Federica DAGHIA
with: Marc Olive, Livio Di Gennaro, Alexandre Lagache

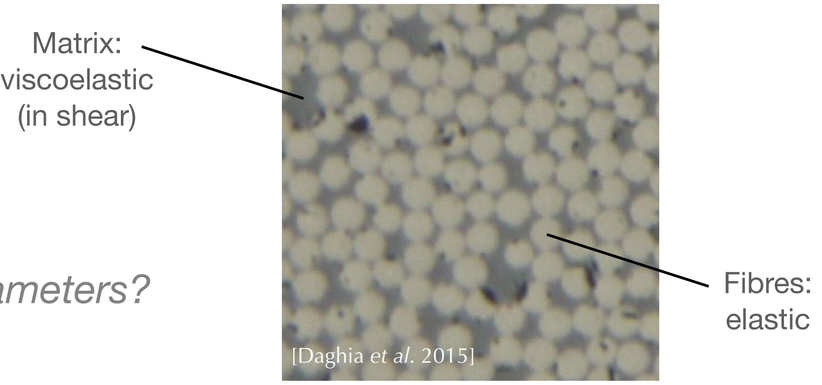
GDR Géométrie Différentielle et Mécanique
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Using the Cartan decomposition to formulate a physics-based viscoelastic law for transversely isotropic composites

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Context

- **Formulation of a viscoelastic model for unidirectional carbon fibres / polymer matrix composites**
  - Constituents' behaviour (microscale):
    > *Fibres: elastic, stiff*
    > *Matrix: viscoelastic (shear), compliant*
  - Composite's behaviour (mesoscale):
    > *Transversely isotropic elasticity (5 material parameters)*
    > *How does the single microscale mechanism translates into the mesoscale model parameters?*



- **Literature: a phenomenological relaxation tensor**
  - The different terms of the stiffness tensor generally have different relaxation behaviours
  - Many material parameters to be identified without a clear link to the original mechanism at the microscale

- **Here: a geometrical formulation of transverse isotropy**
  - An appropriate choice of the elastic parameters clarifies the link with the underlying constituents
  - A simple viscoelastic law affecting only certain parameters can be formulated at the mesoscale
  - Analytical and numerical homogenisation approaches enable us to identify and validate the proposed model
  - [Di Gennaro *et al.*, 2021], [Daghia *et al.*, in preparation]

Outline

- **Modelling the transverse isotropy through a Cartan decomposition**
  - Define a Cartan decomposition of the stress and strain tensors
  - Deduce the minimal integrity basis
  - Formulate the free energy
  - Derive the elastic constitutive law

- **A new transversely isotropic viscoelastic model for polymer matrix composites**
  - An ansatz on the link between the new elastic parameters and the constituents' response
  - Verification via analytical homogenisation results
  - Formulation of the viscoelastic behaviour

- **Numerical homogenisation for identification and validation**
  - Periodic homogenisation for general loading paths
  - Relaxation tests: identification of the transversely isotropic model
  - Creep tests: validation of the transversely isotropic model

- **Conclusions and Perspectives**

A Cartan decomposition of the stress and strain tensors

Modelling the transverse isotropy

- $\mathbf{v}_f$ unit vector in the fibres' direction, $(\mathbf{v}_2, \mathbf{v}_3)$ transverse isotropy plane
- The transverse isotropy is modelled on the group O(2):

  Rotations around $\mathbf{v}_f$
  Change of direction of $\mathbf{v}_f$

Starting from geometry, we have an irreducible decomposition for the stress and strain tensors

$$\boldsymbol{\sigma} = s_f \mathbf{M}_f + s_h \mathbf{M}_h + (s_{f2}\mathbf{M}_{f2} + s_{f3}\mathbf{M}_{f3}) + (s_d \mathbf{M}_d + s_{23}\mathbf{M}_{23})$$

scalar scalar vector vector

$$\mathbf{M}_f = \mathbf{v}_f \otimes \mathbf{v}_f, \qquad \mathbf{M}_{f2} = \frac{1}{\sqrt{2}}\left(\mathbf{v}_f \otimes \mathbf{v}_2 + \mathbf{v}_2 \otimes \mathbf{v}_f\right), \qquad \mathbf{M}_d = \frac{1}{\sqrt{2}}\left(\mathbf{v}_2 \otimes \mathbf{v}_2 - \mathbf{v}_3 \otimes \mathbf{v}_3\right),$$

$$\mathbf{M}_h = \frac{1}{\sqrt{2}}\left(\mathbf{v}_2 \otimes \mathbf{v}_2 + \mathbf{v}_3 \otimes \mathbf{v}_3\right), \qquad \mathbf{M}_{f3} = \frac{1}{\sqrt{2}}\left(\mathbf{v}_f \otimes \mathbf{v}_3 + \mathbf{v}_3 \otimes \mathbf{v}_f\right), \qquad \mathbf{M}_{23} = \frac{1}{\sqrt{2}}\left(\mathbf{v}_2 \otimes \mathbf{v}_3 + \mathbf{v}_3 \otimes \mathbf{v}_2\right).$$

$$\mathbf{M}_\bullet : \mathbf{M}_\bullet = 1, \mathbf{M}_\bullet : \mathbf{M}_\circ = 0 \text{ if } \bullet \neq \circ$$

