) has been derived using the following relation for the Dirac-delta function  $\delta_{\Gamma_d}$  (Stakgold 1979):

$$\int_{\Omega} \left( \boldsymbol{\nabla} \delta_{\Gamma_d} \right) \phi \ d\Omega = - \int_{\Gamma_d} \boldsymbol{\nabla} \phi \ d\Gamma.$$
 (21)

Using Gauss' theorem and after the application of the boundary conditions, the two variational statements generated from equation (18) can be rewritten in the final form:

$$\int_{\Omega} \hat{w}_{e} \hat{e} \, d\Omega + \int_{\Omega^{+}} \hat{w}_{e} \tilde{e} \, d\Omega + c \int_{\Omega} \nabla \hat{w}_{e} \cdot \nabla \hat{e} \, d\Omega$$
$$+ c \int_{\Omega^{+}} \nabla \hat{w}_{e} \cdot \nabla \tilde{e} \, d\Omega = \int_{\Omega} \hat{w}_{e} \varepsilon_{\text{eq}} \, d\Omega \quad (22a)$$

$$\int_{\Omega^{+}} \tilde{w}_{e} \hat{e} \, d\Omega + \int_{\Omega^{+}} \tilde{w}_{e} \tilde{e} \, d\Omega + c \int_{\Omega^{+}} \nabla \tilde{w}_{e} \cdot \nabla \hat{e} \, d\Omega$$
$$+ c \int_{\Omega^{+}} \nabla \tilde{w}_{e} \cdot \nabla \tilde{e} \, d\Omega = \int_{\Omega^{+}} \tilde{w}_{e} \varepsilon_{\text{eq}} \, d\Omega. \quad (22b)$$

Finally, using a Bubnov-Galerkin approach and the engineering notation for  $\boldsymbol{\sigma}$  and  $\boldsymbol{\varepsilon}$  and following standard procedures (Peerlings et al. 1996), the discretised boundary value problem can be written in matrix form as:

$$\begin{bmatrix} \mathbf{K}_{aa,t} & \mathbf{K}_{ab,t} & \mathbf{K}_{ap,t} & \mathbf{K}_{aq,t} \\ \mathbf{K}_{ba,t} & \mathbf{K}_{bb,t} & \mathbf{K}_{bp,t} & \mathbf{K}_{bq,t} \\ \mathbf{K}_{pa,t} & \mathbf{K}_{pb,t} & \mathbf{K}_{pp} & \mathbf{K}_{pq} \\ \mathbf{K}_{qa,t} & \mathbf{K}_{qb,t} & \mathbf{K}_{qp} & \mathbf{K}_{qq} \end{bmatrix} \begin{bmatrix} \Delta \mathbf{a} \\ \Delta \mathbf{b} \\ \Delta \mathbf{p} \\ \Delta \mathbf{q} \end{bmatrix}$$
$$= \begin{bmatrix} \mathbf{f}_{\text{ext},a,t+dt} \\ \mathbf{f}_{\text{ext},b,t+dt} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix} - \begin{bmatrix} \mathbf{f}_{\text{int},a,t} \\ \mathbf{f}_{\text{int},p,t} \\ \mathbf{f}_{\text{int},q,t} \end{bmatrix}, \quad (23)$$

where  $\Delta(\cdot)$  indicates an increment of  $(\cdot)$ , **a** and **b** are regular and enhanced displacement degrees of freedom, **p** and **q** are regular and enhanced non-local equivalent strain degrees of freedom and with the symmetries  $\mathbf{K}_{ba} = \mathbf{K}_{ab}$ ,  $\mathbf{K}_{bp} = \mathbf{K}_{bq} = \mathbf{K}_{aq}$ ,  $\mathbf{K}_{qa} =$  $\mathbf{K}_{qb} = \mathbf{K}_{pb}$ ,  $\mathbf{K}_{qp} = \mathbf{K}_{qq} = \mathbf{K}_{pq}$ , and

$$\mathbf{K}_{aa} = \int_{\Omega} \mathbf{B}_{u}^{\mathrm{T}} (1 - \omega) \mathbf{D} \mathbf{B}_{u} \, d\Omega \qquad (24a)$$

$$\mathbf{K}_{ab} = \int_{\Omega^+} \mathbf{B}_u^{\mathrm{T}} (1 - \omega) \mathbf{D} \mathbf{B}_u \, d\Omega \qquad (24b)$$

$$\mathbf{K}_{ap} = -\int_{\Omega} \mathbf{B}_{u}^{\mathrm{T}} \left[ \frac{\partial \omega}{\partial \kappa} \right] \left[ \frac{\partial \kappa}{\partial e} \right] \mathbf{D} \boldsymbol{\varepsilon} \mathbf{N}_{e} \, d\Omega \qquad (24c)$$

$$\mathbf{K}_{aq} = -\int_{\Omega^+} \mathbf{B}_u^{\mathrm{T}} \left[ \frac{\partial \omega}{\partial \kappa} \right] \left[ \frac{\partial \kappa}{\partial e} \right] \mathbf{D} \boldsymbol{\varepsilon} \mathbf{N}_e \, d\Omega \qquad (24\mathrm{d})$$

