Propagation of uncertainties using probabilistic multi-scale models

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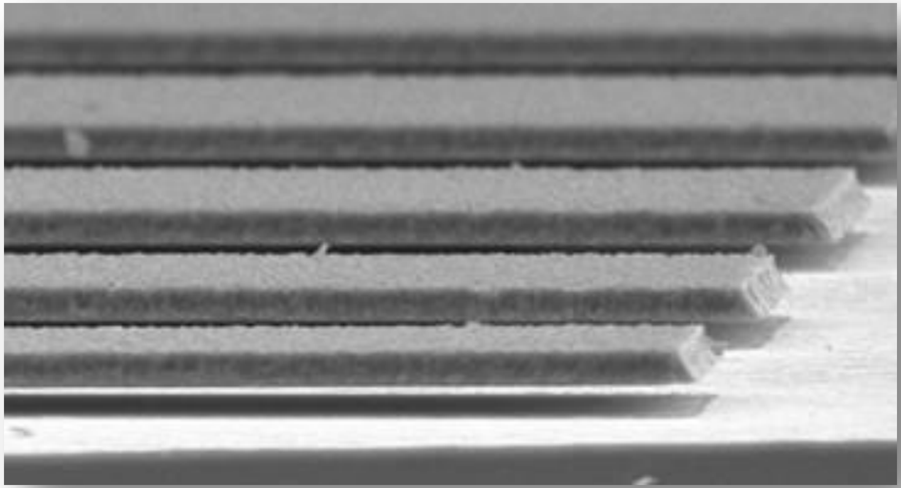
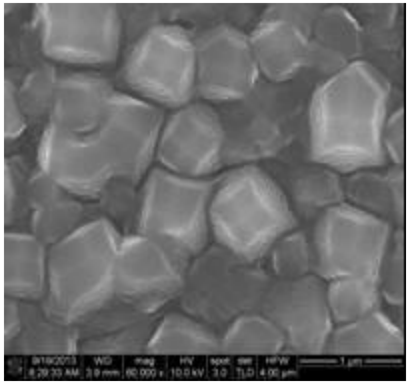
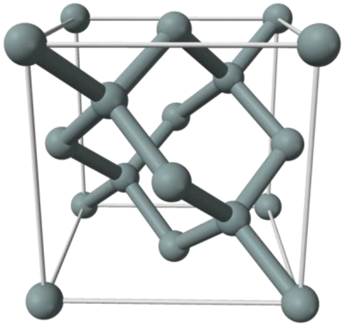


3SMVIB: The research has been funded by the Walloon Region under the agreement no 1117477 (CT-INT 2011-11-14) in the context of the ERA-NET MNT framework.
Robust design of MEMS: Financial support from F. R. S. - F. N. R. S. under the project number FRFC 2.4508.11

Motivations



- MEMS structures
  - Not several orders larger than their micro-structure size
  - As a result their properties exhibit a scatter
  - …
- The objective of this work is to estimate this scatter
  - Polycrystalline materials
    - Here we consider Polysilicon
  - Each grain has an anisotropic behaviour
    - Elastic properties
    - Material strength
    - …
  - Interest in the elastic response
    - Eigen frequencies of MEMS resonators

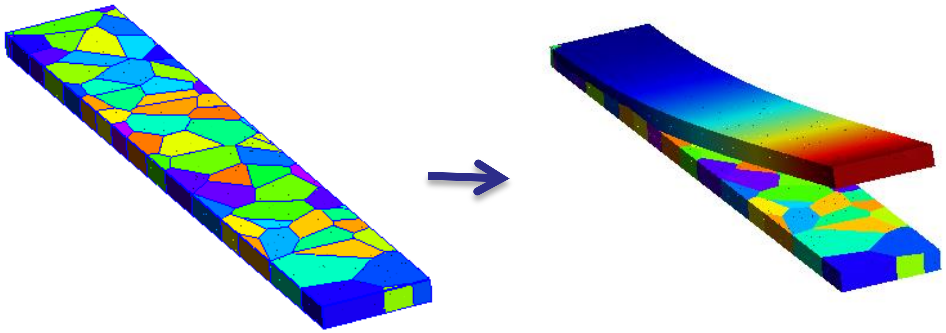


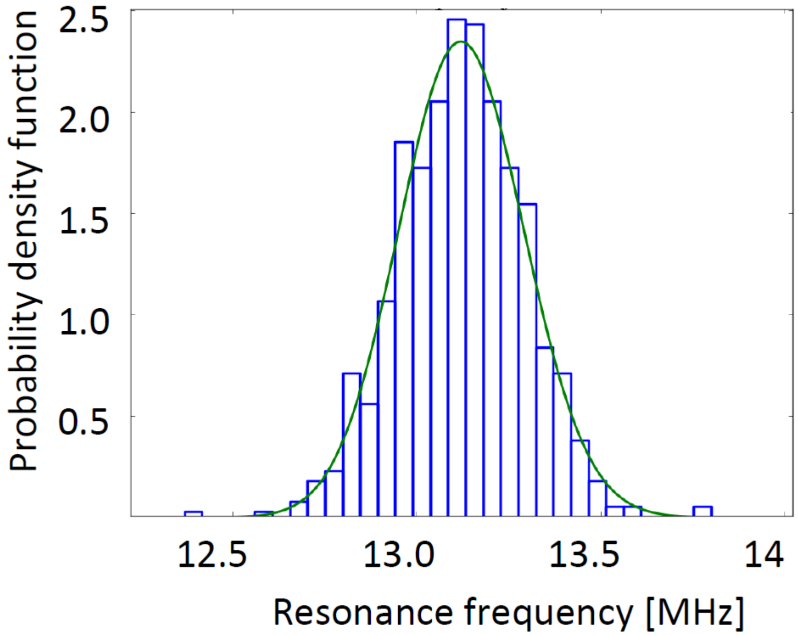
  - Interest in the fracture behaviour
    - Strength, fracture energy, crack path
  - Only uncertainties from the material micro-structure are accounted for

Motivations

- Direct Monte-Carlo simulations
  - Each grain explicitly meshed
    - Poisson Voronoï tessellation
    - Random grain orientation
  - Thousands of simulation required

