DE LA RECHERCHE À L'INDUSTRIE

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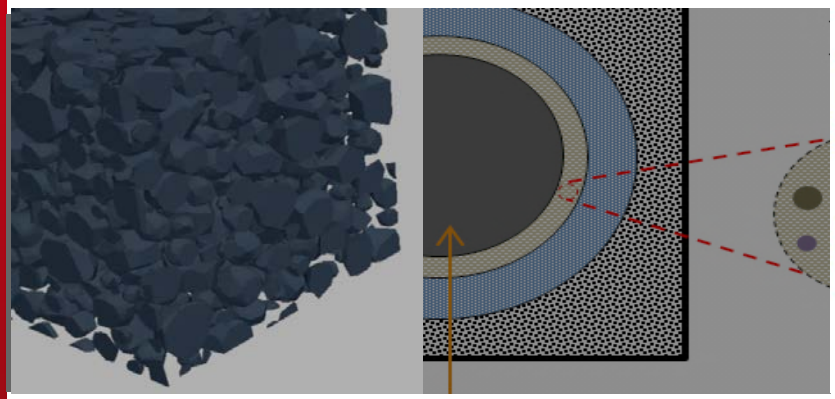
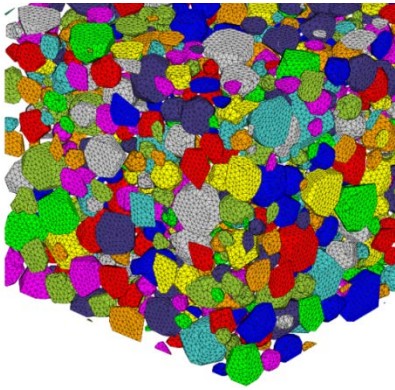
EFFECTIVE AGEING LINEAR VISCOELASTIC PROPERTIES OF COMPOSITES WITH PHASE PRECIPITATION: COMPARISONS BETWEEN NUMERICAL AND ANALYTICAL HOMOGENIZATION APPROACHES





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CONTEXT

Nuclear facilities

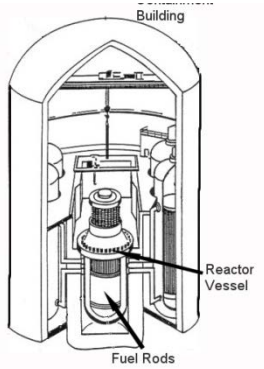
Safety and durability of concrete structures are of particular importance

➔ **Short as well as long term behavior** when submitted to mechanical, hydric and thermal loadings

⇒ **should be precisely characterized**

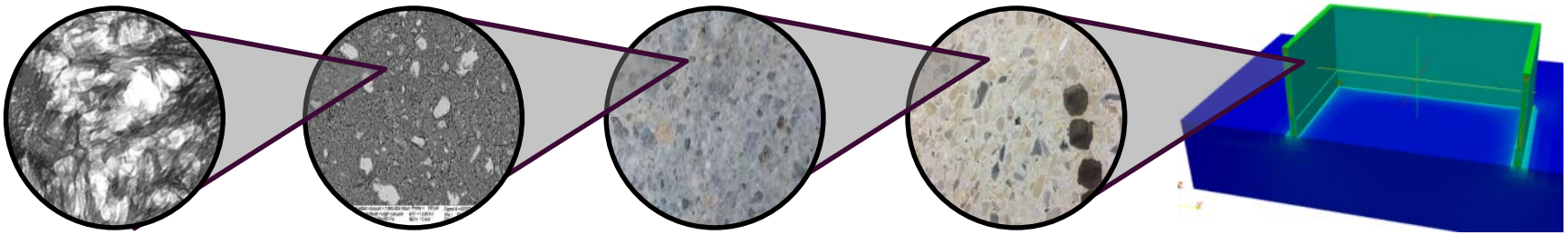
Nuclear waste storage

Confinement building



Focus on the short-term behavior

- Estimation of mechanical properties evolving at early age (hydration)
- Multiscale approach: different phenomena taking place at different time and space scales



Objectives

- Evaluation/validation of a semi-analytical approach for estimating the ageing linear viscoelastic properties of cementitious materials by comparison with 3D numerical simulations

