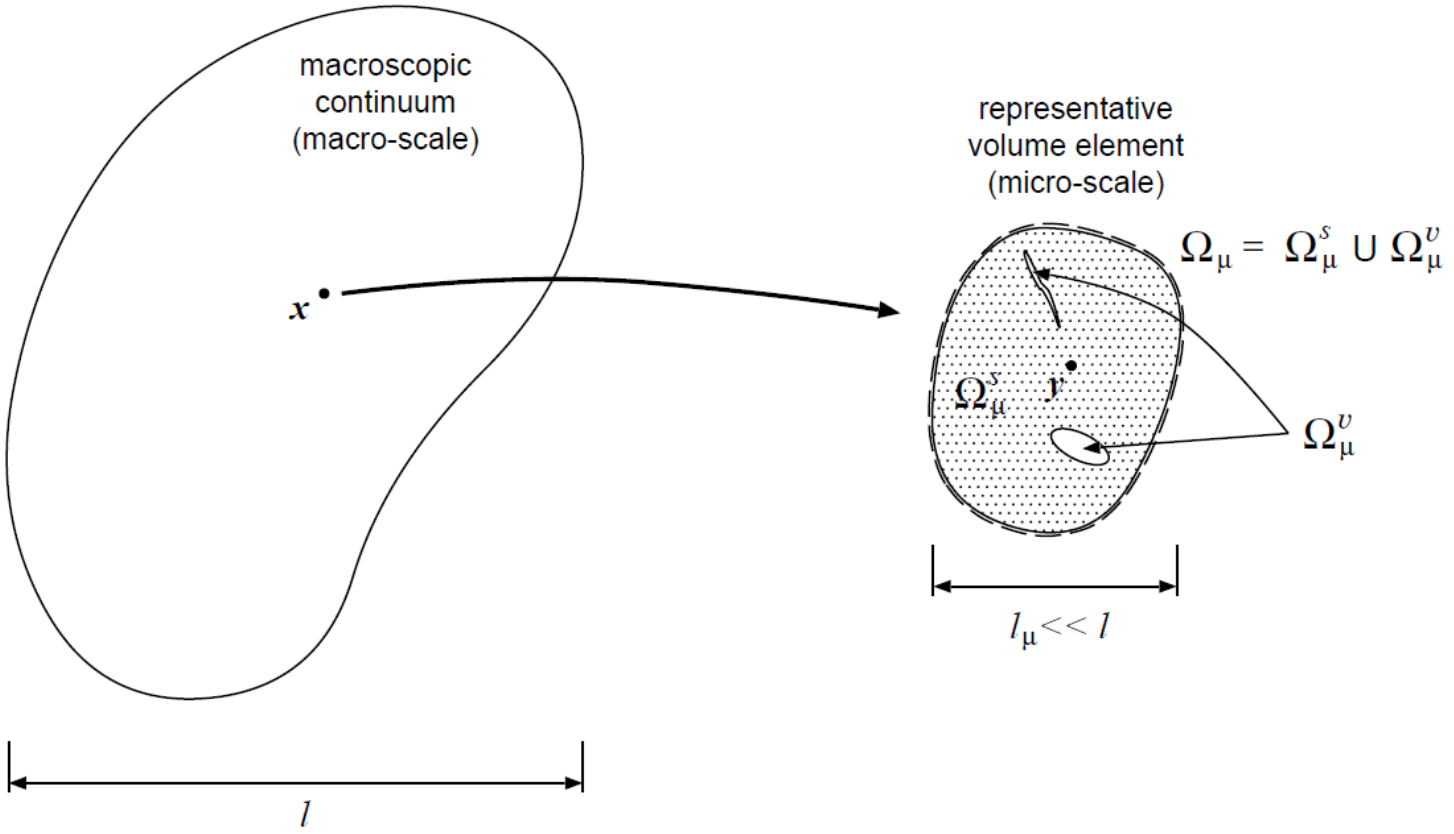
Multiscale Constitutive Modelling of Solids

Topics:

- *Multiscale constitutive theory*
- *Finite element implementation*
- *Applications*



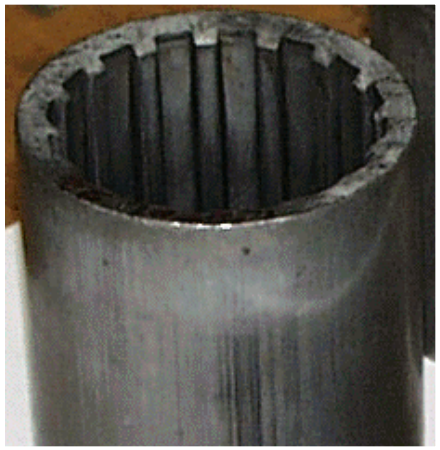
Macro-continuum and the RVE

Multiscale constitutive theory
Background

- Continuum formulation
  - Foundations established by Hill (1960s) and Mandel (1971)
  - Significant contributions, especially related to mathematical concepts, by Sanchez-Palencia and Suquet (1980s)
  - Large number of works related to the estimates of material properties of heterogeneous composites (Nemat-Nasser, Hori, Willis, Ponte-Castaneda and others); still ongoing
- Computational strategies based on FE
  - Feyel and Chaboche (2000): on basic FE methodology
  - Miehe and co-workers (1999,2002,2003): on generic formulation for linear and nonlinear problems
  - Kouznetsova, Brekelmans, Baaijens, Geers (2001,2002): on basic methodology and gradient enhanced models
  - Terada and Kikuchi (2001): generic formulation for linear and nonl. pr.
  - Ladeveze and co-workers (2001): on generic strategies for composites
  - Wriggers and Zohdi (2004): computational estimates of material properties; Wriggers (2007) on homogenisation of particulate materials
  - Ibrahimbegovic and co-workers (2004)
  - Ramm and co-workers (2005):localised failure analysis
  - Belytschko et al. (2007): failure at micro-level; aggregation discontinuities

Why multiscale constitutive models ?

real workpiece



Underlying model:
Lemaitre's ductile damage model with tensile/ compressive
damage growth distinction

Why multiscale constitutive models ?

- Improve predictive capability in numerical simulations
  - Coupled multiscale FE analysis (FE^2)
  - Calibration of phenomenological (macroscopic) models
  - Devising new macroscopic models
- Understanding microscopic mechanisms and their impact on macroscopic behaviour
- Design of new materials

Multiscale Constitutive Theory

Classical internal variable-based constitutive theory

$$\boldsymbol{\sigma}(t) = \mathfrak{F}(\boldsymbol{\varepsilon}^t)$$

Simplest model (linear elasticity – non-dissipative)

$$\boldsymbol{\sigma}(t) = \mathsf{D}^e : \boldsymbol{\varepsilon}(t)$$

A simple dissipative model (Norton's creep law)

$$\begin{cases} \boldsymbol{\sigma} = \mathsf{D}^e : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^p\right) \\ \dot{\boldsymbol{\varepsilon}}^p = \left(\dfrac{\|\operatorname{dev}\boldsymbol{\sigma}\|}{\lambda}\right)^N \operatorname{dev}\boldsymbol{\sigma} \end{cases}$$

$$\longrightarrow \quad \dot{\boldsymbol{\sigma}}(t) = \mathsf{D}^e : \left[\dot{\boldsymbol{\varepsilon}}(t) - \left(\frac{\|\operatorname{dev}\boldsymbol{\sigma}(t)\|}{\lambda}\right)^N \operatorname{dev}\boldsymbol{\sigma}(t)\right]$$

Multiscale constitutive theory

$$\boldsymbol{\sigma}(t) = \mathfrak{F}(\boldsymbol{\varepsilon}^t)$$

… history dependence concept same as in classical theory, BUT

The evolution of the stress is generally described by an initial boundary value problem at the so-called microscopic (RVE) level !!

(as opposed to ODEs in the classical case)

Multiscale constitutive theory

Basic axioms *(EA de Souza Neto & RA Feijoo, 2010)*

(i) Strain/deformation gradient averaging;

(ii) Functional set of admissible fluctuations is a subspace of the minimally constrained space of displacement fields compatible with the deformation gradient averaging;

(iii) Equilibrium of the RVE (principle of virtual work);

(iv) Stress averaging; and

(v) Hill-Mandel Principle of Macro-homogeneity.

(i) Strain averaging

$$\boldsymbol{\varepsilon}(\boldsymbol{x},t) = \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu(\boldsymbol{y},t)\,\mathrm{d}V \qquad\qquad \boldsymbol{\varepsilon}_\mu \equiv \nabla^s \boldsymbol{u}_\mu$$

Consequence Minimally constrained set of RVE displacements fields

$$\boldsymbol{u}_\mu \in \mathscr{K}^*_\mu \equiv \left\{ \boldsymbol{v},\ \text{sufficiently regular} \ \middle|\ \int_{\partial\Omega_\mu} \boldsymbol{v}\otimes_s \boldsymbol{n}\,\mathrm{d}A = V_\mu\,\boldsymbol{\varepsilon} \right\}$$

In terms of displacements fluctuations,

$$\tilde{\boldsymbol{u}}_\mu(\boldsymbol{y},t) \equiv \boldsymbol{u}_\mu(\boldsymbol{y},t) - \{\boldsymbol{u}(\boldsymbol{x},t) + \boldsymbol{\varepsilon}\,\boldsymbol{y}\}$$

$$\tilde{\boldsymbol{u}}_\mu \in \tilde{\mathscr{K}}^*_\mu \equiv \left\{ \boldsymbol{v},\ \text{sufficiently regular} \ \middle|\ \int_{\partial\Omega_\mu} \boldsymbol{v}\otimes_s \boldsymbol{n}\,\mathrm{d}A = \boldsymbol{0} \right\}$$

(ii) The actual kinematical constraints are such that

$$\tilde{\mathcal{K}}_\mu \subset \tilde{\mathcal{K}}_\mu^*$$

is a *subspace* of $\tilde{\mathcal{K}}_\mu^*$

Consequence Space of virtual displacements coincides with the space of admissible fluctuations

$$\mathcal{V}_\mu = \tilde{\mathcal{K}}_\mu$$

(iii) Equilibrium of the RVE

$$\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu(\boldsymbol{y},t) : \nabla^s \boldsymbol{\eta}\, \mathrm{d}V - \int_{\Omega_\mu} \boldsymbol{b}(\boldsymbol{y},t)\cdot\boldsymbol{\eta}\, \mathrm{d}V - \int_{\partial\Omega_\mu} \boldsymbol{t}^e(\boldsymbol{y},t)\cdot\boldsymbol{\eta}\, \mathrm{d}A = 0 \qquad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu$$

(iv) Stress averaging

$$\boldsymbol{\sigma}(\boldsymbol{x},t) \equiv \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu(\boldsymbol{y},t)\, \mathrm{d}V$$

(v) Hill-Mandel Principle

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} = \frac{1}{V_\mu}\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu : \dot{\boldsymbol{\varepsilon}}_\mu\, \mathrm{d}V$$

Consequences

- **Body force** and **external traction fields** are **orthogonal to** $\mathcal{V}_\mu$ (**reactive load systems to the chosen kinematical constraints**)

$$\int_{\partial\Omega_\mu} \boldsymbol{t}^e \cdot \boldsymbol{\eta}\ \mathrm{d}A = 0\,; \qquad \int_{\Omega_\mu^s} \boldsymbol{b} \cdot \boldsymbol{\eta}\ \mathrm{d}V = 0 \qquad \forall\, \boldsymbol{\eta} \in \mathcal{V}_\mu$$

- Reduced RVE equilibrium problem

$$G(\boldsymbol{\varepsilon}, \tilde{\boldsymbol{u}}_\mu, \boldsymbol{\eta}) \equiv \int_{\Omega_\mu^s} \mathfrak{F}_y\{[\boldsymbol{\varepsilon}(\boldsymbol{x},t) + \nabla^s \tilde{\boldsymbol{u}}_\mu(\boldsymbol{y},t)]^t\} : \nabla^s \boldsymbol{\eta}\, \mathrm{d}V$$

$$- \int_{\partial\Omega_\mu^v} \boldsymbol{t}^v(\boldsymbol{y},t) \cdot \boldsymbol{\eta}\, \mathrm{d}A \ = \ 0 \qquad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu$$

where it is generally assumed that $\boldsymbol{\sigma}_\mu(\boldsymbol{y},t) = \mathfrak{F}_y(\boldsymbol{\varepsilon}_\mu^t(\boldsymbol{y}))$

The choices of $\mathscr{V}_\mu$

(a) Taylor model

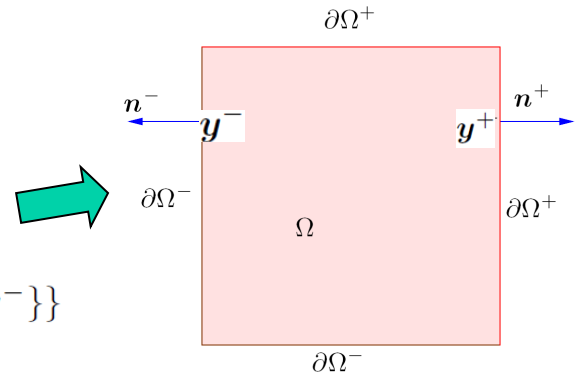
$$\mathscr{V}_\mu = {}^{\text{Taylor}}\mathscr{V}_\mu \equiv \{\mathbf{0}\}$$

(b) Linear boundary displacements model

$$\mathscr{V}_\mu = {}^{\text{lin}}\mathscr{V}_\mu \equiv \{\, \tilde{\boldsymbol{u}}_\mu \in \tilde{\mathscr{K}}^*_\mu \mid \tilde{\boldsymbol{u}}_\mu(\boldsymbol{y},t) = \mathbf{0} \;\; \forall\, \boldsymbol{y} \in \partial\Omega_\mu \}$$

(c) Periodic boundary displacements fluctuations model

$$\begin{aligned} \mathscr{V}_\mu &= {}^{\text{per}}\mathscr{V}_\mu \\ &\equiv \{\, \tilde{\boldsymbol{u}}_\mu \in \tilde{\mathscr{K}}^*_\mu \mid \tilde{\boldsymbol{u}}_\mu(\boldsymbol{y}^+,t) = \tilde{\boldsymbol{u}}_\mu(\boldsymbol{y}^-,t) \;\; \forall \text{ pairs } \{\boldsymbol{y}^+,\boldsymbol{y}^-\} \} \end{aligned}$$



(d) Minimum kinematical constraint (or uniform boundary traction)

$$\mathscr{V}_\mu \equiv \left\{ \boldsymbol{v},\ \text{sufficiently regular} \;\middle|\; \int_{\partial\Omega_\mu} \boldsymbol{v} \otimes_s \boldsymbol{n}\, \mathrm{d}A = \mathbf{0} \right\}$$

Remarks

- Note that

$$\overset{\text{Taylor}}{\mathcal{V}}_\mu \subset \overset{\text{lin}}{\mathcal{V}}_\mu \subset \overset{\text{per}}{\mathcal{V}}_\mu \subset \overset{\text{uni}}{\mathcal{V}}_\mu$$

  That is, the Taylor model results in stiffest response (**upper bound**), while uniform traction results in the softest response (**lower bound**).