A Cartan decomposition of the stress and strain tensors

- **Relation with the classical components: consider** $(\mathbf{v}_f, \mathbf{v}_2, \mathbf{v}_3) = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$

$$\boldsymbol{\sigma} = s_f \mathbf{M}_f + s_h \mathbf{M}_h + (s_{f2} \mathbf{M}_{f2} + s_{f3} \mathbf{M}_{f3}) + (s_d \mathbf{M}_d + s_{23} \mathbf{M}_{23})$$

$$\boldsymbol{\sigma} = \begin{bmatrix} s_f & \frac{\sqrt{2}}{2} s_{f2} & \frac{\sqrt{2}}{2} s_{f3} \\ & \frac{\sqrt{2}}{2}(s_h + s_d) & \frac{\sqrt{2}}{2} s_{23} \\ \text{sym} & & \frac{\sqrt{2}}{2}(s_h - s_d) \end{bmatrix}$$

- s_f normal in the fibres' direction
- $s_{f2}, s_{f3} \rightarrow \mathbf{s}_{fs}$ shear along the fibres' direction
- s_h hydrostatic in the transverse isotropy plane
- $s_d, s_{23} \rightarrow \mathbf{s}_d$ deviatoric in the transverse isotropy plane

- **Similar to the classical hydrostatic/deviatoric decomposition for isotropy, but it concerns the transverse isotropy plane**

Minimal integrity basis

Polynomial invariants: minimal integrity basis

$$\boldsymbol{\sigma} = s_f \mathbb{M}_f + s_h \mathbb{M}_h + \mathbf{s}_{fs} + \mathbf{s}_d$$

- From the Cartan decomposition, we can derive the following minimal integrity basis [Desmorat *et al.,* 2020] (any polynomial invariant can be constructed from these five invariants)

$$\begin{aligned} I_1 &:= s_f, \quad J_1 := s_h, \\ I_2 &:= \|\mathbf{s}_{fs}\|^2, \quad J_2 := \|\mathbf{s}_d\|^2, \\ I_3 &:= \mathrm{tr}\left(\mathbf{s}_{fs}^2 \mathbf{s}_d\right). \end{aligned}$$

- Such a basis is different from the typical invariants used in mechanics (not based on a decomposition *a priori*) - The link between the two sets is not trivial

$$\begin{aligned} \bar{I}_1 &= \mathrm{tr}\ \boldsymbol{\sigma}, \quad \bar{I}_2 = \frac{1}{2}\left(\bar{I}_1^2 - \mathrm{tr}\ \boldsymbol{\sigma}^2\right), \\ \bar{I}_3 &= \det \boldsymbol{\sigma}, \quad \bar{I}_4 = \mathrm{tr}\ \left(\boldsymbol{M}_f \boldsymbol{\sigma}\right), \\ \bar{I}_5 &= \mathrm{tr}\ \left(\boldsymbol{M}_f \boldsymbol{\sigma}^2\right). \end{aligned}$$

Gibbs free energy and elastic constitutive law

- **The Gibbs free energy for linear elasticity can be written as**

$$\begin{aligned}\bar{w} &= \frac{1}{2}S_F I_1^2 + S_{FH} I_1 J_1 + \frac{1}{2}S_H J_1^2 + S_{FS} I_2 + S_D J_2 \\ &= \frac{1}{2}S_F s_f^2 + S_{FH} s_f s_h + \frac{1}{2}S_H s_h^2 + \frac{1}{2\mu_L}\left|\boldsymbol{s}_{fs}\right|^2 + \frac{1}{2\mu_T}\left|\boldsymbol{s}_d\right|^2 .\end{aligned}$$

- **This yields the following elastic constitutive law**

$$\begin{bmatrix} e_f \\ e_h \end{bmatrix} = \begin{bmatrix} S_F & S_{FH} \\ S_{FH} & S_H \end{bmatrix} \begin{bmatrix} s_f \\ s_h \end{bmatrix},$$

$$\mathbf{e}_{fs} = S_{FS}\mathbf{s}_{fs},$$

$$\mathbf{e}_d = S_D\mathbf{s}_d$$

  - It is nicely uncoupled (except f,h due to Poisson's effect)
  - it introduces a new set of 5 material parameters (compliances) $(S_F, S_{FH}, S_H, S_{FS}, S_D)$
  - What is their relation to the typical material parameters for transverse isotropy?

