The simulation of time dependent behaviour of cement bound materials with a micro-mechanical model

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Introduction

Micromechanical models:

- Simple mechanisms considered at micro (meso) scales which are expected to capture the macroscopic behaviour
- Viable alternative to phenomenological models

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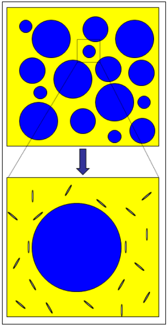
Inelastic strain may derive from:

- shrinkage
- creep
- micro-cracking
- differential thermal expansion
- ageing

Need to simulate inelastic behaviour in the matrix phase alone



Content Outline

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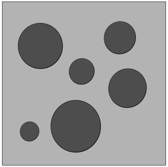
Elastic two-phase composite

Two phase composite idealisation with

- Spherical inclusions(Eshelby solution with modified Mori-Tanaka averaging)
- Penny-shaped micro-cracks(Budiansky and O'Connell)



$$\bar{\boldsymbol{\sigma}} = f_\Omega \cdot \boldsymbol{\sigma}_\Omega + f_M \cdot \boldsymbol{\sigma}_M \quad (1)$$

$$\bar{\boldsymbol{\varepsilon}} = f_\Omega \cdot \boldsymbol{\varepsilon}_\Omega + f_M \cdot \boldsymbol{\varepsilon}_M + \boldsymbol{\varepsilon}_a \quad (2)$$

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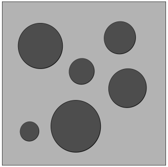


$$\bar{\boldsymbol{\sigma}} = f_\Omega \cdot \boldsymbol{\sigma}_\Omega + f_M \cdot \boldsymbol{\sigma}_M \quad (1)$$

$$\bar{\boldsymbol{\varepsilon}} = f_\Omega \cdot \boldsymbol{\varepsilon}_\Omega + f_M \cdot \boldsymbol{\varepsilon}_M + \boldsymbol{\varepsilon}_a \quad (2)$$

Average stress-strain relationship

$$\bar{\boldsymbol{\sigma}} = \mathbf{D}_{M\Omega} : \bar{\boldsymbol{\varepsilon}}_e = \mathbf{D}_{M\Omega} : (\bar{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}_a) \quad (3)$$

$$\mathbf{D}_{M\Omega} = (f_\Omega \cdot \mathbf{D}_\Omega : \mathbf{T}_\Omega + f_M \cdot \mathbf{D}_M) \cdot (f_\Omega \cdot \mathbf{T}_\Omega + f_M)^{-1}, \quad (4a)$$

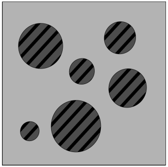
$$\mathbf{T}_\Omega = \mathbf{I}^{2s} + \mathbf{S}_\Omega : \mathbf{A}_\Omega, \quad (4b)$$

$$\mathbf{A}_\Omega = [(\mathbf{D}_\Omega - \mathbf{D}_M) : \mathbf{S}_\Omega + \mathbf{D}_M]^{-1} : (\mathbf{D}_\Omega - \mathbf{D}_M) \quad (4c)$$

Content Outline

Non-linear behaviour within the composite

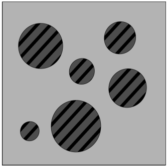
Inelastic strains in the inclusion



$$\mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c + \varepsilon_{IN}) = \mathbf{D}_M : (\varepsilon_o + \varepsilon_c + \varepsilon_{IN} - \varepsilon_\tau) \quad (5a)$$

$$\varepsilon_c = \mathbf{S}_\Omega : (\varepsilon_\tau + \varepsilon_{IN}) \quad (5b)$$

Non-linear behaviour within the composite



Inelastic strains in the inclusion

$$\mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c + \varepsilon_{IN}) = \mathbf{D}_M : (\varepsilon_o + \varepsilon_c + \varepsilon_{IN} - \varepsilon_\tau) \quad (5a)$$

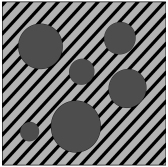
$$\varepsilon_c = \mathbf{S}_\Omega : (\varepsilon_\tau + \varepsilon_{IN}) \quad (5b)$$

