Computational & Multiscale Mechanics of Materials

CM3

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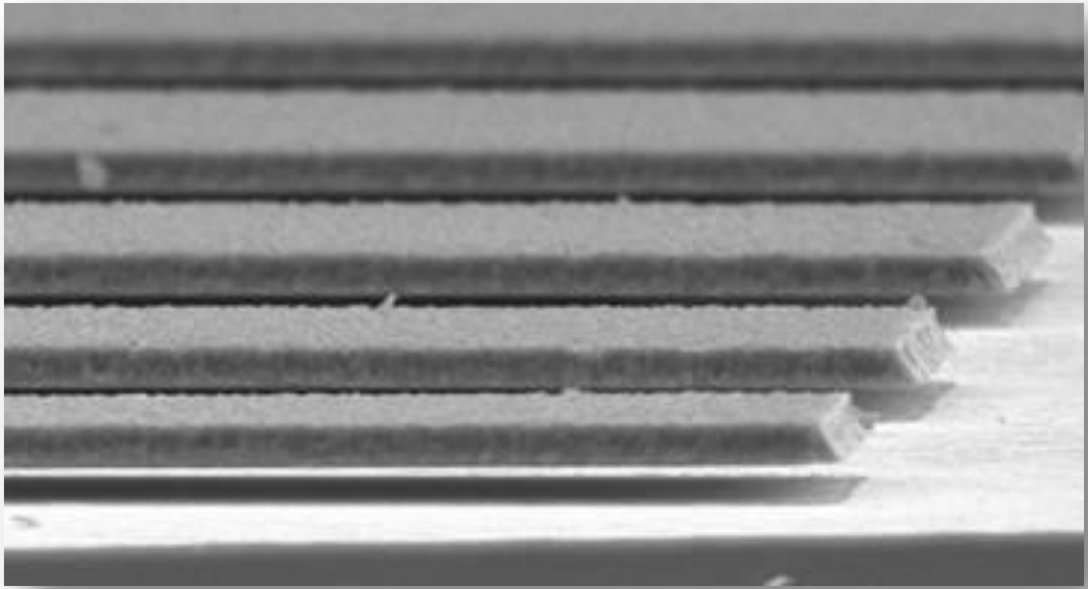
A probabilistic multi-scale model for polycrystalline MEMS resonators



Lucas Vincent
Wu Ling
Paquay Stéphane
Golinval Jean-Claude
Noels Ludovic

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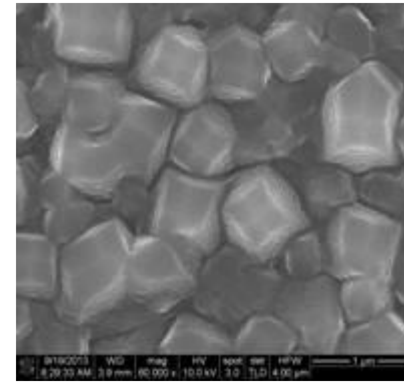
The problem

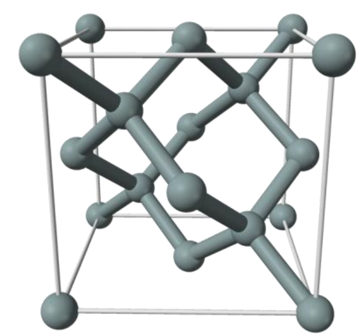


- MEMS structures
  - Are not several orders larger than their micro-structure size
  - As a result, their macroscopic properties can exhibit a **scatter**
    - Due to the fabrication process
    - Due to uncertainties of the material
    - …

→ The objective of this work is to estimate this scatter

- Up to now, the only sources of uncertainty is due to the material
  - Silicon crystals are anisotropic
  - Polysilicon is polycrystalline

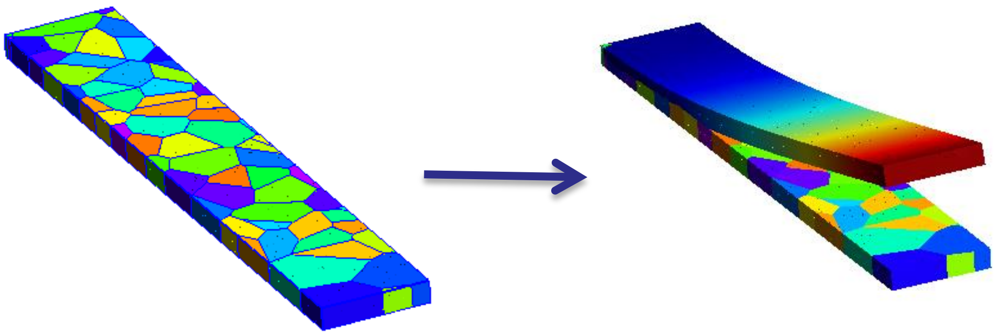
→ **Each grain has a random orientation**

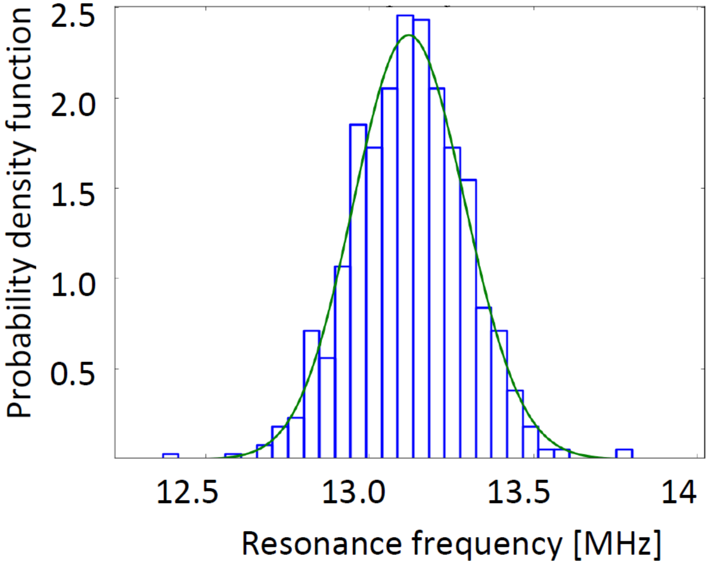


- Characteristics of our model:
  - Clamped microbeam
  - Macroscopic property of interest: first mode eigenfrequency
    - For a MEMS gyroscope for example

Monte-Carlo for a fully modelled beam

- The first mode frequency distribution can be obtained with
  - A 3D beam with each grain modelled
  - and a Monte-Carlo simulation of this model

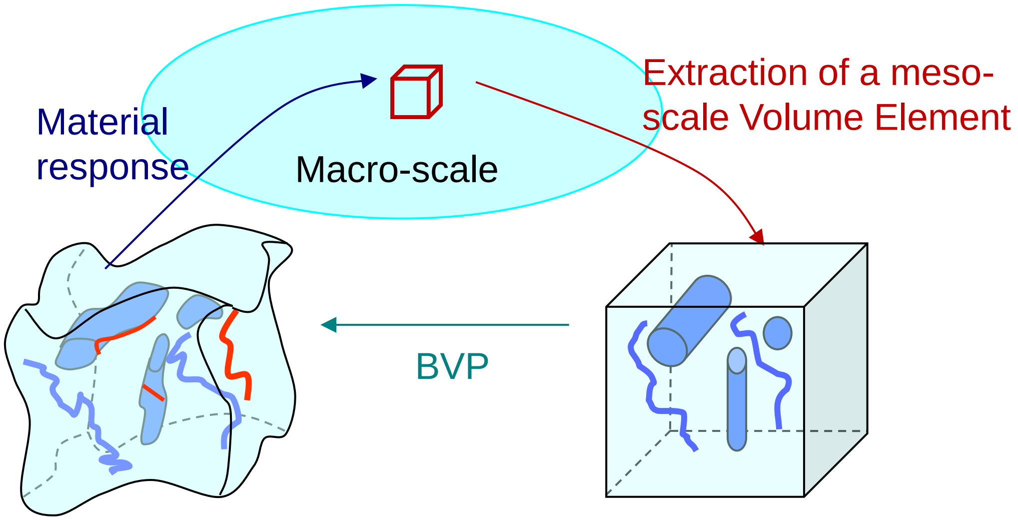




- Considering each grain is expensive and time consuming

  ↳ **Motivation for stochastic multi-scale methods**

- Multi-scale modelling
  - 2 problems are solved concurrently
    - The macro-scale problem
    - The meso-scale problem (on a meso-scale Volume Element)