- The use of different $\mathcal{V}_\mu$ for a given RVE generally produces different estimates.

- The choice of $\mathcal{V}_\mu$ (the **kinematical constraints**) for a given RVE fully **defines the model !**

The macroscopic constitutive tangent tensor

$$\mathbb{C} = \bar{\mathbb{C}} + \tilde{\mathbb{C}}$$

where $\bar{\mathbb{C}}$ is the Taylor (volume average) constitutive tangent tensor and

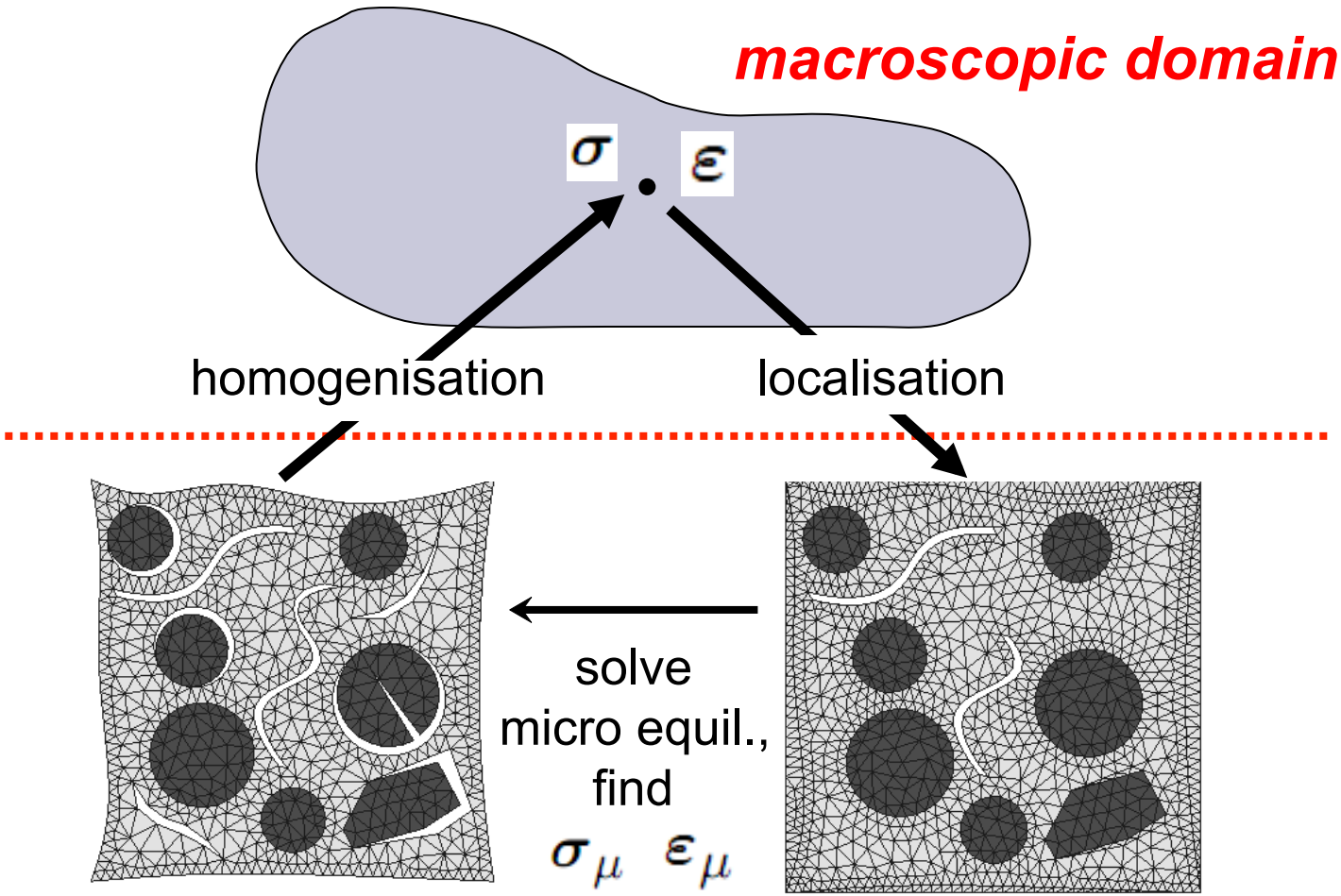
$$\tilde{\mathbb{C}} = \left[\frac{1}{V_\mu} \int_{\Omega_\mu} (\tilde{\mathbf{T}}_{\mu_{kl}})_{ij} \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l) \qquad \tilde{\mathbf{T}}_{\mu_{ij}} = \mathbb{C}_\mu \nabla^{\mathrm{s}} \tilde{\mathbf{u}}_{\mu_{ij}}$$

$$\int_{\Omega_\mu} \mathbb{C}_\mu \nabla^{\mathrm{s}} \tilde{\mathbf{u}}_{\mu_{ij}} \cdot \nabla^{\mathrm{s}} \boldsymbol{\eta} = - \int_{\Omega_\mu} \mathbb{C}_\mu (\mathbf{e}_i \otimes \mathbf{e}_j) \cdot \nabla^{\mathrm{s}} \boldsymbol{\eta} \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu$$

Multiscale constitutive theory
Typical applications

- Coupled multiscale FE analysis (FE^2) → expensive!
- Calibration of phenomenological (macroscopic) models
- Devising new macroscopic models
- Understanding microscopic mechanisms and their impact on macroscopic behaviour
- Design/optimisation of microstructures

Application. ***Fully coupled FE analysis***



discretised macroscopic domain (RVE)

Finite element solution of the RVE equil. problem

Discretised RVE non-linear equilibrium problem

$$G^h(\tilde{\mathbf{u}}_\mu^{n+1}) \equiv \left\{ \int_{\Omega_\mu^h} \mathbf{B}^T \, \hat{\boldsymbol{\sigma}}_y(\boldsymbol{\varepsilon}^{n+1} + \mathbf{B}\, \tilde{\mathbf{u}}_\mu^{n+1}) \, \mathrm{d}V \right\} \cdot \boldsymbol{\eta} = 0$$

$$\forall\, \boldsymbol{\eta} \in \tilde{\mathscr{K}}_\mu^h,$$

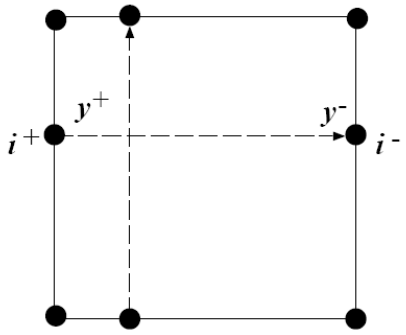
Linearised form. Newton-Raphson iteration

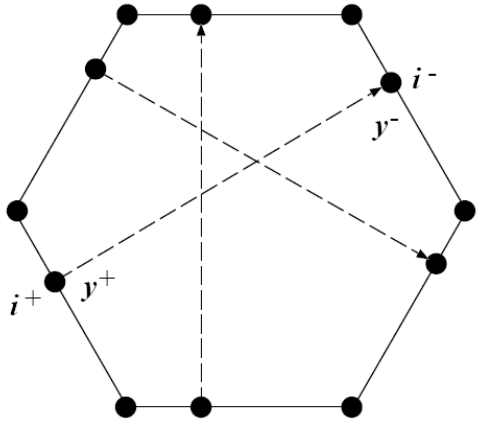
$$\left[\mathbf{F}^{(k-1)} + \mathbf{K}^{(k-1)} \, \delta\tilde{\mathbf{u}}_\mu^{(k)} \right] \cdot \boldsymbol{\eta} = 0 \qquad \forall\, \boldsymbol{\eta} \in \tilde{\mathscr{K}}_\mu^h,$$

$$\mathbf{F}^{(k-1)} \equiv \int_{\Omega_\mu^h} \mathbf{B}^T \, \hat{\boldsymbol{\sigma}}_y(\boldsymbol{\varepsilon}^{n+1} + \mathbf{B}\, \tilde{\mathbf{u}}_\mu^{(k-1)}) \, \mathrm{d}V,$$

$$\mathbf{K}^{(k-1)} \equiv \int_{\Omega_\mu^h} \mathbf{B}^T \, \mathbf{D}^{(k-1)} \, \mathbf{B} \, \mathrm{d}V$$

Periodic boundary fluctuations





$$\tilde{\mathscr{K}}_{\mu}^{h} = \left\{ \mathbf{v} = \begin{bmatrix} \mathbf{v}_i \\ \mathbf{v}_+ \\ \mathbf{v}_- \end{bmatrix} \;\middle|\; \mathbf{v}_+ = \mathbf{v}_- \right\}$$

$$\rightarrow \quad \left\{ \begin{bmatrix} \mathbf{F}_i \\ \mathbf{F}_+ \\ \mathbf{F}_- \end{bmatrix}^{(k-1)} + \begin{bmatrix} \mathbf{k}_{ii} & \mathbf{k}_{i+} & \mathbf{k}_{i-} \\ \mathbf{k}_{+i} & \mathbf{k}_{++} & \mathbf{k}_{+-} \\ \mathbf{k}_{-i} & \mathbf{k}_{-+} & \mathbf{k}_{--} \end{bmatrix}^{(k-1)} \begin{bmatrix} \delta\tilde{\mathbf{u}}_i \\ \delta\tilde{\mathbf{u}}_+ \\ \delta\tilde{\mathbf{u}}_+ \end{bmatrix}^{(k)} \right\} \cdot \begin{bmatrix} \boldsymbol{\eta}_i \\ \boldsymbol{\eta}_+ \\ \boldsymbol{\eta}_+ \end{bmatrix} = 0 \qquad \forall\, \boldsymbol{\eta}_i, \boldsymbol{\eta}_+$$

$$\left\{ \begin{bmatrix} \mathbf{F}_i \\ \mathbf{F}_+ + \mathbf{F}_- \end{bmatrix}^{(k-1)} + \begin{bmatrix} \mathbf{k}_{ii} & \mathbf{k}_{i+} + \mathbf{k}_{i-} \\ \mathbf{k}_{+i} + \mathbf{k}_{-i} & \mathbf{k}_{++} + \mathbf{k}_{+-} + \mathbf{k}_{-+} + \mathbf{k}_{--} \end{bmatrix}^{(k-1)} \begin{bmatrix} \delta\tilde{\mathbf{u}}_i \\ \delta\tilde{\mathbf{u}}_+ \end{bmatrix}^{(k)} \right\} \cdot \begin{bmatrix} \boldsymbol{\eta}_i \\ \boldsymbol{\eta}_+ \end{bmatrix} = 0$$

$$\forall\, \boldsymbol{\eta}_i, \boldsymbol{\eta}_+,$$

Linearised system. Final format

$$\begin{bmatrix} \mathbf{k}_{ii} & \mathbf{k}_{i+} + \mathbf{k}_{i-} \\ \mathbf{k}_{+i} + \mathbf{k}_{-i} & \mathbf{k}_{++} + \mathbf{k}_{+-} + \mathbf{k}_{-+} + \mathbf{k}_{--} \end{bmatrix}^{(k-1)} \begin{bmatrix} \delta\tilde{\mathbf{u}}_i \\ \delta\tilde{\mathbf{u}}_+ \end{bmatrix}^{(k)} = - \begin{bmatrix} \mathbf{F}_i \\ \mathbf{F}_+ + \mathbf{F}_- \end{bmatrix}^{(k-1)}$$