➡ **in the case of a progressive precipitation (solidification) scenario**

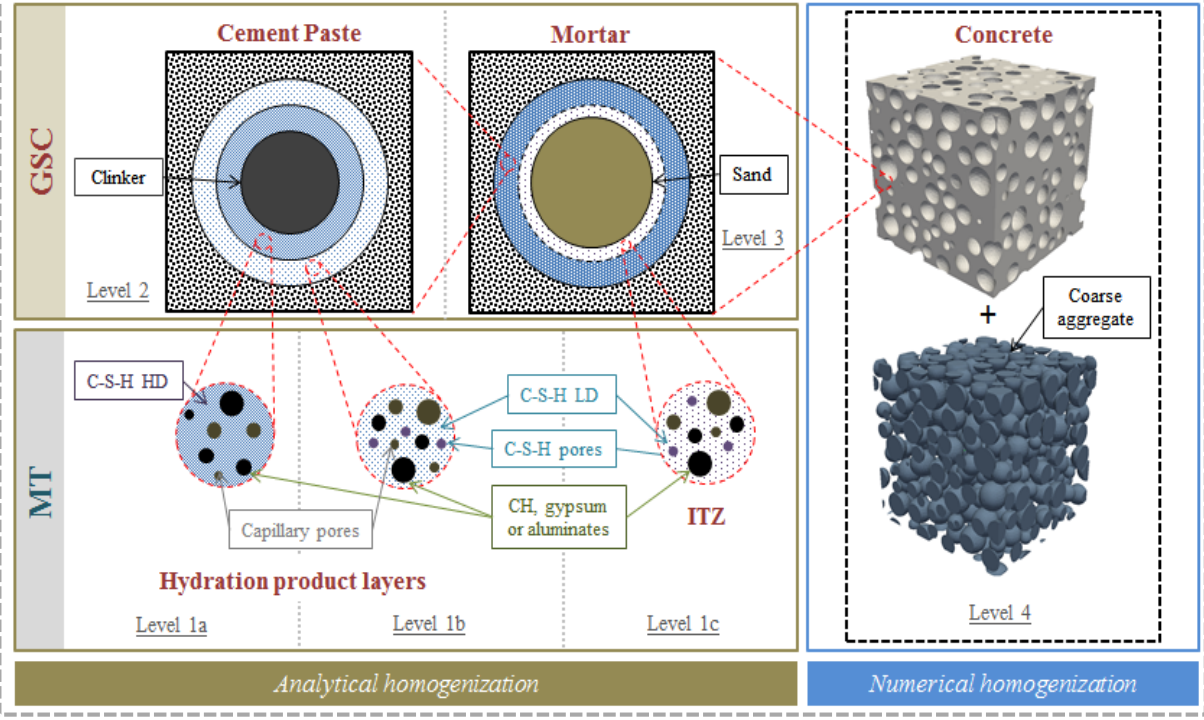
General approach

➔ **Analytical homogenization**:
Estimation of properties at different scales (simplified representation of the microstructure, different phase properties…)

➔ **Numerical homogenization**:
-Validation of analytical approaches
-More complex microstructures
-Analysis of particular aspects: shape of particles, distribution, size…

[Honorio 2015]

Example: analytical homogenization at the cement paste and mortar scale, numerical homogenization at concrete scale



AGEING LINEAR VISCOELASTIC BEHAVIOUR

- Constitutive behaviour in **ageing linear viscoelasticity**:

$$\boldsymbol{\varepsilon}(t) = \int_{t'=-\infty}^{t} \mathbb{S}(t,t') : \mathrm{d}\boldsymbol{\sigma}(t') \qquad \boldsymbol{\sigma}(t) = \int_{t'=-\infty}^{t} \mathbb{R}(t,t') : \mathrm{d}\boldsymbol{\varepsilon}(t')$$

- Ageing aspect → Dependence of the time of loading

- Non-ageing case $\boldsymbol{\varepsilon}(t) = \int_{t'=-\infty}^{t} \mathbb{S}(t-t') : \mathrm{d}\boldsymbol{\sigma}(t')$ $\qquad \boldsymbol{\sigma}(t) = \int_{t'=-\infty}^{t} \mathbb{R}(t-t') : \mathrm{d}\boldsymbol{\varepsilon}(t')$
- *Laplace-Carson transform* → ***Correspondance principle*** → *equivalence to elasticity* [Mandel1966]

- Volterra integral operator : $(f \circ g)(t,\tau) \equiv \int_{t'=-\infty}^{t} f(t,t')\, d_{t'} g(t',\tau)$ [Volterra 1887]

$$\boldsymbol{\varepsilon}(t) = \mathbb{S}(t,.) \overset{\circ}{\vdots} \boldsymbol{\sigma}(.), \qquad \boldsymbol{\sigma}(t) = \mathbb{R}(t,.) \overset{\circ}{\vdots} \boldsymbol{\varepsilon}(.),$$

- Similar form to Elasticity → **Correspondance principle**

- **Numerical method to evaluate Volterra integrals:** [Sanahuja, 2013]
  - ➔ **Time discretization + trapezoidal rule** [Bazant, 1972]

ANALYTICAL HOMOGENIZATION

Derivation of Mori-Tanaka scheme in ageing linear viscoelasticity

- Obtained by Sanahuja [2013]

Derivation of Generalized Self-Consistent scheme (n-layered spherical inclusions)

- Following Herve and Zaoui [1992]

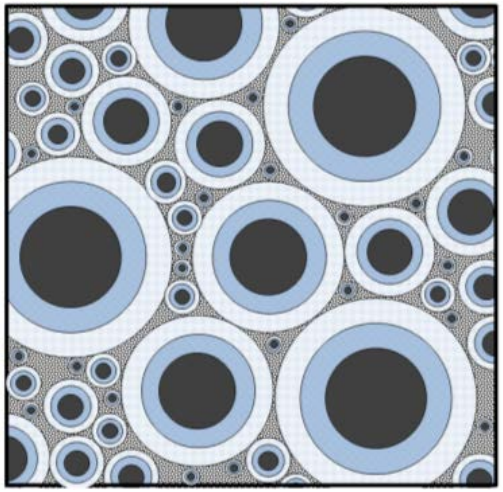
Bulk relaxation function

- For n = 2 (1 layer):

$$k_{(2)}^{eff} = \left[R_2{}^3 k_2 \circ [4\mu_2 + 3k_2]^{-1} \circ [4\mu_2 + 3k_1] - 4\mu_2 \circ [4\mu_2 + 3k_2]^{-1} \circ \left[R_1{}^3 (k_2 - k_1)\right]\right] \circ \left[R_2{}^3 [4\mu_2 + 3k_2]^{-1} \circ [4\mu_2 + 3k_1] + 3[4\mu_2 + 3k_2]^{-1} \circ \left[R_1{}^3 (k_2 - k_1)\right]\right]^{-1}$$

Shear relaxation function

- Problem: Inversion of a matrix with non-commutative elements
  - Schur complement
  - *NCAlgebra* (package for *Mathematica*)