On the different choices of elastic parameters

- **Relation with the classical elastic parameters: consider** $(\mathbf{v}_f, \mathbf{v}_2, \mathbf{v}_3) = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$
  - The compliance tensor reads (stress and strain in Mandel notation)

$$\mathbf{S} = \begin{bmatrix} S_F & \frac{S_{FH}}{\sqrt{2}} & \frac{S_{FH}}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{S_{FH}}{\sqrt{2}} & \frac{S_H+S_D}{2} & \frac{S_H-S_D}{2} & 0 & 0 & 0 \\ \frac{S_{FH}}{\sqrt{2}} & \frac{S_H-S_D}{2} & \frac{S_H+S_D}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_D & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{FS} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{FS} \end{bmatrix} = \begin{bmatrix} \frac{1}{\mathrm{E}_L} & -\frac{\nu_{LT}}{\mathrm{E}_L} & -\frac{\nu_{LT}}{\mathrm{E}_L} & 0 & 0 & 0 \\ -\frac{\nu_{LT}}{\mathrm{E}_L} & \frac{1}{\mathrm{E}_T} & -\frac{\nu_{TT}}{\mathrm{E}_T} & 0 & 0 & 0 \\ -\frac{\nu_{LT}}{\mathrm{E}_L} & -\frac{\nu_{TT}}{\mathrm{E}_T} & \frac{1}{\mathrm{E}_T} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2\mu_T} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2\mu_L} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2\mu_L} \end{bmatrix}$$

  - We have the following correspondence between $(E_l, E_t, \nu_{lt}, \mu_l, \mu_t)$ and $(S_F, S_{FH}, S_H, S_{FS}, S_D)$

$$E_l = \frac{1}{S_F}, \quad E_t = \frac{2}{S_H + S_D}, \quad \nu_{lt} = -\frac{S_{FH}}{\sqrt{2}S_F},$$
$$\mu_l = \frac{1}{2S_{FS}}, \quad \mu_t = \frac{1}{2S_D}.$$

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Ansatz on the micro-meso link

- **Ansatz: how are the new set of elastic parameters influenced by the constituents' behaviour?**
  - Recall that we have very stiff fibres and very compliant matrix in similar proportions

$$\begin{bmatrix} e_f \\ e_h \end{bmatrix} = \begin{bmatrix} S_F & S_{FH} \\ S_{FH} & S_H \end{bmatrix} \begin{bmatrix} s_f \\ s_h \end{bmatrix},$$

$$\mathbf{e}_{fs} = S_{FS}\mathbf{s}_{fs},$$

$$\mathbf{e}_d = S_D\mathbf{s}_d$$

- S_F axial response in the fibres' direction - fibres
- S_H hydrostatic response in the transverse isotropy plane - fibres, matrix bulk response
- S_{FH} coupling term - fibres, matrix bulk response

- S_{FS} shear response in the fibres' direction - matrix shear response
- S_D shear response in the transverse isotropy plane - matrix shear response

- **Approximation: the viscoelastic shear response of the matrix affects only the terms S_{FS}, S_D**

Verification: analytical homogenisation results

How to check the pertinence of this approximation? Analytical homogenisation results

- A cylindrical model yields closed form expressions for the transversely isotropic elastic properties based on the constituents' properties [Hashin, 1970]

- Two sets of parameters with different behaviours for $\mu_m \to 0$:

  > $S_{FS}, S_D \to \infty$
  > S_F, S_{FH}, S_H *remain finite*

- All of the terms evolve with μ_m … how significant is this evolution?

  > *Possible simplifications depend on the ratio between the constituents' material properties and volume fractions*

$$\mu_l = \mu_m \left[1 + \frac{v_f}{\frac{\mu_m}{\mu_f - \mu_m} + \frac{v_m}{2}} \right],$$

$$\mu_t = \mu_m \frac{\left(1 + \alpha v_f^3\right)(\rho + \beta_m v_f) - 3 v_f v_m^2 \beta_m^2}{\left(1 + \alpha v_f^3\right)(\rho - v_f) - 3 v_f v_m^2 \beta_m^2},$$