Minimum constraint (uniform traction)

$$\tilde{\mathscr{K}_\mu}^h \equiv \left\{ \mathbf{v} = \begin{bmatrix} \mathbf{v}_i \\ \mathbf{v}_b \end{bmatrix} \mid \int_{\partial\Omega_\mu^h} \mathbf{N}_b \mathbf{v}_b \otimes_s \boldsymbol{n} \, \mathrm{d}A = \mathbf{0} \right\}$$

$$\mathbf{C}\,\mathbf{v}_b = \mathbf{0}$$

Global constraint matrix

$$\mathbf{C} = \begin{bmatrix} \int_{\partial\Omega_\mu^h} N_{k+1}\, n_1 \,\mathrm{d}A & 0 & \cdots & \int_{\partial\Omega_\mu^h} N_{k+m}\, n_1 \,\mathrm{d}A & 0 \\ 0 & \int_{\partial\Omega_\mu^h} N_{k+1}\, n_2 \,\mathrm{d}A & \cdots & 0 & \int_{\partial\Omega_\mu^h} N_{k+m}\, n_2 \,\mathrm{d}A \\ \int_{\partial\Omega_\mu^h} N_{k+1}\, n_2 \,\mathrm{d}A & \int_{\partial\Omega_\mu^h} N_{k+1}\, n_1 \,\mathrm{d}A & \cdots & \int_{\partial\Omega_\mu^h} N_m\, n_2 \,\mathrm{d}A & \int_{\partial\Omega_\mu^h} N_m\, n_1 \,\mathrm{d}A \end{bmatrix}$$

Elemental constraint matrix (for an 8-noded isoparametric quad)

$$\mathbf{C}^{(e)} = l^{(e)} \begin{bmatrix} \frac{1}{6} & 0 & \frac{2}{3} & 0 & \frac{1}{6} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{6} & 0 & \frac{2}{3} & 0 & \frac{1}{6} \end{bmatrix}$$

$$[\,\mathbf{C}_f\;\mathbf{C}_d\;\mathbf{C}_p\,]\begin{bmatrix}\mathbf{v}_f\\ \mathbf{v}_d\\ \mathbf{v}_p\end{bmatrix}=\mathbf{0}\qquad\qquad \mathbf{v}_p=\mathbf{0}, \text{ (no rigid body motion)}$$

$$\rightarrow\quad [\,\mathbf{C}_f\;\mathbf{C}_d\,]\begin{bmatrix}\mathbf{v}_f\\ \mathbf{v}_d\end{bmatrix}=\mathbf{0}$$

$$\rightarrow\quad \mathbf{v}_d=\mathbf{R}\,\mathbf{v}_f\qquad \mathbf{R}\equiv-\mathbf{C}_d^{-1}\,\mathbf{C}_f$$

$$\rightarrow\quad \tilde{\mathscr{K}}_\mu^{\,h}\equiv\left\{\mathbf{v}=\begin{bmatrix}\mathbf{v}_i\\ \mathbf{v}_f\\ \mathbf{v}_d\end{bmatrix}\;\middle|\;\mathbf{v}_d=\mathbf{R}\,\mathbf{v}_f\right\}$$

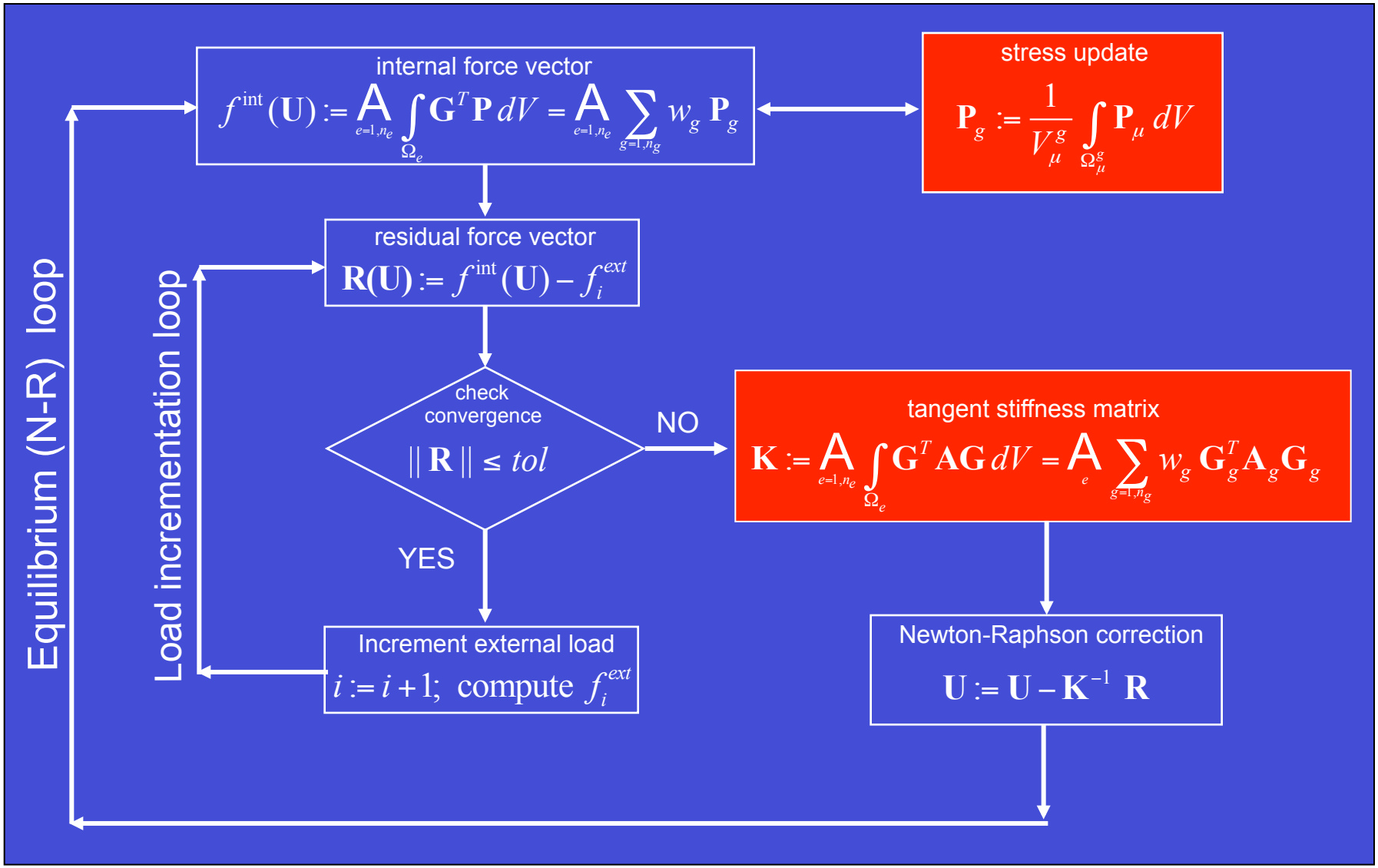
Linearised system

$$\left\{ \begin{bmatrix} \mathbf{F}_i \\ \mathbf{F}_f \\ \mathbf{F}_d \end{bmatrix}^{(k-1)} + \begin{bmatrix} \mathbf{k}_{ii} & \mathbf{k}_{if} & \mathbf{k}_{id} \\ \mathbf{k}_{fi} & \mathbf{k}_{ff} & \mathbf{k}_{fd} \\ \mathbf{k}_{di} & \mathbf{k}_{df} & \mathbf{k}_{dd} \end{bmatrix}^{(k-1)} \begin{bmatrix} \delta\tilde{\mathbf{u}}_i \\ \delta\tilde{\mathbf{u}}_f \\ \mathbf{R}\,\delta\tilde{\mathbf{u}}_f \end{bmatrix}^{(k)} \right\} \cdot \begin{bmatrix} \boldsymbol{\eta}_i \\ \boldsymbol{\eta}_f \\ \mathbf{R}\,\boldsymbol{\eta}_f \end{bmatrix} = 0 \qquad \forall\, \boldsymbol{\eta}_i, \boldsymbol{\eta}_f$$

Final format

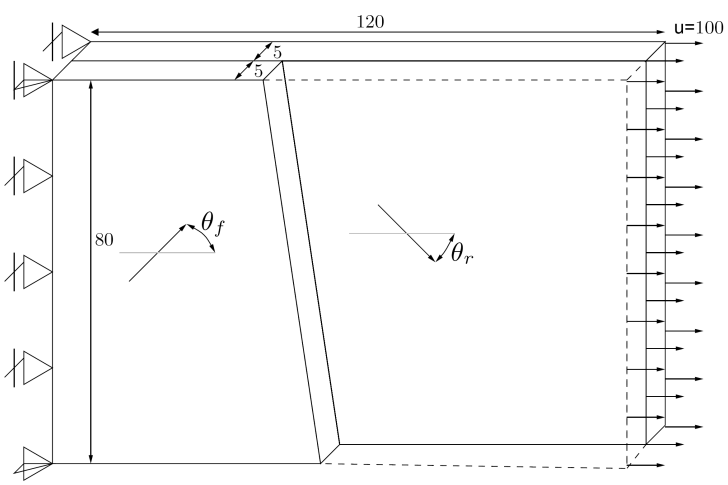
$$\begin{bmatrix} \mathbf{k}_{ii} & \mathbf{k}_{if}+\mathbf{k}_{id}\mathbf{R} \\ \mathbf{k}_{fi}+\mathbf{R}^T\mathbf{k}_{di} & \mathbf{k}_{ff}+\mathbf{k}_{fd}\mathbf{R}+\mathbf{R}^T\mathbf{k}_{df}+\mathbf{R}^T\mathbf{k}_{dd}\mathbf{R} \end{bmatrix}^{(k-1)} \begin{bmatrix} \delta\tilde{\mathbf{u}}_i \\ \delta\tilde{\mathbf{u}}_f \end{bmatrix}^{(k)} = -\begin{bmatrix} \mathbf{F}_i \\ \mathbf{F}_f+\mathbf{R}^T\mathbf{F}_d \end{bmatrix}^{(k-1)}$$

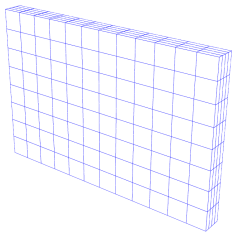
Fully coupled multiscale analysis

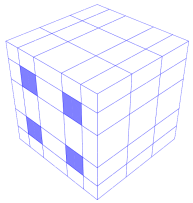


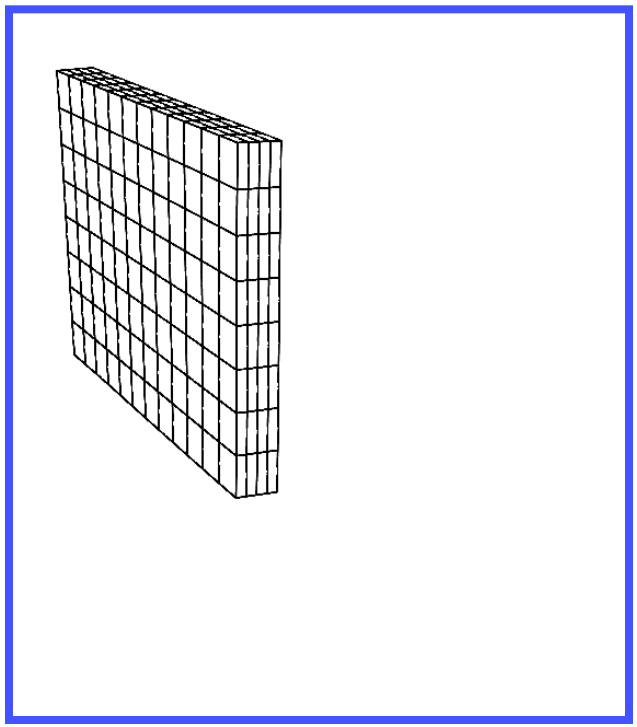
Fully coupled FE analysis. Example

Hyperelastic composite. Two-ply laminate









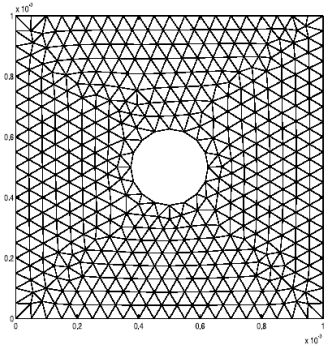
Multiscale constitutive theory
Typical applications

- Coupled multiscale FE analysis (FE^2)
- **Calibration of phenomenological (macroscopic) models**
- Devising new macroscopic models
- Understanding microscopic mechanisms and their impact on macroscopic behaviour
- Design/optimisation of microstructures

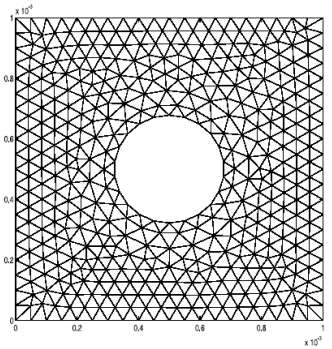
Linear elastic microstructures

No need for coupled analysis as the homogenised constitutive tensor defines completely the macroscopic behaviour !