Inelastic strains in the matrix

- Secant moduli method (Weng)

$$\mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c) = \mathbf{D}_{Secant} : (\varepsilon_o + \varepsilon_c - \varepsilon_\tau) \quad (6a)$$

$$\varepsilon_c = \mathbf{S}_{secant} : \varepsilon_\tau \quad (6b)$$



- Elastic constraint method (Weng)

$$\mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c + \varepsilon_{IN}) = \mathbf{D}_M : (\varepsilon_o + \varepsilon_c + \varepsilon_{IN} - \varepsilon_\tau) \quad (7a)$$

$$\varepsilon_c = \mathbf{S}_\Omega : (\varepsilon_\tau - \varepsilon_{IN}) \quad (7b)$$

(Nemat Nasser and Hori(1993), Mura (1987) and Weng (1988))

Content Outline

Two material problem with matrix undergoing transformation strain ε_{IN}. Ω remains elastic.

Matrix phase

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : \varepsilon_M = \mathbf{D}_M : (\varepsilon_o + \varepsilon_c - \varepsilon_{IN}) \quad (8)$$

Inclusion phase

$$\boldsymbol{\sigma}_\Omega = \mathbf{D}_\Omega : \varepsilon_\Omega = \mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c) \quad (9)$$

Consistency equation

$$\mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c) = \mathbf{D}_M : (\varepsilon_o + \varepsilon_c - \varepsilon_\tau) \quad (10)$$

Constrained strain

$$\varepsilon_c = \mathbf{S}_\Omega : (\varepsilon_\tau - \varepsilon_{IN}) \quad (11)$$

Transformation eigenstrain

$$\varepsilon_\tau = \mathbf{A}_\Omega : (\varepsilon_o - \mathbf{S}_\Omega : \varepsilon_{IN}) \quad (12)$$

Individual phase and composite equations

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : \varepsilon_{Mel} = \mathbf{D}_M : (\varepsilon_M - \varepsilon_{IN}) \tag{13}$$

$$\boldsymbol{\sigma}_\Omega = \mathbf{D}_\Omega : \mathbf{T}_\Omega : (\varepsilon_M - \mathbf{S}_\Omega : \varepsilon_{IN}) \tag{14}$$

Substitution and rearranged total strain equation

$$\varepsilon_M = (f_\Omega \cdot \mathbf{T}_\Omega + f_M)^{-1} : (\bar{\varepsilon} + f_\Omega \cdot \mathbf{T}_\Omega \cdot \mathbf{S}_\Omega : \varepsilon_{IN}) \tag{15}$$

Constitutive equation

$$\bar{\boldsymbol{\sigma}} = \mathbf{D}_{M\Omega} : (\bar{\varepsilon} - \varepsilon_{INEQ}) \tag{16}$$

where

$$\varepsilon_{INEQ} = \mathbf{D}_{M\Omega}{}^{-1} \cdot (f_\Omega \cdot \mathbf{D}_\Omega \cdot \mathbf{T}_\Omega : \mathbf{S}_\Omega + f_M \cdot \mathbf{D}_M - f_\Omega \cdot \mathbf{D}_{M\Omega} \cdot \mathbf{T}_\Omega : \mathbf{S}_\Omega) : \varepsilon_{IN} \tag{18}$$

Individual phase and composite equations

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : \varepsilon_{Mel} = \mathbf{D}_M : (\varepsilon_M - \varepsilon_{IN}) \quad (13)$$

$$\boldsymbol{\sigma}_\Omega = \mathbf{D}_\Omega : \mathbf{T}_\Omega : (\varepsilon_M - \mathbf{S}_\Omega : \varepsilon_{IN}) \quad (14)$$

Substitution and rearranged total strain equation

$$\varepsilon_M = (f_\Omega \cdot \mathbf{T}_\Omega + f_M)^{-1} : (\bar{\varepsilon} + f_\Omega \cdot \mathbf{T}_\Omega \cdot \mathbf{S}_\Omega : \varepsilon_{IN}) \quad (15)$$

Constitutive equation

$$\bar{\boldsymbol{\sigma}} = \mathbf{D}_{M\Omega} : (\bar{\varepsilon} - \varepsilon_{INEQ} - \varepsilon_a) \quad (17)$$

where

$$\varepsilon_{INEQ} = \mathbf{D}_{M\Omega}{}^{-1} \cdot (f_\Omega \cdot \mathbf{D}_\Omega \cdot \mathbf{T}_\Omega : \mathbf{S}_\Omega + f_M \cdot \mathbf{D}_M - f_\Omega \cdot \mathbf{D}_{M\Omega} \cdot \mathbf{T}_\Omega : \mathbf{S}_\Omega) : \varepsilon_{IN} \quad (18)$$