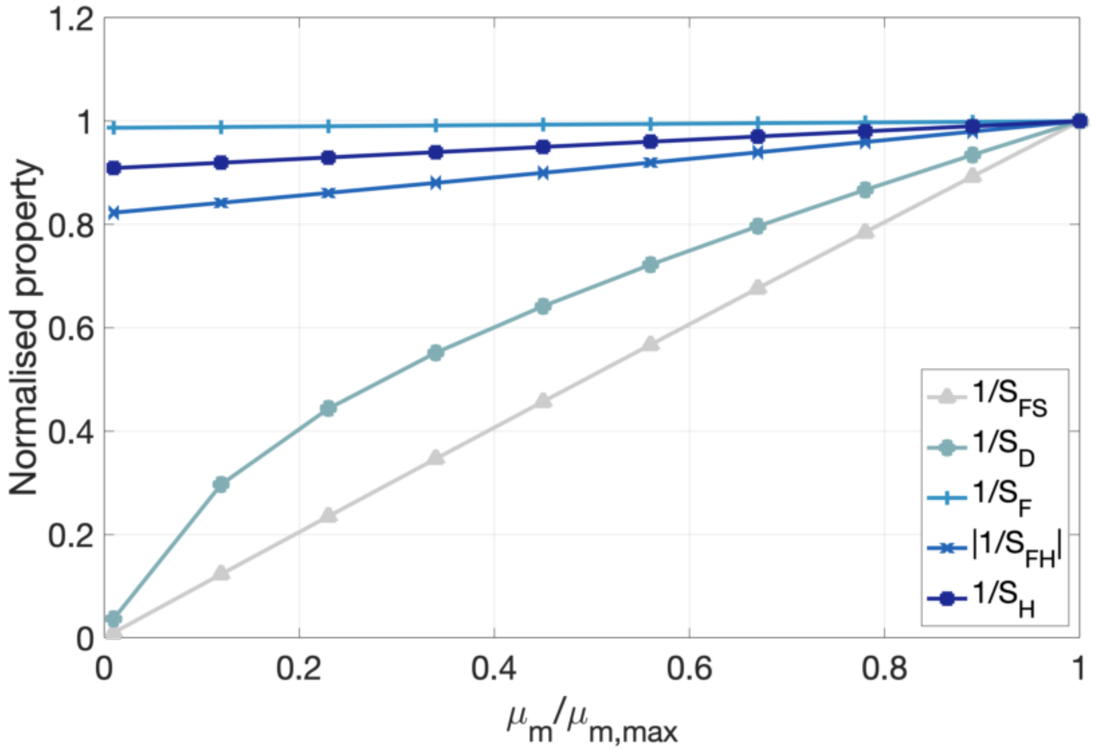
$$E_l = E_m v_m + E_f v_f + \frac{4 v_m v_f (\nu_f - \nu_m)^2}{\frac{v_m}{k_f} + \frac{v_f}{k_m} + \frac{1}{\mu_m}},$$

$$\nu_{lt} = \nu_m v_m + \nu_f v_f + \frac{v_m v_f (\nu_f - \nu_m)\left(\frac{1}{k_m} - \frac{1}{k_f}\right)}{\frac{v_m}{k_f} + \frac{v_f}{k_m} + \frac{1}{\mu_m}},$$

$$k_t = k_m \left[1 + \frac{v_f}{\frac{k_m}{k_f - k_m} + \frac{k_m v_m}{k_m + \mu_m}} \right].$$