- Length-scales separation

$$L_{macro} >> L_{VE} >> L_{micro}$$

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

To be statistically representative: Size of the meso-scale volume element larger than the characteristic length of the micro-structure

Motivations

- For structures not several orders larger than the micro-structure size

$$L_{macro} >> L_{VE} >\sim L_{micro}$$

For accuracy: Size of the meso-scale volume element smaller than the characteristic length of the macro-scale loading

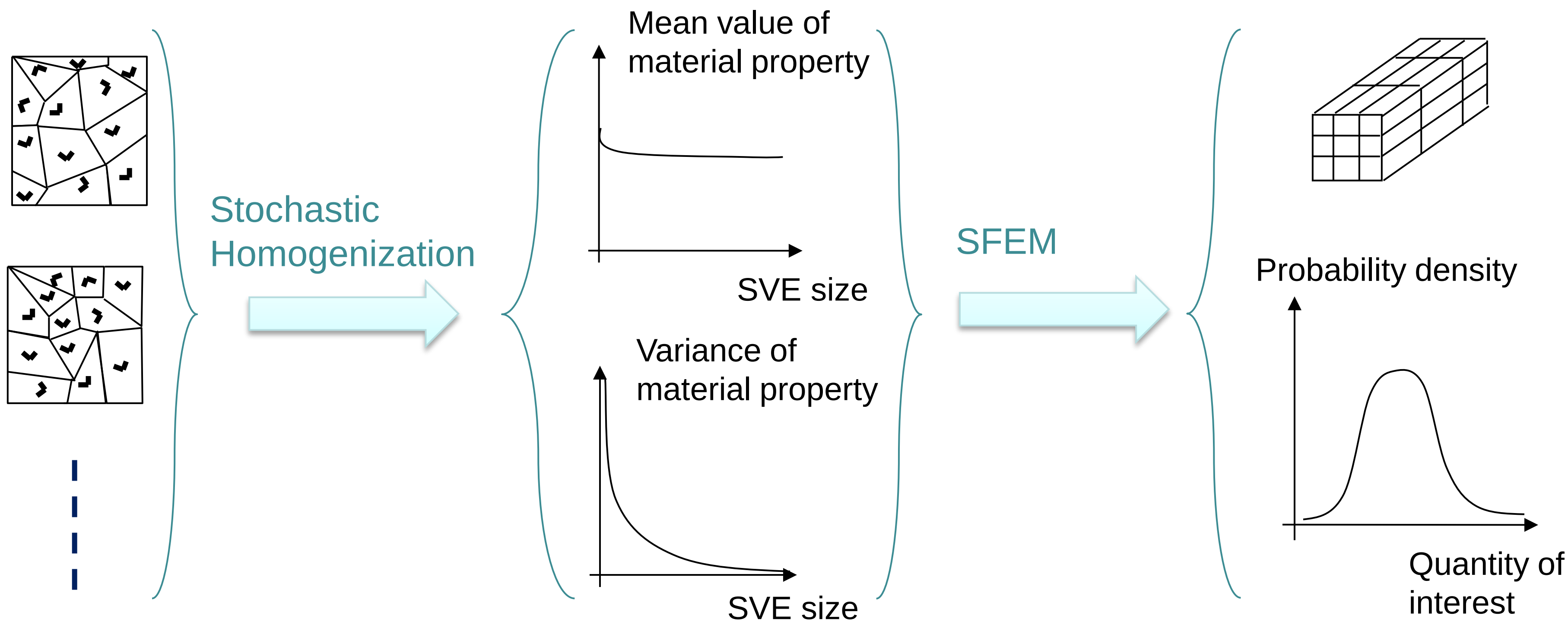
Meso-scale volume element no longer statistically representative: Stochastic Volume Elements*

- Possibility to propagate the uncertainties from the micro-scale to the macro-scale

**M Ostoja-Starzewski, X Wang, 1999*
P Trovalusci, M Ostoja-Starzewski, M L De Bellis, A Murrali, 2015
X. Yin, W. Chen, A. To, C. McVeigh, 2008
J. Guilleminot, A. Noshadravan, C. Soize, R. Ghanem, 2011
….

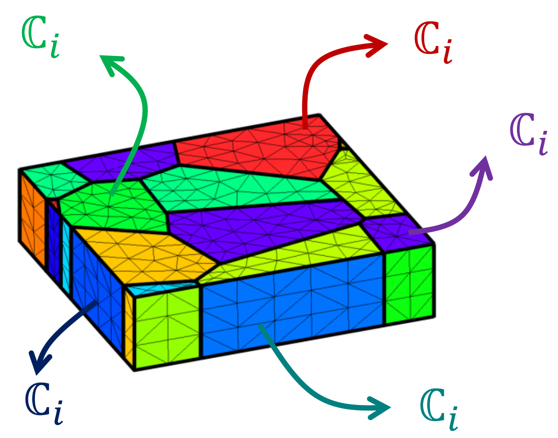
A 3-scale procedure

Grain-scale or micro-scale	Meso-scale	Macro-scale
➢ Samples of the microstructure (volume elements) are generated ➢ Each grain has a random orientation	➢ Intermediate scale ➢ The distribution of the material property $\mathbb{P}(C)$ is defined	➢ Uncertainty quantification of the macro-scale quantity ➢ E.g. the first mode frequency $\mathbb{P}(f_1)$



From the micro-scale to the meso-scale

- Definition of Stochastic Volume Elements (SVEs)
  - Poisson Voronoï tessellation
  - Each grain i is assigned an elasticity tensor $\mathbb{C}_i$
  - $\mathbb{C}_i$ defined from silicon crystal properties
  - Each $\mathbb{C}_i$ is assigned a random rotation
  - Mixed BCs



- Stochastic homogenization
  - Several realizations

$$\boldsymbol{\sigma}_{m^i} = \mathbb{C}_i : \boldsymbol{\epsilon}_{m^i} \quad , \forall i \quad \longrightarrow \quad \boldsymbol{\sigma}_M = \mathbb{C}_M : \boldsymbol{\epsilon}_M$$

Computational homogenization

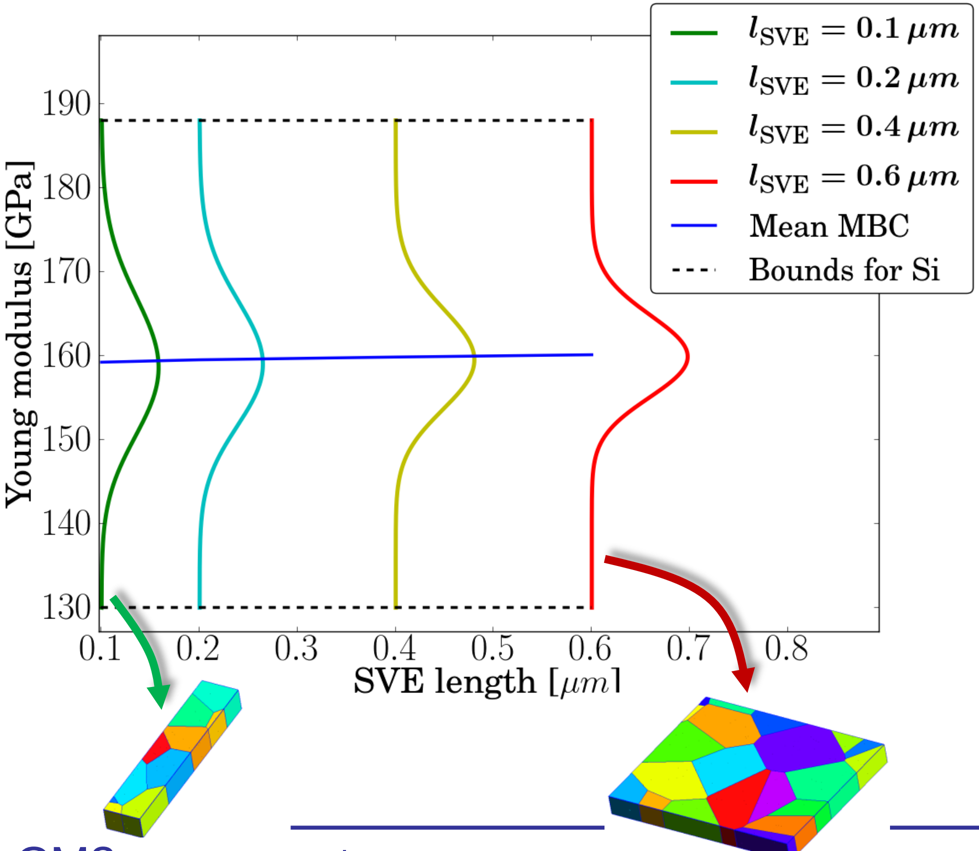
Samples of the meso-scale homogenized elasticity tensors