    → Time consuming

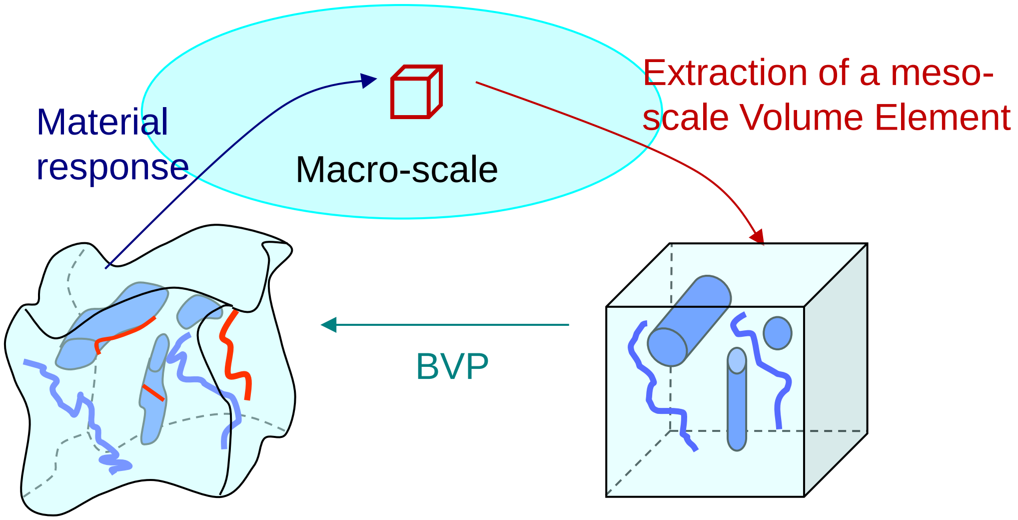




- Motivations for stochastic multi-scale methods

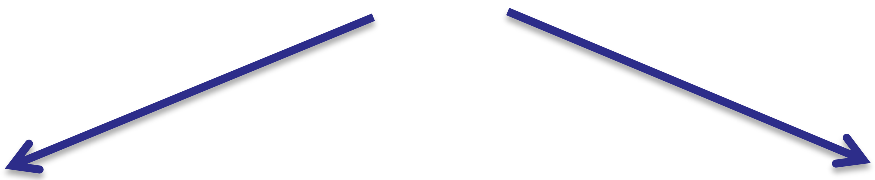
Motivations

- 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

*"*Stochastic finite elements as a bridge between random material microstructure and global response*", M Ostoja-Starzewski, X Wang *Computer methods in applied mechanics and engineering (1999)*
"Scale-dependent homogenization of random composites as micropolar continua", P Trovalusci, M Ostoja-Starzewski, M L De Bellis, A Murrali, European Journal of Mechanics - A/Solids (2015)
"Statistical volume element method for predicting micro-structure constitutive property relations", X. Yin, W. Chen, A. To, C. McVeigh, Computer Methods in Applied Mechanics and Engineering (2008)
"Computational nonlinear stochastic homogenization using a nonconcurrent multiscale approach for hyperelastic heterogeneous microstructures analysis". A. Clement, C. Soize, J. Yvonnet, International Journal for Numerical Methods in Engineering (2012)
"A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures", J. Guilleminot, A. Noshadravan, C. Soize, R. Ghanem Computer Methods in Applied Mechanics and Engineering (2011)
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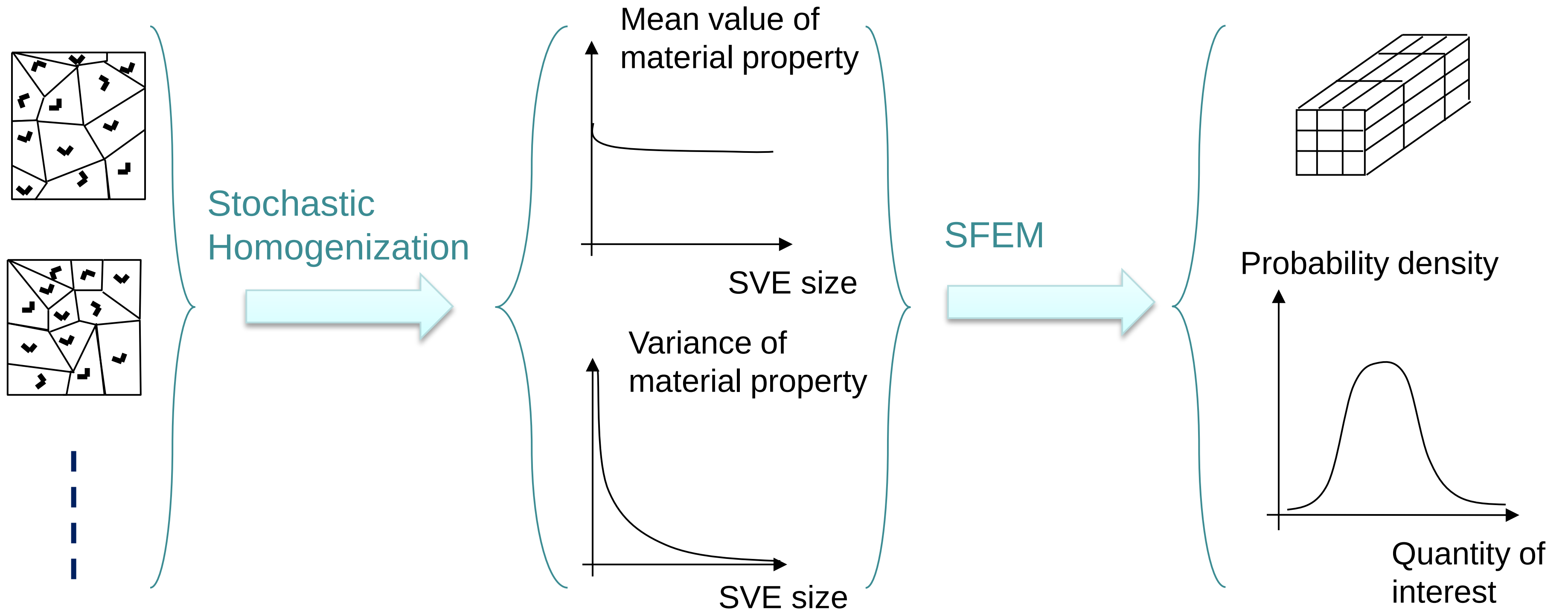
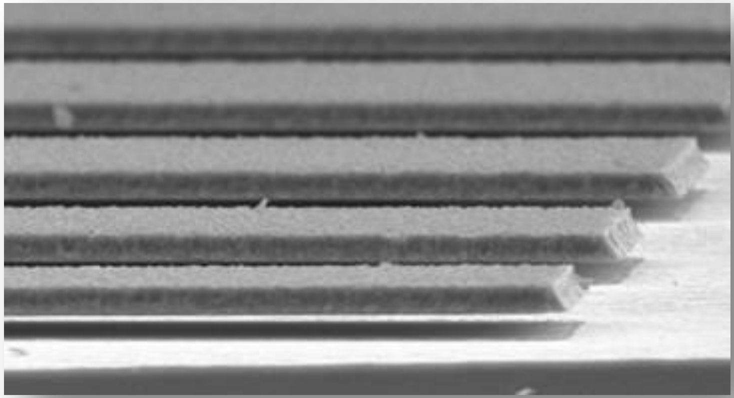
A 3-scale process

Grain-scale or micro-scale	Meso-scale	Macro-scale
➢ Samples of the microstructure (SVE) ➢ Each grain has a random orientation	➢ Intermediate scale ➢ Distribution of the meso-scale material property $\mathbb{P}(C)$	➢ Uncertainty quantification of the macro-scale quantity

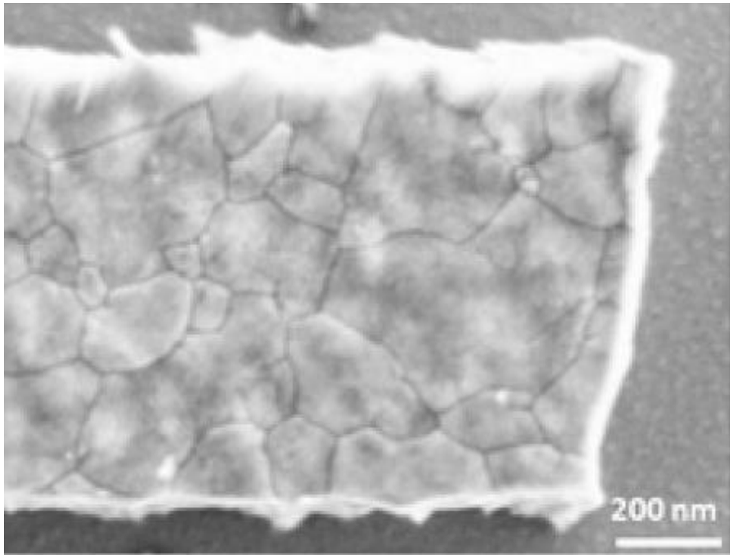


A 3-scale process

- Application to MEMS resonators: resonance frequencies distribution

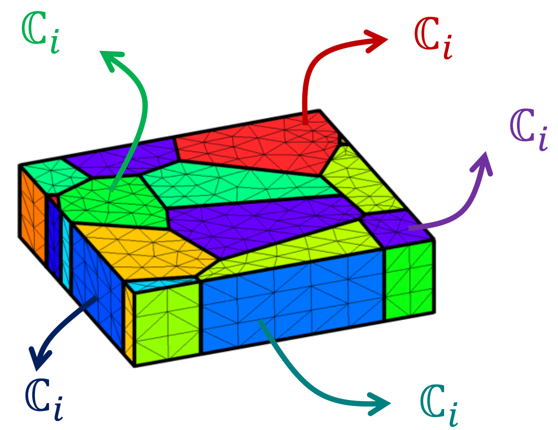


- Application to the fracture of MEMS



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

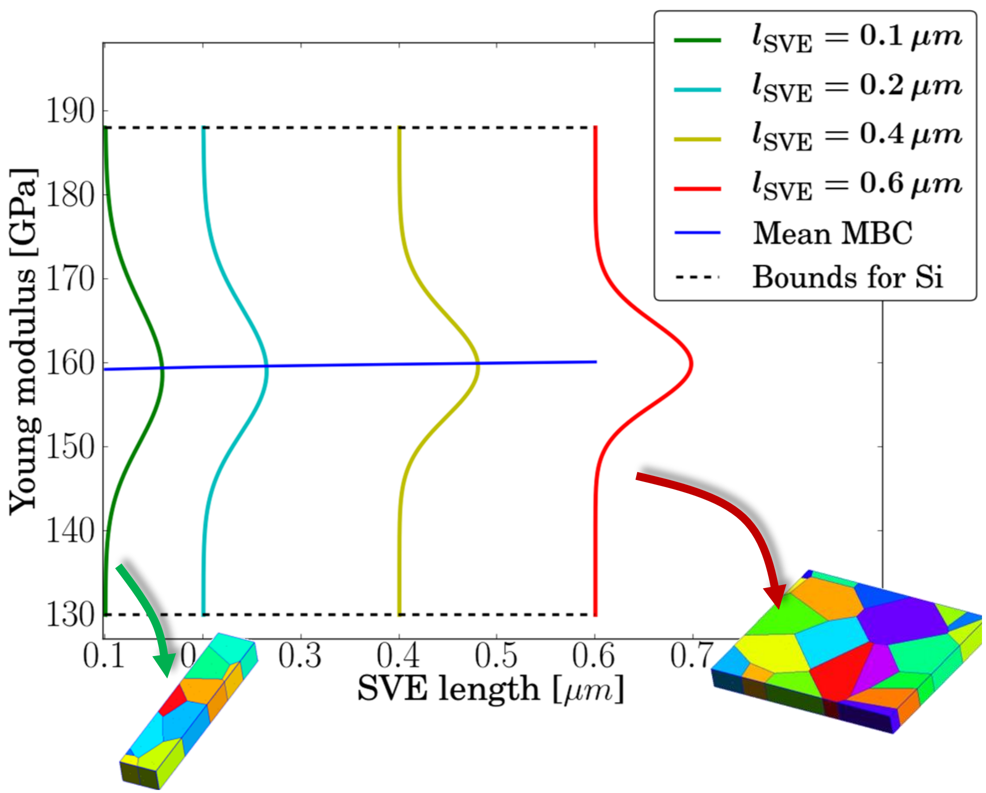
Samples of the meso-scale homogenized elasticity tensors

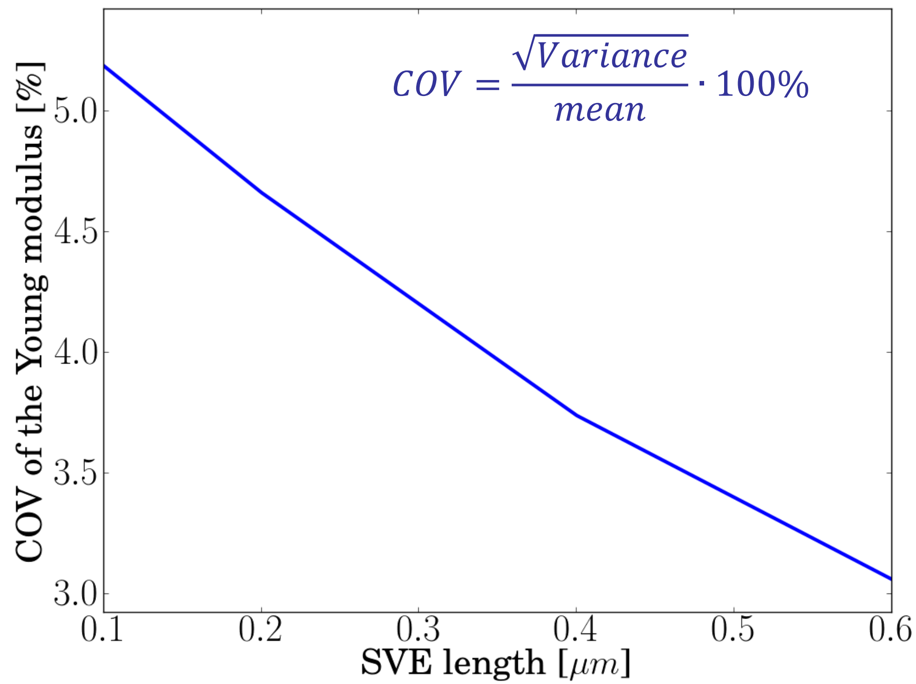
  - Homogenized elasticity tensor not unique as statistical representativeness is lost*
    - It is thus called apparent elasticity tensor

