On the thermodynamics of gradient regularization of continuum damage models

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Introduction

In 1958 Kachanov introduced a model to describe continuous degradation of a material.

He introcuded a single variable - damage index or integrity - which continuosly reduces the elastic properties.

For the evolution of the integrity ϕ, he proposed the following kinetic law (modified by Rabotnov 1959)

$$\dot{\phi} = -\frac{A}{\phi^p}\left(\frac{\sigma}{\phi}\right)^n, \qquad \sigma = \phi E \varepsilon \tag{1}$$

For an undamaged material $\phi = 1$ and at fully damaged state $\phi = 0$.

Thermodynamic formulation

- The spesific free energy ψ (per unit mass) depends on strain $\boldsymbol{\varepsilon}$ and damage $D = 1 - \phi$: Videly used simple form of the free energy is

$$\rho\psi(\boldsymbol{\varepsilon}, D) = \frac{1}{2}(1-D)\boldsymbol{C}\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} = (1-D)W_{\mathrm{e}}. \tag{2}$$

- The dissipative behaviour is modelled using the dual form of the dissipation potential depending on the dissipative force $Y_{\mathrm{d}} = -Y_{\mathrm{e}} = W_{\mathrm{e}}$ as

$$\varphi^*(Y_{\mathrm{d}}; D) = \frac{1}{r+1}\frac{Y_{\mathrm{r}}}{(1-D)^p t_{\mathrm{d}}}\left(\frac{Y_{\mathrm{d}}}{Y_{\mathrm{r}}}\right)^{r+1}, \quad Y_{\mathrm{r}} = \frac{1}{2}E\varepsilon_{\mathrm{r}}^2 = \frac{\sigma_{\mathrm{r}}^2}{2E} \tag{3}$$

- The following constitutive equations are obtained:

$$\boldsymbol{\sigma} = \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}} = (1-D)\boldsymbol{C} : \boldsymbol{\varepsilon} \quad \text{and} \quad \dot{D} = \frac{\partial\varphi^*}{\partial Y_{\mathrm{d}}} = \frac{1}{t_{\mathrm{d}}(1-D)^p}\left(\frac{Y_{\mathrm{d}}}{Y_{\mathrm{r}}}\right)^r. \tag{4}$$

Motivation - understand the model behaviour

Uniaxial constant strain rate loading $\varepsilon(t) = \dot{\varepsilon}_0 t$. Stress-strain and dispersion behaviour of damaging bar.

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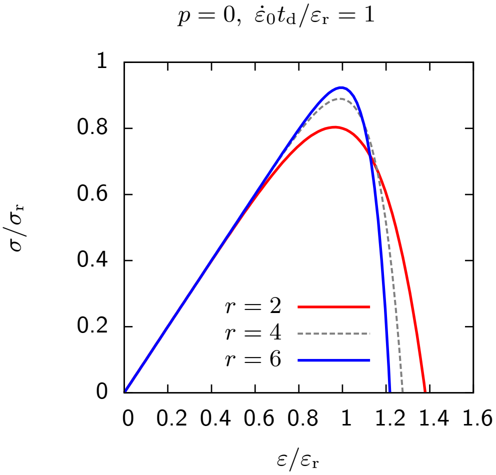
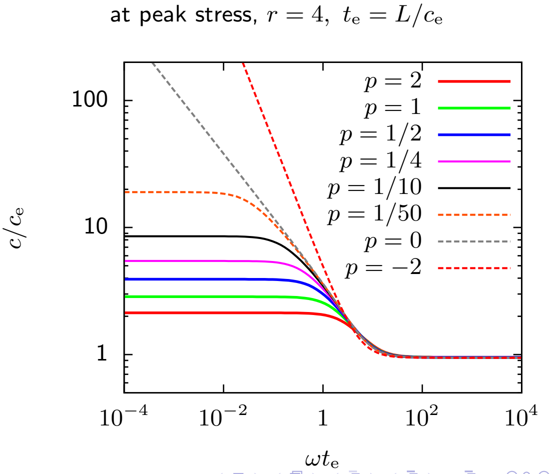




Localisation study

Definition:

$$\text{localisation width:} \quad l_{\mathrm{loc}} = \mathrm{meas}\left\{x | D^* \leq D \leq 1\right\} \tag{5}$$