Content Outline

Penny-shaped micro-cracks in the matrix

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : (\boldsymbol{\varepsilon}_M - \boldsymbol{\varepsilon}_{IN} - \boldsymbol{\varepsilon}_{FRM}) \quad (19)$$

$$\boldsymbol{\sigma}_\Omega = \mathbf{D}_\Omega : \boldsymbol{\varepsilon}_\Omega = \mathbf{D}_\Omega : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c) \quad (20)$$

Consistency equation

$$\mathbf{D}_\Omega : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c) = (1-\omega)\mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_\tau) \quad (21)$$

Constrained strain

$$\boldsymbol{\varepsilon}_c = \mathbf{S}_\Omega : (\boldsymbol{\varepsilon}_\tau - \boldsymbol{\varepsilon}_{IN}) \quad (23)$$

Penny-shaped micro-cracks in the matrix

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : (\boldsymbol{\varepsilon}_M - \boldsymbol{\varepsilon}_{IN} - \boldsymbol{\varepsilon}_{FRM}) \quad (19)$$

$$\boldsymbol{\sigma}_\Omega = \mathbf{D}_\Omega : \boldsymbol{\varepsilon}_\Omega = \mathbf{D}_\Omega : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c) \quad (20)$$

Consistency equation

$$\mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c) = \mathbf{D}_M : (\varepsilon_o + \varepsilon_c - \varepsilon_\tau - \varepsilon_{FRM\Omega}) \quad (22)$$

Constrained strain

$$\varepsilon_c = \mathbf{S}_\Omega : (\varepsilon_\tau - \varepsilon_{IN}) \quad (23)$$

Penny-shaped micro-cracks in the matrix

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : (\boldsymbol{\varepsilon}_M - \boldsymbol{\varepsilon}_{IN} - \boldsymbol{\varepsilon}_{FRM}) \quad (19)$$

$$\boldsymbol{\sigma}_\Omega = \mathbf{D}_\Omega : \boldsymbol{\varepsilon}_\Omega = \mathbf{D}_\Omega : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c) \quad (20)$$

Consistency equation

$$\mathbf{D}_\Omega : (\varepsilon_o + \varepsilon_c) = \mathbf{D}_M : (\varepsilon_o + \varepsilon_c - \varepsilon_\tau - \varepsilon_{FRM\Omega}) \qquad (22)$$

Constrained strain

$$\varepsilon_c = \mathbf{S}_\Omega : (\varepsilon_\tau - \varepsilon_{IN}) \qquad (23)$$

Transformation eigenstrain

$$\varepsilon_\tau = \mathbf{A}_\Omega : (\varepsilon_o - \mathbf{S}_\Omega : \varepsilon_{IN}) - \mathbf{B}_\Omega : \varepsilon_{FRM\Omega} \qquad (24)$$

where $\mathbf{B}_\Omega = [(\mathbf{D}_\Omega - \mathbf{D}_M : \mathbf{S}_\Omega + \mathbf{D}_M]^{-1} \cdot \mathbf{D}_M$ (25)

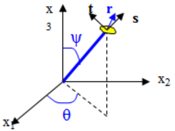
Local model of fracture strain

$$\mathbf{e}_{FRM} = C_{LM} : \mathbf{s}_M \quad (26a)$$

$$\mathbf{s}_M = N \cdot \boldsymbol{\sigma}_M \quad (26b)$$

$$\mathbf{e}_{FRM} = C_{LM} : N \cdot \boldsymbol{\sigma}_M \quad (26c)$$

$$\boldsymbol{\varepsilon}_{FRM} = \int N^T \cdot e_{FRM} \cdot ds \quad (26d)$$



Reference system

$$\boldsymbol{\varepsilon}_{FRM} = (\mathbf{I}^{2s} + \mathbf{C}_{add})^{-1} \cdot \mathbf{C}_{add} : \mathbf{D}_M : (\boldsymbol{\varepsilon}_M - \boldsymbol{\varepsilon}_{IN}) \quad (27a)$$