*"*Application of variational concepts to size effects in elastic heterogeneous bodies*", *C. Huet, Journal of the Mechanics and Physics of Solids(1990)*

From the micro-scale to the meso-scale

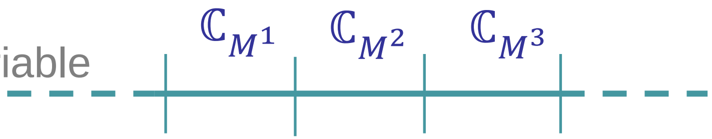
- Distribution of the apparent meso-scale elasticity tensor $\mathbb{C}_M$
  - Depends on the SVE size
    - For large SVEs, the apparent tensor tends to the effective (and unique) one
  - Bounded
    - Bounds do not depend on the SVE size but on the silicon elasticity tensor $\mathbb{C}_i$
    - However, the larger the SVE the lower the probability to be close to the bounds

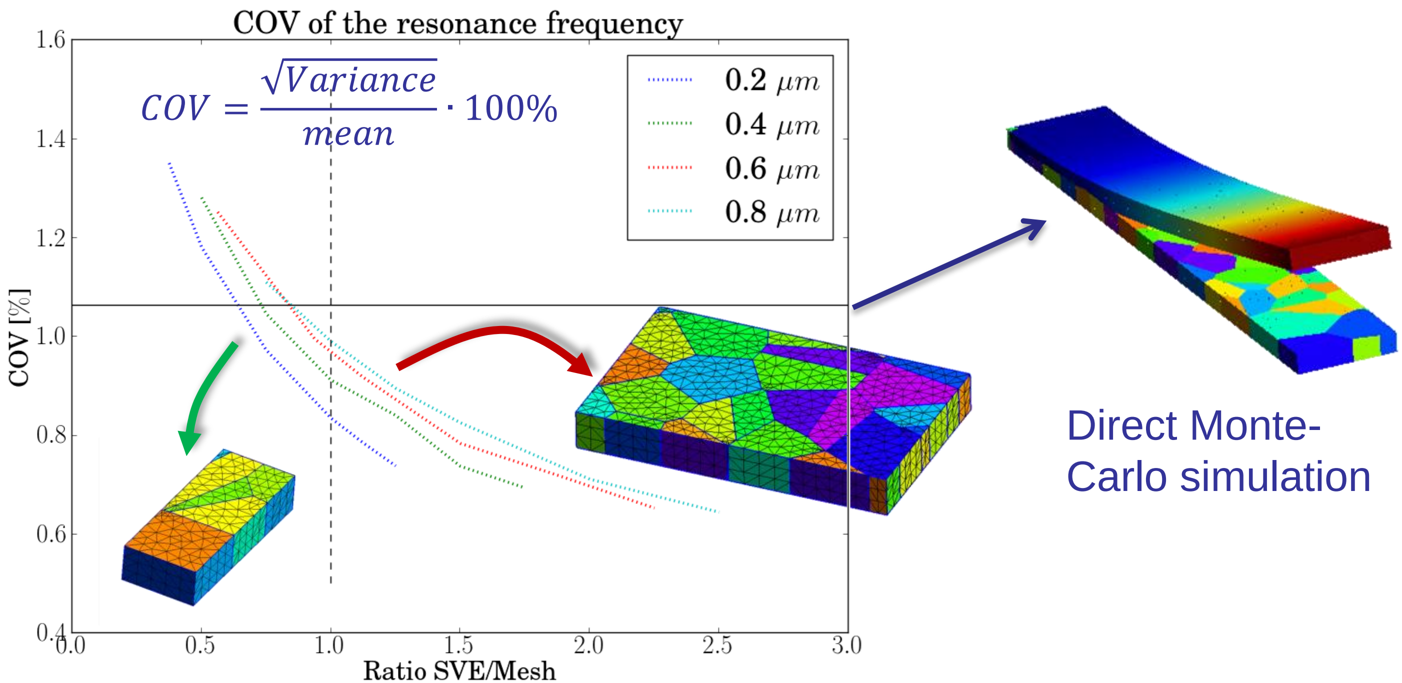




From the micro-scale to the meso-scale

- 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-scale mesh

Fine macro-scale mesh

- Macro-scale distribution (first resonance frequency) depends on SVE and mesh sizes

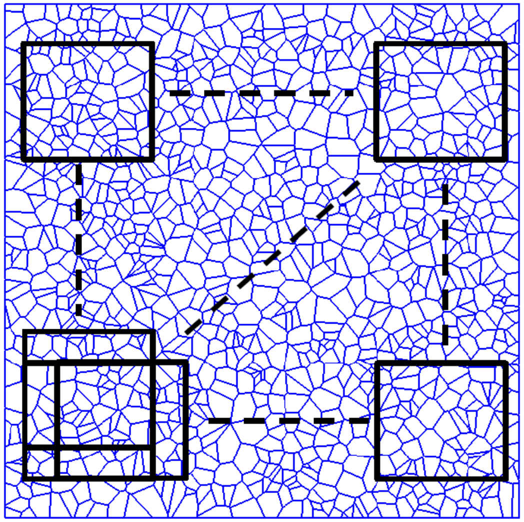
- Introduction of the (meso-scale) spatial correlation
  - SVEs extracted at different distances
  - Spatial correlation of the r^{th} and s^{th} components of the apparent elasticity tensor $\mathbb{C}_M$

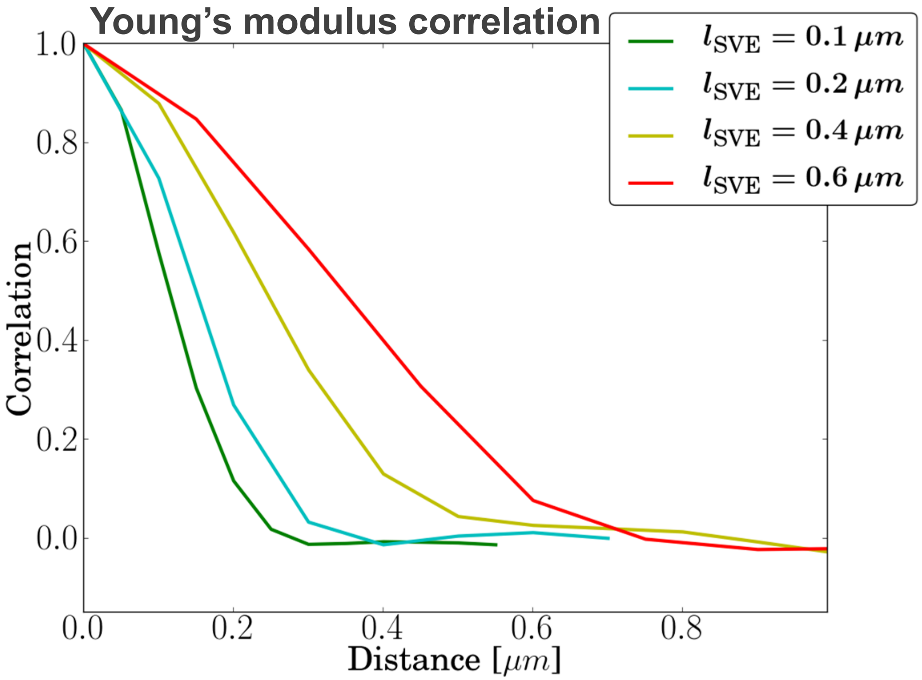
$$R_{\mathbb{C}}^{(rs)}(\boldsymbol{\tau}) = \frac{\mathbb{E}[\mathbb{C}^{(r)}(\boldsymbol{x})\mathbb{C}^{(s)}(\boldsymbol{x}+\boldsymbol{\tau})]}{\mathbb{E}[\mathbb{C}^{(r)}(\boldsymbol{x})]\mathbb{E}[\mathbb{C}^{(s)}(\boldsymbol{x}+\boldsymbol{\tau})]}$$

  - 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



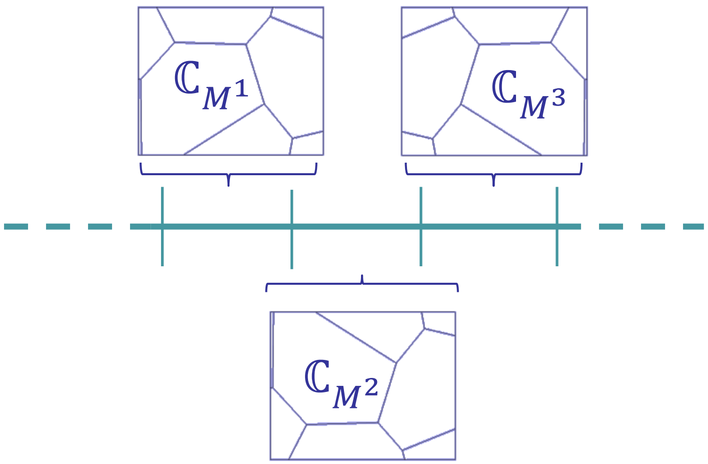


"Characterization of Random Composites Using Moving-Window Technique", S. Baxter, L. Graham, Journal of Engineering Mechanics (2000)