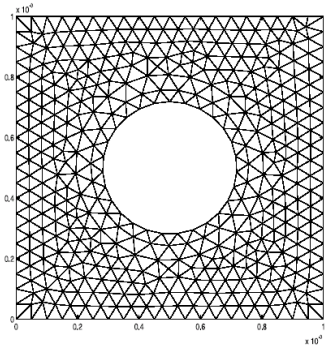
Example:
Linear elastic porous material



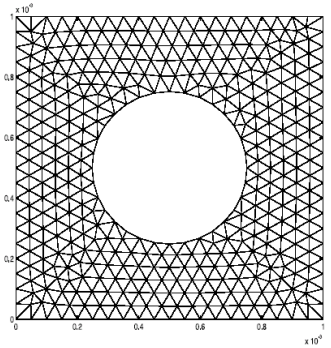
Type 1
5% VVF



Type 2
10% VVF



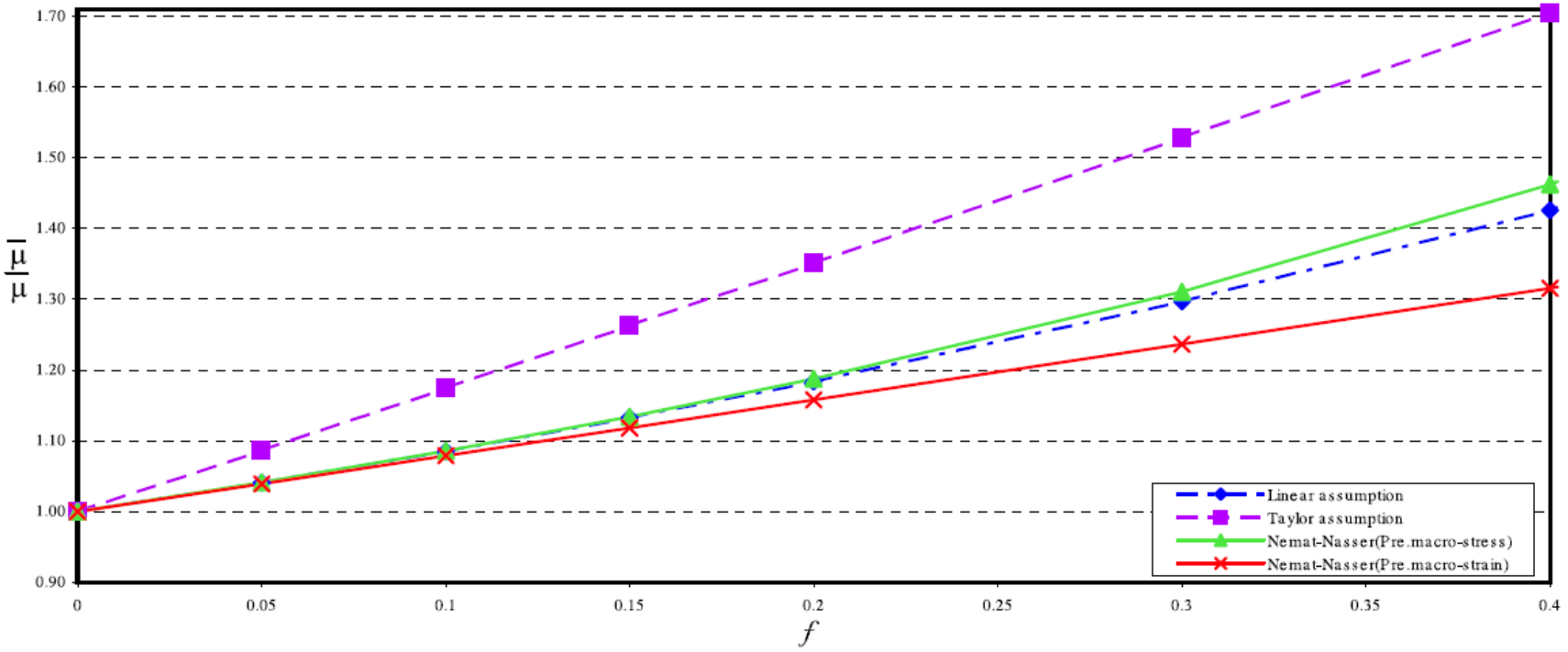
Type 3
15% VVF



Type 4
20% VVF

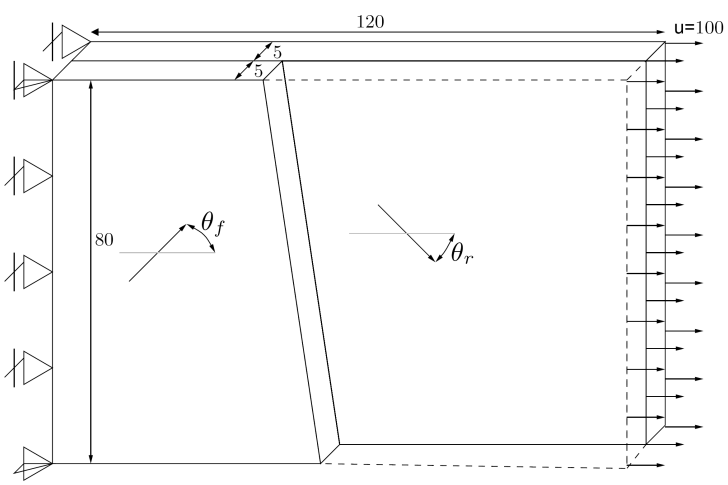
Example: Linear elastic porous material

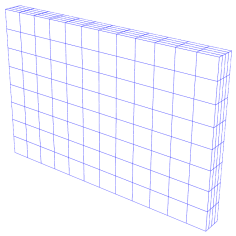
Shear modulus as a function of void volume fraction
(need only compute elasticity tensor)

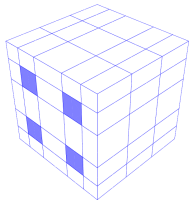


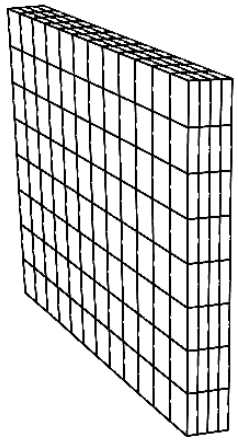
…back to a previous example

Hyperelastic composite. Two-ply laminate









- Single-Scale Transversely Isotropic Continuum Model:

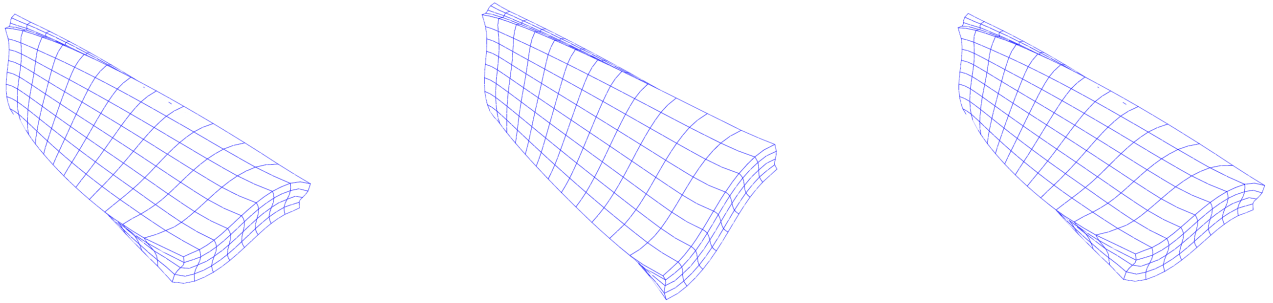
$$\begin{aligned}\Psi_{iso} &= \frac{\mu}{2}(I_1 - 3) - \mu \ln J + \frac{\lambda}{2}(J-1)^2 \\ \Psi_{trn} &= [\alpha + \beta \ln J + \gamma(I_4 - 1)](I_4 - 1) - \frac{\alpha}{2}(I_5 - 1).\end{aligned}$$

Bonet J., Burton AJ., A simple orthotropic, transversely isotropic hyperelastic constitutive equation for large strain computations, *Comput. Methods Appl. Mech. Engrg.*, **162** (1998) 151-164.

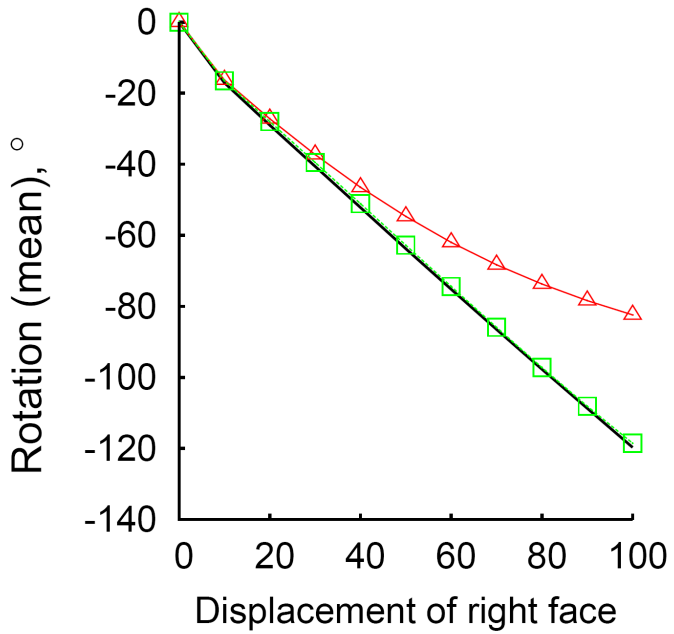
- Multi-Scale Model with Isotropic Neo-Hookean Matrix:

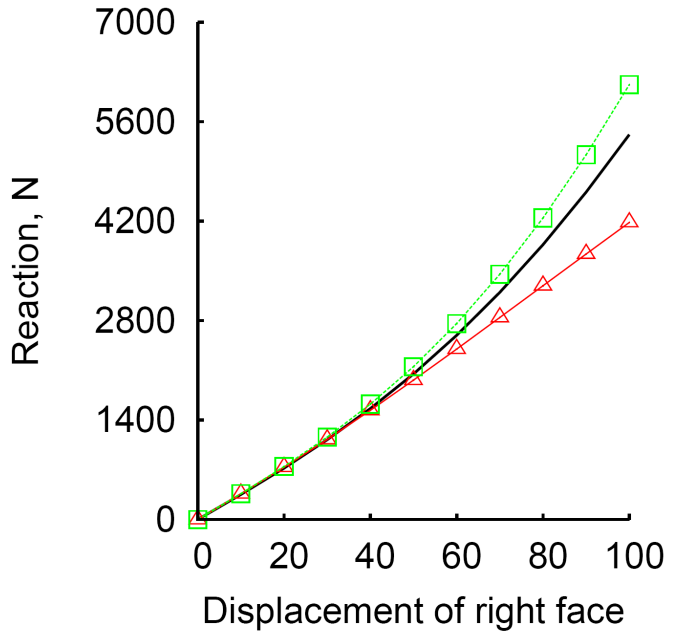
$$\Psi_{mat} = \frac{\mu}{2}(I_1 - 3) - \mu \ln J + \frac{\lambda}{2}(J-1)^2$$

  - Isotropic Neo-Hookean Fiber: $\Psi_{neo} = \Psi_{mat}$
  - Isotropic Ogden Fiber: $\Psi_{ogd} = \sum_{n=1}^{N} \frac{\mu_n}{\alpha_n}(\lambda_1^{\alpha_n} + \lambda_2^{\alpha_n} + \lambda_3^{\alpha_n} - 3)$
    N is a positive integer, $\lambda_{i(i=1,2,3)}$ are the principal stretches and μ_n and α_n are material constants such that $\mu_n \alpha_n > 0\ , \quad n = 1, 2, ..., N$



Single-Scale Model RVE (Neo-Hookean Fibre) RVE (Ogden Fibre)





Multiscale constitutive theory
Typical applications

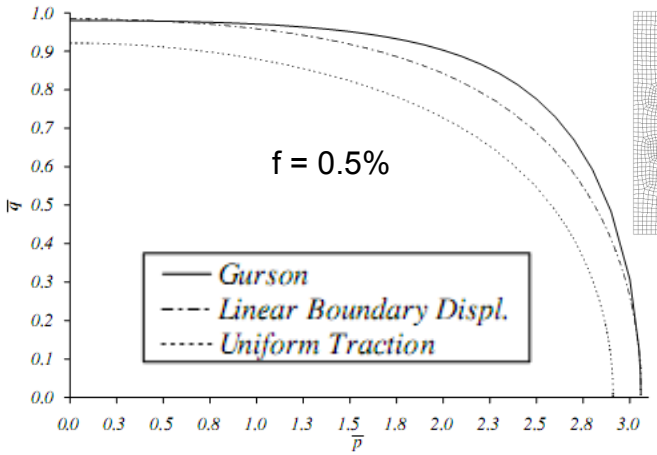
- Coupled multiscale FE analysis (FE^2)
- Calibration of phenomenological (macroscopic) models
- **Devising new macroscopic models**
- Understanding microscopic mechanisms and their impact on macroscopic behaviour
- Design/optimisation of microstructures

