A stochastic 3-Scale approach to study the thermo-mechanical damping of MEMS

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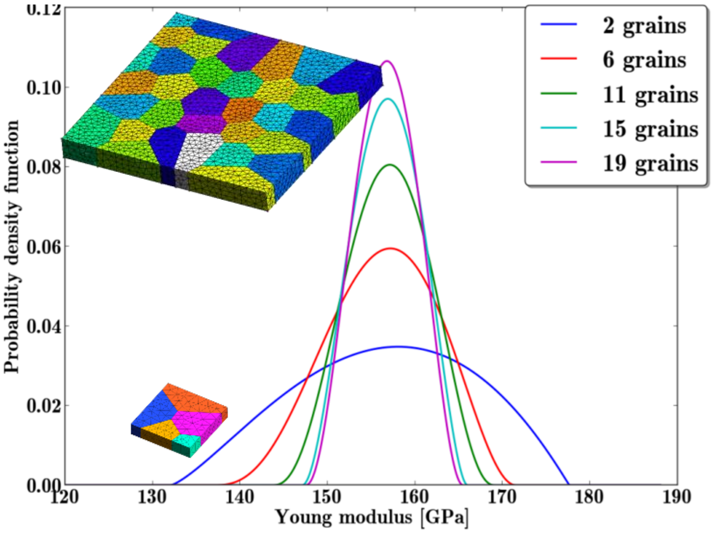

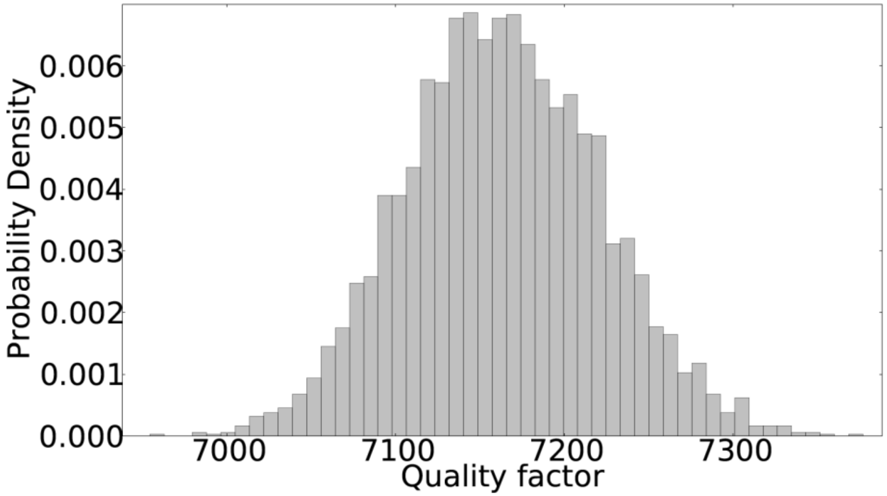

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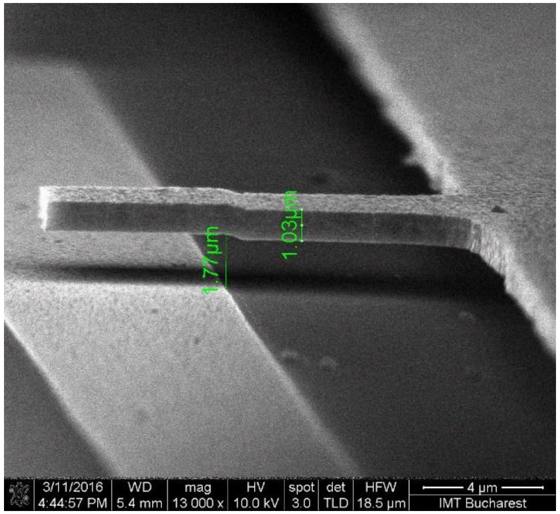
The problem

- MEMS structures
  - Are not several orders larger than their micro-structure size
  - Parameters-dependent manufacturing process
    - Low Pressure Chemical Vapor Deposition (LPCVD)
    - Properties depend on the temperature, time process, and flow gas conditions



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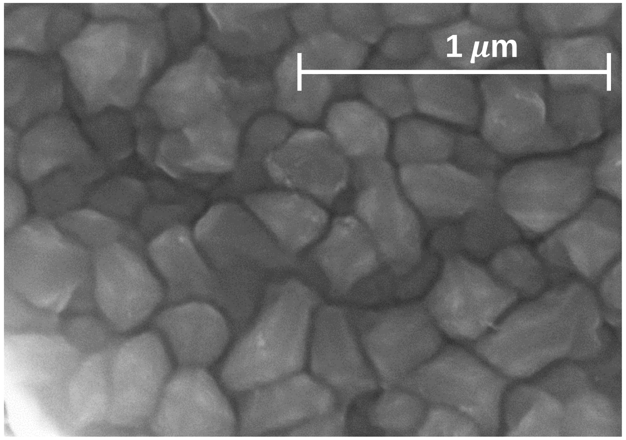
The problem