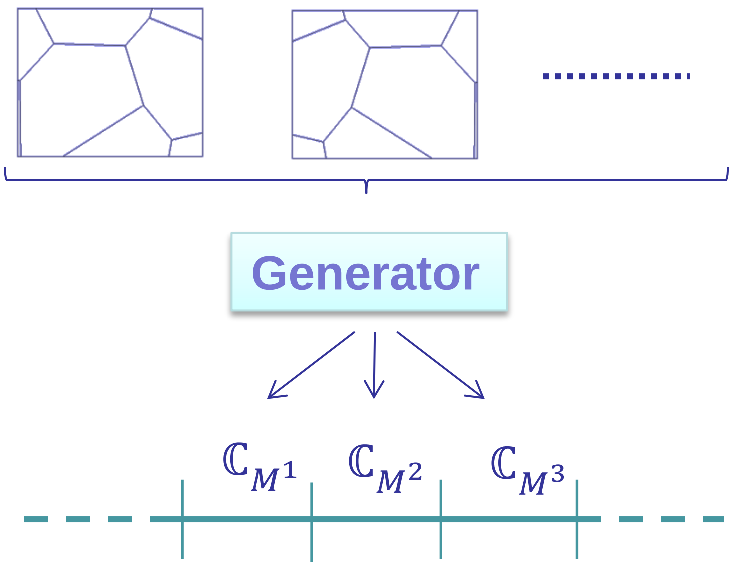
- Use of the meso-scale distribution with stochastic (macro-scale) finite elements
  - Use of the meso-scale correlated distribution as a random field
  - Monte-Carlo simulations
- The meso-scale random field

Direct resolution of SVEs at each (macro-scale) (Gauss) integration-points

Not computationally efficient



Generator of meso-scale elasticity tensors*



*"Maximum entropy approach for modeling random uncertainties in transient elastodynamics", C. Soize, The Journal of the Acoustical Society of America(2001)

"Bounded Random Matrix Approach for Stochastic Upscaling" S. Das, R. Ghanem, Multiscale Modeling & Simulation (2009)

"A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures", J. Guilleminot, A. Noshadravan, C. Soize, R. Ghanem Computer Methods in Applied Mechanics and Engineering (2011)

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The meso-scale random field

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

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

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

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

    - This will ensure the convergence of the Stochastic Finite Element Method*
    - We now need to generate the spatially correlated random field $\Delta\boldsymbol{C}(x,\theta)$
  - Cholesky decomposition

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

Homogeneous random field

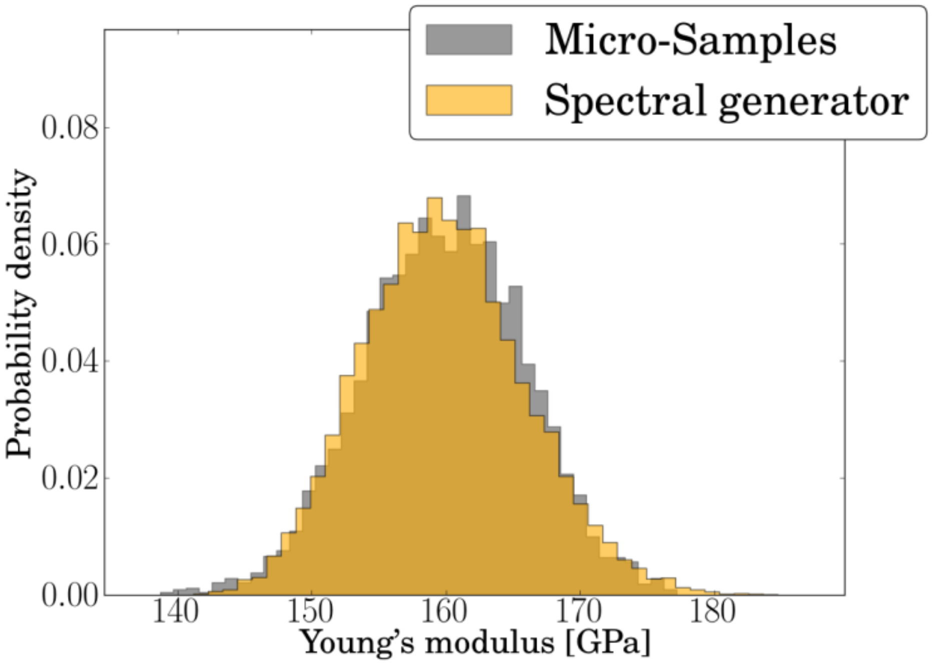
  - $\boldsymbol{A}'(\boldsymbol{x},\boldsymbol{\theta})$ is generated using the spatial correlation matrix $R_{\boldsymbol{A}'}(\tau)$
    - Here we use the spectral method**
    - Assumed Gaussian (can be changed)

*"Bounded Random Matrix Approach for Stochastic Upscaling" S. Das, R. Ghanem, Multiscale Modeling & Simulation (2009)
"A probabilistic model for bounded elasticity tensor random fields with application to polycrystalline microstructures", J. Guilleminot, A. Noshadravan, C. Soize, R. Ghanem Computer Methods in Applied Mechanics and Engineering (2011)
**"The Scale of Correlation for Stochastic Fields– Technical Report, Department of Civil Engineering and Engineering Mechanics", T. Harada, M. Shinozuka, Columbia University, New York, NY