D^* damage value at fracture stress for quasi-static constant strain-rate loading

$$D^* = 1 - \left(\frac{2r - 1}{2r + p + 2}\right)^{1/(p+1)}, \tag{6}$$

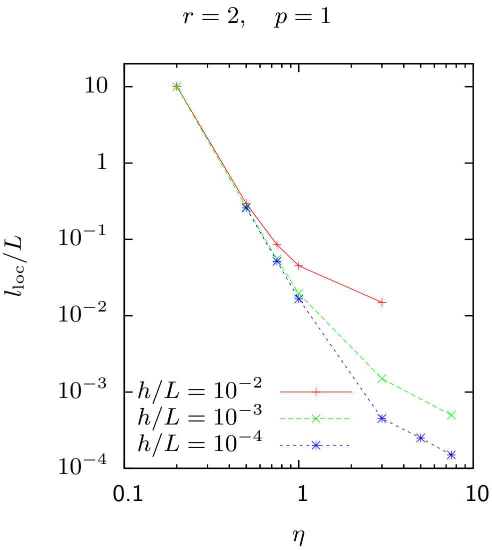
independent of the applied strain-rate.

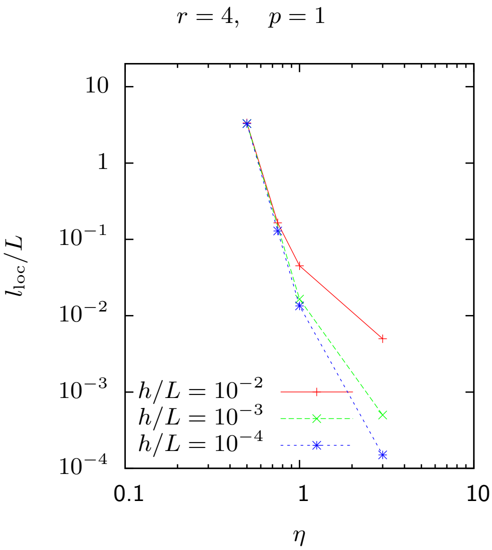
FE-study of a semi-infinite bar with prescribed displacement

$$u(0,t) = \eta \varepsilon_{\mathrm{r}} L t / t_{\mathrm{d}} \quad \text{and} \quad L = c_{\mathrm{e}} t_{\mathrm{d}}, \quad c_{\mathrm{e}} = \sqrt{E/\rho} \tag{7}$$

Linear finite elements, central-difference time integration.

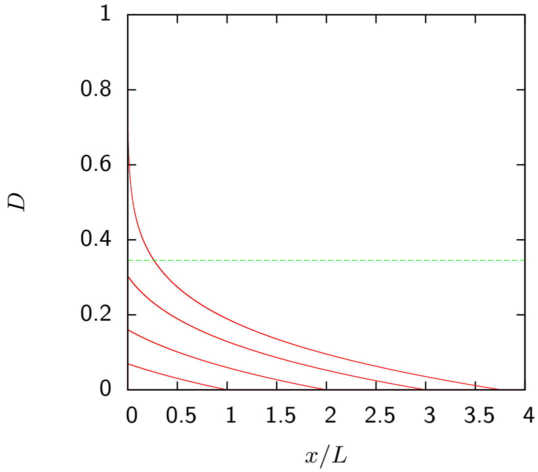
Damage localisation width





Damage profiles

At times $t_\mathrm{d}, 2t_\mathrm{d}, 3t_\mathrm{d}$ and $3.76t_\mathrm{d}$, $p = 1, r = 2, \eta = 0.5$ and $h = L/1000$.



The vertical dashed green line indicates the value D^*.

Gradiend enhancement - balance equations

The generalized principle of virtual power is stated as

$$\mathcal{P}_{\text{int}} + \mathcal{P}_{\text{ine}} + \mathcal{P}_{\text{mech}} = 0 \tag{8}$$

where the power of internal and inertial forces are

$$\mathcal{P}_{\text{int}} = -\int_V \left(\boldsymbol{\sigma} : \text{sym}(\text{grad}\, \boldsymbol{v}) + Y \dot{D} + \boldsymbol{Z} \cdot \text{grad}\, \dot{D} + X \Delta \dot{D} \right) \text{d}V, \qquad \mathcal{P}_{\text{ine}} = -\int_V \rho \dot{\boldsymbol{v}} \cdot \boldsymbol{v} \text{d}V, \tag{9}$$

and the power of external mechanical forces is

$$\mathcal{P}_{\text{mech}} = \int_V \rho \boldsymbol{b} \cdot \boldsymbol{v}\, \text{d}V + \int_S \boldsymbol{t} \cdot \boldsymbol{v}\, \text{d}S + \int_V \rho b_D \dot{D}\, \text{d}V + \int_S t_D \dot{D}\, \text{d}S + \int_S x_D\, \text{grad}\, \dot{D} \cdot \boldsymbol{n}\, \text{d}S \tag{10}$$