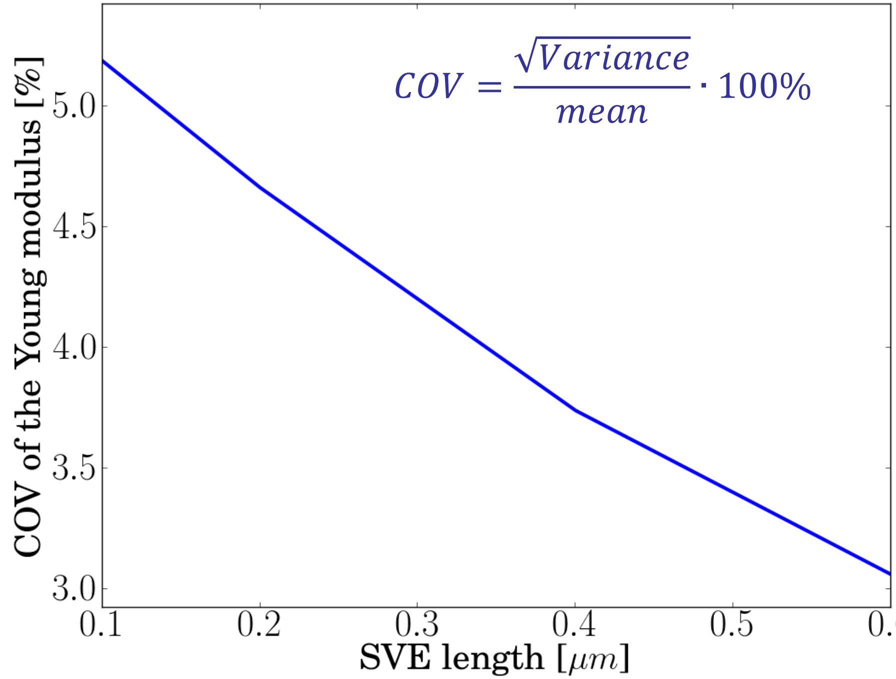
  - Homogenized elasticity tensor not unique as statistical representativeness is lost*
    - It is thus called apparent elasticity tensor

*"C. Huet, 1990

From the micro-scale to the meso-scale

- Distribution of the apparent meso-scale elasticity tensor $\mathbb{C}_M$
  - For large SVEs, the apparent tensor tends to the effective (and unique) one

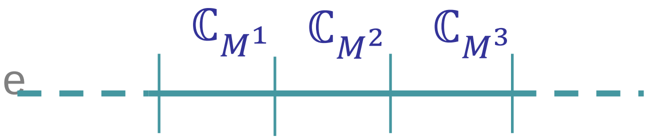


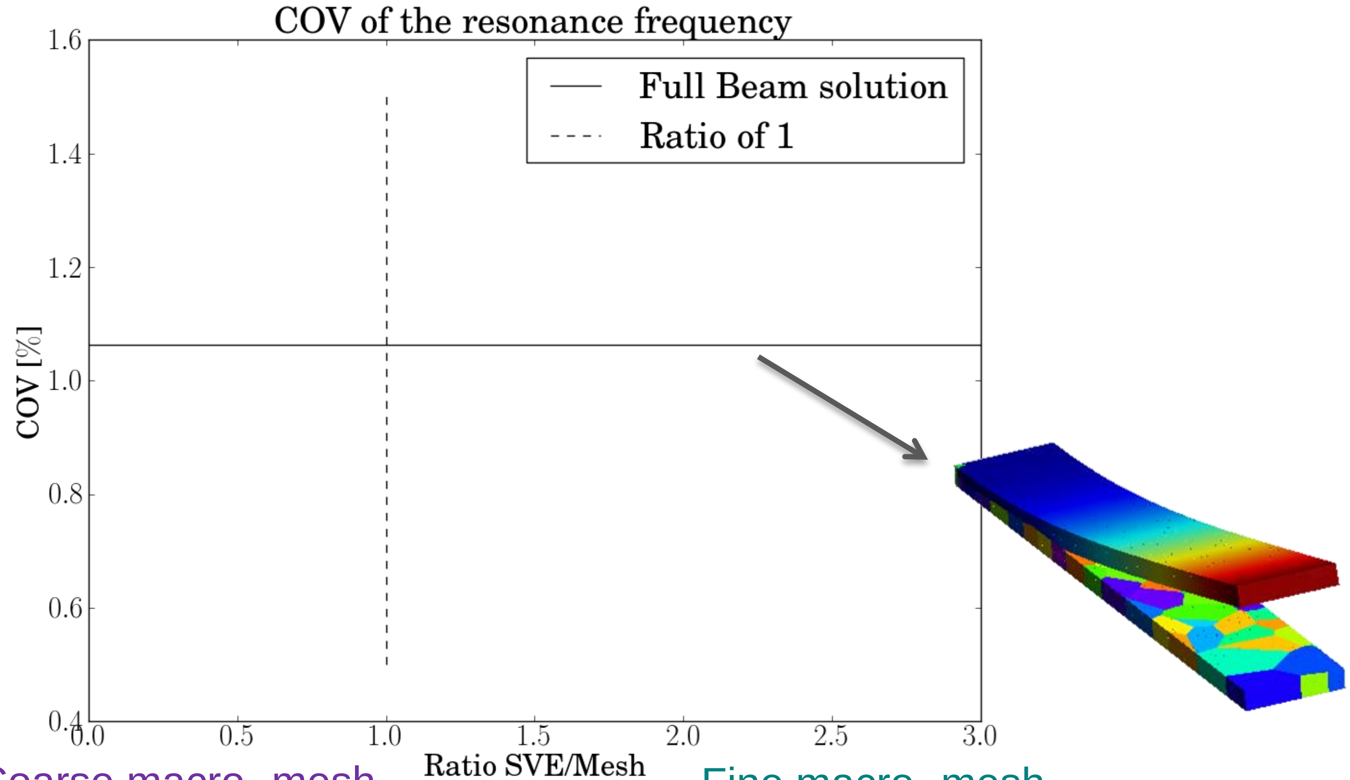


- The bounds do not depend on the SVE size but on the silicon elasticity tensor
- However, the larger the SVE, the lower the probability to be close to the bounds

From the micro-scale to the meso-scale

- Use of the meso-scale distribution with macro-scale finite elements
  - Beam macro-scale finite elements
  - Use of the meso-scale distribution as a random variable
  - Monte-Carlo simulations





Coarse macro- mesh

Fine macro- mesh

From the micro-scale to the meso-scale

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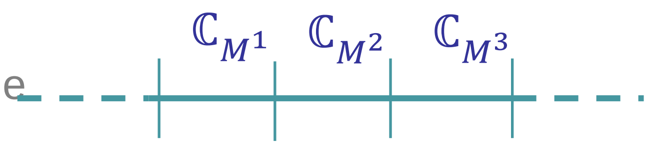