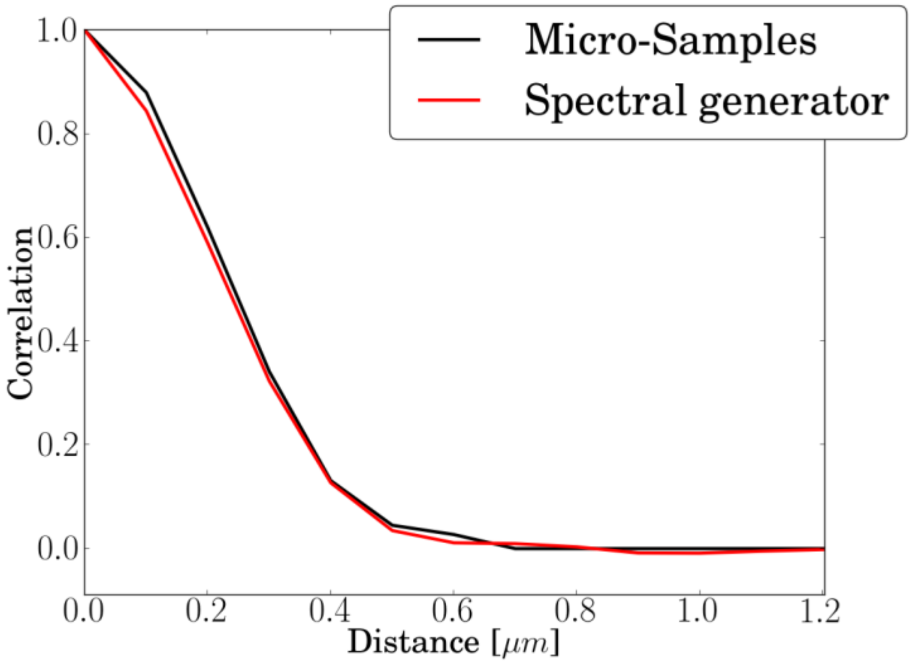
The meso-scale random field

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

Young's modulus distribution

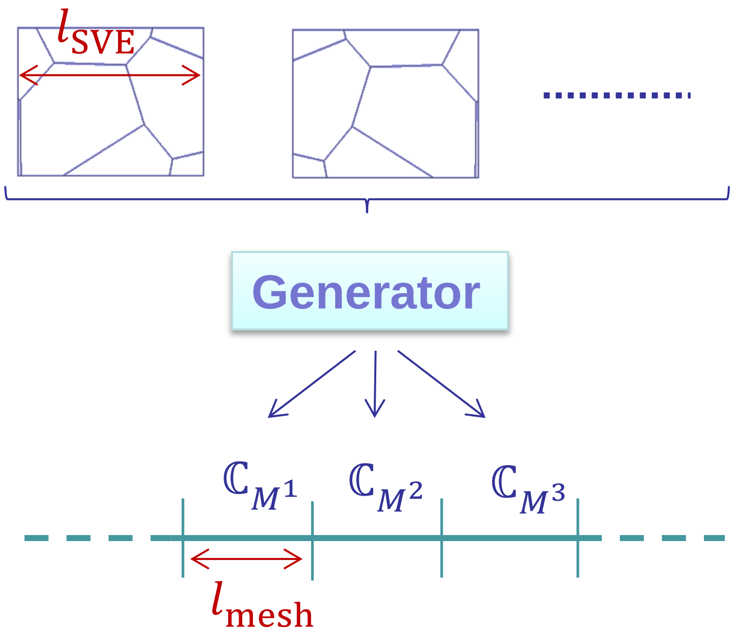


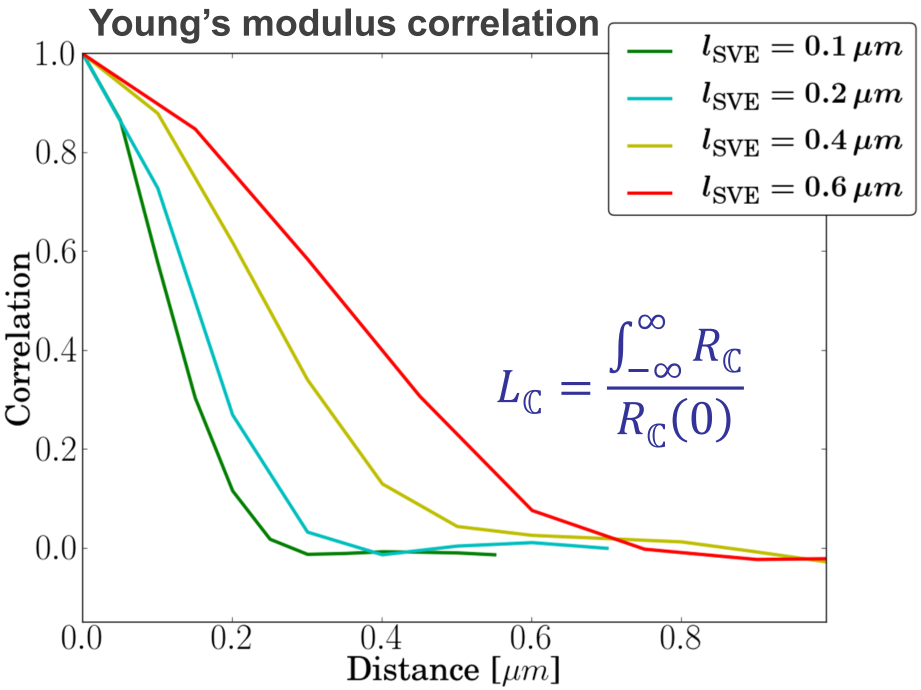
Young's modulus spatial correlation



From the meso-scale to the macro-scale

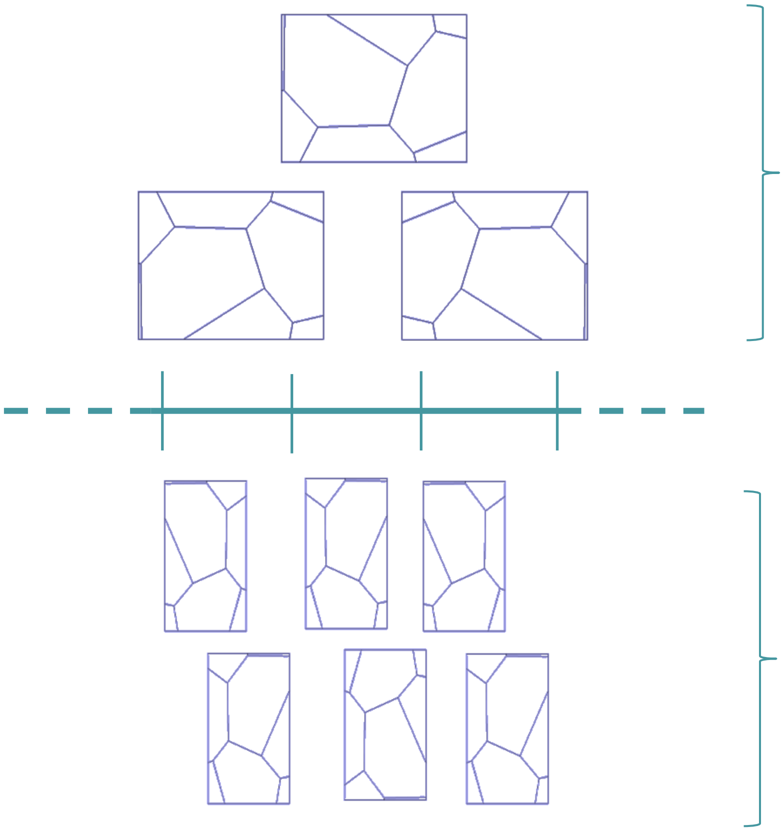
- Stochastic finite element method (SFEM)
  - Macro-scale beam elements of size l_{mesh}
  - Use the meso-scale random field obtained using SVEs of size l_{SVE}
  - The meso-scale random field is characterized by the correlation length $L_{\mathbb{C}}$
- The ratio $\alpha = \frac{L_{\mathbb{C}}}{l_{\mathrm{mesh}}}$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

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

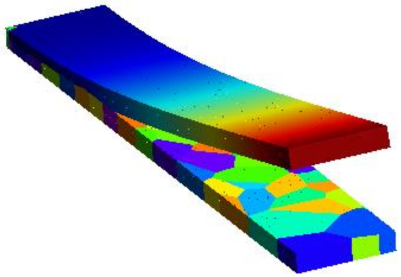


$\alpha = \frac{L_{\mathbb{C}}}{l_{\text{mesh}}} > 1$: The spatial correlation can be accounted for

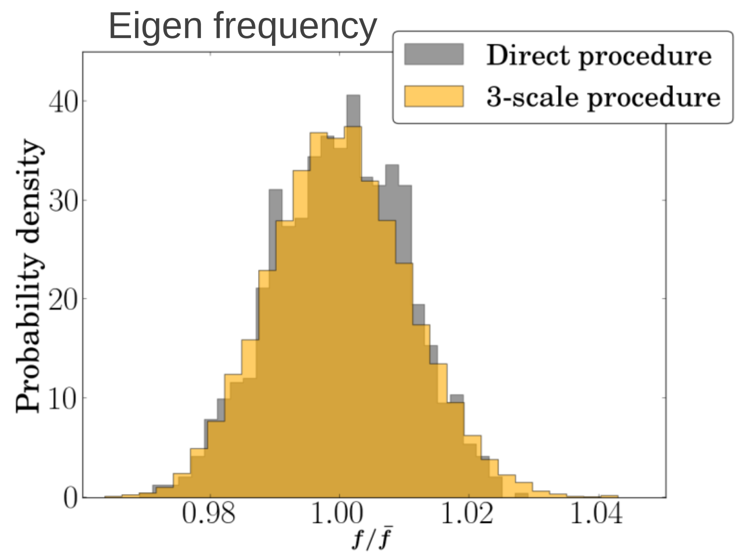
$\alpha = \frac{L_{\mathbb{C}}}{l_{\text{mesh}}} < 1$: For the spatial correlation to be accounted for, we need more integration points

- 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 $L_{\text{SVE}} \sim L_{\text{micro}}$

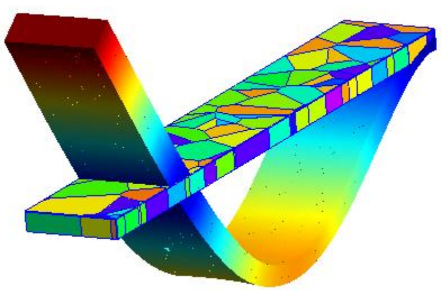
- Verification of the 3-scale process ($\alpha \sim 2$) with direct Monte-Carlo simulations
  - First flexion mode of a 3.2 μm-long beam



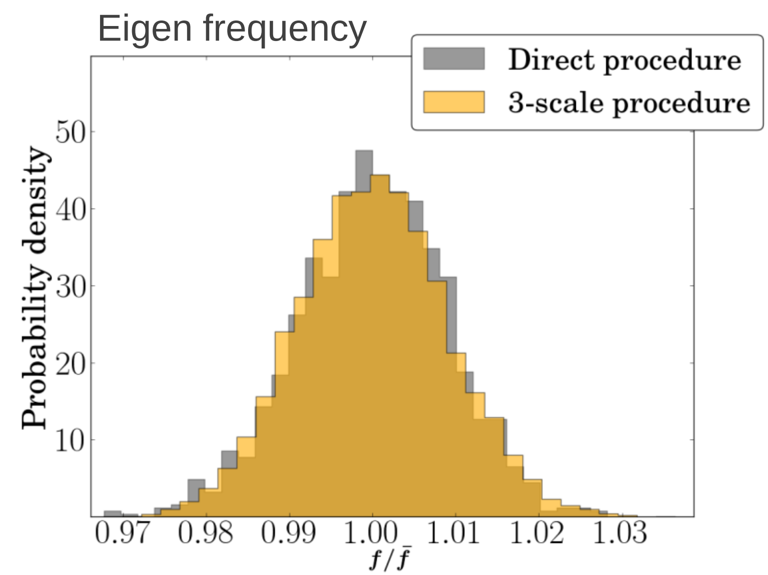
Relative difference
in the mean: 0.57 %



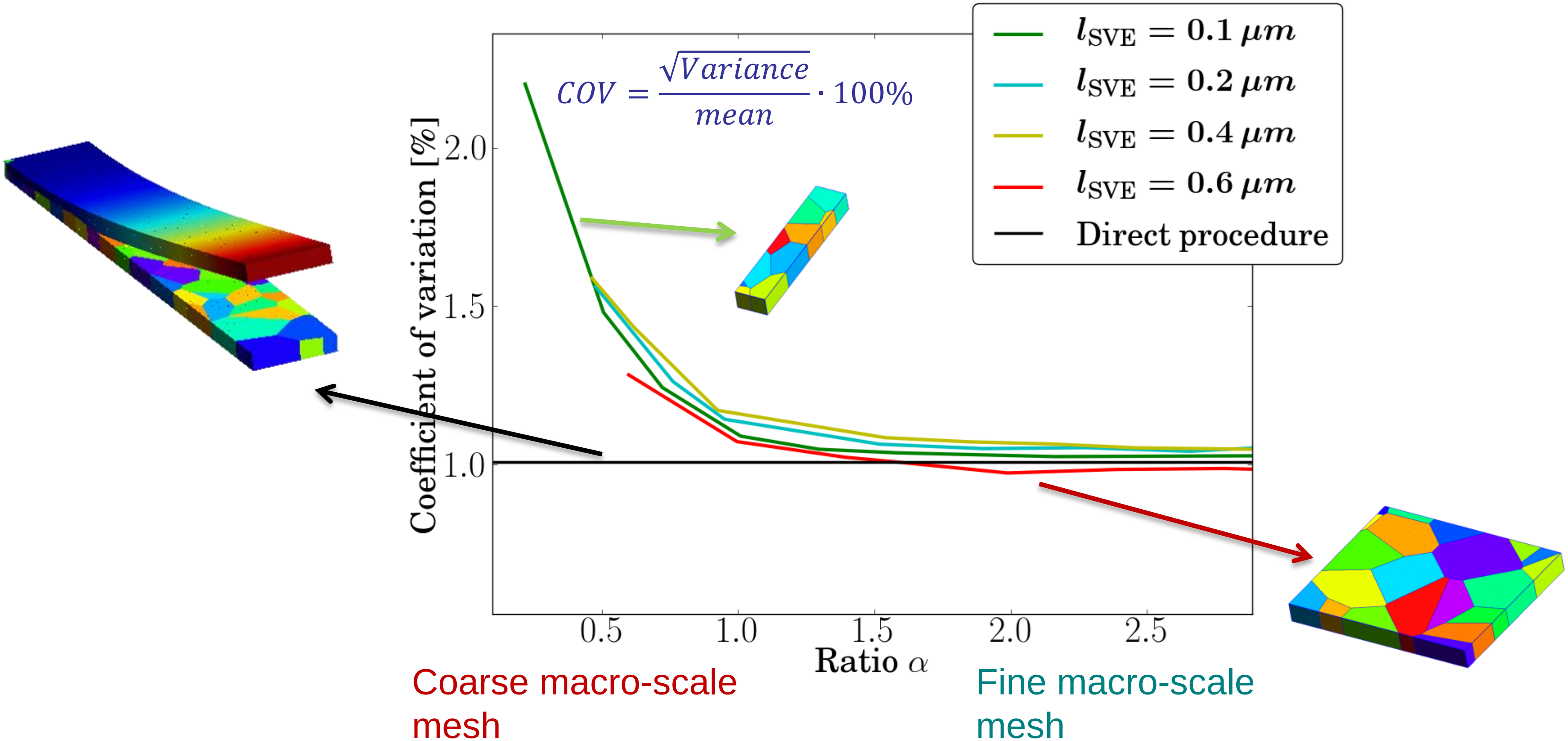
  - Second flexion mode of a 3.2 μm-long beam