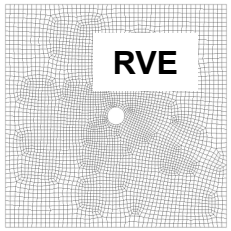
Application. Devising new models

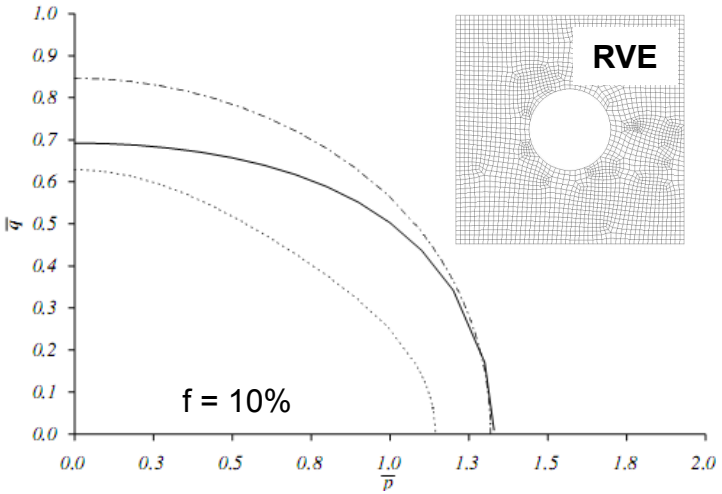
Porous plasticity

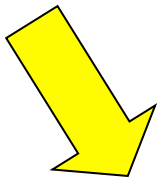
$$\bar{\epsilon} = \alpha \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} + \sqrt{1-\alpha^2} \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

$$\alpha \in [0, 1]$$









Macroscopic yield function

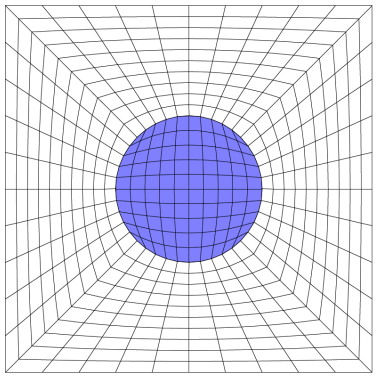
$$\bar{\Phi} = q - C_1 \left[1 - C_2 \sin^2\left(\frac{\pi p}{2P_m}\right)\right] \left\{\frac{1}{C_{\text{eq}}}\left[1 + f^2 - 2fC_3 \cosh\left(\frac{\sqrt{3}C_4 p}{\sigma_Y}\right)\right]\right\}^{\frac{1}{2}} \sigma_Y$$

Application. Devising new models

Plasticity with phase debonding

$$\bar{\boldsymbol{\varepsilon}} = \alpha \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} + \sqrt{1-\alpha^2} \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \quad , \quad \alpha = -1.0, -0.9, ..., 0, ..., 1.0$$

$\Downarrow$



-ideally plastic matrix

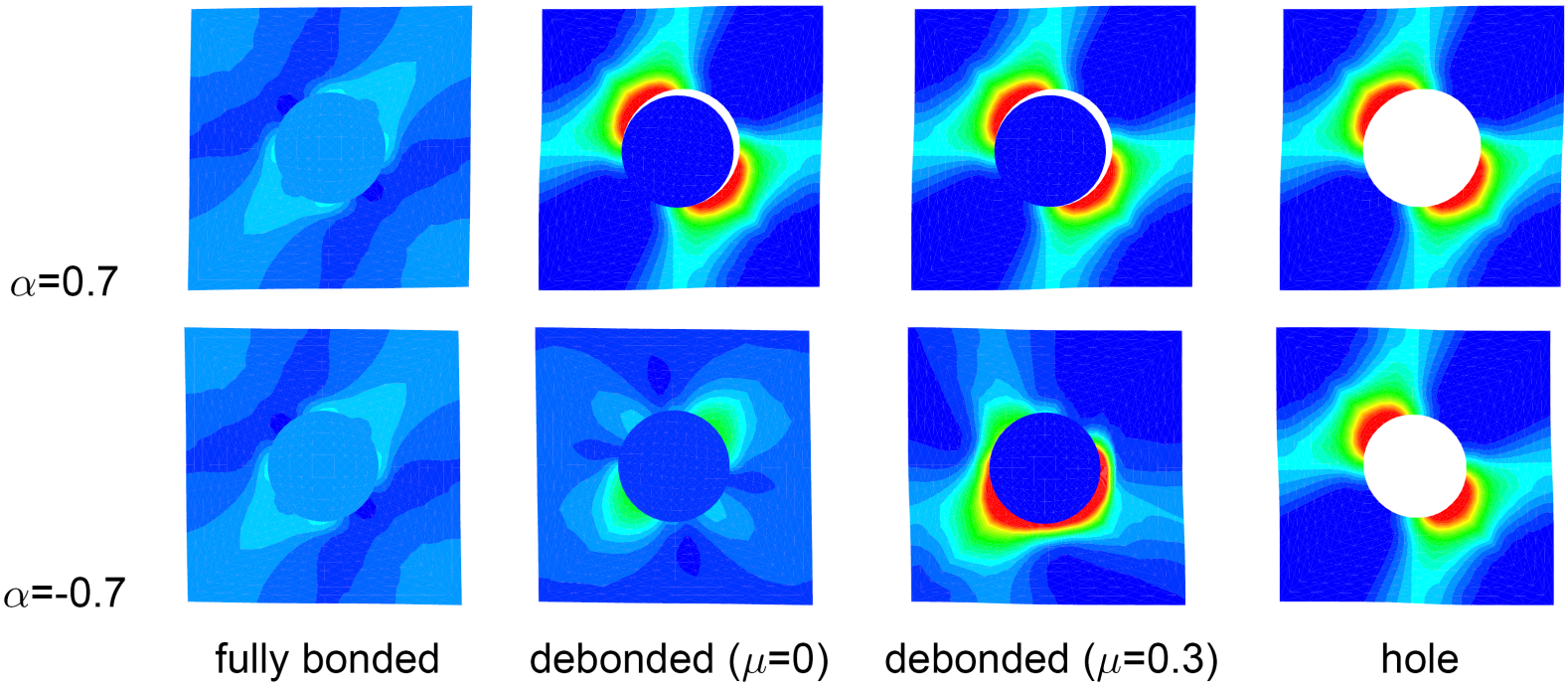
-rigid inclusion

-contact with (μ=0.3) and without (μ=0) friction

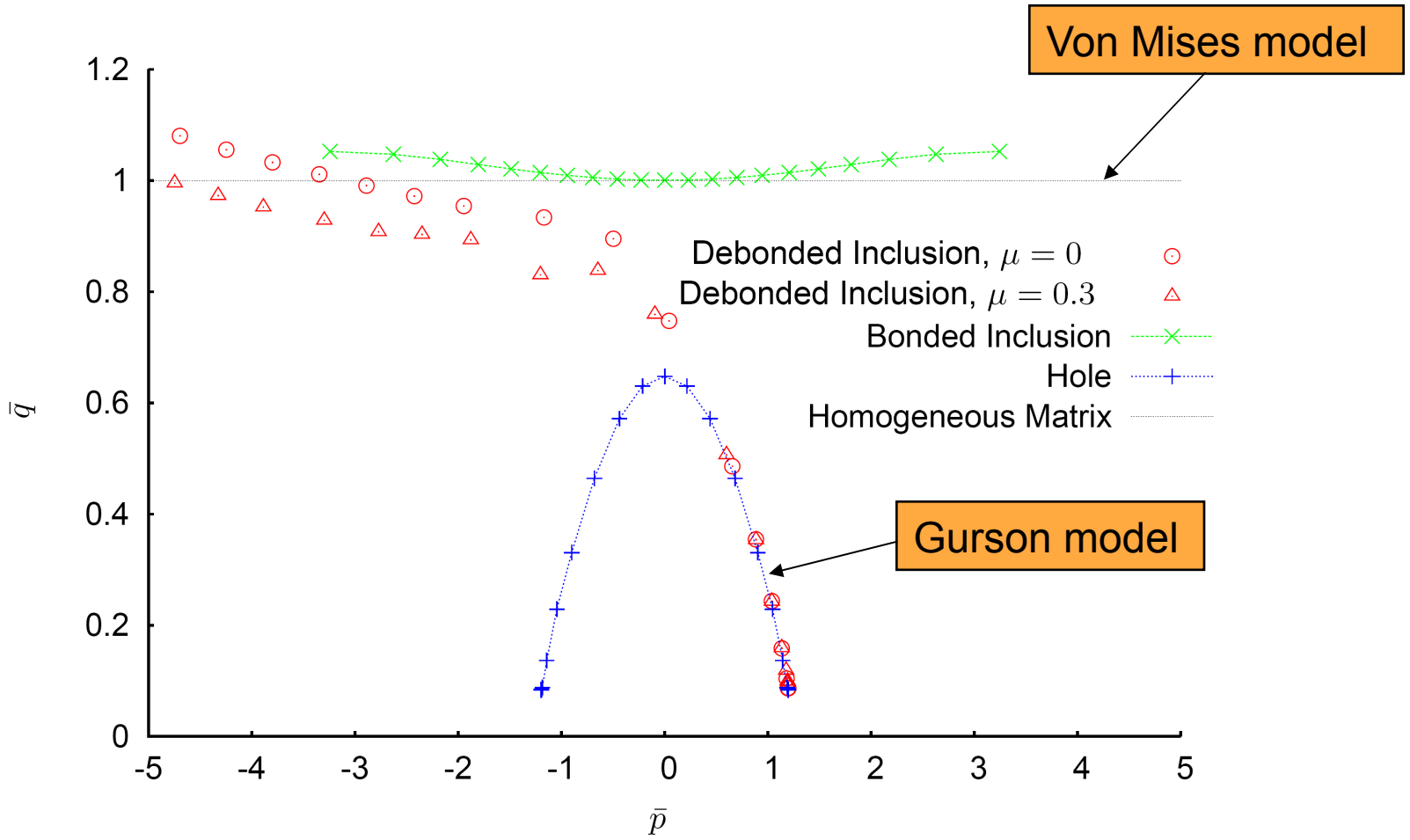
$\Downarrow$

$$\bar{\boldsymbol{\sigma}}^{coll} \Rightarrow \left\{ \begin{array}{c} p^{coll} = \frac{1}{3}\sum_{i=1}^{3} \bar{\boldsymbol{\sigma}}_{ii}^{coll} \\ \\ q^{coll} = \sqrt{\frac{3}{2}(\bar{\boldsymbol{\sigma}}^{coll} - p\boldsymbol{I}) : (\bar{\boldsymbol{\sigma}}^{coll} - p\boldsymbol{I})} \end{array} \right\} \Rightarrow \left\{ \begin{array}{c} \bar{p} = \frac{p^{coll}}{\sigma_Y} \\ \\ \bar{q} = \frac{q^{coll}}{\sigma_Y} \end{array} \right\}$$