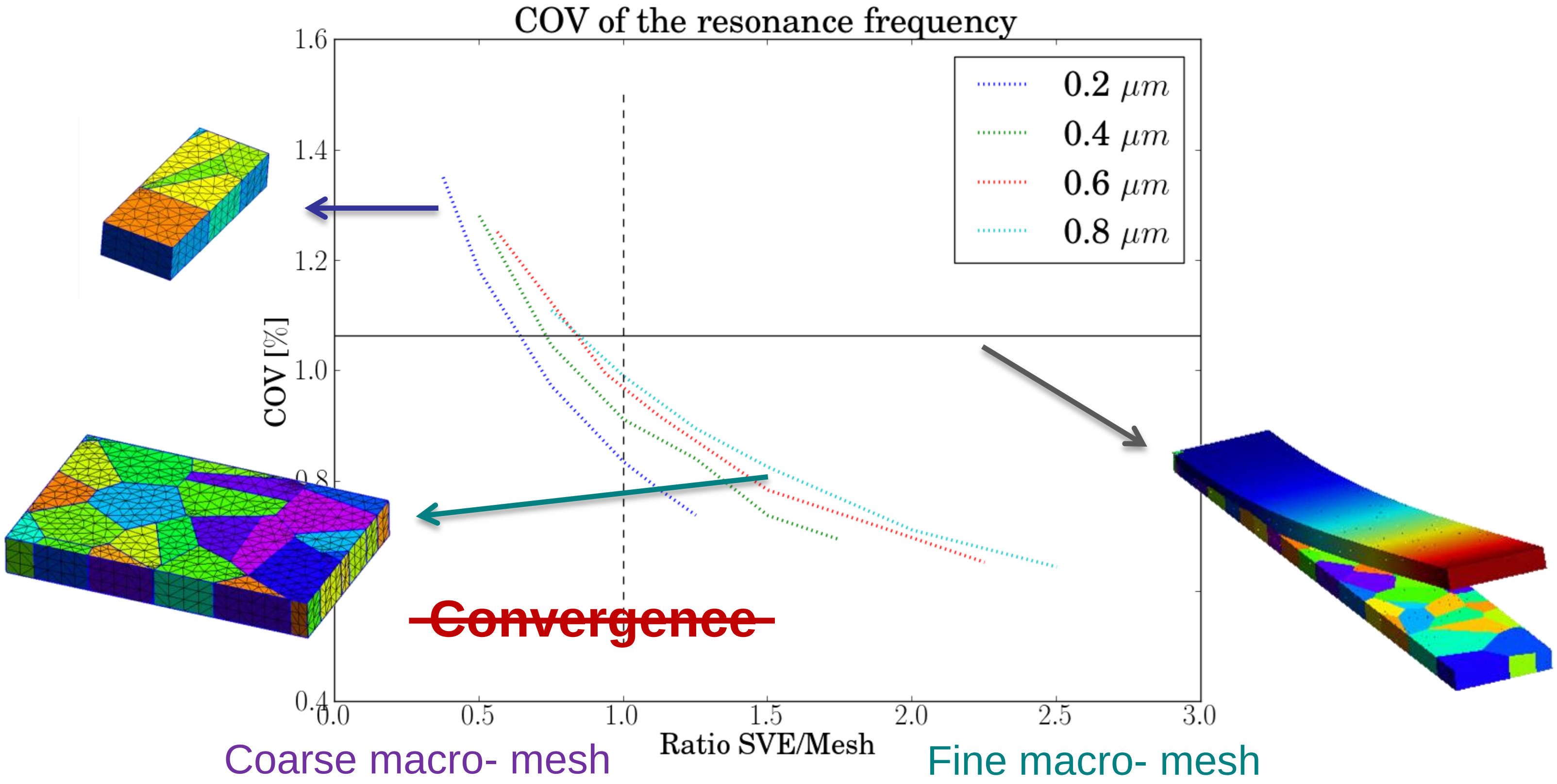

- No convergence: the macro-scale distribution (first resonance frequency) depends on SVE and mesh sizes

From the micro-scale to the meso-scale

- Use of the meso-scale distribution with macro-scale finite elements
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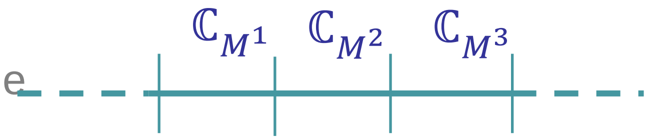
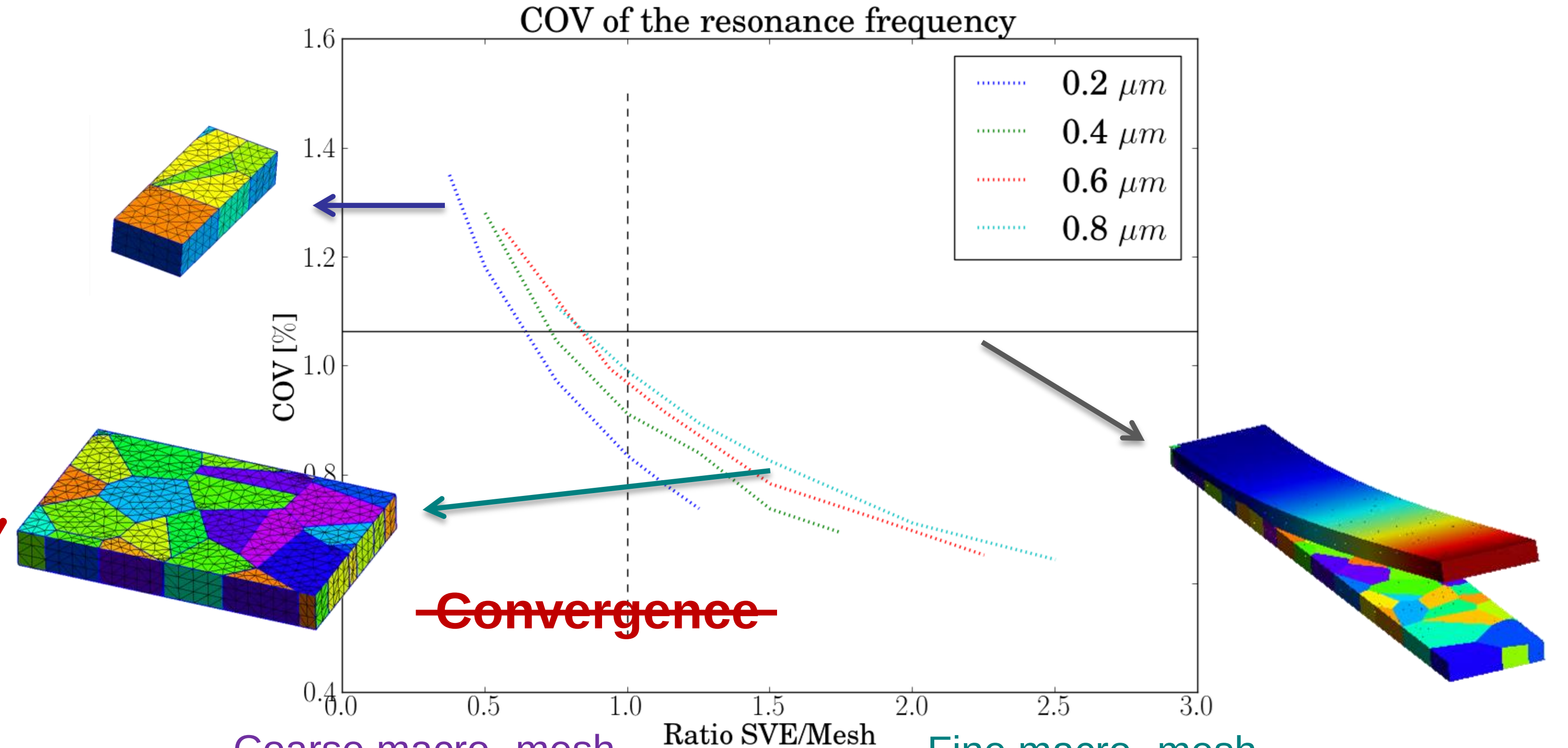