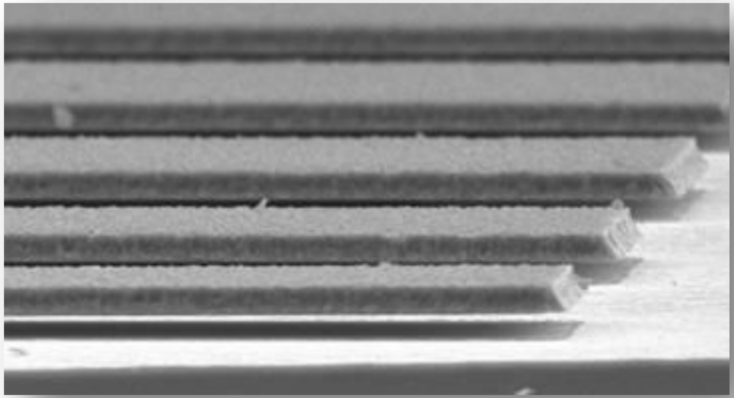
Relative difference
in the mean: 0.44 %



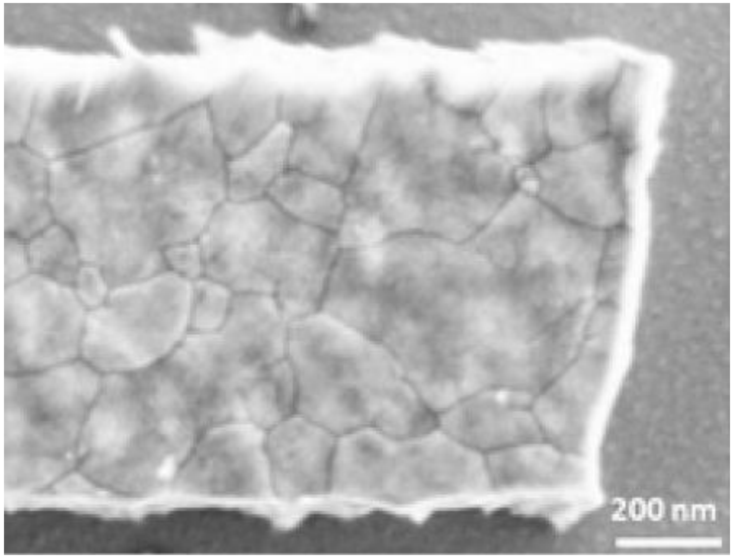
- Convergence of the 3-scale process
  - In terms of $\alpha = \frac{l_{\mathbb{C}}}{l_{\text{mesh}}}$
  - First flexion mode of a 3.2 μm-long beam



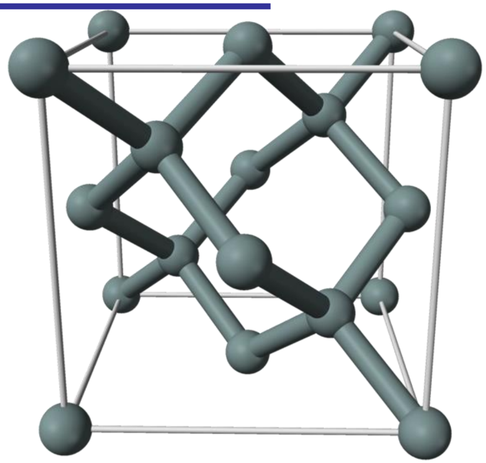
- Application to MEMS resonators: resonance frequencies distribution



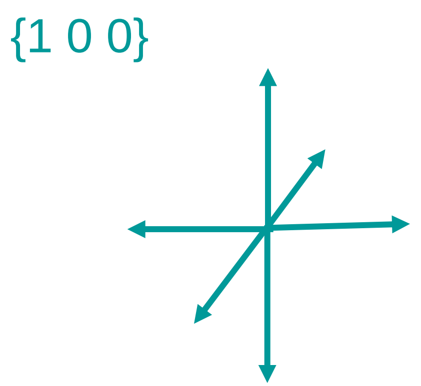
- Application to the fracture of MEMS



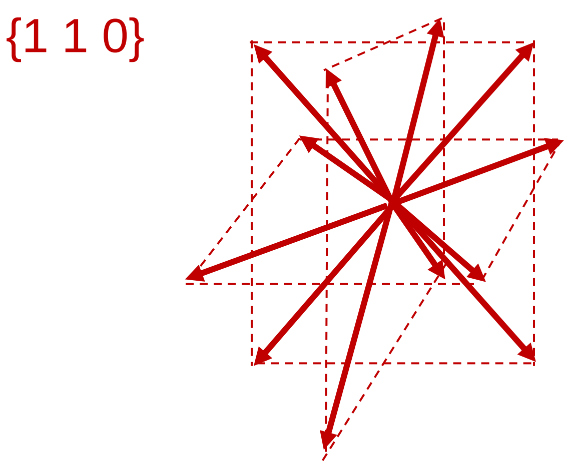
- Silicon Crystal
  - Orthotropic material



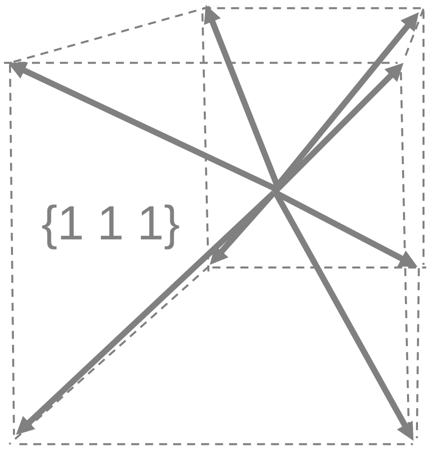
- Different fracture strengths and critical energy release rates
  - 6 {1 0 0}-directions, 12 {1 1 0}-directions, 8 {1 1 1}-directions



$\sigma_{100} = 1.53\ \text{GPa}$



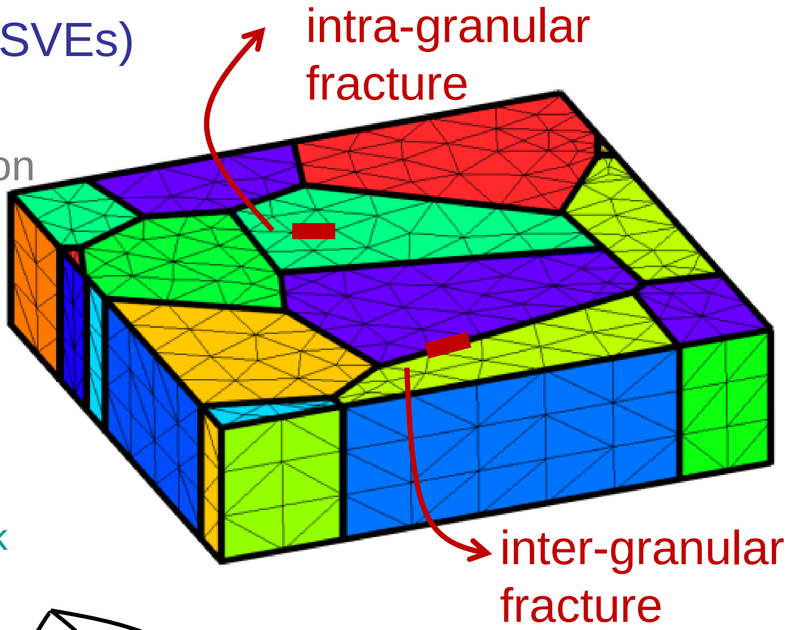
$\sigma_{110} = 1.21\ \text{GPa}$



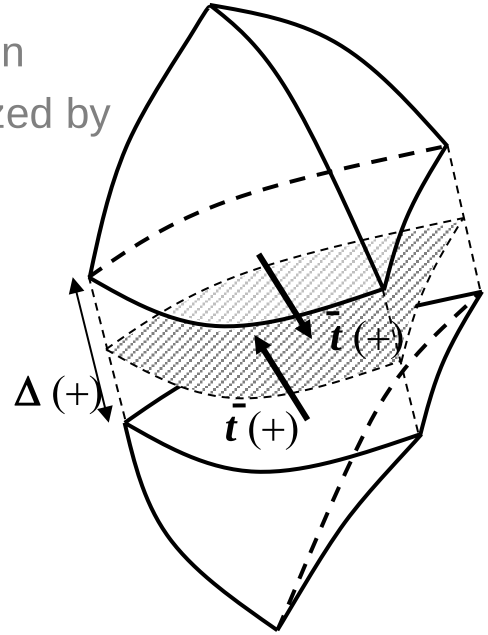
$\sigma_{111} = 0.868\ \text{GPa}$

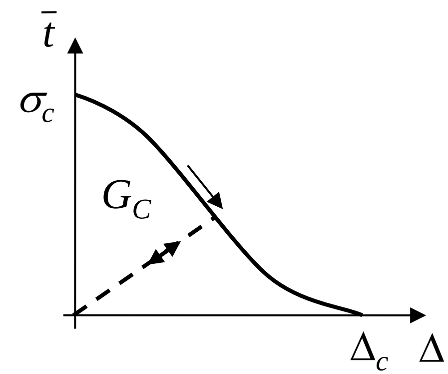
From the micro-scale to the meso-scale

- Definition of Stochastic Volume Elements (SVEs)
  - Voronoï tessellation
  - Each grain i is assigned a random orientation
  - Several realizations