$$\boldsymbol{\varepsilon}_{FRM\Omega} = (\mathbf{I}^{2s} + \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{V}_\Omega)^{-1} \cdot \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{U}_\Omega : (\boldsymbol{\varepsilon}_M - \mathbf{S}_\Omega : \boldsymbol{\varepsilon}_{IN}) \quad (27b)$$

where

$$\mathbf{C}_{add} = \frac{1}{2\pi} \int_{2\pi} \int_{\frac{\pi}{2}} N_\varepsilon : C_{LM} : N \cdot \frac{\omega(\theta,\psi)}{1-\omega(\theta,\psi)} sin(\psi) \mathrm{d}\psi \mathrm{d}\theta \quad (28a)$$

$$\mathbf{U}_\Omega = \mathbf{I}^{2s} + (\mathbf{S}_\Omega - \mathbf{I}^{2s}) : \mathbf{A}_\Omega, \quad (28b)$$

$$\mathbf{V}_\Omega = \mathbf{I}^{2s} + (\mathbf{S}_\Omega - \mathbf{I}^{2s}) : \mathbf{B}_\Omega \quad (28c)$$

Inelastic strain and micro-cracks in the matrix

Constitutive equation

$$\bar{\boldsymbol{\sigma}} = \mathbf{D}_{M\Omega FR} : (\bar{\varepsilon} - \varepsilon_{INFREQ}) \tag{29}$$

where

$$\mathbf{D}_{M\Omega FR} = \mathbf{F} : \mathbf{H} \tag{30a}$$

$$\boldsymbol{\varepsilon}_{INFREQ} = [(\mathbf{D}_{M\Omega FR}{}^{-1} : \mathbf{G}) - \mathbf{J}] : \boldsymbol{\varepsilon}_{IN} \tag{30b}$$

$$\mathbf{F} = f_\Omega \cdot \mathbf{D}_M \mathbf{U}_\Omega - f_\Omega \cdot \mathbf{D}_M : \mathbf{V}_\Omega \cdot (\mathbf{I}^{2s} + \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{V}_\Omega)^{-1} \cdot \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{U}_\Omega + f_M \cdot \mathbf{D}_M - f_M \cdot \mathbf{D}_M \mathbf{C}_{add} \cdot (\mathbf{I}^{2s} + \mathbf{C}_{add} : \mathbf{D}_M)^{-1} \cdot \mathbf{D}_M \tag{30c}$$

$$\mathbf{H} = [f_\Omega \cdot \mathbf{D}_\Omega^{-1} : \mathbf{D}_M : U_\Omega + f_M \cdot \mathbf{I}^{2s} - f_\Omega \cdot \mathbf{D}_\Omega^{-1} : \mathbf{D}_M : V_\Omega \cdot (\mathbf{I}^{2s} + \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{V}_\Omega)^{-1} \cdot \mathbf{C}_{add} : \mathbf{D}_M : U_\Omega]^{-1} \tag{30d}$$

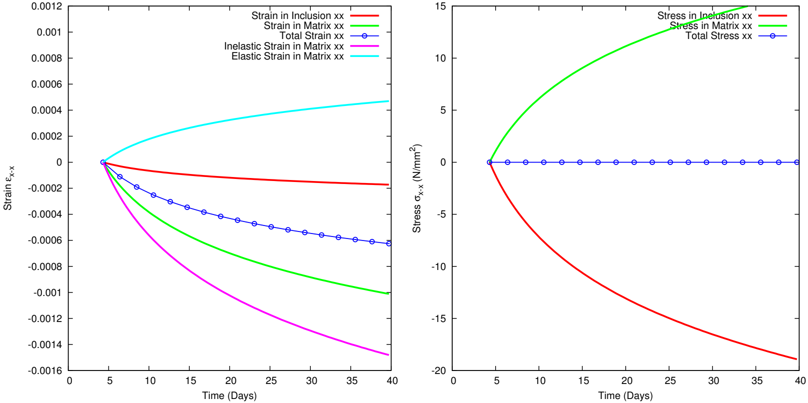
$$\mathbf{G} = f_\Omega \cdot \mathbf{D}_M \mathbf{U}_\Omega : \mathbf{S}_\Omega - f_\Omega \cdot \mathbf{D}_M : \mathbf{V}_\Omega \cdot (\mathbf{I}^{2s} + \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{V}_\Omega)^{-1} \cdot \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{U}_\Omega : \mathbf{S}_\Omega + f_M \cdot \mathbf{D}_M - f_M \cdot \mathbf{D}_M \mathbf{C}_{add} \cdot (\mathbf{I}^{2s} + \mathbf{C}_{add} : \mathbf{D}_M)^{-1} \cdot \mathbf{D}_M \tag{30e}$$