Change of E distribution at each Gauss Point



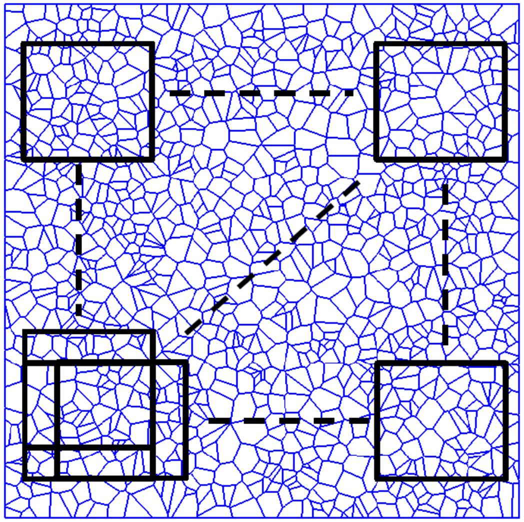
Coarse macro- mesh

Fine macro- mesh

More random variables having the same distribution

From the micro-scale to the meso-scale

- Introduction of the (meso-scale) spatial correlation
  - SVEs extracted at different distances
  - Spatial correlation of the r^{th} and s^{th} components of the apparent (homogeneous) elasticity tensor $\mathbb{C}_M$

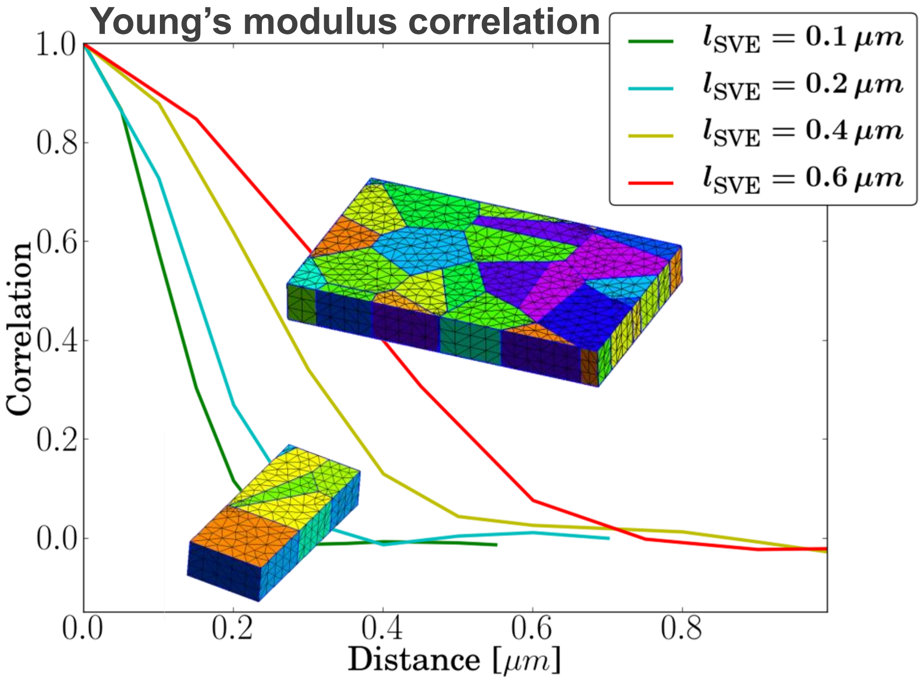


$$R_{\mathbb{C}}^{(rs)}(\boldsymbol{\tau}) = \frac{\mathbb{E}\left[\left(\mathbb{C}^{(r)}(\boldsymbol{x}) - \mathbb{E}\left(\mathbb{C}^{(r)}\right)\right)\left(\mathbb{C}^{(s)}(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}\left(\mathbb{C}^{(s)}\right)\right)\right]}{\sqrt{\mathbb{E}[(\mathbb{C}^{(r)} - \mathbb{E}(\mathbb{C}^{(r)}))^2]\mathbb{E}[(\mathbb{C}^{(s)} - \mathbb{E}(\mathbb{C}^{(s)}))^2]}}$$

  - Represented by the correlation length:

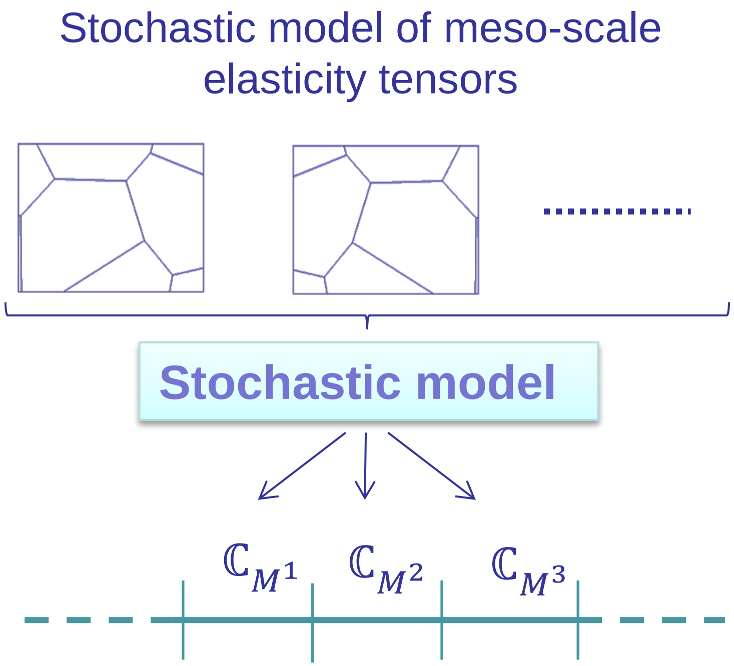
$$L_{\mathbb{C}}^{(rs)} = \frac{\int_{-\infty}^{\infty} R_{\mathbb{C}}^{(rs)}}{R_{\mathbb{C}}^{(rs)}(0)}$$

    - The correlation length increases with the SVE size



The meso-scale random field

- Use of the meso-scale distribution with stochastic (macro-scale) finite elements
  - Use of the meso-scale correlated distribution as a random field
  - Meso-scale random field from a generator
  - Monte-Carlo simulations at the macro-scale



The meso-scale random field

- Generation of the elasticity tensor $\mathbb{C}_M(x,\theta)$ (matrix $\boldsymbol{C}_M$) spatially correlated field*
  - Define a lower isotropic lower bound $\boldsymbol{C}_L$ from the silicon crystal tenor $\boldsymbol{C}_S$

$$\min_{E,\nu} \|\boldsymbol{C}_L(E,\nu) - \boldsymbol{C}_S\| \text{ with} \boldsymbol{C}_L(E,\nu) \leq \boldsymbol{C}_S$$

  - Define the positive semi-definite tensor $\Delta\boldsymbol{C}(x,\theta)$such that

$$\boldsymbol{C}_M(x,\theta) = \boldsymbol{C}_{\boldsymbol{L}} + \Delta\boldsymbol{C}(x,\theta)$$

    - This will ensure the existence of the expectation of ${\boldsymbol{C}_M}^{-\mathbf{1}}$
    - We now need to generate the spatially correlated random field $\Delta\boldsymbol{C}(x,\theta)$

  - Cholesky decomposition

$$\Delta\boldsymbol{C}(x,\theta) = \boldsymbol{A}(x,\theta)\boldsymbol{A}(x,\theta)^{\mathrm{T}} \quad \text{with} \quad \boldsymbol{A}(x,\theta) = \overline{\boldsymbol{A}} + \boldsymbol{A}'(x,\theta)$$