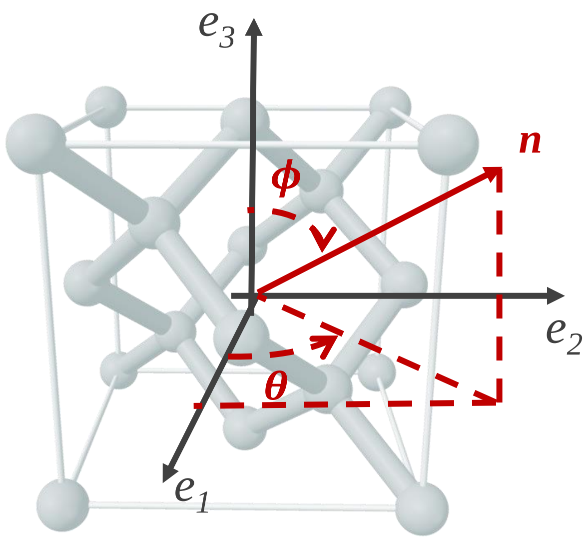


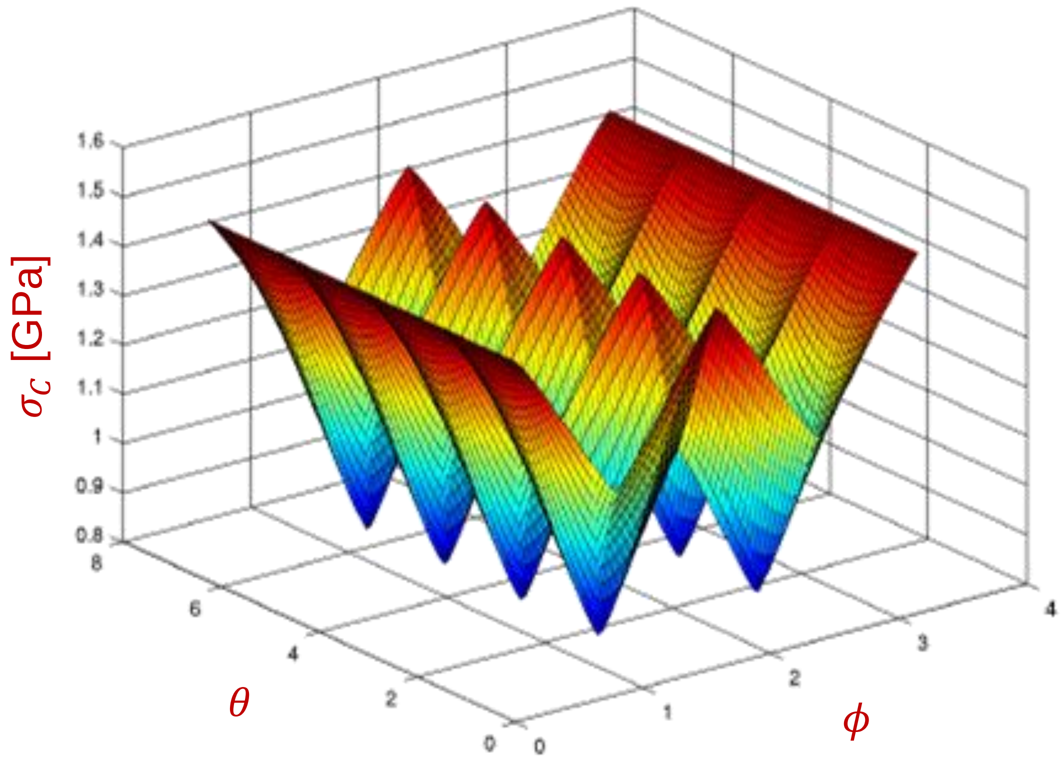
- Fracture models
  - Cohesive elements inserted between two bulk elements
    - Consistent discontinuous Galerkin framework
  - They integrate the cohesive Traction Separation Law (TSL) characterized by
    - Strength σ_C &
    - Critical energy release rate G_C
  - Can be tailored for
    - Intra/inter granular failure
    - Different orientations





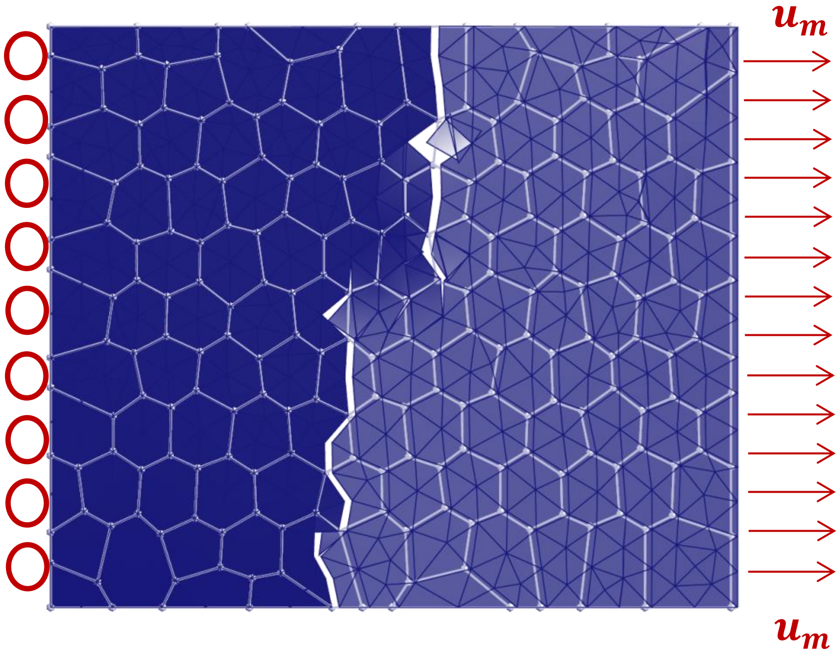
- Intra-granular failure
  - TSL depends on
    - Grain orientation
    - Interface orientation
  - Assumption: FE mesh > silicon crystal cell size (5.43 Å)
    - Compute effective fracture strength for the interface element of normal ***n***
    - Use polar coordinates in the crystal referential