$$\mathbf{J} = [f_\Omega \cdot \mathbf{D}_\Omega^{-1} : \mathbf{D}_M : U_\Omega - f_\Omega \cdot \mathbf{D}_\Omega^{-1} : \mathbf{D}_M : V_\Omega \cdot (\mathbf{I}^{2s} + \mathbf{C}_{add} : \mathbf{D}_M : \mathbf{V}_\Omega)^{-1} \cdot \mathbf{C}_{add} : \mathbf{D}_M : U_\Omega] : \mathbf{S}_\Omega \tag{30f}$$

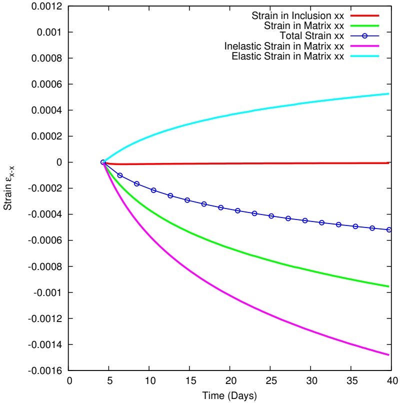
(30g)

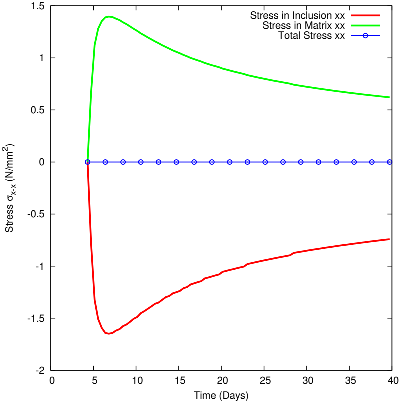
Content Outline

Free shrinkage with inelastic strain in matrix only with no micro-cracking

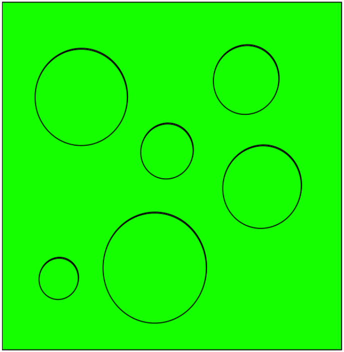


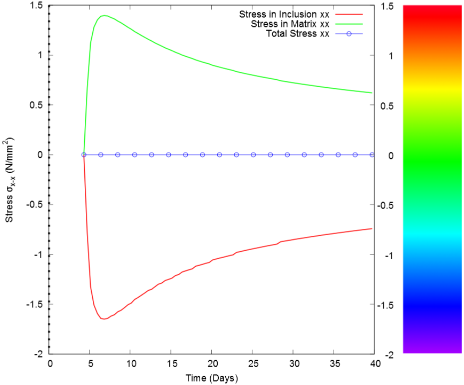
Free shrinkage with inelastic strain in matrix with micro-cracking