Homogeneous random field

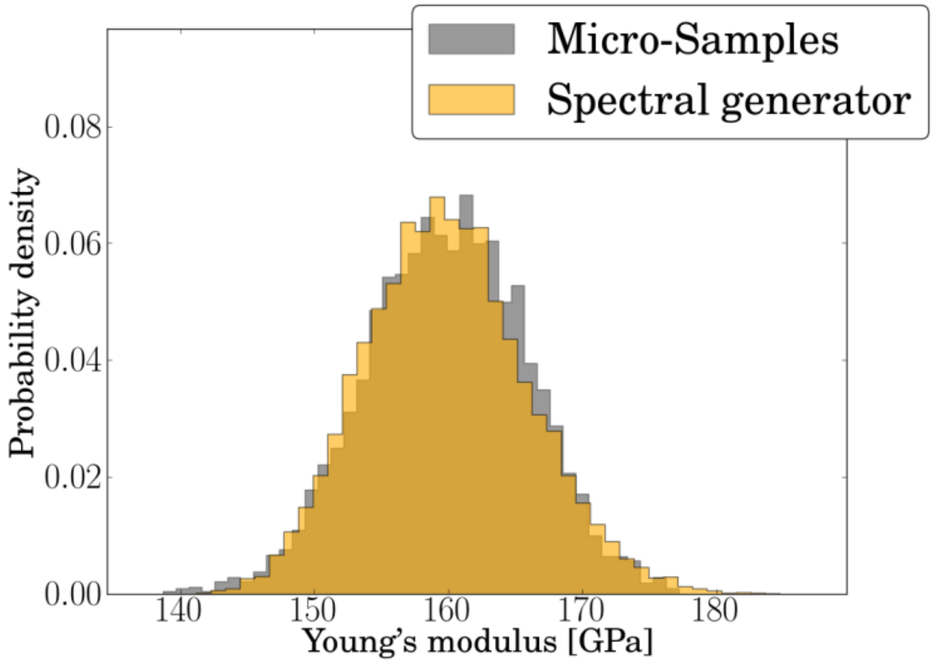
  - $\boldsymbol{A}'(\boldsymbol{x},\boldsymbol{\theta})$ is generated using the spatial correlation matrix $R_{\boldsymbol{A}'}(\tau)$
    - Here we use the spectral method*
    - Assumed Gaussian (can be changed)

* *Lucas, Golinval, Paquay, Nguyen, Noels, Wu, 2016*

The meso-scale random field

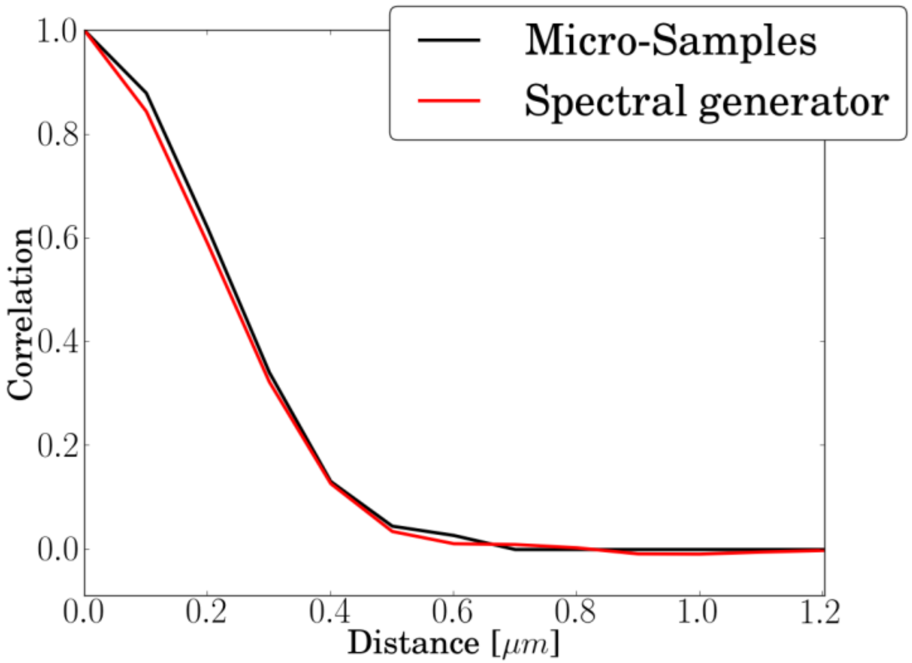
- Good agreement between:
  - The **samples** of elasticity tensors computed from the homogenization
  - The **generated** elasticity tensors

Young's modulus distribution



	Relative error [%]
mean of E	0,026
variance of E	0,97

Young's modulus spatial correlation



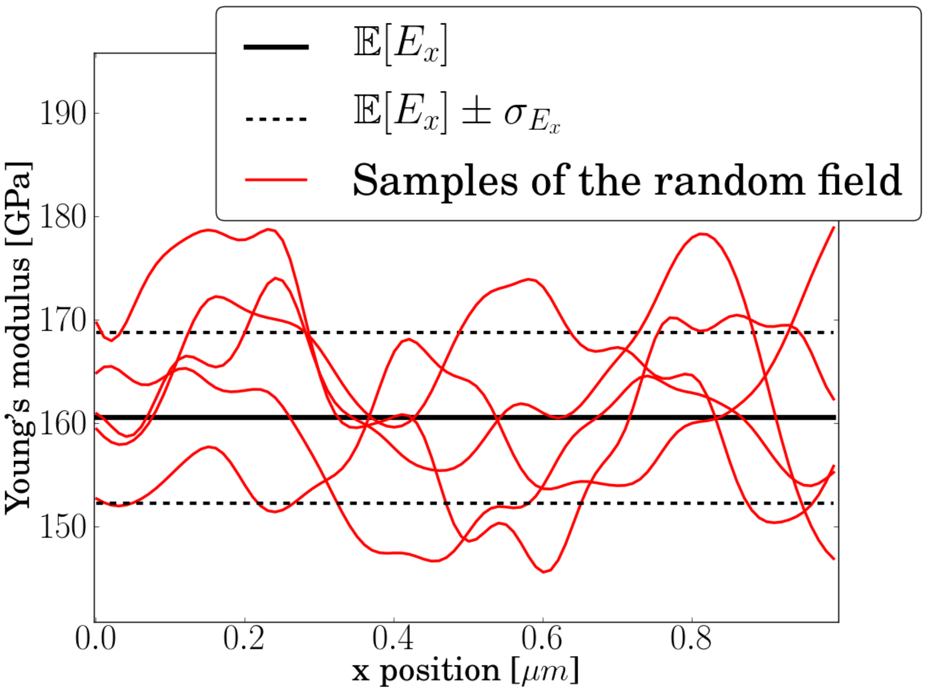
	Micro-samples	Generator
Skewness of E	−0,11	0,26
Kurtosis of E	2,93	3,02

From the meso-scale to the macro-scale

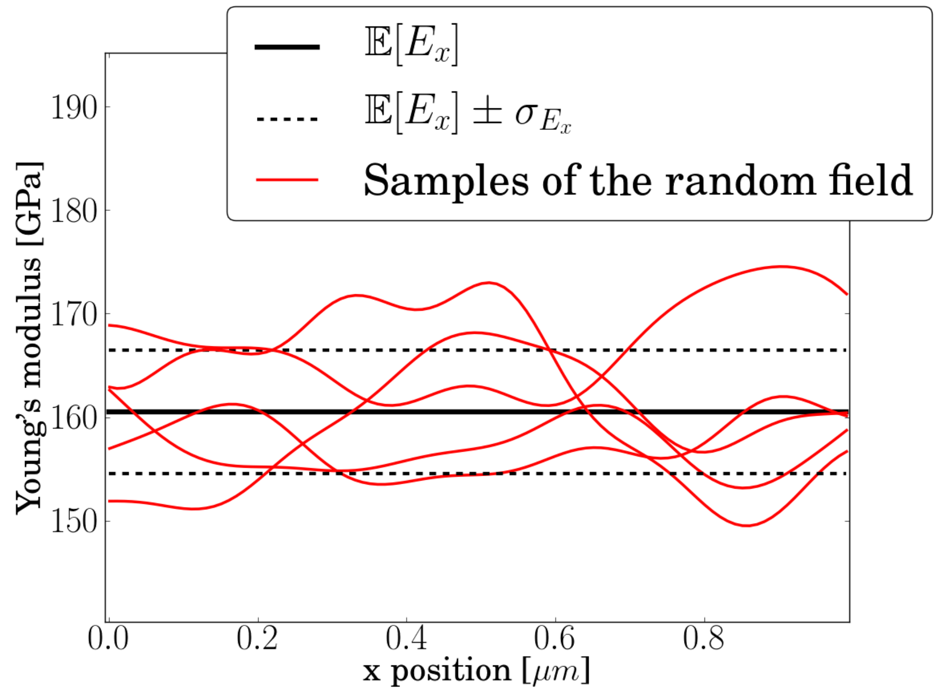
- Stochastic finite element method (SFEM)
  - Macro-scale beam elements of size l_{mesh}
  - Use the meso-scale random field obtained using SVEs of size l_{SVE}
  - The meso-scale random field is characterized by the correlation length $L_{\mathbb{C}}$