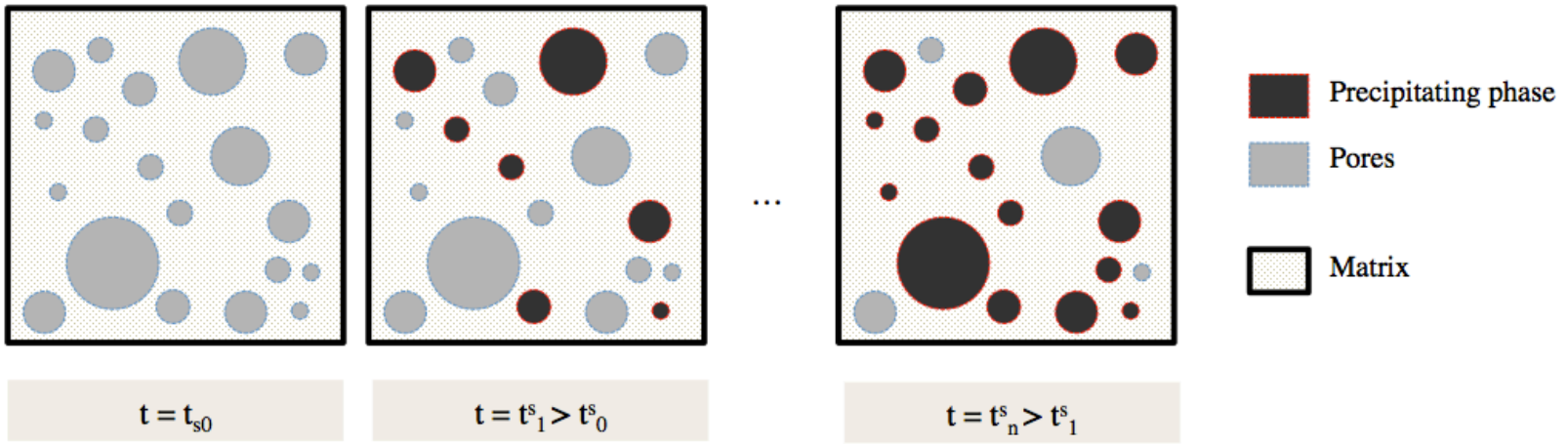


[Honorio et al., under review]

EXTENSION : SOLIDIFICATION CASE

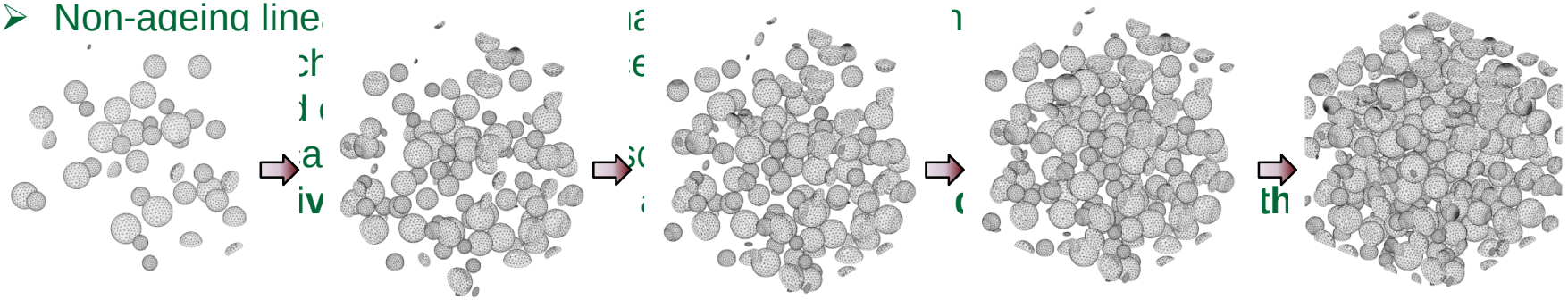
- **Progressive precipitation of phases** ➔ ageing of the material (including in the case of non-ageing behavior of phases [Bazant 1977])

- **Simplified scenario considered in this study:**



Example: precipitation of 30% spherical inclusions

- Microstructures = matrix + 1 inclusion phase
- Non-ageing line



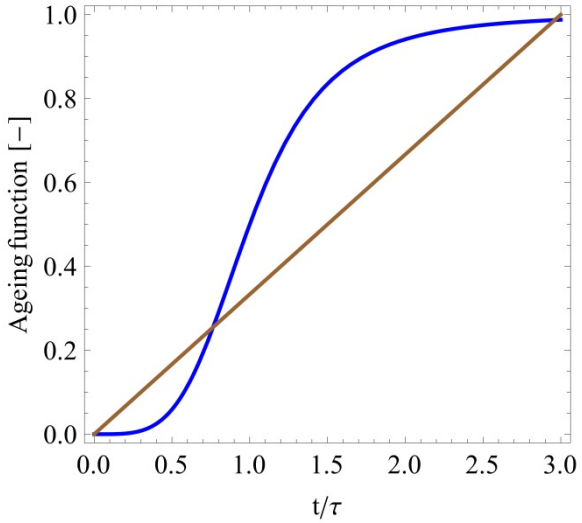
PARAMETERS

To simplify the comparison ➔ use of idealized behaviors

➢ **Two ageing functions are studied:**

Linear $f_{age}^{B}(t) = \min\left(1, \frac{1}{3}t\right) f_{age}^{\infty}$

Sigmoidal $f_{age}^{A}(t) = \frac{t^4}{1+t^4} f_{age}^{\infty}$



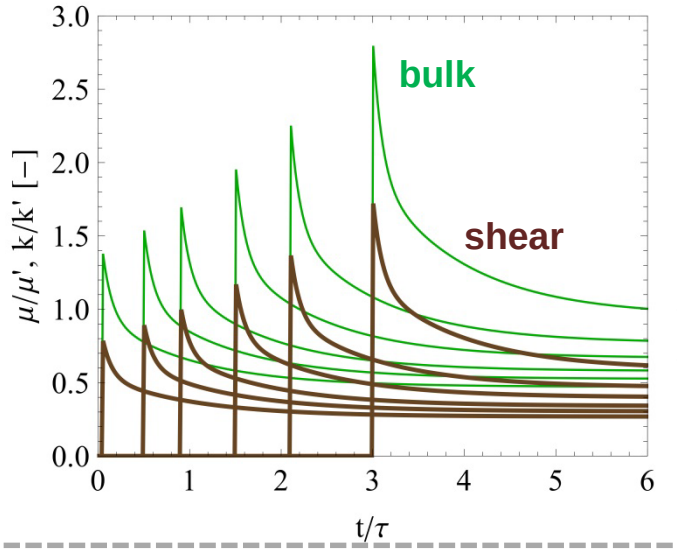
➢ **Linear viscoelastic behavior for the phases:**