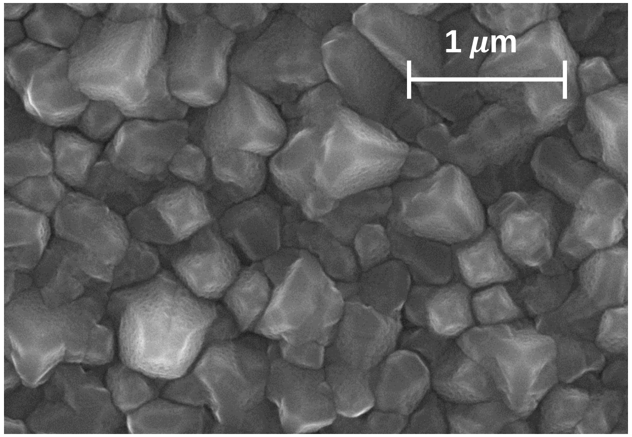
- Material structure: grain size distribution

  Measurement of SEM (Scanning electron microscope)

  - Grain size dependent on the LPCVD temperature process
  - 2 µm-thick poly-silicon films



Deposition temperature: 580 °C

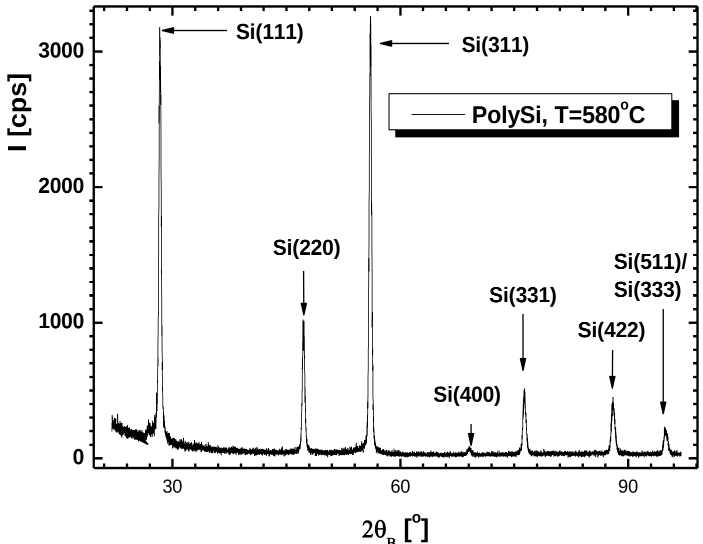


Deposition temperature: 650 °C

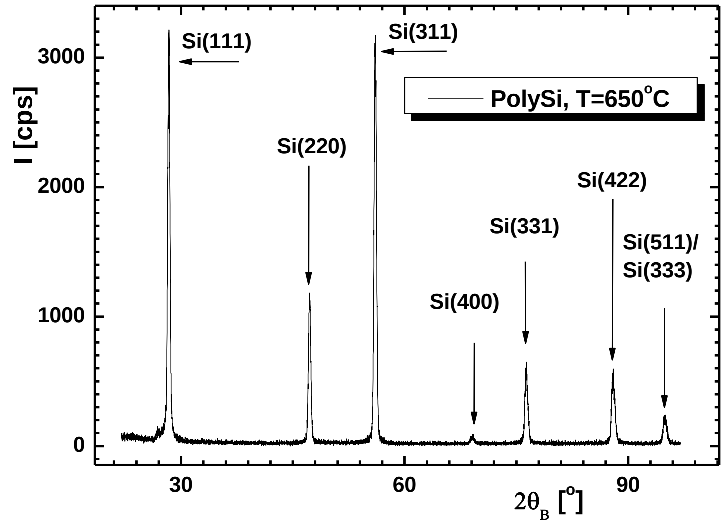
Temperature [°C]	580	610	630	650
Average grain diameter [µm]	0.21	0.45	0.72	0.83

SEM images provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

- Material structure: grain orientation distribution
  - Grain orientation by XRD (X-ray Diffraction) measurements on 2 µm-thick poly-silicon films



Deposition temperature: 580 °C



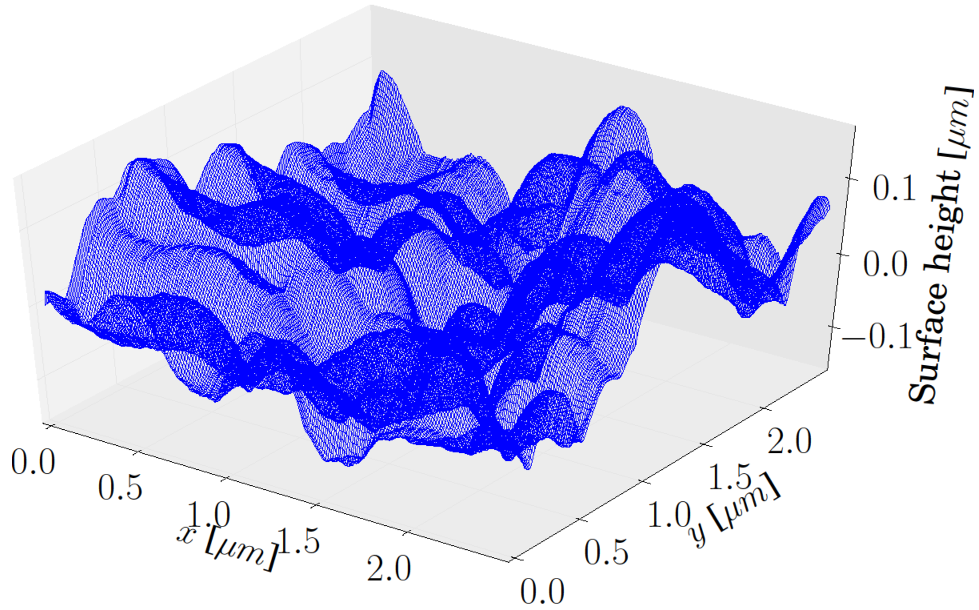
Deposition temperature: 630 °C

Temperature [°C]	580	610	630	650
<111> [%]	12.57	19.96	12.88	11.72
<220> [%]	7.19	13.67	7.96	7.59
<311> [%]	42.83	28.83	39.08	38.47
<400> [%]	4.28	5.54	3.13	3.93
<331> [%]	17.97	18.14	21.32	20.45
<422> [%]	15.15	13.86	15.63	17.84