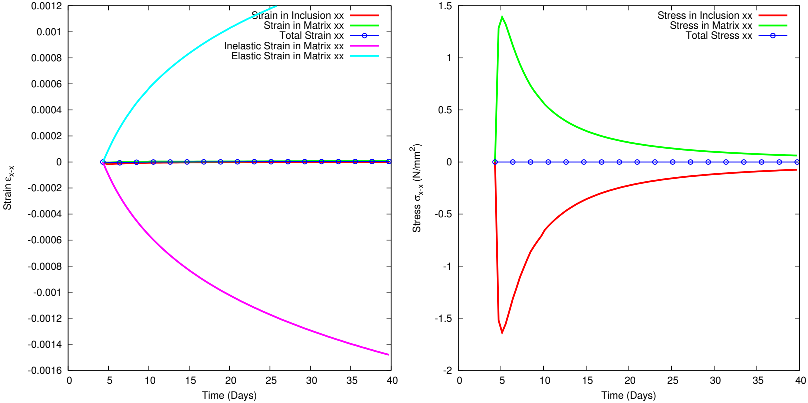


Free shrinkage with inelastic strain in matrix with micro-cracking

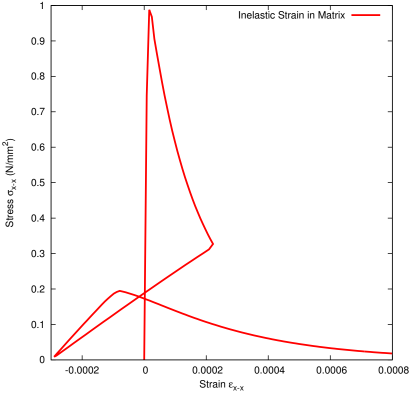


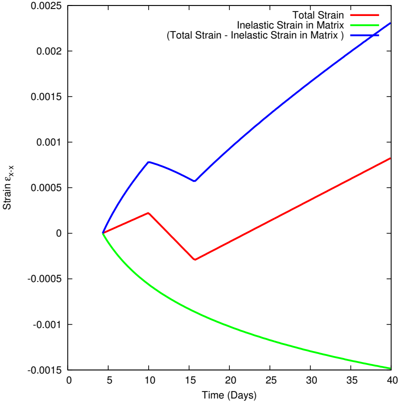


Free shrinkage comparison with elastic constraint method (early results)



Uni-axial tension strain path with inelastic strain in matrix





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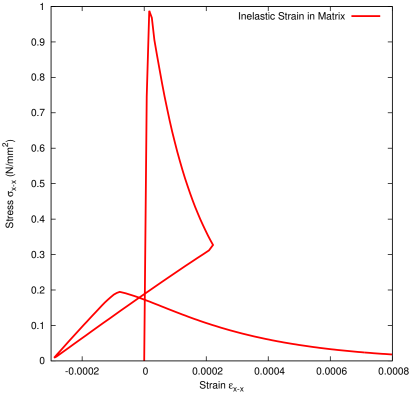
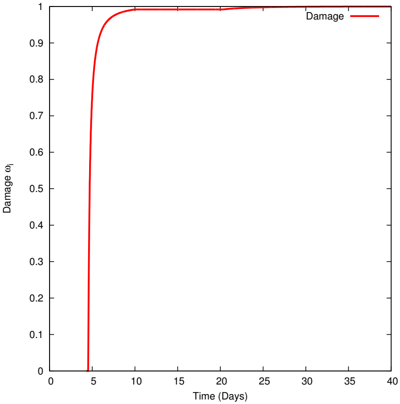
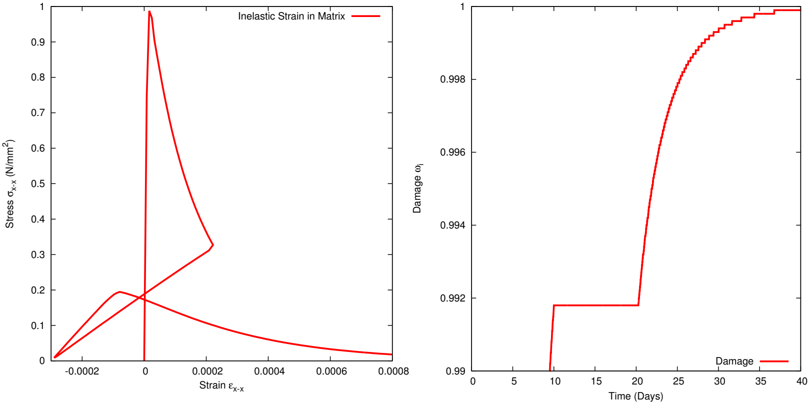
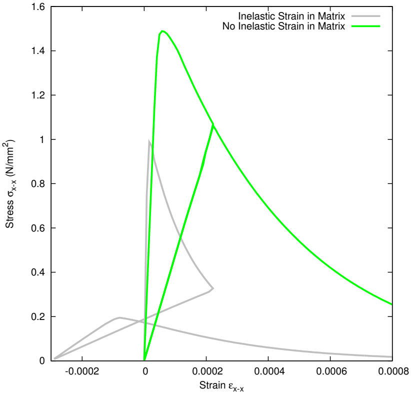