Verification: analytical homogenisation results

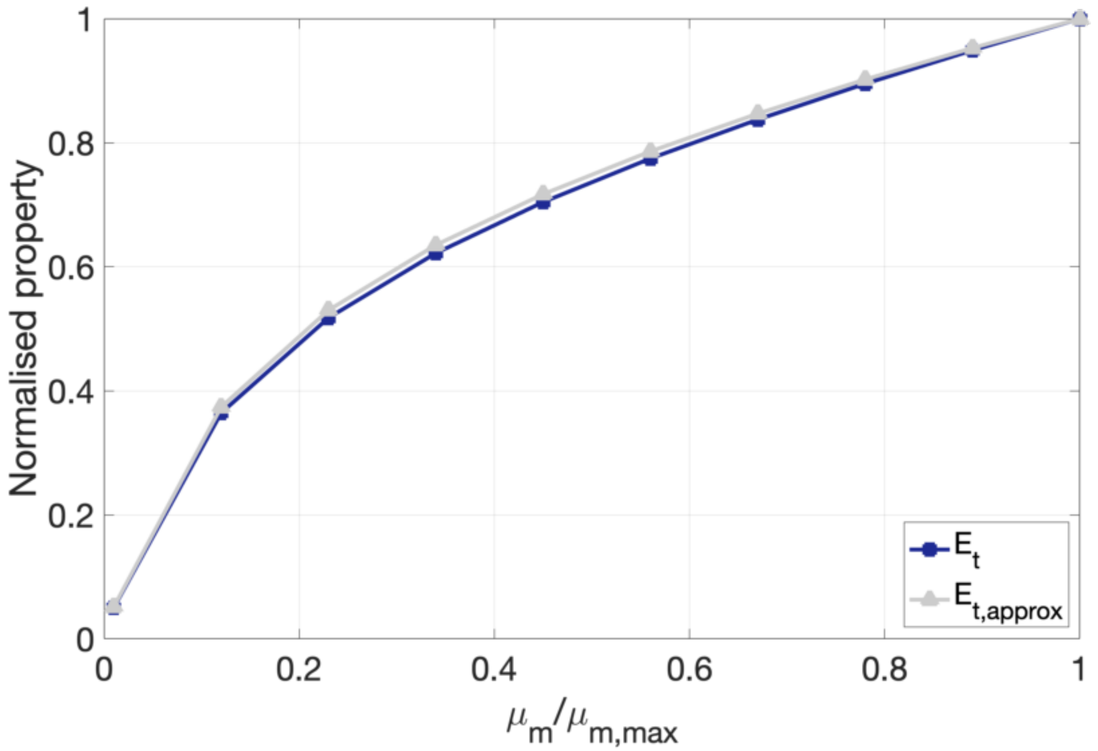
- **How to check the pertinence of this approximation? Analytical homogenisation results**
  - Evolution of the composite's properties as μ_m decreases
  - Constituents' properties and volume fractions for a typical carbon fibres / polymer matrix composite
    - E_f = 248 GPa, υ_f = 0.2
    - E_m = 3.24 GPa, υ_m = 0.4
    - v_f = 0.5



Verification: analytical homogenisation results

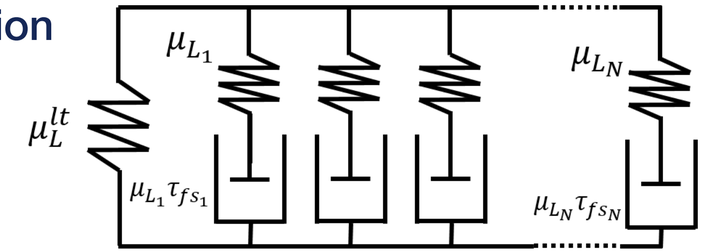
- **How to check the pertinence of this approximation? Analytical homogenisation results**
  - Neglecting the evolution of S_H, we can still capture E_t quite accurately

$$E_t = \frac{2}{S_H + S_D}$$



Formulation of the viscoelastic model

- **Many possible formulations for viscoelasticity.**
  Here, we choose a Generalised Maxwell (GM) model with integral formulation
  - Rheological representation



  - Model equation

$$\mathbf{s}_\bullet(t) = \int_0^t \Gamma_\bullet\left(t - t'\right) \frac{\mathrm{d}\mathbf{e}_\bullet(t')}{\mathrm{d}t'} \mathrm{d}t',$$

$$\Gamma_\bullet = \left(\frac{1}{S_\bullet}\right)_{lt} + \sum_{j=1}^{N} \left(\frac{1}{S_\bullet}\right)_j \exp\left(-\frac{t - t'}{(\tau_\bullet)_j}\right).$$

  - Reasons behind these choices:

> *Generalised Maxwell vs Generalised Kelvin-Voigt: GM elements are uncoupled with strain-driven integration (FEM)*
> *Integral vs Differential formulation: an efficient and accurate integration algorithm is available for the former [Taylor et al. 1970]*

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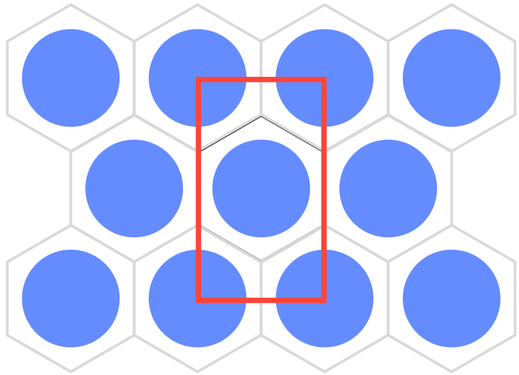
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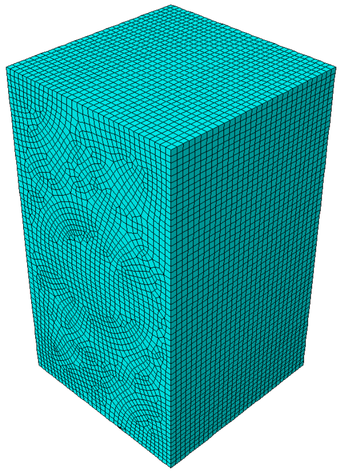
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- **Conclusions and Perspectives**