XRD images provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

The problem

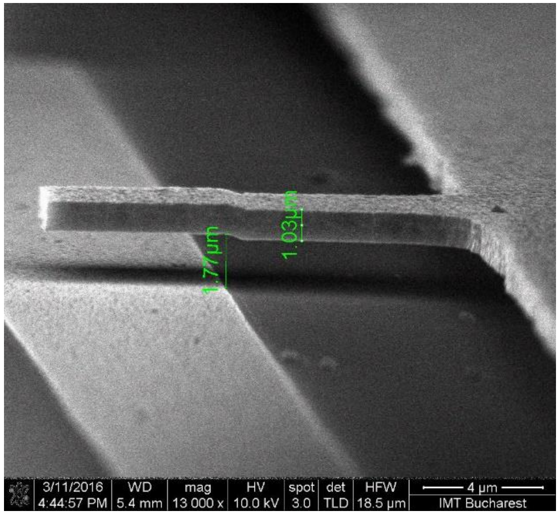
- Surface topology: asperity distribution
  - Upper surface topology by AFM (Atomic Force Microscope) measurements on 2 µm-thick poly-silicon films



Temperature [ºC]	580	610	630	650
Std deviation [nm]	35.6	60.3	90.7	88.3

AFM data provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

The problem

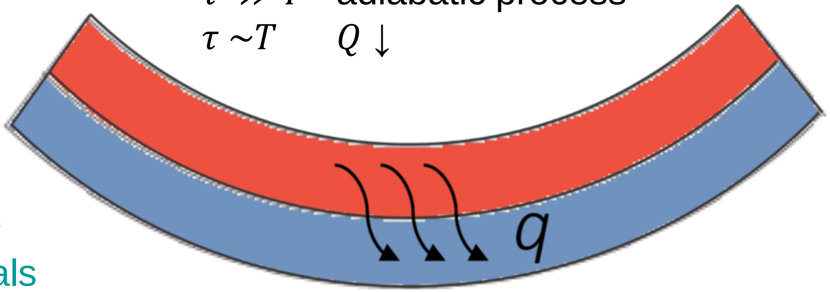


- MEMS structures
  - Are not several orders larger than their micro-structure size
  - Parameters-dependent manufacturing process
    - Low Pressure Chemical Vapor Deposition (LPCVD)
    - Properties depend on the temperature, time process, and flow gas conditions
  - As a result, their macroscopic properties can exhibit a **scatter**
    - Due to the fabrication process (photolithography, wet and dry etching)
    - Due to uncertainties of the material
    - …

→ The objective of this work is to estimate this scatter

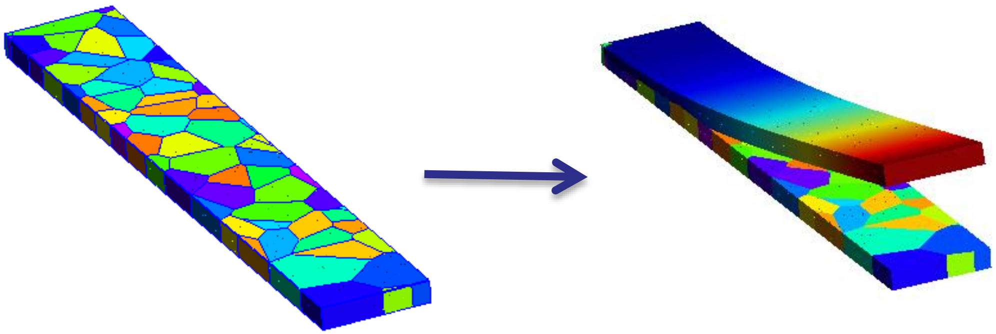
- Application example
  - Poly-silicon resonators
  - Quantities of interest
    - Eigen frequency
    - Quality factor due to thermo-elastic damping Q ~ $W/\Delta W$
    - Thermoelastic damping is a source of intrinsic material damping present in almost all materials

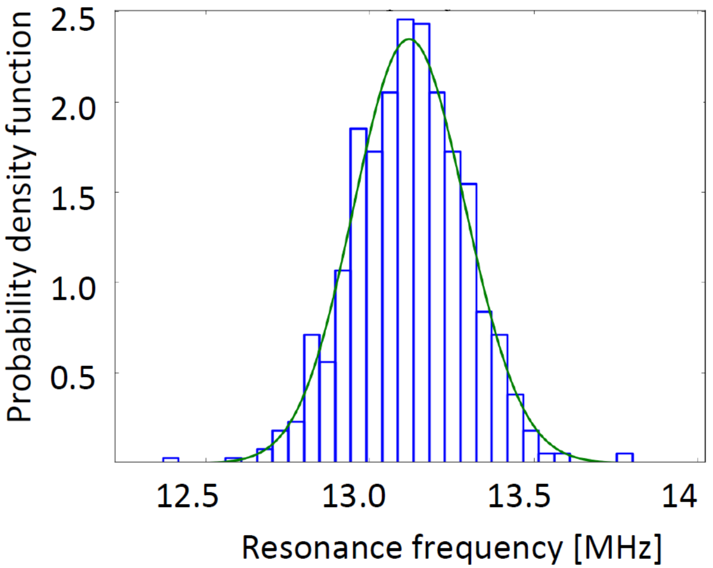
$\tau \ll T$ isothermal process
$\tau \gg T$ adiabatic process
$\tau \sim T$ $Q \downarrow$