gives the balance equations

$$\text{div}\, \boldsymbol{\sigma} + \rho \boldsymbol{b} = \rho \dot{\boldsymbol{v}}, \quad \text{in } V, \quad \text{and} \quad \boldsymbol{\sigma} \cdot \boldsymbol{n} = \boldsymbol{t} \quad \text{in } S, \tag{11}$$

and

$$-\Delta X + \text{div}\, \boldsymbol{Z} - Y + \rho b_D = 0, \quad \text{in } V, \quad \text{and} \quad (\boldsymbol{Z} - \nabla X) \cdot \boldsymbol{n} = t_D, \quad X = x_D \quad \text{in } S. \tag{12}$$

Gradiend enhancement - potential functions and power of dissipation

Assume now that the specific Helmholtz free energy is expressed as

$$\psi(\boldsymbol{\varepsilon}, D, \operatorname{grad} D, \Delta D) \tag{13}$$

and the thermodynamic forces are additively decomposed into energetic and dissipative components as

$$Y = Y_\mathrm{e} + Y_\mathrm{d}, \quad \boldsymbol{Z} = \boldsymbol{Z}_\mathrm{e} + \boldsymbol{Z}_\mathrm{d}, \quad X = X_\mathrm{e} + X_\mathrm{d}, \tag{14}$$

where the energetic parts are

$$Y_\mathrm{e} = \rho \frac{\partial \psi}{\partial D}, \quad \boldsymbol{Z}_\mathrm{e} = \rho \frac{\partial \psi}{\partial \operatorname{grad} D}, \quad X_\mathrm{e} = \rho \frac{\partial \psi}{\partial \Delta D}. \tag{15}$$

The dual form of the dissipation potential

$$\varphi^*(Y_\mathrm{d}, \boldsymbol{Z}_\mathrm{d}, X_\mathrm{d}; D, \operatorname{grad} D, \Delta D) \tag{16}$$

and the dissipation power can be expressed in the forms

$$\gamma = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} + Y\dot{D} + \boldsymbol{Z} \cdot \operatorname{grad} \dot{D} + X \Delta \dot{D} - \rho \dot{\psi} = \frac{\partial \varphi^*}{\partial Y_\mathrm{d}} Y_\mathrm{d} + \frac{\partial \varphi^*}{\partial \boldsymbol{Z}_\mathrm{d}} \cdot \boldsymbol{Z}_\mathrm{d} + \frac{\partial \varphi^*}{\partial X_\mathrm{d}} X_\mathrm{d} \geq 0. \tag{17}$$

Gradiend enhancement - specification

If we assume the simplest form of the free energy as

$$\begin{aligned}\rho\psi &= \frac{1}{2}(1-D)\boldsymbol{C}_{\mathrm{e}}\boldsymbol{\varepsilon}:\boldsymbol{\varepsilon}+\frac{1}{2}k_1E\ell_1^2(\operatorname{grad}D)^2+\frac{1}{2}k_2E\ell_1^4(\Delta D)^2\\ &= (1-D)W_{\mathrm{e}}+\frac{1}{2}k_1E\ell_1^2(\operatorname{grad}D)^2+\frac{1}{2}k_2E\ell_1^4(\Delta D)^2.\end{aligned} \tag{18}$$

Further assume that in addition to stress also $\boldsymbol{Z}$ and X are energetic, thus

$$\boldsymbol{Z}_{\mathrm{e}} = k_1\operatorname{grad}D, \quad X_{\mathrm{e}} = k_2\ell_1^2\Delta D \tag{19}$$

and

$$Y_{\mathrm{d}} = -\Delta X_{\mathrm{e}} + \operatorname{div}\boldsymbol{Z}_{\mathrm{e}} - Y_{\mathrm{e}} = -\Delta(k_2\ell_1^2\Delta D) + \operatorname{div}(k_1\operatorname{grad}D) + W_{\mathrm{e}}. \tag{20}$$

Now we consider the dual form of the dissipation potential in the form

$$\varphi^*(Y_{\mathrm{d}}; D, \operatorname{grad}D, \Delta D) \tag{21}$$

Gradiend enhancement - specification (cont'd)