Random field with different SVEs sizes

$\boldsymbol{L_{\text{SVE}} = 0.1\ \mu m}$

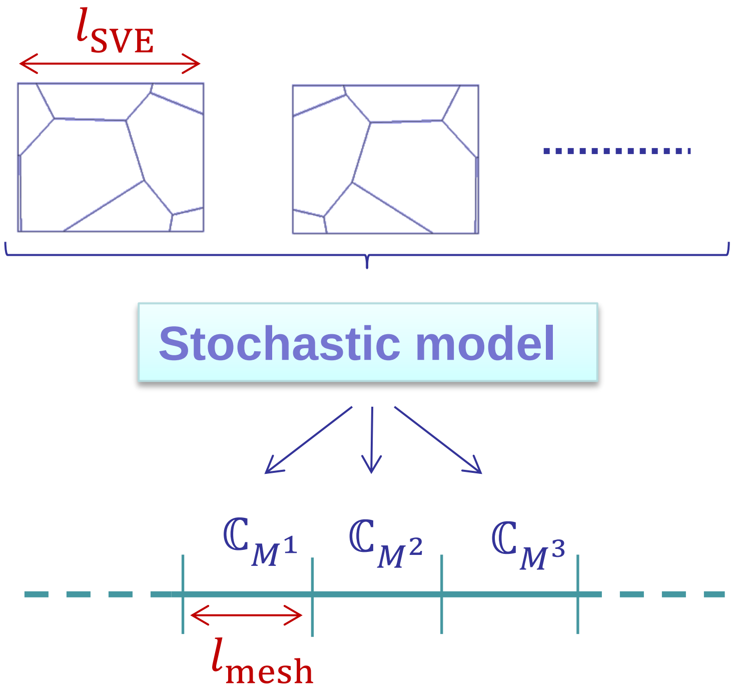


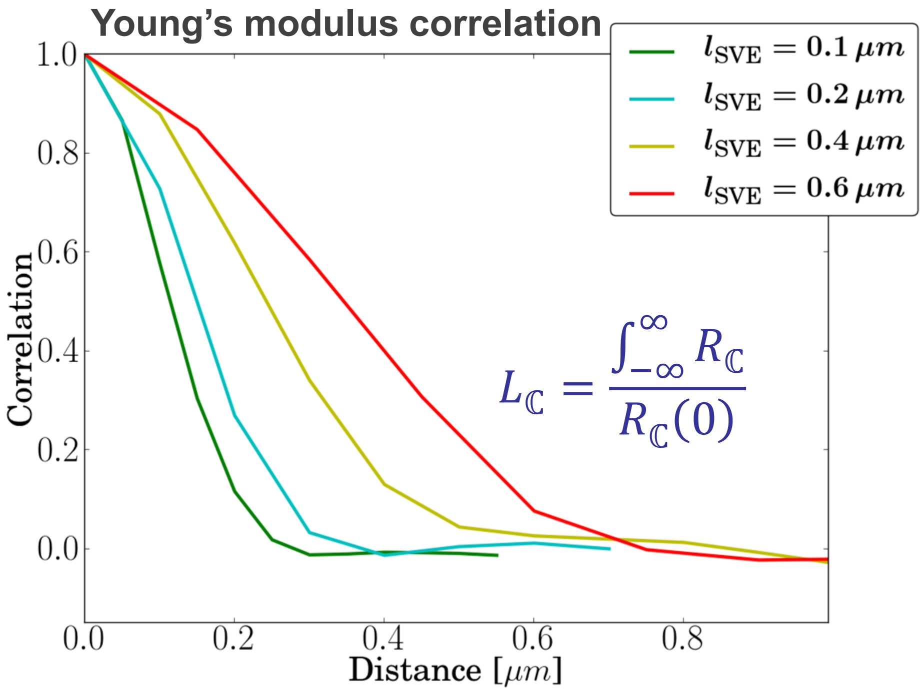
$\boldsymbol{L_{\text{SVE}} = 0.4\ \mu m}$



From the meso-scale to the macro-scale

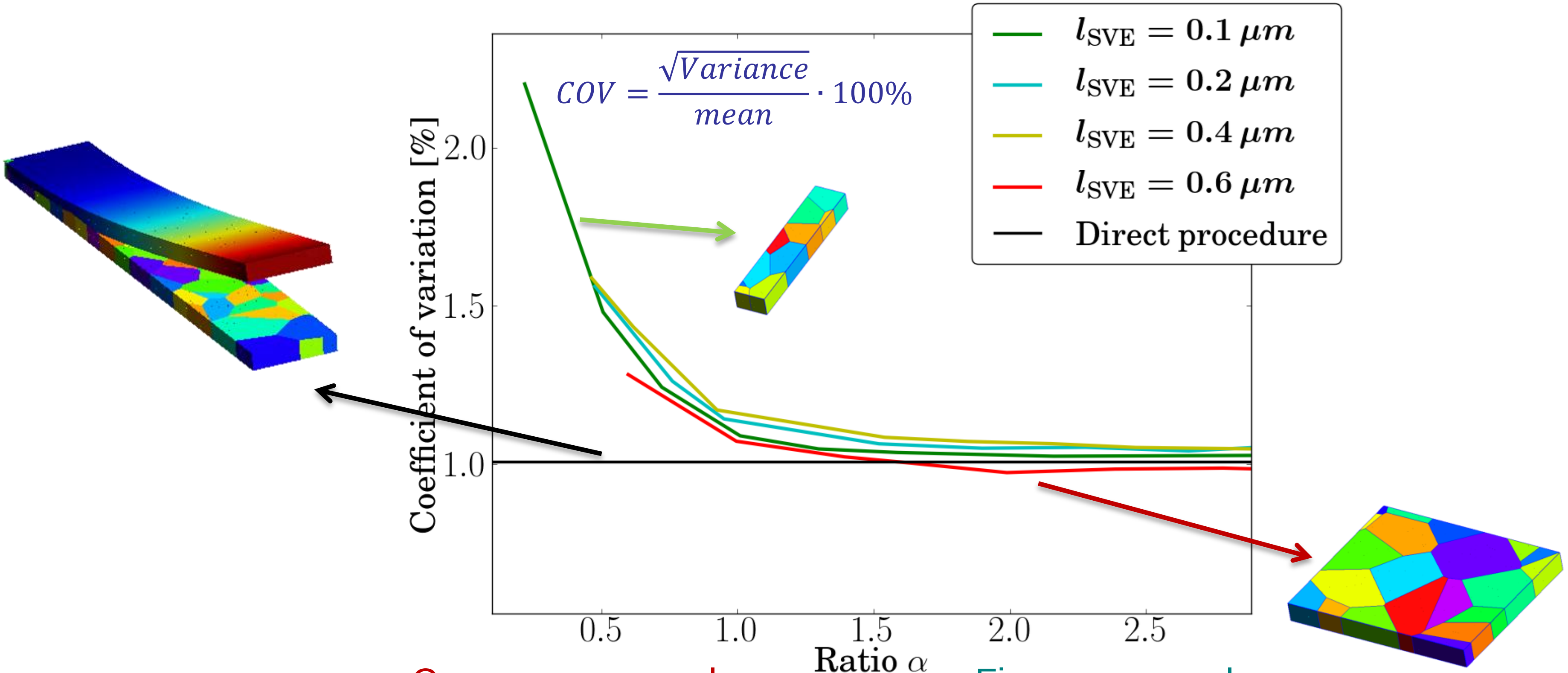
- The ratio $\alpha = \frac{L_{\mathbb{C}}}{l_{\text{mesh}}}$
  - Links the (macro-scale) finite element size to the correlation length
  - Is related to the SVE size thought the correlation length