Monte-Carlo for a fully modelled beam

- The first mode frequency distribution can be obtained with
  - A 3D beam with each grain modelled
  - Grains according to experimental measurements
  - Monte-Carlo simulations



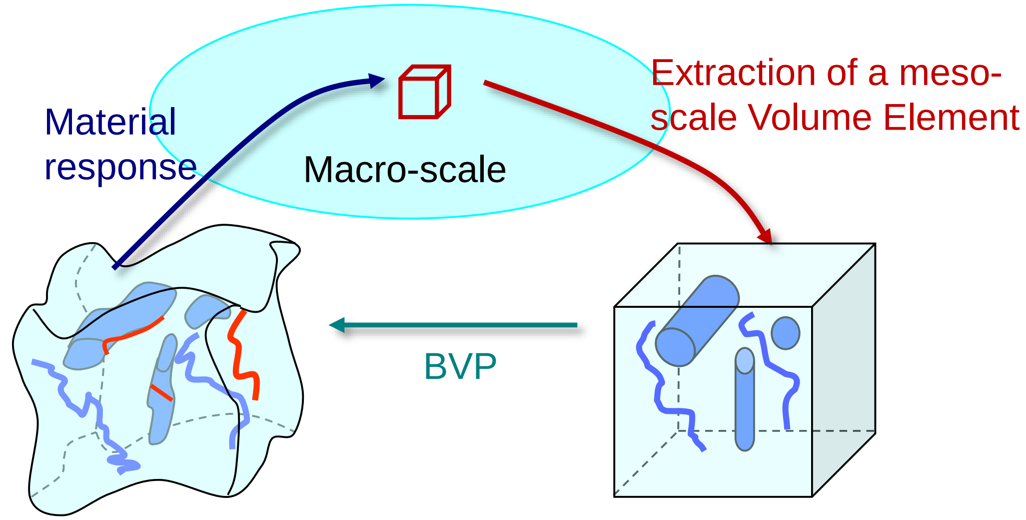


- Considering each grain is expensive and time consuming

→ **Motivation 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

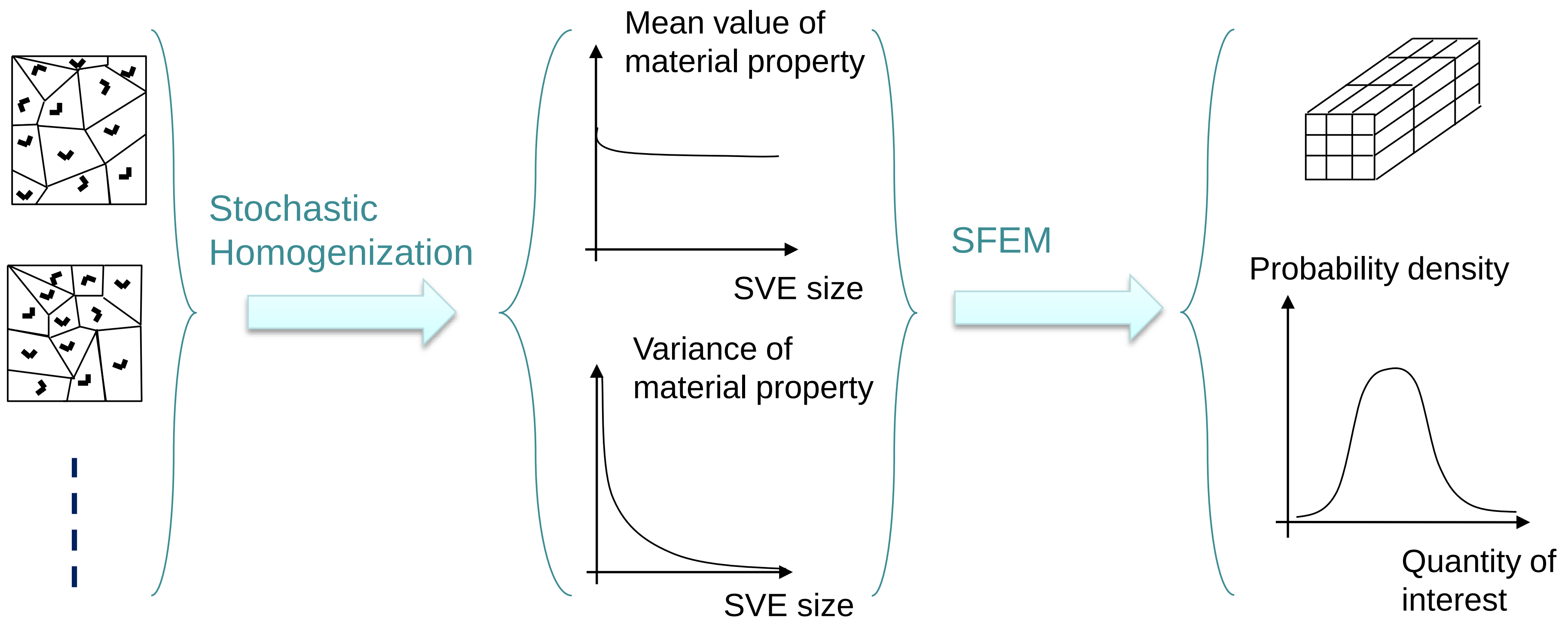
Meso-scale volume element no longer statistically representative: Stochastic Volume Elements*