Generalized Maxwell model for bulk and shear moduli

➡ $X(t-t') = x_0 + \sum_i x_i \exp[-(t-t')/\chi_i]$

Parameters

	x_0	x_1	x_2
k/k'	1	1	1
μ/μ'	1/2	1/2	1/2
χ/τ	-	0.1	1



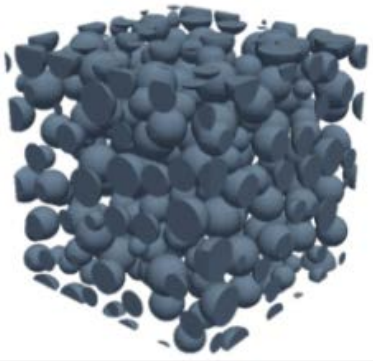
➔ Evolutions of bulk and shear moduli, linear ageing function, 30% inclusions

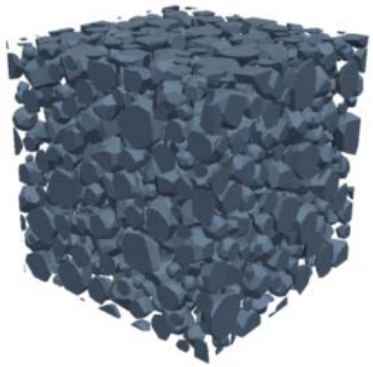
3D SIMULATIONS : DISCRETIZATION OF THE INCLUSION PHASE

Numerical samples considered ➔ Generation with CAD code **salome** (www.salome-platform.org)

- Randomly distributed inclusions
- Various shapes and sizes
- Periodic meshes

- 360 spherical aggregates of different sizes
- 30%
- 1.75 10^6 finite elements





- 1124 Voronoi aggregates of different sizes
- 40%
- 2.37 10^6 finite elements

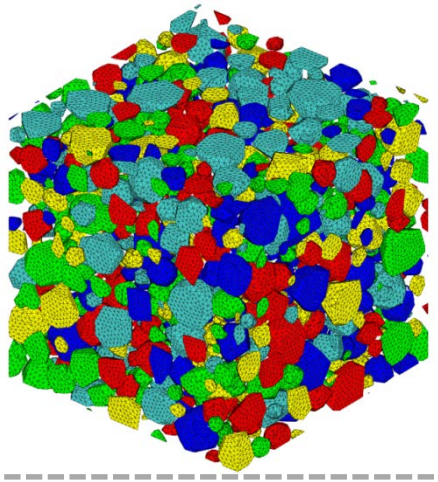
Discretization in FE simulations (Cast3M) ➔ random repartition of inclusions

➔ Random repartition in a prescribed number of sub-families as a function of the volumes of each aggregate

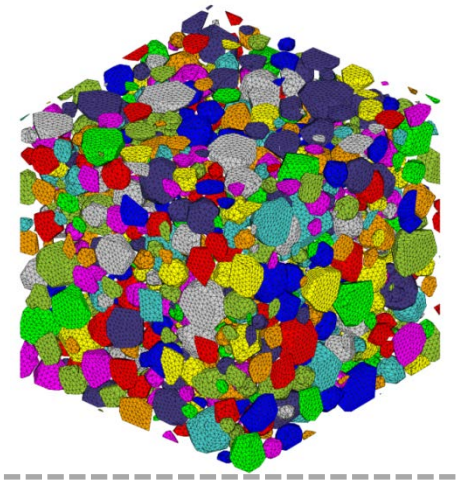
➔ Calculation of the exact precipitation time for each sub-family