Assume now

$$\varphi^*(Y_\mathrm{d}; D, \mathrm{grad}\, D, \Delta D) = \frac{Y_\mathrm{r}}{r+1} \frac{\langle 1 + \ell_2^2 \|\mathrm{grad}\, D\|^2 + \ell_3^2 \Delta D \rangle}{t_\mathrm{d}(1-D)^p} \left(\frac{Y_\mathrm{d}}{Y_\mathrm{r}} \right)^{r+1}, \tag{22}$$

then the damage rate is

$$\dot{D} = \frac{1}{t_\mathrm{d}(1-D)^p} \left(\frac{Y_\mathrm{d}}{Y_\mathrm{r}} \right)^r \langle 1 + \ell_2^2 \|\mathrm{grad}\, D\|^2 + \ell_3^2 \Delta D \rangle, \tag{23}$$

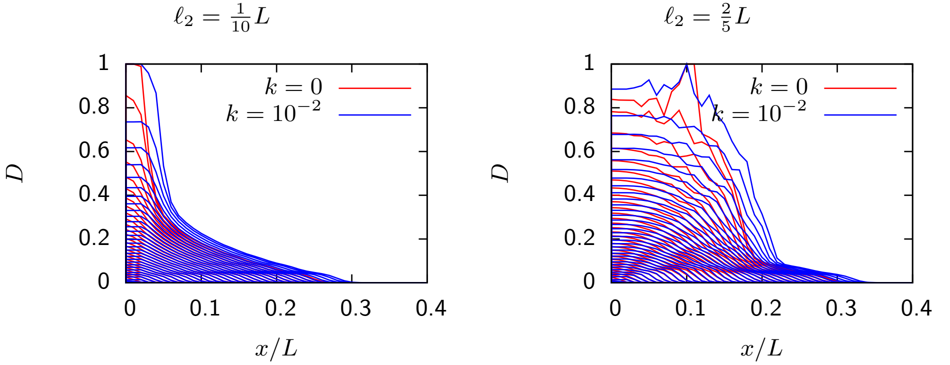
with

$$Y_\mathrm{d} = W_\mathrm{e} - \Delta(k_2 \ell_1^2 \Delta D) + \mathrm{div}\,(k_1 \mathrm{grad}\, D). \tag{24}$$

Gradiend enhancement - example 1 - only first order gradients

$$\rho\psi(\boldsymbol{\varepsilon}, D, \mathrm{grad}\, D) = (1-D)W_{\mathrm{e}} + \frac{1}{2}k_1 E \ell_1^2 (\mathrm{grad}\, D)^2, \quad \varphi^*(Y_{\mathrm{d}}; D, \mathrm{grad}\, D) = \frac{Y_{\mathrm{r}}}{r+1} \frac{\langle 1 + \ell_2^2 \|\mathrm{grad}\, D\|^2 \rangle}{t_{\mathrm{d}}(1-D)^p} \left(\frac{Y_{\mathrm{d}}}{Y_{\mathrm{r}}}\right)^{r+1}$$

As before - **dynamic study of a semi-infinite bar** with prescribed displ. - FD also for spatial discretisation:
$u(0,t) = \eta\varepsilon_{\mathrm{r}} L t / t_{\mathrm{d}}, \quad L = c_{\mathrm{e}} t_{\mathrm{d}}, \quad c_{\mathrm{e}} = \sqrt{E/\rho}, \quad h = L/100, \quad k_1 > 0.$

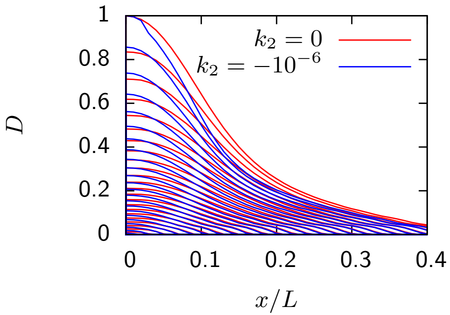


Gradiend enhancement - example 2 - only second order gradients

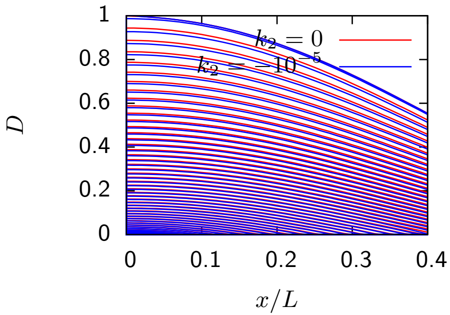
$$\rho\psi(\boldsymbol{\varepsilon}, D, \Delta D) = (1-D)W_{\mathrm{e}} + \frac{1}{2}k_2 E \ell_1^4 (\Delta D)^2, \quad \varphi^*(Y_{\mathrm{d}}; D, \Delta D) = \frac{Y_{\mathrm{r}}}{r+1}\frac{\langle 1+\ell_3^2\|\Delta D\|^2\rangle}{t_{\mathrm{d}}(1-D)^p}\left(\frac{Y_{\mathrm{d}}}{Y_{\mathrm{r}}}\right)^{r+1}$$