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

**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 process

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 $\mathbb{P}(f_1)$ /Quality factor $\mathbb{P}(Q)$



Content

- Thermo-mechanical problems
  - Governing equations
  - Macro-scale stochastic finite element
  - Meso-scale volume elements
- From the micro-scale to the meso-scale
  - Thermo-mechanical homogenization
  - Definition of Stochastic Volume Elements (SVEs) & Stochastic homogenization
  - Need for a meso-scale random field
- The meso-scale random field
  - Definition of the thermo-mechanical meso-scale random field
  - Stochastic model of the random field: Spectral generator & non-Gaussian mapping
- From the meso-scale to the macro-scale
  - 3-Scale approach verification
  - Application to extract the quality factor
- Extension to stochastic-plate finite elements
  - Second-order stochastic homogenization
  - Rough Stochastic Volume Elements
  - Topology uncertainties effects

Thermo-mechanical problem

- Governing equations
  - Thermo-mechanics
    - Linear balance $\rho\ddot{\mathbf{u}} - \nabla\cdot\boldsymbol{\sigma} - \rho\boldsymbol{b} = 0$
    - Clausius-Duhem inequality in terms of volume entropy rate $\dot{S} = -\dfrac{\nabla\cdot\boldsymbol{q}}{T}$
    - Helmholtz free energy

$$\begin{cases} \mathcal{F}(\boldsymbol{\varepsilon},T) = \mathcal{F}_0(T) - \boldsymbol{\varepsilon}:\dfrac{\partial^2\psi}{\partial\boldsymbol{\varepsilon}\partial\boldsymbol{\varepsilon}}:\alpha(T-T_0) + \psi(\boldsymbol{\varepsilon}) \\ \boldsymbol{\sigma} = \left(\dfrac{\partial\mathcal{F}}{\partial\boldsymbol{\varepsilon}}\right)_T \quad , \quad S = \left(\dfrac{\partial\mathcal{F}}{\partial T}\right)_{\boldsymbol{\varepsilon}} \quad \& \quad \left(\dfrac{\partial^2\mathcal{F}_0}{\partial T\partial T}\right) = \rho C_v \end{cases}$$

  - Strong form in terms of the displacements $\boldsymbol{u}$ and temperature change ϑ (linear elasticity)

$$\hookrightarrow \begin{cases} \rho\ddot{\mathbf{u}} - \nabla\cdot(\mathbb{C}:\dot{\boldsymbol{\varepsilon}} - \mathbb{C}:\boldsymbol{\alpha}\vartheta) - \rho\boldsymbol{b} = 0 \\ \rho C_v\dot{\vartheta} + T_0\boldsymbol{\alpha}:\mathbb{C}:\dot{\boldsymbol{\varepsilon}} - \nabla\cdot(\boldsymbol{\kappa}\nabla\vartheta) = 0 \end{cases}$$

  - Finite element discretization

$$\hookrightarrow \begin{bmatrix} \mathbf{M}(\rho) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}\begin{bmatrix} \ddot{\mathbf{u}} \\ \ddot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{\vartheta\mathrm{u}}(\boldsymbol{\alpha},\mathbb{C}) & \mathbf{D}_{\vartheta\vartheta}(\rho C_v) \end{bmatrix}\begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{\mathrm{uu}}(\mathbb{C}) & \mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\alpha},\mathbb{C}) \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\kappa}) \end{bmatrix}\begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_{\mathrm{u}} \\ \boldsymbol{F}_{\vartheta} \end{bmatrix}$$

- Macro-scale stochastic finite element method
  - Meso-scale material properties subjected to uncertainties
    - Elasticity tensor $\mathbb{C}_M(\boldsymbol{\theta})$,
    - Heat conductivity tensor $\boldsymbol{\kappa}_M(\boldsymbol{\theta})$, and
    - Thermal expansion tensors $\boldsymbol{\alpha}_M(\boldsymbol{\theta})$

    in the sample space $\boldsymbol{\theta} \in \boldsymbol{\Omega}$

$$\begin{bmatrix} \mathbf{M}(\rho_\mathrm{M}) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{u}} \\ \ddot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{\vartheta\mathrm{u}}(\boldsymbol{\alpha}_\mathrm{M}, \mathbb{C}_\mathrm{M}) & \mathbf{D}_{\vartheta\vartheta}(\rho_\mathrm{M} C_{v\mathrm{M}}) \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{\mathrm{uu}}(\mathbb{C}_\mathrm{M}) & \mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\alpha}_\mathrm{M}, \mathbb{C}_\mathrm{M}) \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\kappa}_\mathrm{M}\ ) \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_\mathrm{u} \\ \boldsymbol{F}_\vartheta \end{bmatrix}$$

$$\hookrightarrow \begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{u}} \\ \ddot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{\vartheta\mathrm{u}}(\boldsymbol{\theta}) & \mathbf{D}_{\vartheta\vartheta} \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{\mathrm{uu}}(\boldsymbol{\theta}) & \mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\theta}) \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\theta}) \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_\mathrm{u} \\ \boldsymbol{F}_\vartheta \end{bmatrix}$$