Example : with the 1124 Voronoi aggregates microstructure

5 sub-families

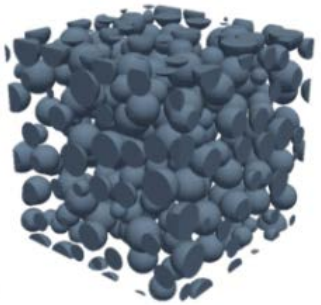


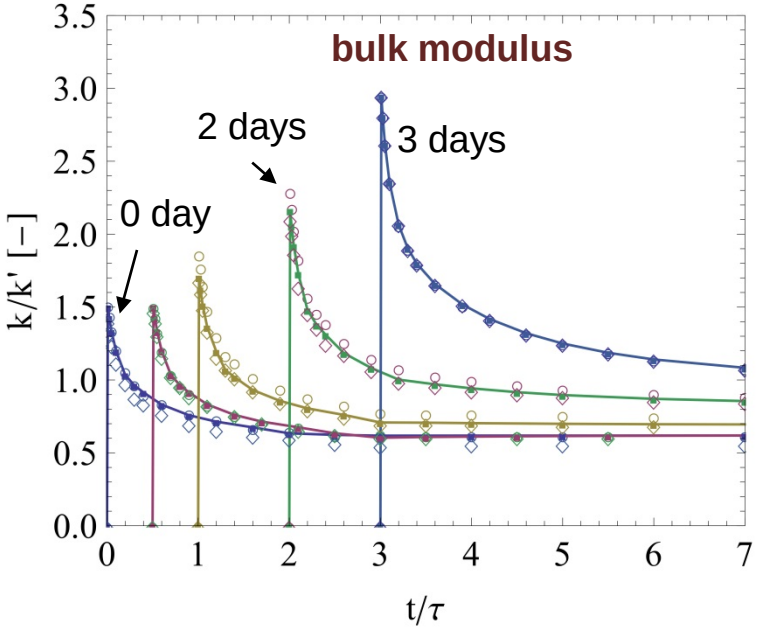
10 sub-families

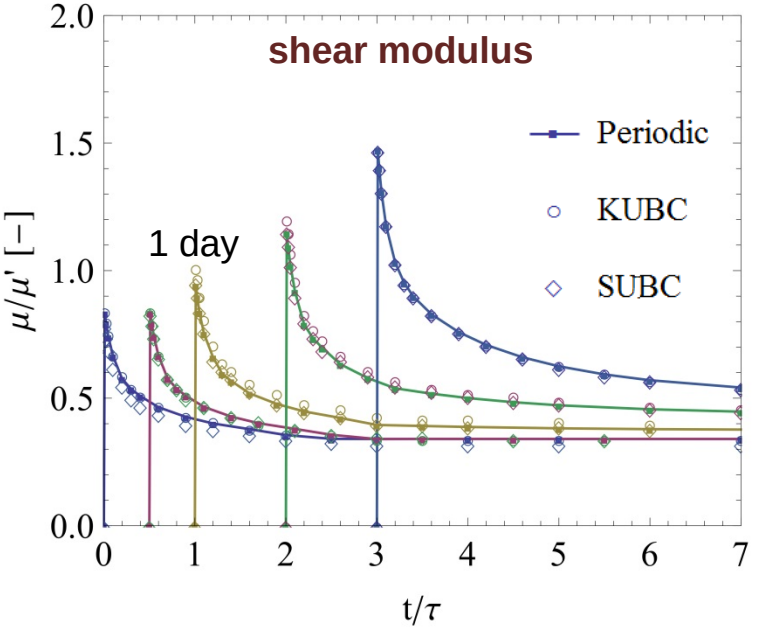


INFLUENCE OF THE BOUNDARY CONDITIONS

- **Numerical simulation results of Representative Element Volumes are known to be dependent on boundary conditions**
  - Linear ageing function
  - Age of loading: 0.0, 0.5, 1, 2, 3 days, discretization=10 sub-families
  - Boundary conditions considered: static uniform (SUBC), kinematic uniform (KUBC) and periodic (PBC)



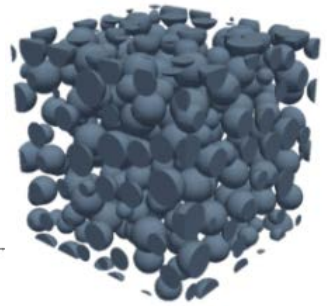


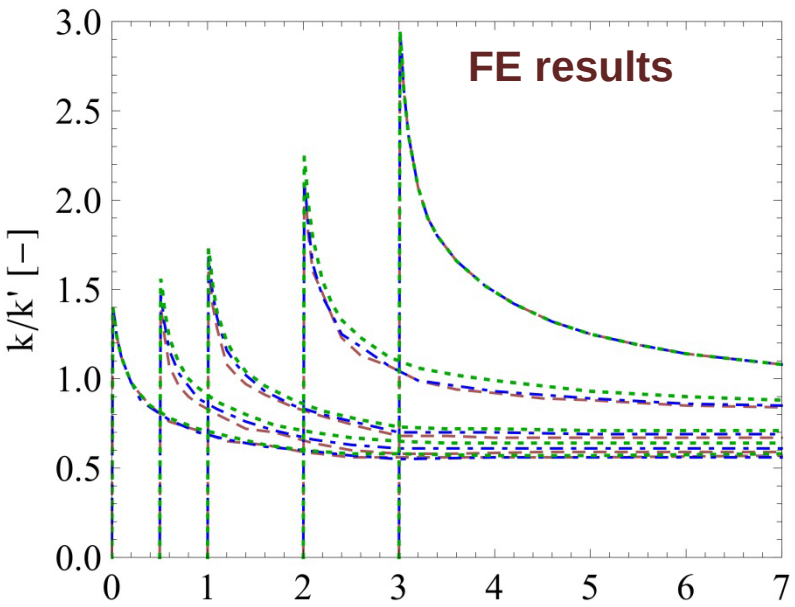


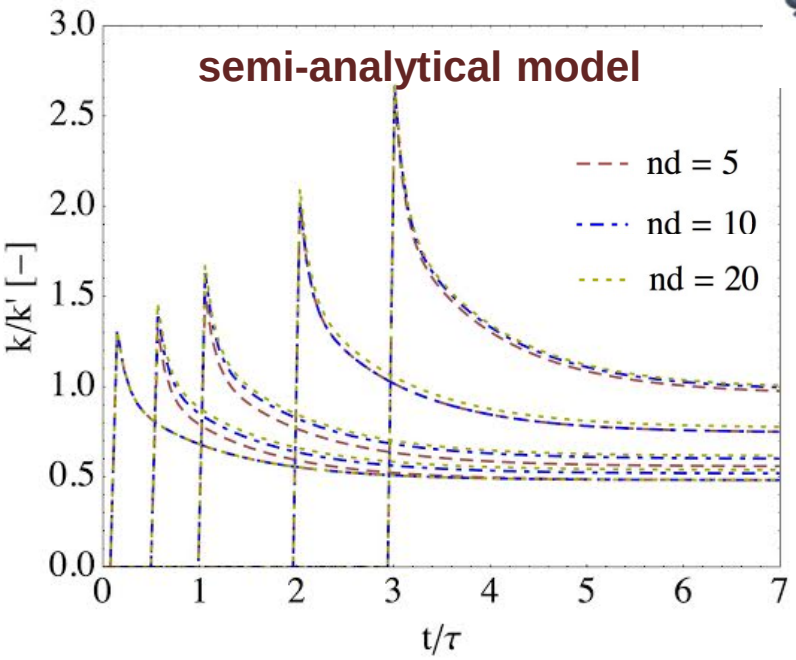
➔ Relatively small differences between the BC
➔ SUBC close to PBC (taken as reference)
➔ Computation time with SUBC (1.5-2 hours for 20 time steps) about 2.5 times less than PBC ➔ in the following **results are shown with SUBC**

INFLUENCE OF THE DISCRETIZATION

- **Discretization to reproduce a progressive precipitation** :
  - Discretization of the inclusion phase influences both FE and semi-analytical methods
  - Example on bulk modulus obtained with 3 discretization levels: 5, 10 and 20 sub-families, 30% spherical inclusion case