Plasticity with phase debonding



Plasticity with phase debonding. Homogenised yield surfaces



Multiscale constitutive theory
Typical applications

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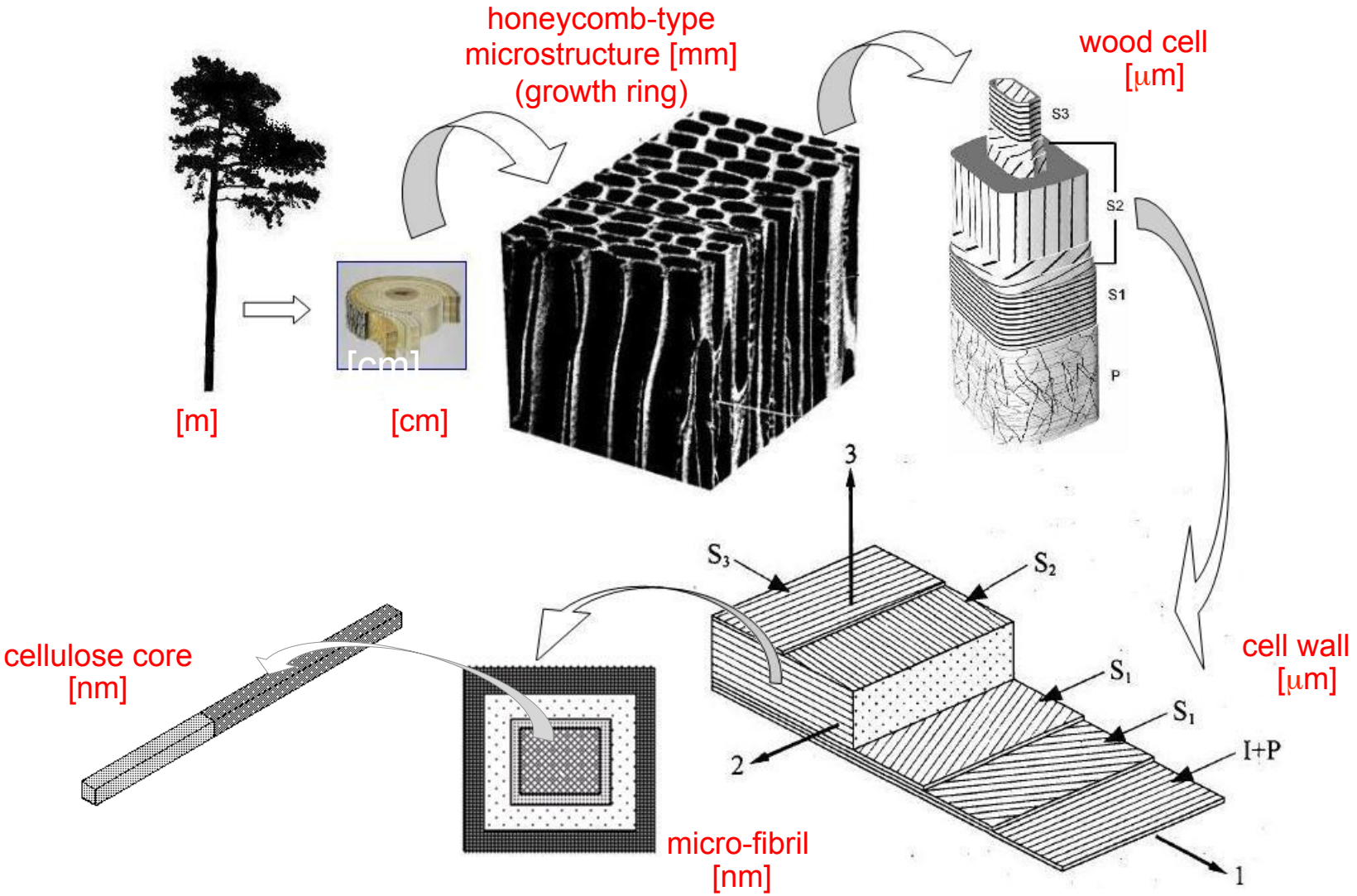
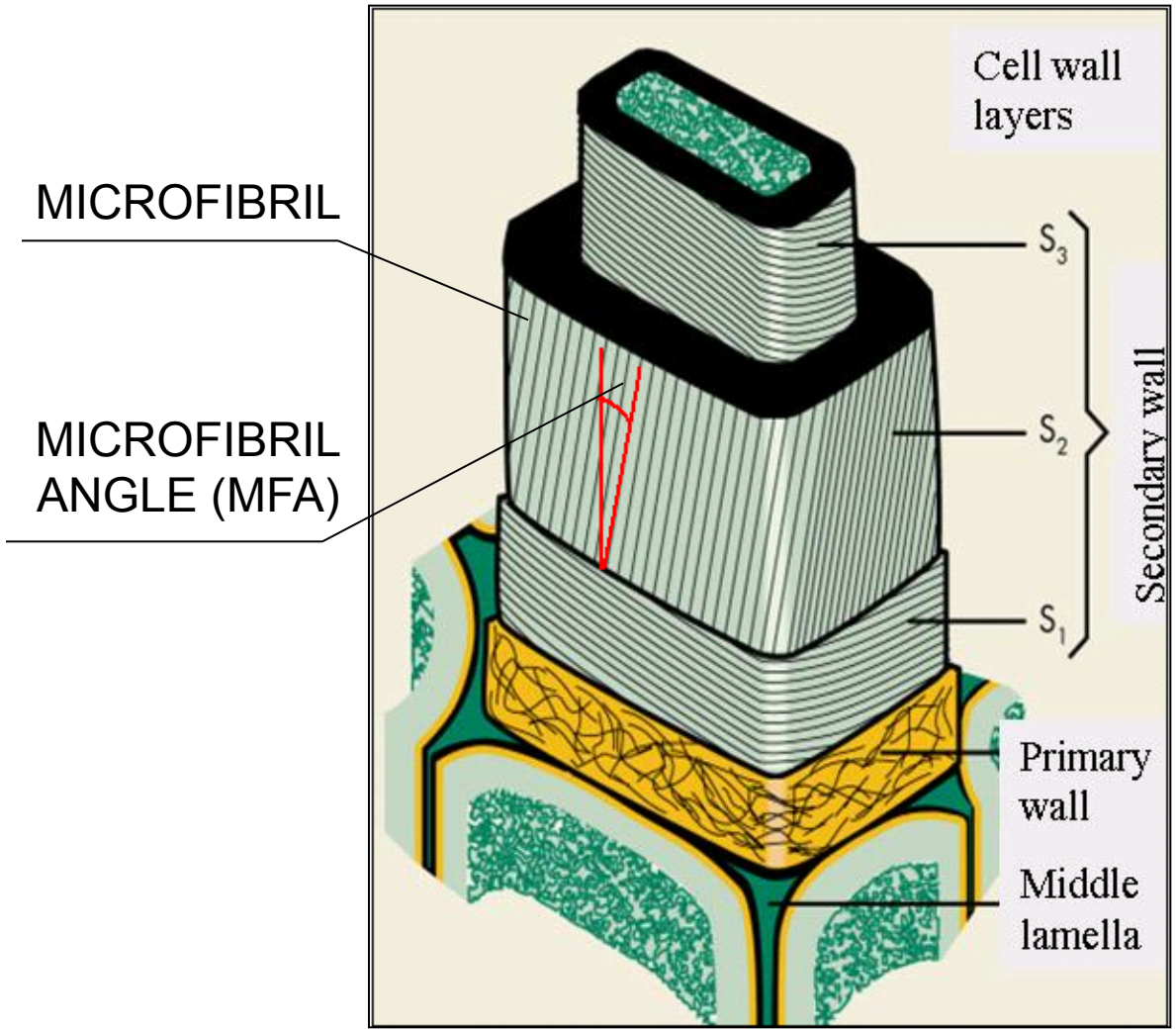
- Calibration of phenomenological (macroscopic) models
- Devising new macroscopic models
- **Understanding microscopic mechanisms and their impact on macroscopic behaviour**
- Design/optimisation of microstructures

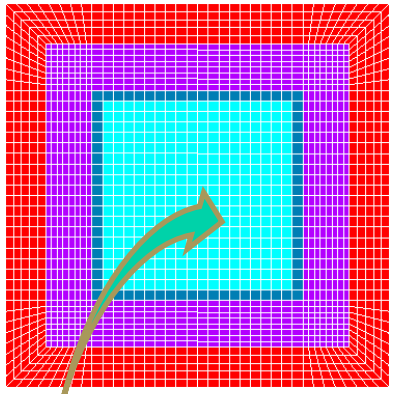
Application. Understanding dissipative behaviour Wood cell-wall



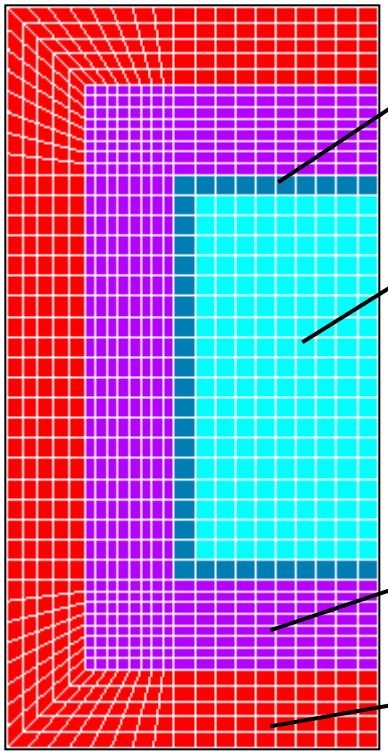
Application. Understanding dissipative behaviour Wood cell-wall



2-scale 3-D microfibril (cell-wall level) RVE



symmetry



non-crystalline (amorphous) cellulose

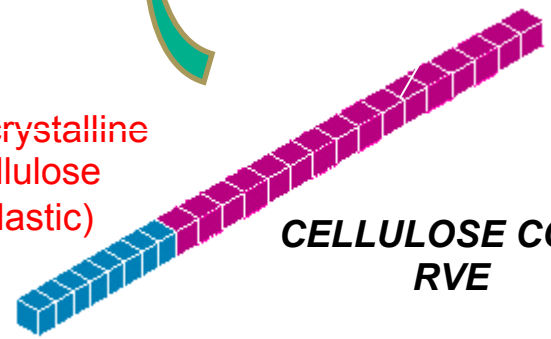
crystalline + non-crystalline cellulose

hemicellulose (visco-plastic)

lignin (visco-plastic)

crystalline cellulose (elastic)

non-crystalline cellulose (plastic)

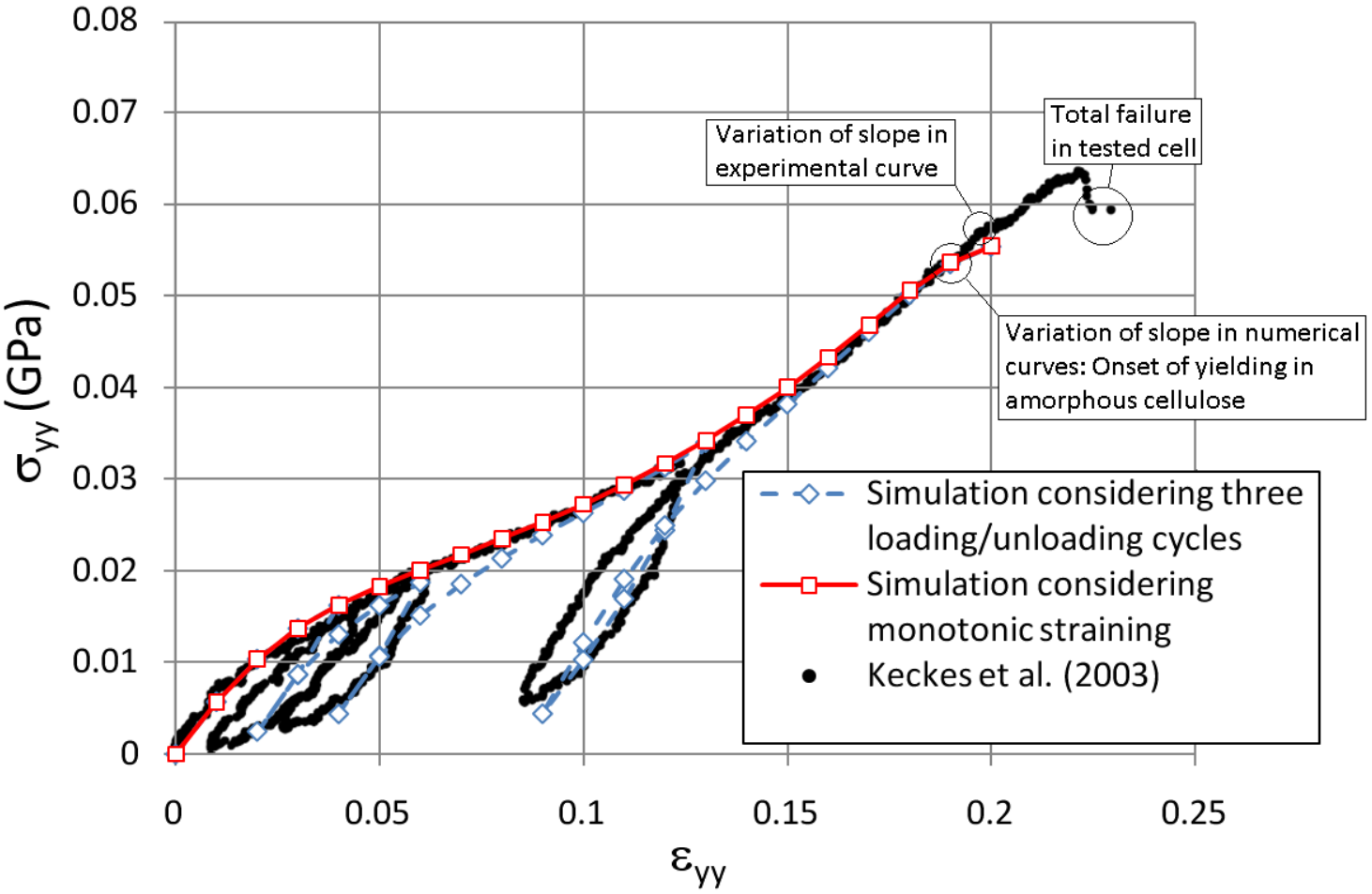


CELLULOSE CORE RVE

All parameters experimental,
except for hemicellulose yield stress
and hemicellulose/lignin viscosity parameter

Application. Understanding dissipative behaviour Wood cell-wall

(Saavedra Flores, de Souza Neto, Comput. Mat. Sci., 2011)



Multiscale constitutive theory
Typical applications

- Coupled multiscale FE analysis (FE^2)
- Calibration of phenomenological (macroscopic) models
- Devising new macroscopic models
- Understanding microscopic mechanisms and their impact on macroscopic behaviour
- **Design/optimisation of microstructures**

Application
Microstructural design/optimisation

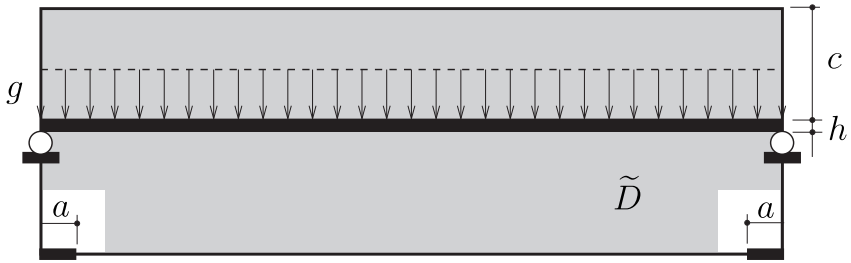
The idea

- To develop a **topological derivative-based** algorithm for the optimisation/design of elastic microstructures

The reason

- Success of the approach in the optimisation of load-bearing structures – **simple algorithms**
- Current methods of topological optimisation rely heavily on artificial algorithmic parameters and ad-hoc post-processing techniques