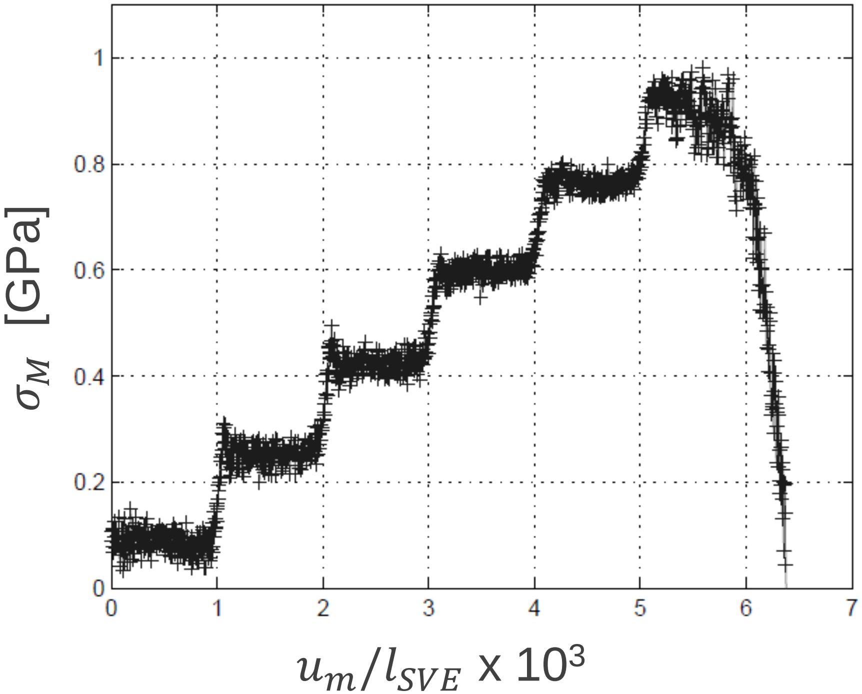




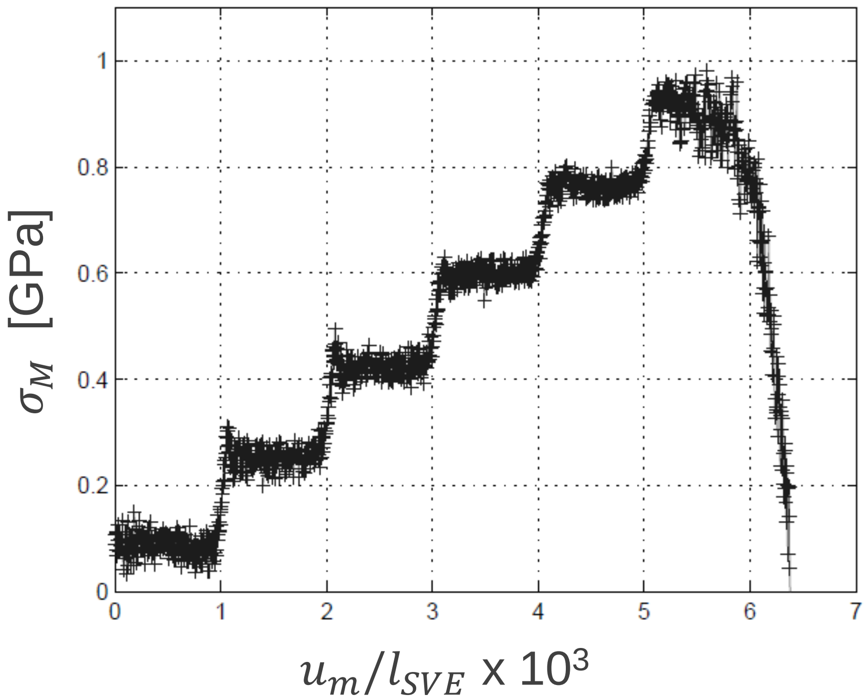
From the micro-scale to the meso-scale

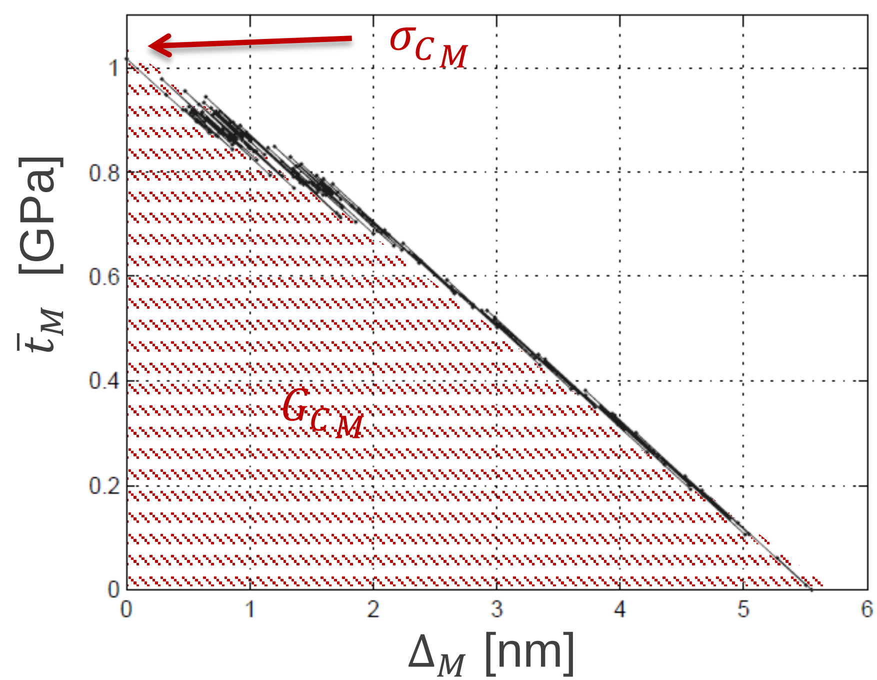
- SVEs computation
  - Extraction of the SVE response
  - Several realizations





- Extraction of the meso-scale TSL ($\bar{t}_M$ vs. Δ_M)
  - Following [Verhoosel et al.*]
  - Mesoscopic surface traction increment: $\delta\bar{\boldsymbol{t}}_M = \boldsymbol{\delta\sigma_M} \cdot \boldsymbol{e}_X$
  - Mesoscopic opening increment: $\delta\boldsymbol{\Delta}_M = \delta\boldsymbol{u}^m - L_{\text{cell}}\boldsymbol{C_M}^{-1}: \boldsymbol{e}_X \otimes \boldsymbol{e}_X \cdot \boldsymbol{\delta\bar{t}}_M$

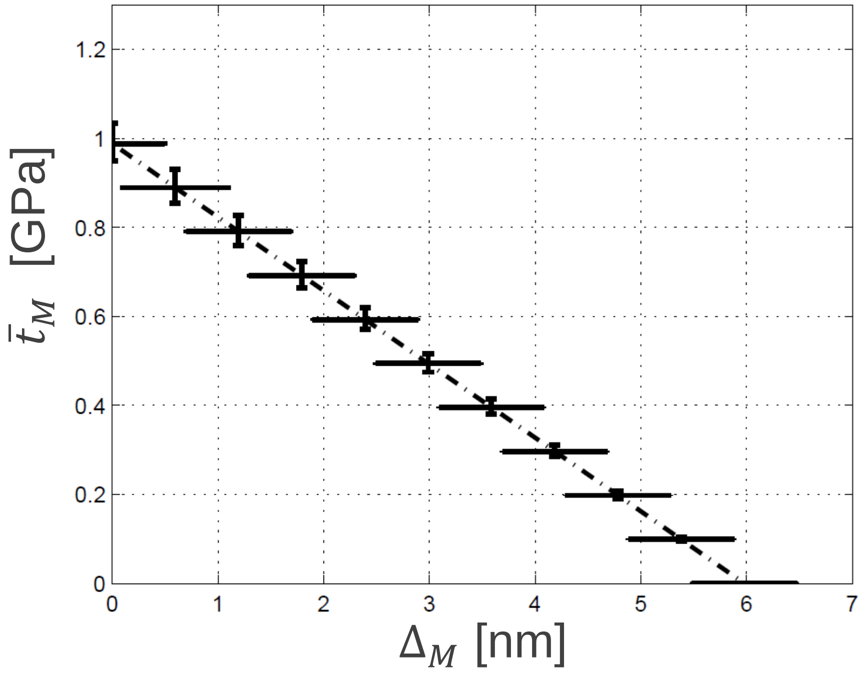




*"Computational homogenization for adhesive and cohesive failure in quasi-brittle solids" C.V. Verhoosel, J.J.C. Remmers, M.A. Gutiérrez, R. de Borst, International Journal for Numerical Methods in Engineering (2010)

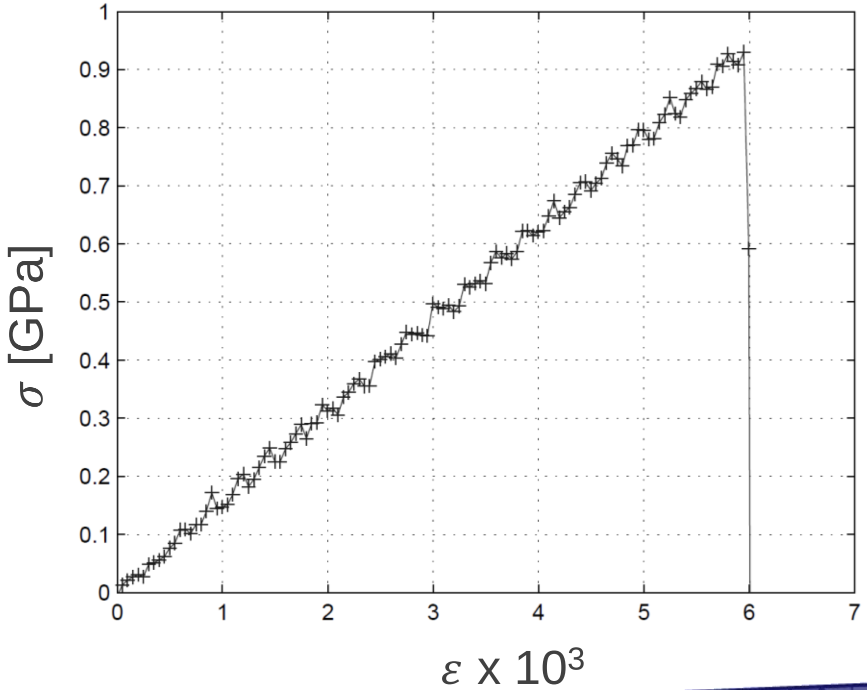
The meso-scale random cohesive law

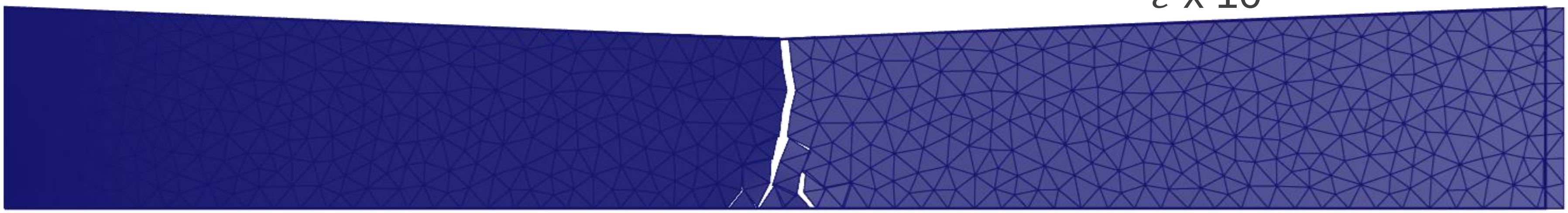
- Probabilistic TSL
  - Several SVE realizations
  - For each realization, extraction of (the correlated):
    - Meso-scopic strength σ_{c_M}
    - Meso-scopic critical energy release rate G_{c_M}
  - Generation of meso-scopic TSLs



From the meso-scale to the macro-scale

- Macro-scale simulations
  - Do not require discretization of the grains
  - Coarser meshes can be used (~size of the SVEs)
- Example of one realization





Conclusions & Perspectives

- Stochastic 3-scale methodology for poly-crystalline materials
  - Use of a meso-scale random field obtained from SVE resolutions
  - Propagation of the meso-scale uncertainties using SFEM

- In the future
  - Accounting for preferred crystallographic orientations
  - Accounting for other sources of uncertainties
    - Roughness
    - Grooves
    - Full MEMS geometry (clamping…)
  - Study of the influence of the amorphous phase
  - ….