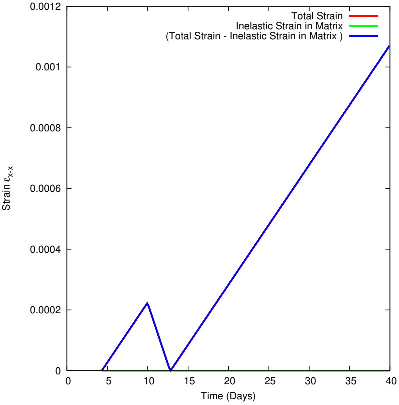


Uni-axial tension strain path with inelastic strain in matrix

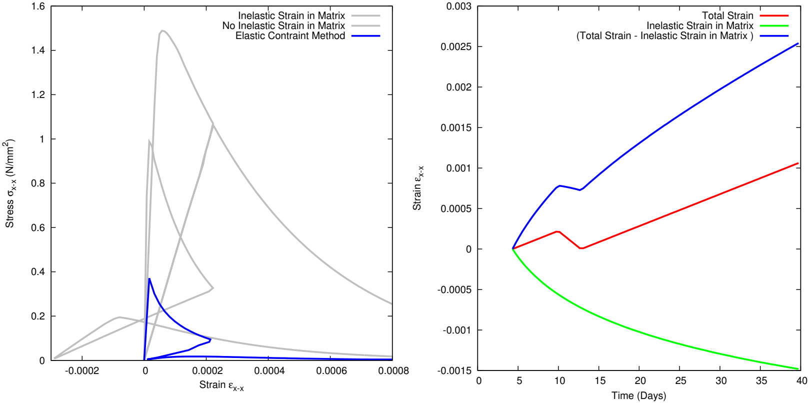


Uni-axial tension strain path no inelastic strain in matrix





Uni-axial tension strain path comparison with Elastic Constraint Method (early results)



Content Outline

1. Elastic two-phase composite
2. Non-linear behaviour within the composite
3. A two-phase composite with inelastic strain in the matrix only
4. Micro-cracks in the matrix
5. Damage predictions
6. Concluding remarks

Concluding remarks

- A new way of introducing inelastic strains into the matrix
- Introducing micro-cracking into the matrix
- Models predict an expected inelastic and micro-cracking response
- Basic framework for simulating real behaviour of cementitious materials

Future work

- Inelastic creep strain using solidification theory
- Integration of new thermo-hygro model
- Modelling self-healing processes
- Experimental work for model validation

Thank you for your attention.

I now welcome your questions.

First principle derivation

1. One material ellipsoid undergoes a transformation

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c) \qquad \boldsymbol{\sigma}_{Mi} = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_i) \text{ where } \boldsymbol{\varepsilon}_c = \mathbf{S}_\Omega : \boldsymbol{\varepsilon}_i$$

2. Standard two material problem

$$\boldsymbol{\sigma}_\Omega = \mathbf{D}_\Omega : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c) = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_\tau) \text{ where } \boldsymbol{\varepsilon}_c = \mathbf{S}_\Omega : \boldsymbol{\varepsilon}_\tau$$

3. Standard two material problem with ε_i in the Ω

$$\mathbf{D}_\Omega : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_i) = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_\tau - \boldsymbol{\varepsilon}_i) \text{ where } \boldsymbol{\varepsilon}_c = \mathbf{S}_\Omega : (\boldsymbol{\varepsilon}_\tau + \boldsymbol{\varepsilon}_i)$$

4. One material problem with M undergoing ε_i

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c) \qquad \boldsymbol{\sigma}_{Mi} = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_i) \text{ where } \boldsymbol{\varepsilon}_c = \mathbf{S}_\Omega : \boldsymbol{\varepsilon}_i$$

transformation strain on outside (added to both sides)

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c + \boldsymbol{\varepsilon}_i) \qquad \boldsymbol{\sigma}_{Mi} = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_i + \boldsymbol{\varepsilon}_i) \text{ where } \boldsymbol{\varepsilon}_c = \mathbf{S}_\Omega : \boldsymbol{\varepsilon}_i$$

Ω undergoing -ve strain to start with (removed to both sides)

$$\boldsymbol{\sigma}_M = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c - \boldsymbol{\varepsilon}_i) \qquad \boldsymbol{\sigma}_{Mi} = \mathbf{D}_M : (\boldsymbol{\varepsilon}_o + \boldsymbol{\varepsilon}_c + \boldsymbol{\varepsilon}_i - \boldsymbol{\varepsilon}_i) \text{ where } \boldsymbol{\varepsilon}_c = -\mathbf{S}_\Omega : \boldsymbol{\varepsilon}_i$$