Example of topological derivative-based design optimisation



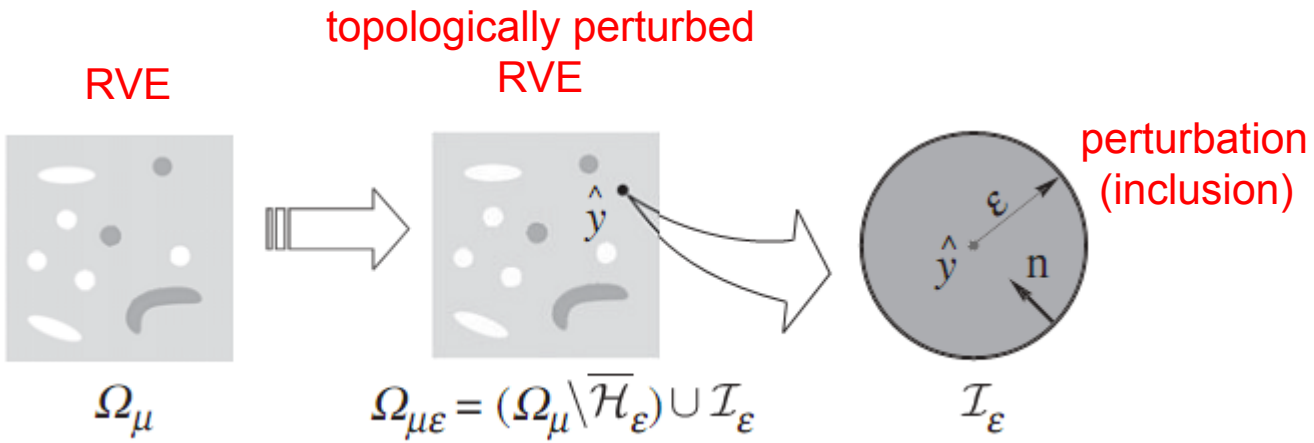
Initial bridge design guess

Optimum design – von Mises stress constraint

Optimum design – Drucker-Prager stress constraint

Topological optimisation/design of elastic microstructures

The ***topological derivative*** (Sokolowski & Zochowski, 1999) here will be associated with the following topological perturbation of the microscopic domain:



topological asymptotic expansion of a functional

$$\psi\left(\Omega_{\mu\varepsilon}(\widehat{\boldsymbol{y}})\right) = \psi\left(\Omega_\mu\right) + f\left(\varepsilon\right) D_T\psi(\widehat{\boldsymbol{y}}) + o\left(f\left(\varepsilon\right)\right)$$

$$\text{where } f\left(\varepsilon\right) \to 0, \text{ when } \varepsilon \to 0^+.$$

topological derivative

$$D_T\psi = \lim_{\varepsilon \to \mathbf{0}} \frac{\psi\left(\Omega_{\mu\varepsilon}\right) - \psi\left(\Omega_\mu\right)}{f\left(\varepsilon\right)}$$

$$f\left(\varepsilon\right) = |B_\varepsilon|$$

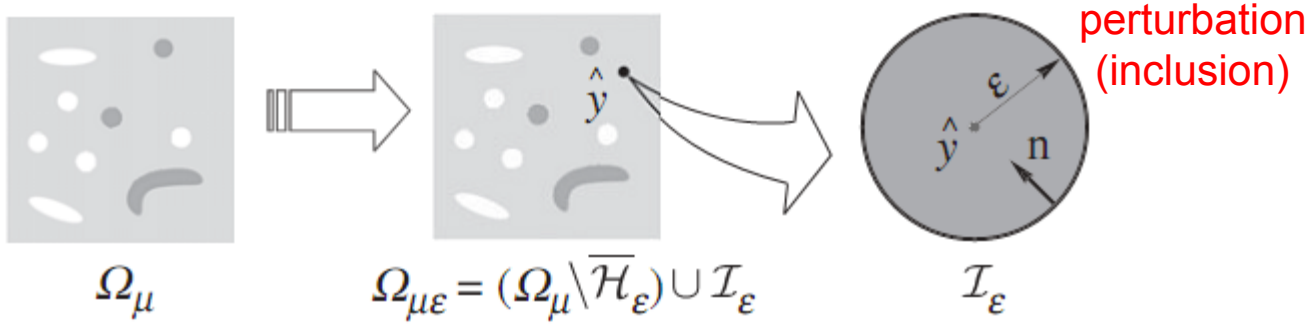
Topological optimisation/design of elastic microstructures

Problem definition

RVE

topologically perturbed RVE

perturbation (inclusion)



macroscopic elasticity tensor

$\mathbb{C}$

macroscopic elasticity tensor

$\mathbb{C}_\varepsilon$

RVE elasticity tensor field:

$$\mathbb{C}_\mu^* = \begin{cases} \mathbb{C}_\mu & \forall \boldsymbol{y} \in \Omega_\mu \backslash \overline{\mathcal{H}_\varepsilon} \\ \gamma \mathbb{C}_\mu & \forall \boldsymbol{y} \in \mathcal{I}_\varepsilon \end{cases}$$

Topological optimisation/design of elastic microstructures

The macroscopic elasticity tensor

$$\mathbb{C} = \bar{\mathbb{C}} + \tilde{\mathbb{C}}$$

where $\bar{\mathbb{C}}$ is the Taylor (volume average) elasticity tensor and

$$\tilde{\mathbb{C}} = \left[\frac{1}{V_\mu} \int_{\Omega_\mu} (\tilde{\mathbf{T}}_{\mu_{kl}})_{ij} \right] (\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l) \qquad \tilde{\mathbf{T}}_{\mu_{ij}} = \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}}$$

$$\int_{\Omega_\mu} \mathbb{C}_\mu \nabla^s \tilde{\mathbf{u}}_{\mu_{ij}} \cdot \nabla^s \boldsymbol{\eta} = - \int_{\Omega_\mu} \mathbb{C}_\mu (\mathbf{e}_i \otimes \mathbf{e}_j) \cdot \nabla^s \boldsymbol{\eta} \quad \forall \boldsymbol{\eta} \in \mathcal{V}_\mu$$

Topological optimisation/design of elastic microstructures

Topological asymptotic expansion of the macro elasticity tensor
(Giusti, Novotny & de Souza Neto. *Proc. R. Soc. A*, 2010)

$$\psi(\varepsilon) := \mathcal{J}_{\Omega_{\mu\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu\varepsilon}} \mathbf{T}_{\mu_\varepsilon} \cdot \nabla^{\mathrm{S}} \mathbf{u}_{\mu_\varepsilon}$$

$$D_{\mathrm{T}}\psi = \lim_{\varepsilon \to 0} \frac{1}{f'(\varepsilon)} \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \mathcal{J}_{\Omega_{\mu\varepsilon}}(\mathbf{u}_{\mu_\varepsilon})$$

$$\frac{\mathrm{d}}{\mathrm{d}\varepsilon} \mathcal{J}_{\Omega_{\mu\varepsilon}}(\mathbf{u}_{\mu_\varepsilon}) = \int_{\Omega_{\mu\varepsilon}} \boldsymbol{\Sigma}_{\mu_\varepsilon} \cdot \nabla \mathbf{v} \qquad \boldsymbol{\Sigma}_{\mu_\varepsilon} = (\mathbf{T}_{\mu_\varepsilon} \cdot \mathbf{E}_{\mu_\varepsilon})\mathbf{I} - 2(\nabla \tilde{\mathbf{u}}_{\mu_\varepsilon})^{\mathrm{T}} \mathbf{T}_{\mu_\varepsilon}$$

$$\mathbf{T}^{\varepsilon} \cdot \mathbf{E} = \mathbf{T} \cdot \mathbf{E} - v(\varepsilon) \mathbb{H} \mathbf{T}_{\mu} \cdot \mathbf{T}_{\mu} + o(v(\varepsilon))$$

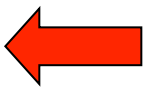
$$v(\varepsilon) := \pi \varepsilon^2 / V_{\mu}$$

Topological optimisation/design of elastic microstructures

Topological asymptotic expansion of $\mathbb{C}$

$$\mathbb{C}_\varepsilon = \mathbb{C} - v(\varepsilon)\mathbb{D}_{\mathrm{T}\mu} + o(v(\varepsilon))$$

$$\mathbb{D}_{\mathrm{T}\mu} = \mathbb{H}\tilde{\mathbf{T}}_{\mu_{ij}} \cdot \tilde{\mathbf{T}}_{\mu_{kl}}(\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_l)$$



topological derivative of $\mathbb{C}$

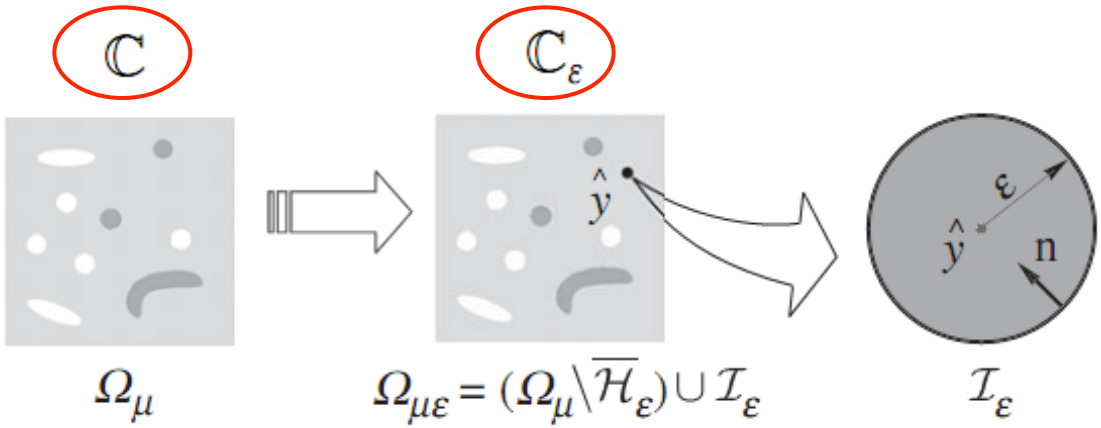
$$\mathbb{H} := \frac{1}{E}\left(\frac{1-\gamma}{1+\alpha\gamma}\right)\left[4\mathbb{I} + \frac{\gamma(\alpha-2\beta)-1}{1+\beta\gamma}(\mathbf{I}\otimes\mathbf{I})\right] \qquad \alpha := \frac{3-\nu}{1+\nu} \qquad \beta := \frac{1+\nu}{1-\nu}$$

Limits:

$\gamma \to 0$ *(insertion of void)* $\qquad \gamma \to \infty$ *(rigid inclusion)*

$$\mathbb{H} = \frac{1}{E}[4\mathbb{I} - (\mathbf{I}\otimes\mathbf{I})] \qquad \mathbb{H} = -\frac{1}{E\alpha}\left[4\mathbb{I} + \frac{\alpha-2\beta}{\beta}(\mathbf{I}\otimes\mathbf{I})\right]$$

Topological optimisation/design of elastic microstructures



The field $\mathbb{D}_{T\mu}$ at each point $\hat{y}$ of the RVE represents the derivative of $\mathbb{C}$ with respect to the volume fraction of inclusion inserted at that point.

Topological optimisation/design of elastic microstructures

The optimisation problem (bi-material micro-structure)

$$\underset{\Omega_\mu^1 \subset \Omega_\mu}{\text{Minimize}}\, J\left(\Omega_\mu^1\right) = h(\mathbb{C}) + r_i \left[\frac{|\Omega_\mu^1|}{V_\mu} - \frac{|\Omega_\mu^{1^*}|}{V_\mu}\right]^2$$

Topological derivative-based optimisation algorithm
(Amstutz, Giusti, Novotny, de Souza Neto. IJNME, 2010)

$$D_T J(y) = \langle Dh(\mathbb{C}),\, D_T\mathbb{C}(y)\rangle + 2r_i(V_j^1 - V^{1^*})$$

topological derivative of cost function *J*

$$\Omega_\mu^1 = \{y \in \Omega_\mu, \psi(y) < 0\}$$
$$\Omega_\mu^2 = \{y \in \Omega_\mu, \psi(y) > 0\}$$

level-set domain representation

$$\exists\, \tau > 0 \quad \text{s.t.} \quad g = \tau\, \psi \qquad g(y) = \begin{cases} -D_T J(\Omega_\mu^1)(y) & \text{if} \quad y \in \Omega_\mu^1 \\ D_T J(\Omega_\mu^1)(y) & \text{if} \quad y \in \Omega_\mu^2 \end{cases}$$

Sufficient optimality condition

$$D_T J(y) > 0 \quad \forall y \in \Omega_\mu$$

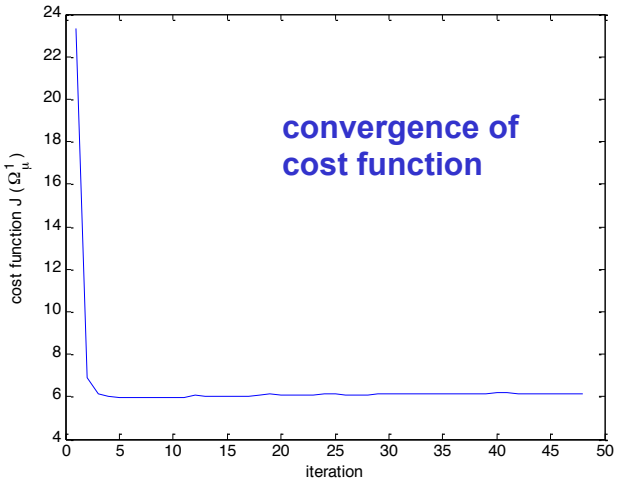
$$\psi_0 \in \mathcal{S}$$

$$\psi_{n+1} = \frac{1}{\sin\theta_n}\left[\sin((1-\kappa_n)\theta_n)\psi_n + \sin(\kappa_n\theta_n)\frac{g_n}{\|g_n\|_{L^2}}\right]$$