From the meso-scale to the macro-scale

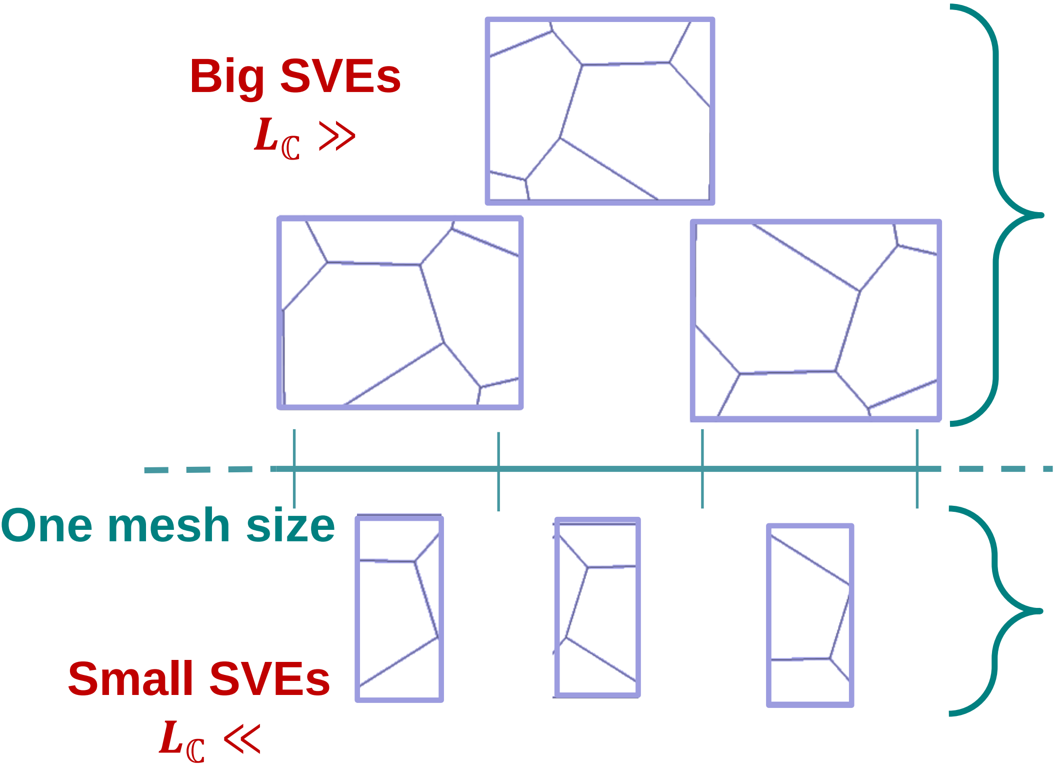
- Convergence of the 3-scale process
  - In terms of $\alpha = \frac{l_{\mathbb{C}}}{l_{\text{mesh}}}$
  - First flexion mode of a 3.2 μm-long beam



Coarse macro-scale mesh

Fine macro-scale mesh

- Effect of the ratio $\alpha = \frac{l_{\mathbb{C}}}{l_{\text{mesh}}}$



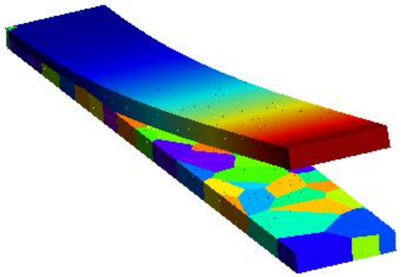
$\alpha = \frac{L_{\mathbb{C}}}{l_{\text{mesh}}} > 1 \rightarrow$ The spatial correlation can be accounted for

$\alpha = \frac{L_{\mathbb{C}}}{l_{\text{mesh}}} < 1 \rightarrow$ For the spatial correlation to be accounted for, we need more integration points

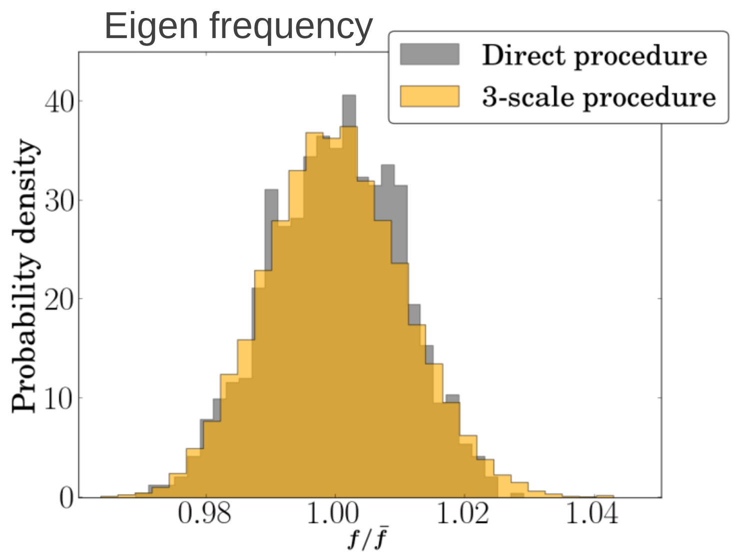
- For extreme values of α:
  - $\alpha \gg 1$: no more scale separation if $L_{\text{SVE}} \sim L_{\text{macro}}$
  - $\alpha \ll 1$: loss of microstructural details if $L_{\text{SVE}} \sim L_{\text{micro}}$

From the meso-scale to the macro-scale

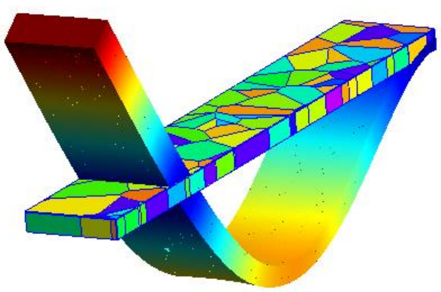
- Verification of the 3-scale process ($\alpha\sim 2$) with direct Monte-Carlo simulations
  - First bending mode of a 3.2 μm-long beam



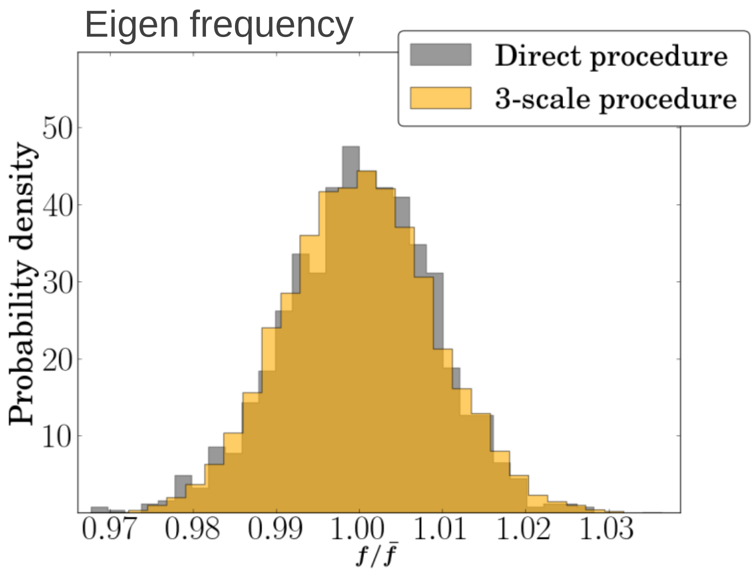
Relative difference in the mean: 0.57 %



  - Second bending mode of a 3.2 μm-long beam



Relative difference in the mean: 0.44 %



Perspectives

- Validate the 1D model on a bigger beam with experimental results
  - Measures for appropriate data as inputs: grain sizes, preferred direction, …
  - Samples of 1st mode frequency
  - Is the grain orientation the main contribution to the scatter of the first mode?
- Extend the model to 3D
  - Extension to 3D macroscale SFEM (generator already 3D)
  - Extension to thermoelasticity
  - Will permit to study the influence of the **clamp** and **thermoelastic damping**
- Study geometric uncertainties

Thank you for your attention !