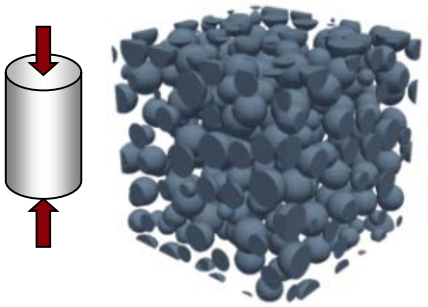


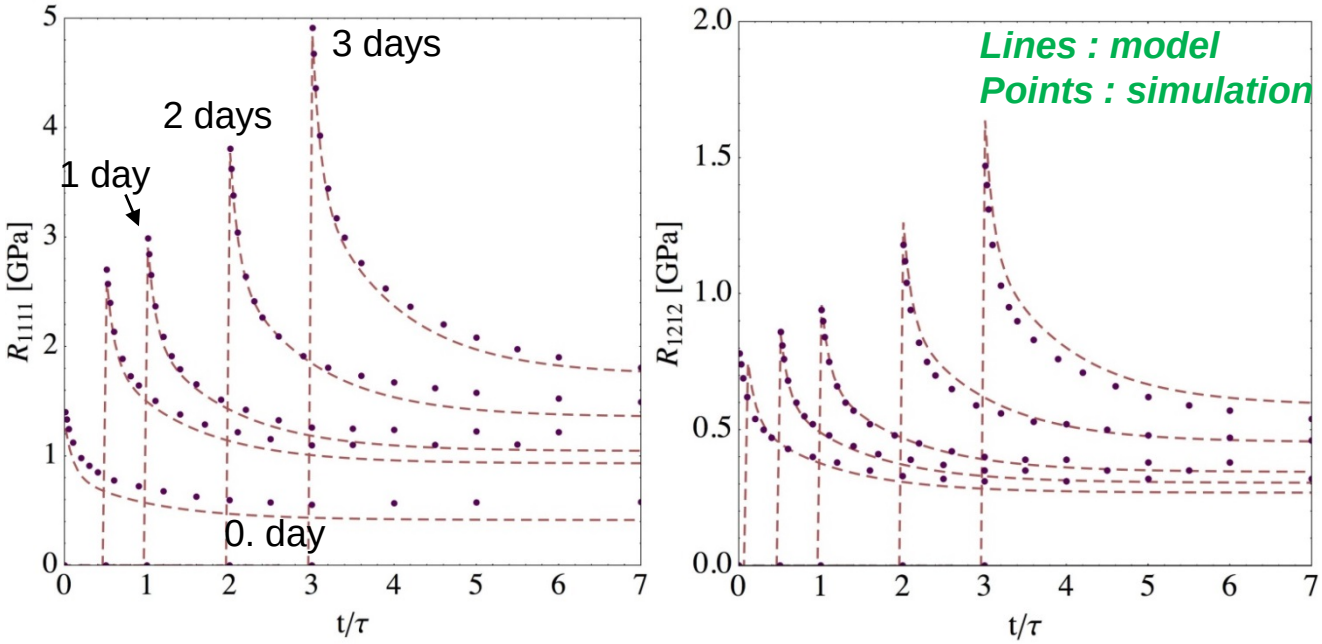
➔ Some limited differences are observed as a function of the discretization
➔ Discrepancies are of the same order for the FE and model results
➔ **At least 10 sub-families for both FE simulations and model**

RESULTS: FE/MODEL COMPARISON (1)

- **Relaxation tensor, 30% spherical inclusion case**
  - Linear ageing function
  - Different loading ages: 0.0, 0.5, 1, 2, 3 days

creep

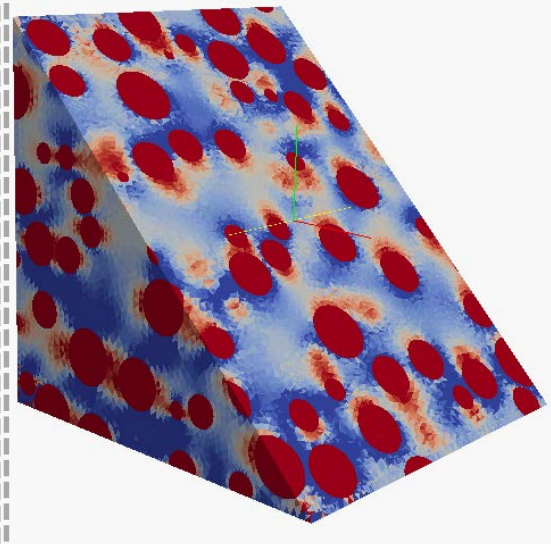




➔ Relatively good agreement between FE and semi-analytical results

➔ **Validation of the analytical procedure**

Evolution of the longitudinal stresses in the microstructure



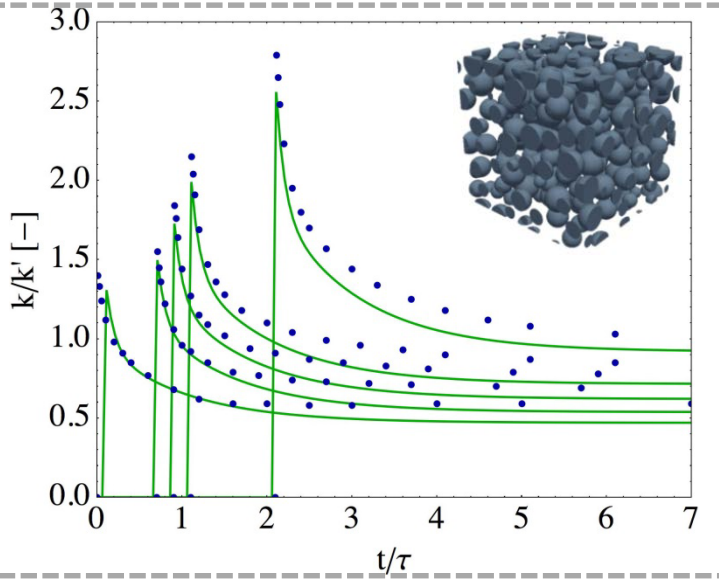
Age of loading: 1 day

RESULTS: FE/MODEL COMPARISON (2)