- Defining the random properties at the meso-scale by
  - Using micro-scale information (SEM, XRD, images)
  - Homogenization method

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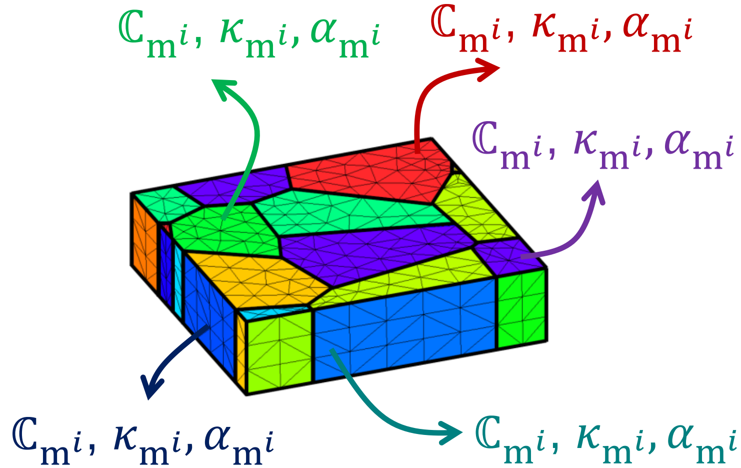
Thermo-mechanical problem

- Meso-scale Volume Elements (VE)
  - Micro-scale material properties
    - Elasticity tensor $\mathbb{C}_m$,
    - Heat conductivity tensor $\boldsymbol{\kappa}_m$, and
    - Thermal expansion tensors $\boldsymbol{\alpha}_m$

    defined on each phase/heterogeneity



  - Length scales separation assumptions
    - VE small enough for the time for strain wave to propagate in the SVE to remain negligible
    - VE small enough for the time variation of heat storage to remain negligible

$$\begin{bmatrix} \mathbf{M}(\rho_{\mathrm{m}}) & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{u}} \\ \ddot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{D}_{\vartheta\mathrm{u}}(\boldsymbol{\alpha}_{\mathrm{m}}, \mathbb{C}_{\mathrm{m}}) & \mathbf{D}_{\vartheta\vartheta}(\rho_{\mathrm{m}} C_{v\mathrm{m}}) \end{bmatrix} \begin{bmatrix} \dot{\mathbf{u}} \\ \dot{\boldsymbol{\vartheta}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{\mathrm{uu}}(\mathbb{C}_{\mathrm{m}}) & \mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\alpha}_{\mathrm{m}}, \mathbb{C}_{\mathrm{m}}) \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\kappa}_{\mathrm{m}}\ ) \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_{\mathrm{u}} \\ \boldsymbol{F}_{\vartheta} \end{bmatrix}$$

$$\hookrightarrow \quad \begin{bmatrix} \mathbf{K}_{\mathrm{uu}} & \mathbf{K}_{\mathrm{u}\vartheta} \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_{\mathrm{u}} \\ \boldsymbol{F}_{\vartheta} \end{bmatrix}$$

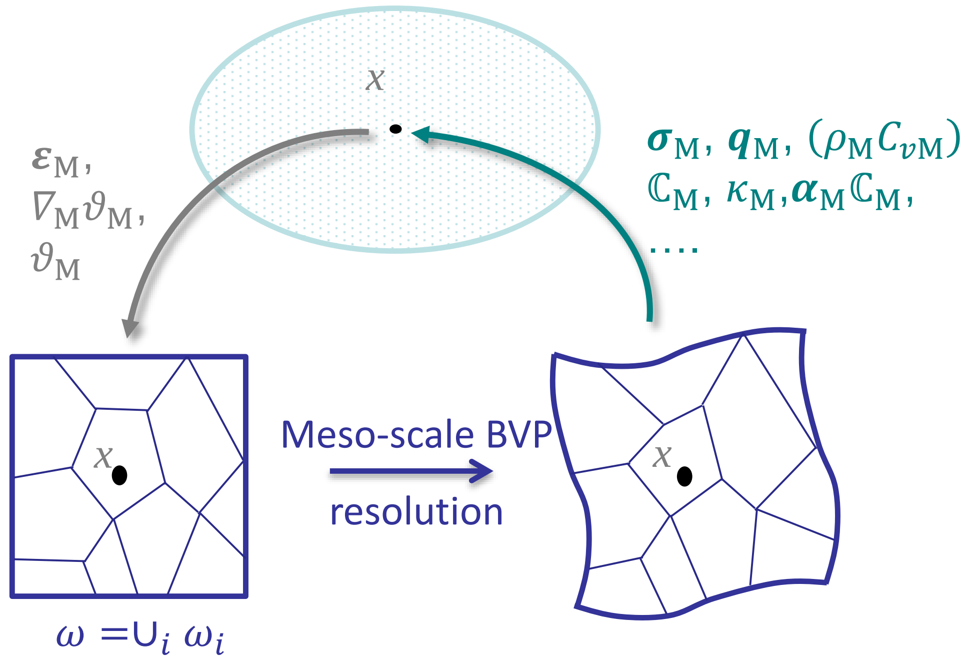
- Transition from meso-scale BVP realizations to the meso-scale random properties