As before - **dynamic study of a semi-infinite bar** with prescribed displ. - FD also for spatial discretisation:
$u(0,t) = \eta\varepsilon_{\mathrm{r}} L t/t_{\mathrm{d}}, \quad L = c_{\mathrm{e}} t_{\mathrm{d}}, \quad c_{\mathrm{e}} = \sqrt{E/\rho}, \quad \ell_1 = L/10, \quad h = L/100, \quad k_2^* < k_2 < 0.$

$\ell_3 = \frac{1}{10}L$



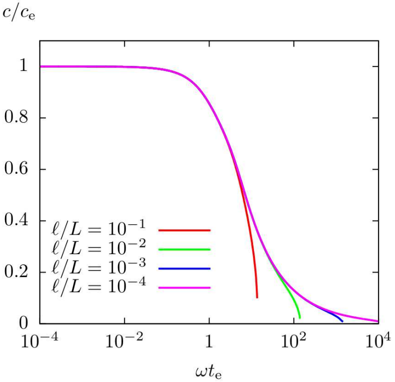
$\ell_3 = \frac{2}{5}L$

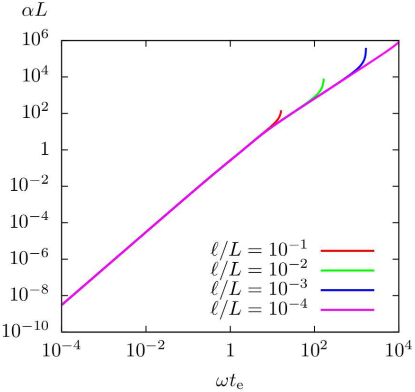


Dispersion analysis - Laplacian only in the dissipation potential

$$\rho\psi(\boldsymbol{\varepsilon}, D) = (1-D)W_{\mathrm{e}}, \quad \varphi^*(Y_{\mathrm{d}}; D, \Delta D) = \frac{Y_{\mathrm{r}}}{r+1}\frac{\langle 1+\ell_3^2\|\Delta D\|^2\rangle}{t_{\mathrm{d}}(1-D)^p}\left(\frac{Y_{\mathrm{d}}}{Y_{\mathrm{r}}}\right)^{r+1}$$

Assuming $u(x,t) = A\sin\left[\mathrm{i}(kx+\omega t)\right], \quad D(x,t) = B\sin\left[\mathrm{i}(kx+\omega t)\right]$, and $k = k_{\mathrm{r}} + \alpha\mathrm{i}$.
In the figures below $\ell = \ell_3$.





Some references

- Askes H., Sluys, L.J. Explicit and implicit gradient series in damage mechanics. *Eur. J. Mech. A/Solids*, **21**, 2002, 379–390.
- Comi C. Computational modelling of gradient-enhanced damage in quasi-brittle materials. *Mech. Cohes.-Frict. Mater.*, **4**, 1999, 17–36.
- Comi C., Corigliano A. On uniqueness of the dynamic finite-step problem in gradient-dependent softening plasticity. *Int. J. Sol. Struct.*, **33**, 1996, 3881–3902.
- Frémond M., Nedjar B. Damage, gradient of damage and principle of virtual power. *Int. J. Sol. Struct.*, **33**, 1996, 1083–1104.
- Liebe T., Steinmann P., Benallal A. Theoretical and computational aspects of a thermodynamically consistent framework for geometrically linear damage. *Comp. Methods Appl. Mech. Engng*, **190**, 2001, 6555–6576.
- Nguyen Q.S. On standard gradient plasticity and visco-plasticity. *Int. J. Sol. Struct.*, **225**, 2021, 111038.
- Polizotto C. Unified thermodynamic framework of nonlocal/gradient continuum theories. *Eur. J. Mech. A/Solids*, **22**, 2003, 651–668.

Concluding remarks

- Numerical study of the localisation properties of the Kachanov-Rabotnov damage model.
- Localisation width depends strongly on the loading rate and the r-pararameter.
- Decrasing the loading rate increases the localisation zone width which is in contrast to strain-softening viscoplasticity.
- Gradient damage? Further studies needed, e.g. dispersion and stabiliy analysis.

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Thank you for your attention!

Riikka Soininen - Flow. Oil and gilded metal leaf on canvas, 2021