- **Results with sigmoidal ageing function**
  - 30% spherical inclusions
  - Loading times: 0.0, 0.7, 0.9, 1.1, 2 days

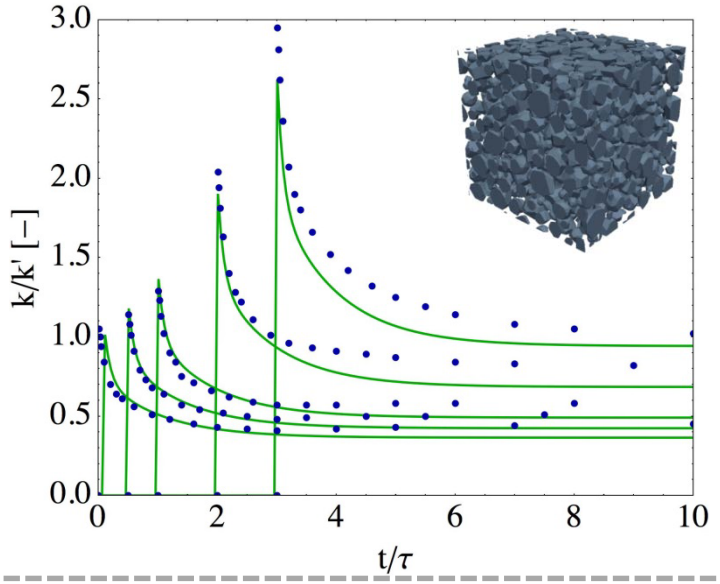
➔ Relatively good agreement between FE and semi-analytical results of overall moduli

Lines : model
Points : simulation



- **Results with the 40% Voronoi aggregate microstructure**
  - Linear ageing function
  - Different loading times: 0.0, 0.5, 1, 2, 3 days

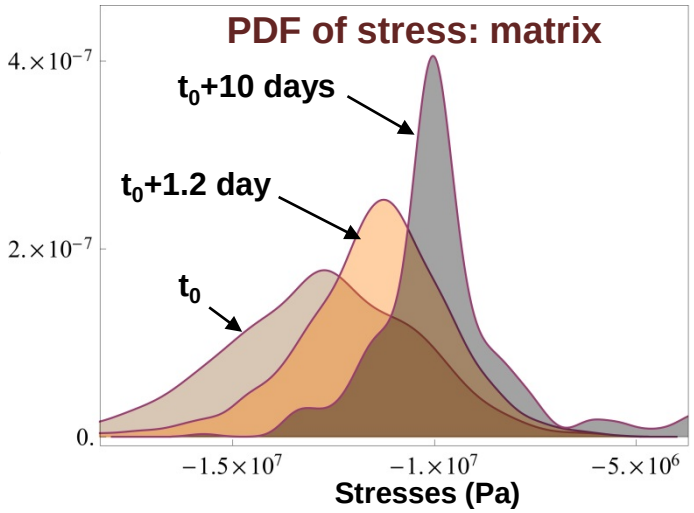
➔ Correct agreement between FE and semi-analytical results, with greater volume fraction of inclusions
➔ *Negligible effects of the random discretization process through several realizations (not shown)*
➔ *Effects of the aggregate shape are to be analyzed specifically*

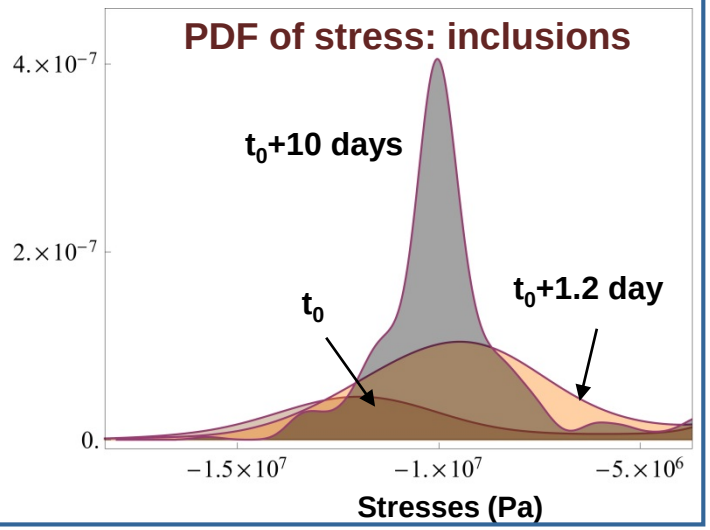


LOCAL RESULTS: DISPERSION

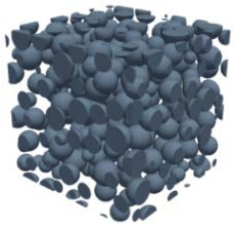
❑ Evaluation of the dispersion in the aggregates and matrix

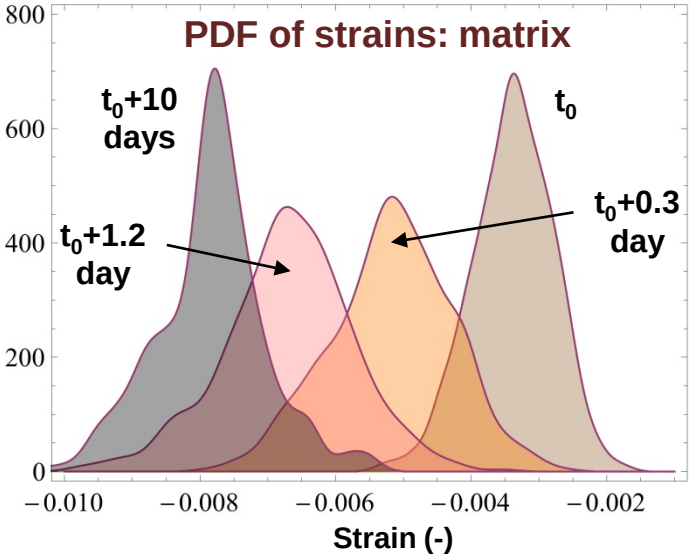
- **Example**: average longitudinal stress and strains within aggregates and matrix subvolumes
- Probability Distribution Functions at different times
- **t_0 at loading = 1 day**