$$\mathbf{K}_{bb} = \int_{\Omega^+} \mathbf{B}_u^{\mathrm{T}} (1 - \omega) \mathbf{D} \mathbf{B}_u \, d\Omega \qquad (24\mathrm{e})$$

$$\mathbf{K}_{pa} = -\int_{\Omega} \mathbf{N}_{e}^{\mathrm{T}} \left[ \frac{\partial \varepsilon_{\mathrm{eq}}}{\partial \boldsymbol{\varepsilon}} \right]^{\mathrm{T}} \mathbf{B}_{u} \, d\Omega \qquad (24\mathrm{f})$$

$$\mathbf{K}_{pb} = -\int_{\Omega^+} \mathbf{N}_e^{\mathrm{T}} \left[ \frac{\partial \boldsymbol{\varepsilon}_{\mathrm{eq}}}{\partial \boldsymbol{\varepsilon}} \right]^{\mathrm{T}} \mathbf{B}_u \, d\Omega \qquad (24\mathrm{g})$$

$$\mathbf{K}_{pp} = \int_{\Omega} \left( \mathbf{N}_{e}^{\mathrm{T}} \mathbf{N}_{e} + \mathbf{B}_{e}^{\mathrm{T}} c \mathbf{B}_{e} \right) \, d\Omega \qquad (24\mathrm{h})$$

$$\mathbf{K}_{pq} = \int_{\Omega^+} \left( \mathbf{N}_e^{\mathrm{T}} \mathbf{N}_e + \mathbf{B}_e^{\mathrm{T}} c \mathbf{B}_e \right) \, d\Omega.$$
 (24i)

As in the standard gradient damage formulation, the total stiffness matrix is not symmetric. In equations (24),  $\mathbf{N}$  is a matrix containing the usual finite element shape functions,  $\mathbf{B}$  is a matrix containing spatial

derivatives of the shape functions and  $\kappa$  is the maximum value of the non-local equivalent strain (Peerlings et al. 1996). The terms in the RHS of the discretised boundary value problem read:

$$\mathbf{f}_{\text{int},a} = \int_{\Omega} \mathbf{B}_{u}^{\mathrm{T}} \boldsymbol{\sigma} \, d\Omega \tag{25a}$$

$$\mathbf{f}_{\text{int},b} = \int_{\Omega^+} \mathbf{B}_u^{\mathrm{T}} \boldsymbol{\sigma} \, d\Omega \tag{25b}$$

$$\mathbf{f}_{\text{int},p} = \int_{\Omega} \left( \mathbf{N}_{e}^{\mathrm{T}} \mathbf{N}_{e} \mathbf{p} + \mathbf{B}_{e}^{\mathrm{T}} c \mathbf{B}_{e} \mathbf{p} - \mathbf{N}_{e}^{\mathrm{T}} \varepsilon_{\text{eq}} \right) d\Omega$$
$$+ \int_{\Omega^{+}} \left( \mathbf{N}_{e}^{\mathrm{T}} \mathbf{N}_{e} \mathbf{q} + \mathbf{B}_{e}^{\mathrm{T}} c \mathbf{B}_{e} \mathbf{q} \right) d\Omega \quad (25c)$$

$$\mathbf{f}_{\text{int},q} = \int_{\Omega^+} \left( \mathbf{N}_e^{\mathrm{T}} \mathbf{N}_e \mathbf{p} + \mathbf{B}_e^{\mathrm{T}} c \mathbf{B}_e \mathbf{p} - \mathbf{N}_e^{\mathrm{T}} \varepsilon_{\text{eq}} \right) \, d\Omega + \int_{\Omega^+} \left( \mathbf{N}_e^{\mathrm{T}} \mathbf{N}_e \mathbf{q} + \mathbf{B}_e^{\mathrm{T}} c \mathbf{B}_e \mathbf{q} \right) \, d\Omega.$$
(25d)

The finite element implementations follows mainly the one proposed in Peerlings et al. (1996) for the gradient-enhanced model and the one in Wells and Sluys (2001) and Wells et al. (2002) for the discontinuous modelling.

A discontinuity can be introduced when the average value of the damage in an element reaches a critical value. As a discontinuity propagates, the activity of the non-local equivalent strain is mobilised at the discontinuity tip and ceases behind it. Spurious growth of damage can thus be prevented. The direction of the discontinuity can be determined by computing the direction of maximum accumulation of the non-local equivalent strain.

#### 5 CONCLUSIONS

A discontinuous gradient-enhanced damage model for fracture has been presented. A gradient-enhanced damage model is coupled to a discontinuous model based on the partition of unity concept. The discretisation procedure for the combined model has been fully described. By introducing a discontinuity at a fully damaged material point, macroscopic cracks can be realistically described. Spurious growth of damage can thus be prevented since non-local interaction between the two sides of the discontinuity is avoided.

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