$\longrightarrow$ Stochastic thermo-mechanical homogenization

From the micro-scale to the meso-scale

- Thermo-mechanical homogenization
  - Down-scaling

$$\begin{cases} \boldsymbol{\varepsilon}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\varepsilon}_{\mathrm{m}} d\omega \\ \nabla_{\mathrm{M}} \vartheta_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \nabla_{\mathrm{m}} \vartheta_{\mathrm{m}} d\omega \\ \vartheta_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \dfrac{\rho_{\mathrm{m}} C_{v\mathrm{m}}}{\rho_{\mathrm{M}} C_{v\mathrm{M}}} \vartheta_{\mathrm{m}} d\omega \end{cases}$$



  - Meso-scale BVP fluctuation fields

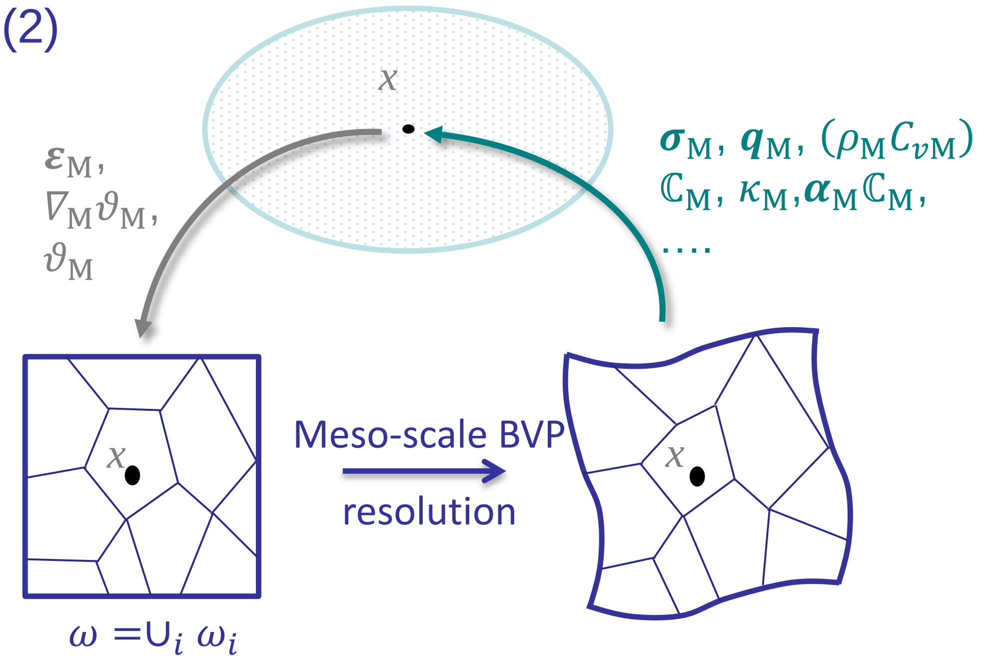
$$\begin{cases} \boldsymbol{u}_{\mathrm{m}} = \boldsymbol{\varepsilon}_{\mathrm{M}} \cdot \boldsymbol{x} + \boldsymbol{u}' \\ \vartheta_{\mathrm{m}} = \nabla_{\mathrm{M}} \vartheta_{\mathrm{M}} \cdot \boldsymbol{x} + \vartheta'_{\mathrm{m}} \end{cases} \longrightarrow \begin{cases} 0 = \displaystyle\int_{\partial\omega} \boldsymbol{u}' \otimes \boldsymbol{n} \, d\partial\omega \\ 0 = \displaystyle\int_{\partial\omega} \boldsymbol{n} \vartheta' \, d\partial\omega \end{cases}$$

$\longrightarrow$ Satisfied by periodic boundary conditions

From the micro-scale to the meso-scale

- Thermo-mechanical homogenization (2)
  - Upscaling

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} d\omega \\ \boldsymbol{q}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{q}_{\mathrm{m}} d\omega \\ \rho_{\mathrm{M}} C_{v\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int \rho_{\mathrm{m}} C_{v\mathrm{m}} dV \end{cases}$$