Numerical homogenisation

- **Numerical homogenisation: a convenient tool for identification and validation**
- **Elements of numerical homogenisation:**
  - Representative Volume Element - RVE (random or periodic)





  - Boundary Value Problem on the RVE:

> *Kinematic Uniform Boundary Conditions (KUBC) - too stiff*
> *Static Uniform Boundary Conditions (SUBC) - too compliant*
> *Periodic Boundary Conditions (PBC) - the best*

Field equations (Ω) + Boundary Conditions ($\partial\Omega$)

$$\boldsymbol{\varepsilon} = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla^{\mathrm{T}}\mathbf{u}\right),$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}\left(\boldsymbol{\varepsilon}\right), \qquad \mathbf{u}_N - \mathbf{u}_M = \mathbf{E}_0 \cdot (\mathbf{ON} - \mathbf{OM}).$$

$$\nabla \cdot \boldsymbol{\sigma} = \mathbf{0}.$$

  - Obtain the macroscopic stress and strain by averaging over the RVE

$$\boldsymbol{\Sigma} = \langle\boldsymbol{\sigma}\rangle = \frac{1}{V}\int_V \boldsymbol{\sigma}\mathrm{d}\Omega, \quad \mathbf{E} = \langle\boldsymbol{\varepsilon}\rangle = \frac{1}{V}\int_V \boldsymbol{\varepsilon}\mathrm{d}\Omega.$$

Numerical homogenisation

- **Numerical homogenisation for elasticity**
  - Compute 6 elementary problems (for PBC, in macroscopic strain control)
  - Identify the stiffness matrix and the elastic parameters
- **Numerical homogenisation for viscoelasticity: different strategies**
  - Laplace domain:
    > *Analogous to an elastic problem, BUT need the reverse Laplace transform [Suquet 1985]*
  - Time domain:
    > *Reformulation as a variational problem with internal variables [Lahellec, Suquet 2007]*
    > *Compute 6 elementary problems in macroscopic strain control and identify a general relaxation tensor [Tran et al. 2011]*
    > *...*
- **Here: we use the RVE as a virtual testing machine**
  - General driving strategy (macroscopic strain OR stress components)
  - Relaxation tests: identification of the transversely isotropic GM model parameters
  - Creep tests: validation of the transversely isotropic GM model assumptions

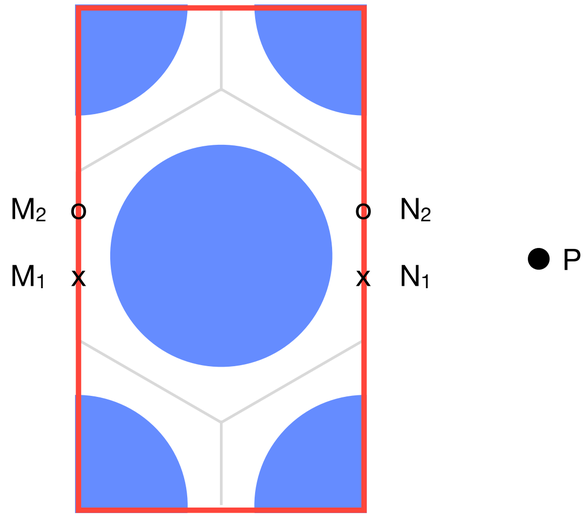
A general driving strategy for PBC

How to implement a general driving strategy for Periodic Boundary Conditions (PBC)?

- Formulation of the PBC via dummy nodes:
  for each side, add a list of linear constraints as follows

$$\mathbf{u}_{N_1} - \mathbf{u}_{M_1} = \mathbf{u}_P$$
$$\mathbf{u}_{N_2} - \mathbf{u}_{M_2} = \mathbf{u}_P$$
$$\dots$$

- All couple of nodes are related to the same dummy node,
  so the stiffness associated to this node corresponds to the macroscopic RVE stiffness



- The force and displacement at this node
  are related to the macroscopic strain and stress

$$\mathbf{E}_0 \cdot \mathbf{n} = \frac{\mathbf{u}_P}{L_n}$$
$$\mathbf{\Sigma}_0 \cdot \mathbf{n} = \frac{\mathbf{F}_P}{S_n}$$

- For each component, either the macroscopic strain or the macroscopic stress can be controlled