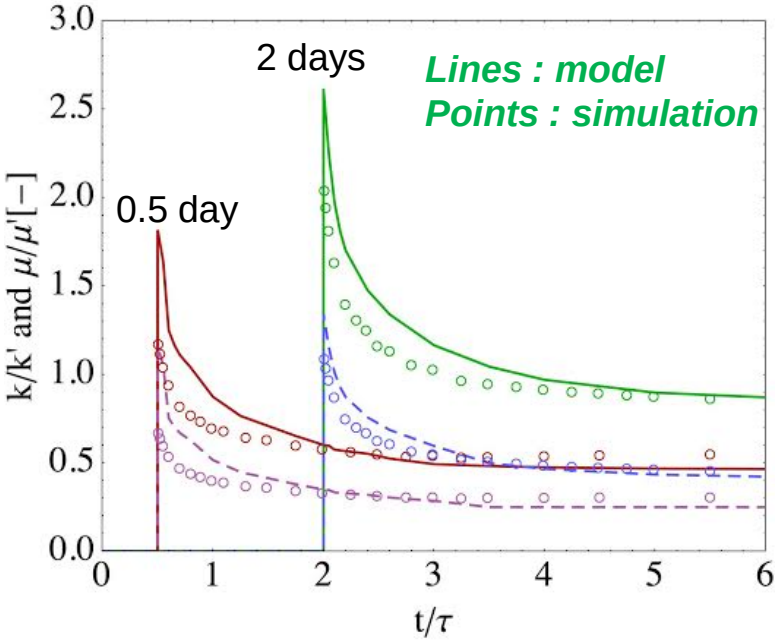
- Large dispersion of stresses in both matrix and inclusion, which decreases for greater times
- Stress distribution appears more disperse in the aggregates than in matrix subvolumes
- Significant dispersion in the matrix strains; the mean strain in the matrix decreases with time

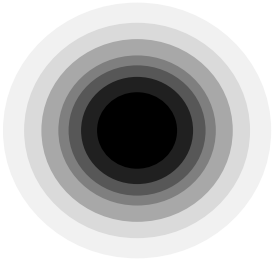




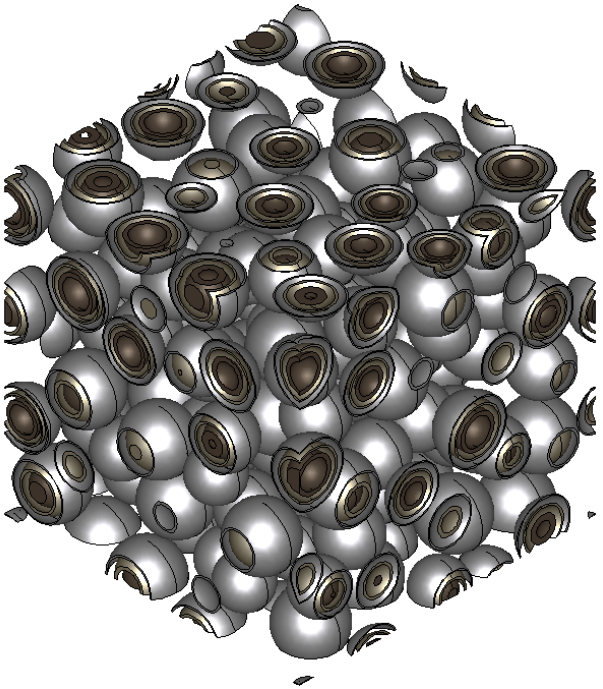
IN PROGRESS: MULTILAYER INCLUSIONS

- **First results with 40% multilayer inclusions**
  - Progressive precipitation from the external layer to the core
  - 120 inclusions composed of 1 core and 9 layers
  - 3.57 millions of finite elements
  - Use of the GSCS for the analytical estimations

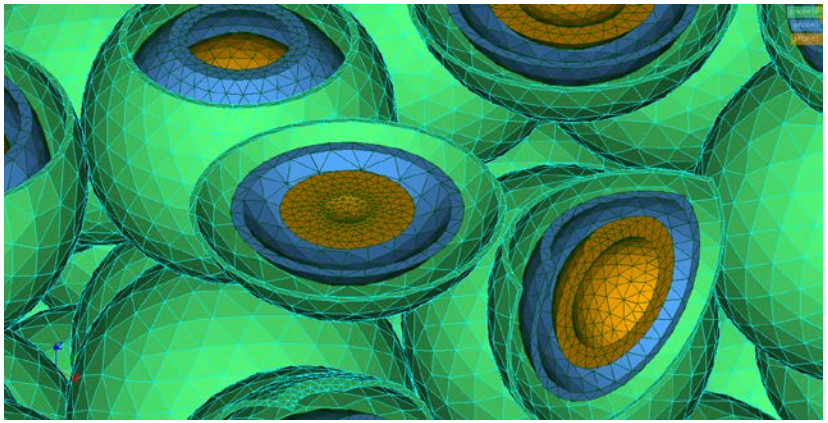




Multilayer inclusion



Details of the mesh



- Correct, but more discrepancies with respect to the MT case
- Aspects to be addressed in the future: effects of the mesh refinement

CONCLUSIONS AND PERPECTIVES

- 3D FE numerical simulations with scenarios of progressive precipitation of inclusions
- Confrontation with a semi-analytical model for estimating the ageing linear viscoelastic properties of cement-based materials
- The comparison shows generally a correct agreement between FE and analytical results, which validates the analytical procedure

Perspectives:

- Extension and application to the hydration of cement particles
- Introduction of an ageing viscoelastic behaviour of the phases (C-S-H)
- Other precipitation scenarios (multilayer inclusions) to be analyzed
- Extension to other physical properties: coefficient of thermal expansion (in progress)…