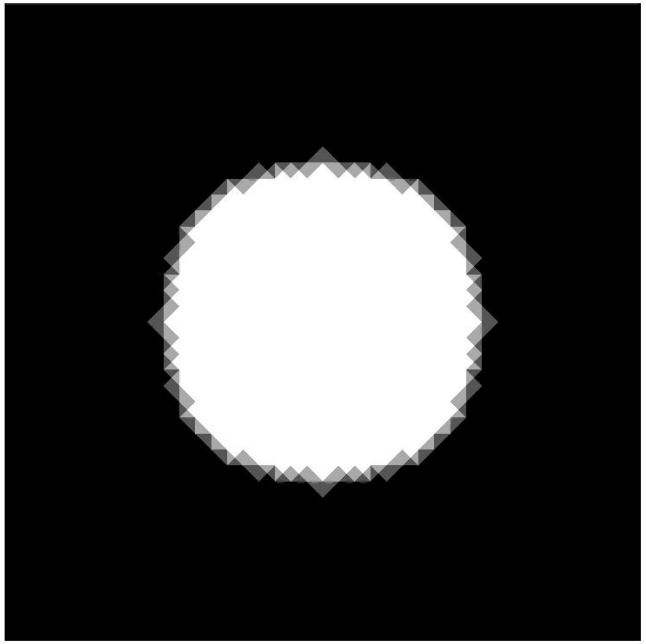
fixed point iteration

EXAMPLE 1 – Maximisation of Bulk modulus with specified volume fraction

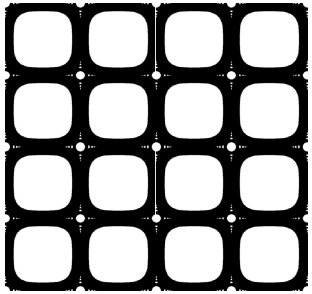
Target volume fraction of phase 1 = 0.44



$$h(\mathbb{C}) = (\mathbb{C}^{-1})_{1111} + 2(\mathbb{C}^{-1})_{1122} + (\mathbb{C}^{-1})_{2222}$$



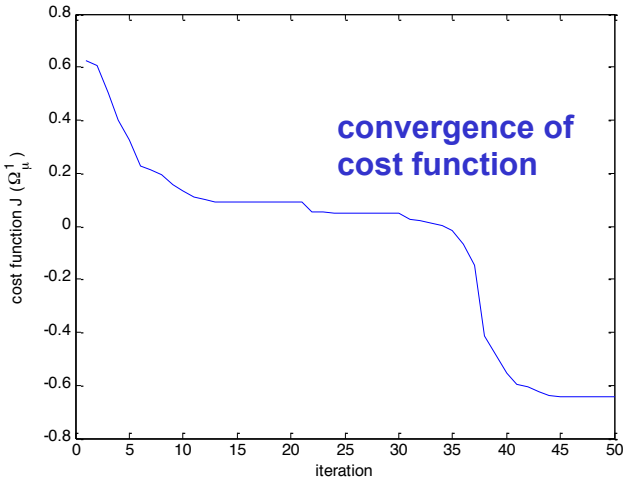
designed microstructure

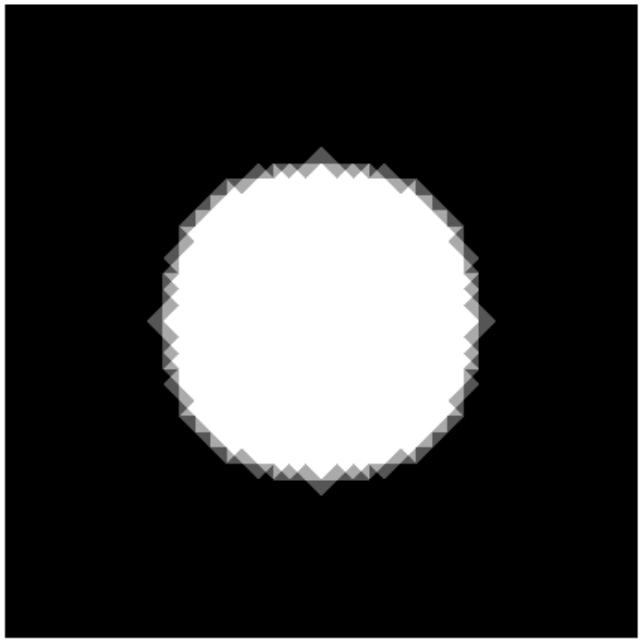


K = 0.1640
Vf = 0.4444

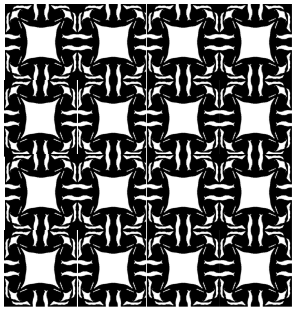
EXAMPLE 2 – Minimisation of Poisson ratio with specified volume fraction

Target volume fraction of phase 1 = 0.66



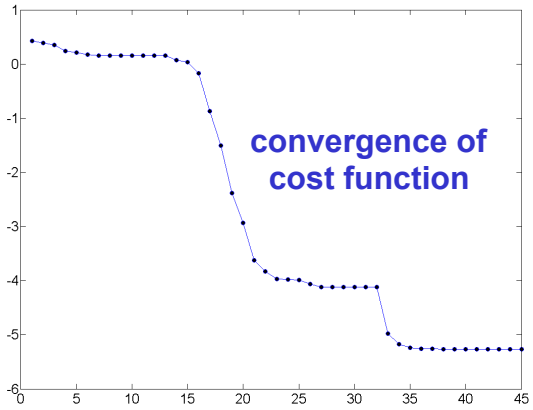


designed microstructure

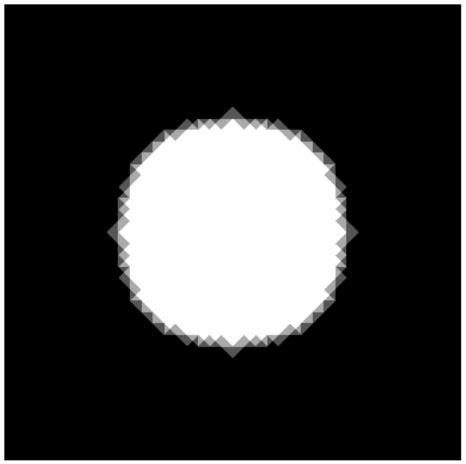


Poiss = -0.322
Vf = 0.655

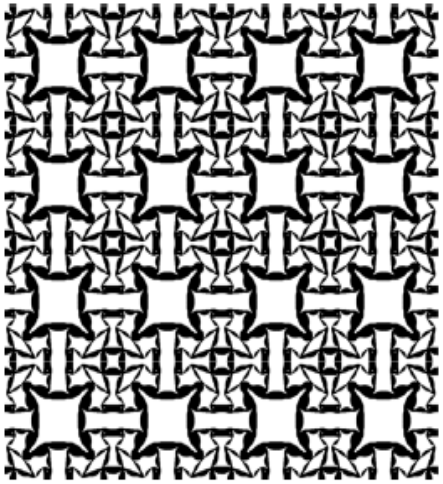
EXAMPLE 3 – Poisson ratio minimisation



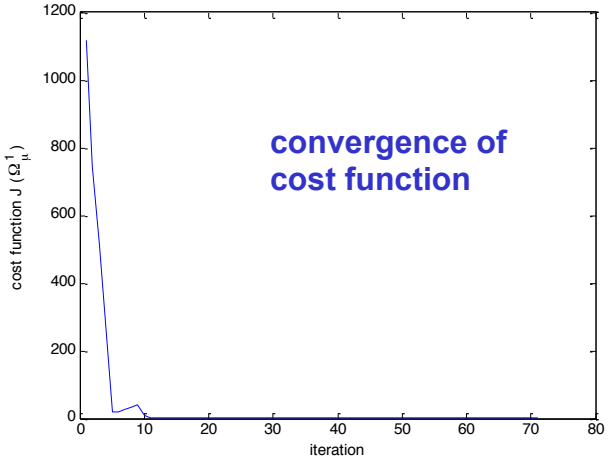
$$h(\mathbb{C}) = -(\mathbb{C}^{-1})_{1122}$$

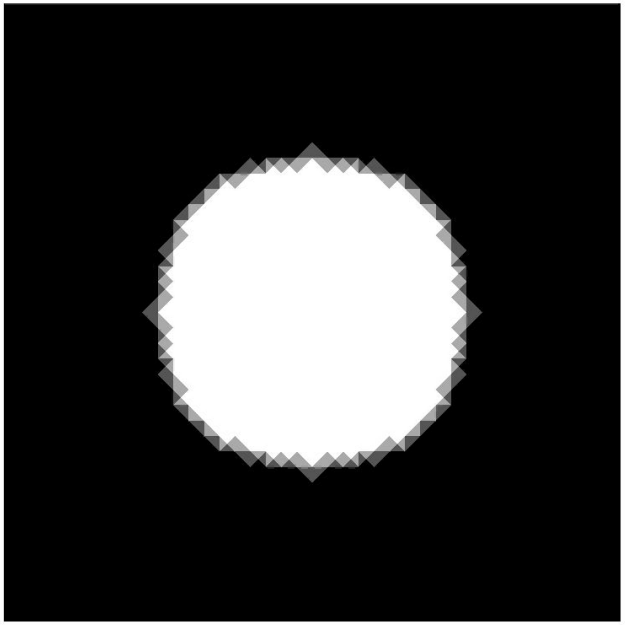


optimised
microstructure

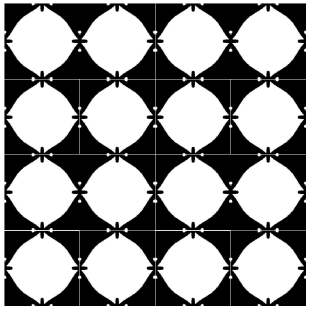


EXAMPLE 4 – Microstructure design to specified property
Target Bulk Modulus = 0.1
Target volume fraction of phase 1 = 0.44



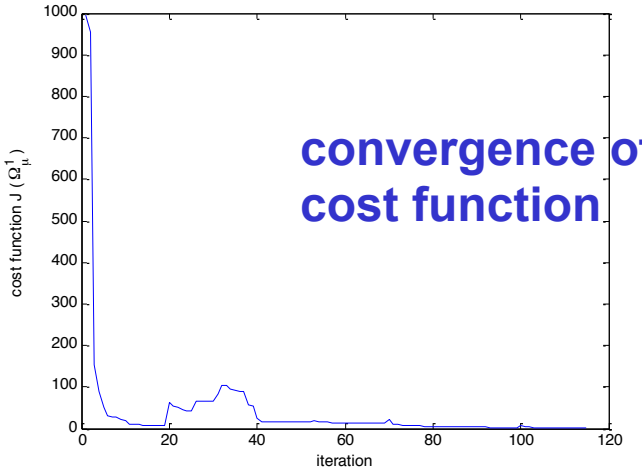


designed microstructure

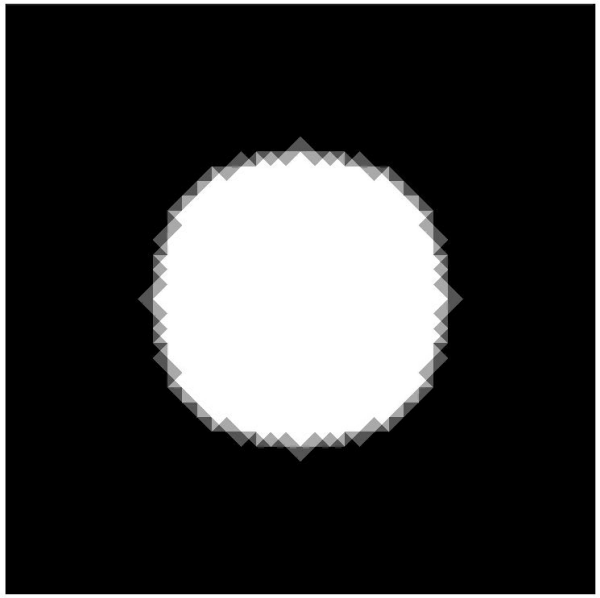


K = 0.1003
Vf = 0.4401

EXAMPLE 5 – Microstructure design to specified property
Target in-plane Poisson ratio = 0.8
Target volume fraction of phase 1 = 0.48

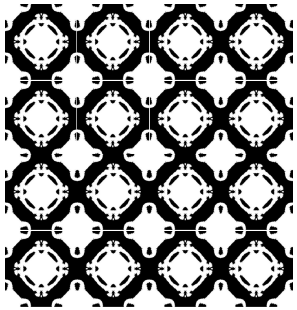


convergence of cost function



designed microstructure

Poiss = 0.7899
Vf = 0.4803



Multiscale modelling
Current challenges and ongoing work

- Multiscale modelling/analysis:
  - Alloys (phenomena such as grain boundary sliding, etc)
  - Hydrogen enbrittlement/hydrogen diffusion
- Microstructural design/optimisation:
  - Manufacturing constraints
  - Bio-inspired materials
  - Biocompatible materials
  - Stress intensity factor constraints (?)
  - Metamaterials (?)