Results

- **Elastic tests on the RVE: identification of the instantaneous properties**
  - The analytical results by [Hashin 1970] are extremely accurate for most parameters
  - Discrepancies are observed for the (2,3) shear response (upper bound) - and on the transverse Young's modulus

Table 1: Comparison between analytical and numerical homogenisation results for linear elastic constituents ($E_f = 248$ GPa, $\nu_f = 0.2$, $E_m = 3.24$ GPa, $\nu_m = 0.4$, $v_f = 0, .5$)

Parameter	units	Analytical	Numerical
$E_l = 1/S_F$	GPa	125.72	125.56
E_t	GPa	12.917	10.385
ν_{lt}	-	0.29119	0.29128
$\mu_l = 1/(2S_{FS})$	GPa	3.373	3.376
$\mu_t = 1/(2S_D)$	GPa	4.445	3.330
k_t	GPa	12.200	12.189
$1/S_{FH}$	GPa	-305.291	-304.810
$1/S_H$	GPa	23.622	23.594

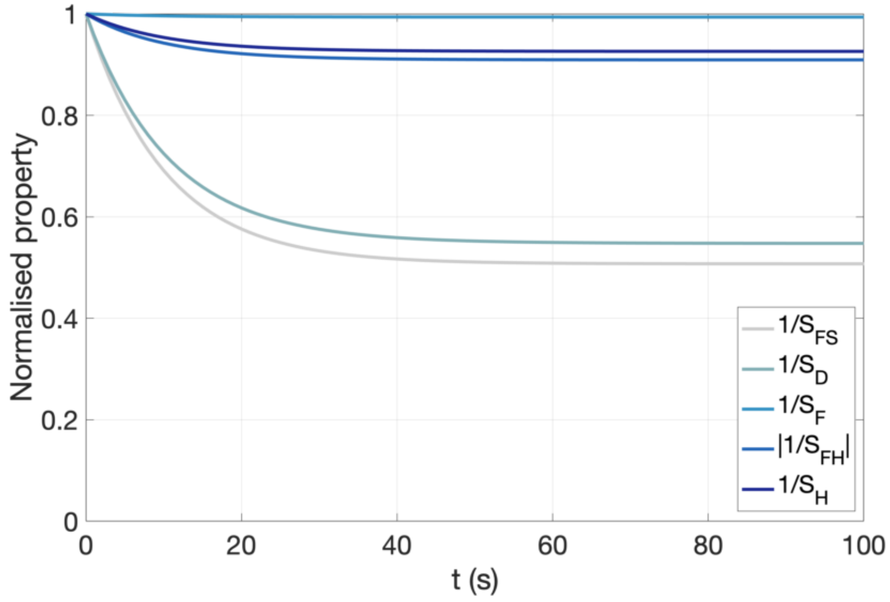
Relaxation tests on the RVE: identification of the viscoelastic response

- Tests at constant macroscopic strain enable us to identify the relaxation tensor

$$\mathbf{E}(t) = H(t)\mathbf{E}_0$$

$$\mathbf{\Sigma}(t) = \int_0^t \mathbf{\Gamma}\left(t - t'\right) \frac{\mathrm{d}\mathbf{E}\left(t'\right)}{\mathrm{d}t'} \mathrm{d}t' = \int_0^t \mathbf{\Gamma}\left(t - t'\right) \delta(t') \mathbf{E}_0 \mathrm{d}t' = \mathbf{\Gamma}(t)\mathbf{E}_0$$

- For a simple matrix relaxation behaviour
  (max relaxation 50% of the instantaneous response, characteristic time 10s)
  we have the following homogenised response



- Identification:

  We neglect relaxation of S_F, S_{FH}, S_H
  For the other two parameters, we get

$$\left(\frac{1}{S_{FS}}\right)_1 = 0.4926 \left(\frac{1}{S_{FS}}\right)_{inst}, \tau_1 = 10.14\ s;$$

$$\left(\frac{1}{S_D}\right)_1 = 0.4523 \left(\frac{1}{S_D}\right)_{inst}, \tau_1 = 10.77\ s.$$

Results

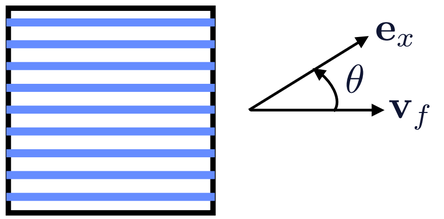
Creep tests on the RVE: validation of the proposed model

- Comparison of the RVE response and the transversely isotropic model response for creep tests in different directions

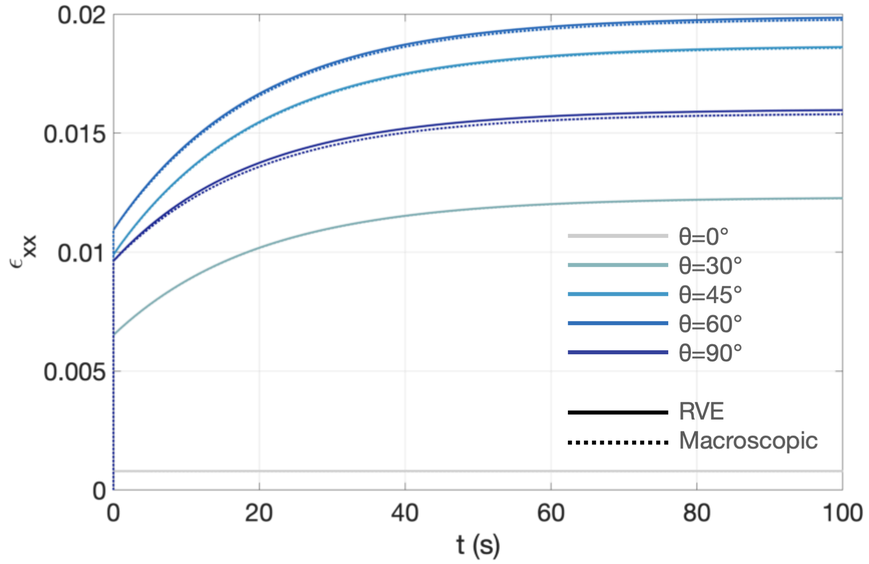
Unconstrained: $\boldsymbol{\Sigma}_0(t) = \Sigma_0 \mathbf{e}_x \otimes \mathbf{e}_x$

Constrained: $\boldsymbol{\Sigma}_0(t) = \Sigma_0 \mathbf{e}_x \otimes \mathbf{e}_x + \Sigma_{yy}(t)\mathbf{e}_y \otimes \mathbf{e}_y + \Sigma_{zz}(t)\mathbf{e}_z \otimes \mathbf{e}_z;$

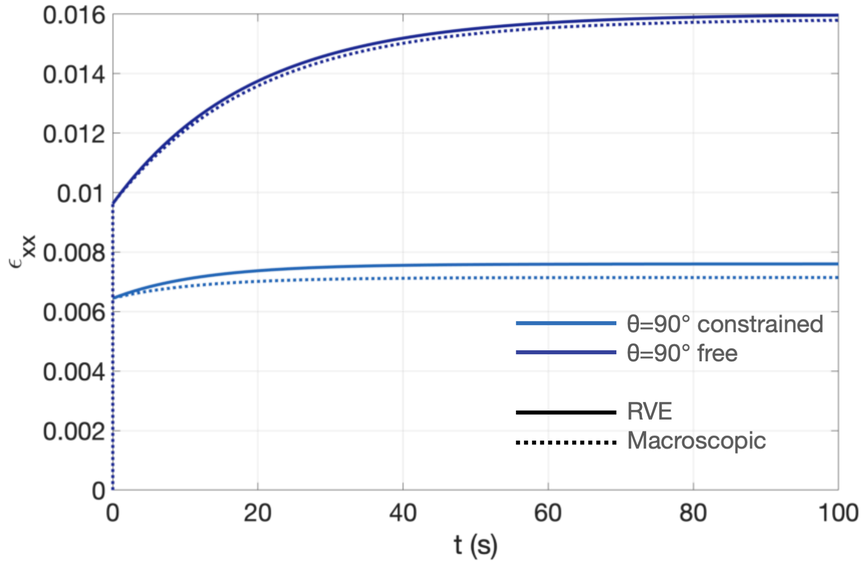
$$E_{yy,0}(t) = E_{zz,0}(t) = 0.$$



- Unconstrained uniaxial creep tests
  - very good agreement



- Constrained uniaxial creep tests
  - the approximation is more visible but still acceptable



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Conclusions and perspectives

A geometrical description of the constitutive behaviour

- The Cartan decomposition, based on the geometric modelling of the transverse isotropy, yields uncoupled constitutive laws with a clearer link to the underlying constituents' properties
- An ansatz on the properties affected by the viscoelastic response results in a good approximation of the Representative Volume Element response
- A better description can be obtained by introducing viscoelasticity on the other parameters (but more material parameters are required!)

Perspectives

- For transverse isotropy:

  > *Damage modelling in laminated composites?*
  > *Finite transformation modelling with the new set of invariants?*

- For orthotropy / other material symmetries:

  > *How do the formulated laws change?*
  > *What can these formulations teach us about the underlying mechanics?*

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Thank you for your attention!
Questions?

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