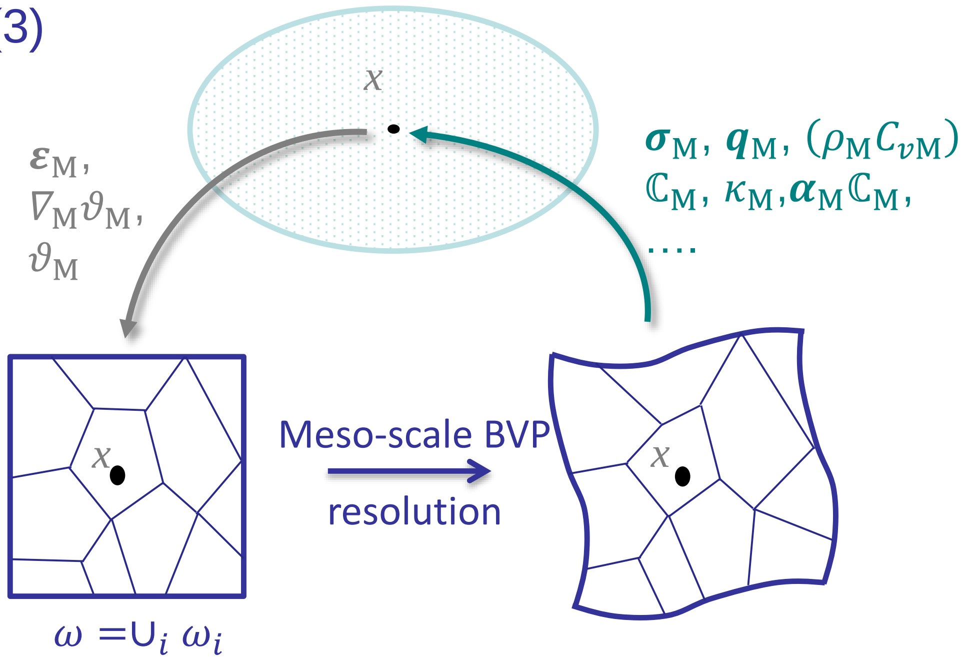
  - Consistency

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} : \delta\boldsymbol{\varepsilon}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} : \delta\boldsymbol{\varepsilon}_{\mathrm{m}} d\omega \\ \dfrac{\boldsymbol{q}_{\mathrm{M}} \cdot \nabla_{\mathrm{M}} \delta\vartheta_{\mathrm{M}}}{T_{\mathrm{M}}} \simeq \dfrac{1}{T_{\mathrm{M}} V(\omega)} \displaystyle\int_{\omega} \boldsymbol{q}_{\mathrm{m}} \cdot \nabla_{\mathrm{m}} \delta\vartheta_{\mathrm{m}} d\omega \\ \rho_{\mathrm{M}} C_{v\mathrm{M}} \vartheta_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \rho_{\mathrm{m}} C_{v\mathrm{m}} \vartheta_{\mathrm{m}} d\omega \end{cases} \longrightarrow \begin{cases} 0 = \displaystyle\int_{\partial\omega} (\boldsymbol{\sigma}_{\mathrm{m}} \cdot \boldsymbol{n}) \cdot \boldsymbol{u}' \, d\partial\omega \\ 0 = \displaystyle\int_{\partial\omega} (\boldsymbol{q}_{\mathrm{m}} \cdot \boldsymbol{n}) \vartheta' \, d\partial\omega \\ \vartheta_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \dfrac{\rho_{\mathrm{m}} C_{v\mathrm{m}}}{\rho_{\mathrm{M}} C_{v\mathrm{M}}} \vartheta_{\mathrm{m}} d\omega \end{cases}$$

$\longrightarrow$ Satisfied by periodic boundary conditions & volume constraint

- Thermo-mechanical homogenization (3)
  - Micro-scale BVP

$$\begin{cases} \begin{bmatrix} \mathbf{K}_{\mathrm{uu}} & \mathbf{K}_{\mathrm{u}\vartheta} \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{F}_{\mathrm{u}} \\ \boldsymbol{F}_{\vartheta} \end{bmatrix} \\ \mathbf{C} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} = \mathbf{S} \begin{bmatrix} \nabla_{\mathrm{M}} \boldsymbol{u}_{\mathrm{M}} \\ \nabla_{\mathrm{M}} \vartheta_{\mathrm{M}} \\ \vartheta_{\mathrm{M}} \end{bmatrix} \end{cases}$$

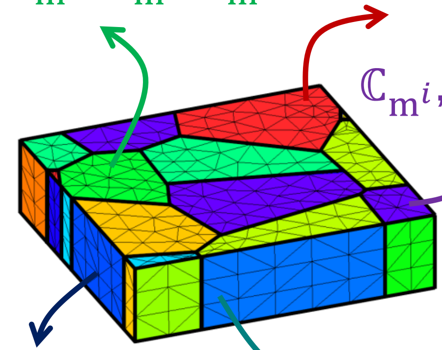


  - Solution is the stationary point of $\Psi = \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix}^T \begin{bmatrix} \mathbf{K}_{\mathrm{uu}} & \mathbf{K}_{\mathrm{u}\vartheta} \\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} - \boldsymbol{\lambda}^T \left[\mathbf{C} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\vartheta} \end{bmatrix} - \mathbf{S} \begin{bmatrix} \nabla_{\mathrm{M}} \boldsymbol{u}_{\mathrm{M}} \\ \nabla_{\mathrm{M}} \vartheta_{\mathrm{M}} \\ \vartheta_{\mathrm{M}} \end{bmatrix} \right]$

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \dfrac{\partial \Psi}{\partial \boldsymbol{u}_{\mathrm{M}} \otimes \boldsymbol{\nabla}_{\mathrm{M}}} \\ \boldsymbol{q}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \dfrac{\partial \Psi}{\partial \nabla_{\mathrm{M}} \vartheta_{\mathrm{M}}} \end{cases} \longrightarrow \begin{cases} \mathbb{C}_{\mathrm{M}} = \dfrac{\partial \boldsymbol{\sigma}_{\mathrm{M}}}{\partial \boldsymbol{u}_{\mathrm{M}} \otimes \boldsymbol{\nabla}_{\mathrm{M}}} \quad \& \quad \boldsymbol{\alpha}_{\mathrm{M}} : \mathbb{C}_{\mathrm{M}} = -\dfrac{\partial \boldsymbol{\sigma}_{\mathrm{M}}}{\partial \vartheta_{\mathrm{M}}} \\ \boldsymbol{\kappa}_{\mathrm{M}} = -\dfrac{\partial \boldsymbol{q}_{\mathrm{M}}}{\partial \nabla_{\mathrm{M}} \vartheta_{\mathrm{M}}} \end{cases}$$

From the micro-scale to the meso-scale

- Definition of Stochastic Volume Elements (SVEs)
  - Poisson Voronoï tessellation realizations
    - SVE realization ω_j
  - Each grain ω_i is assigned material properties
    - $\mathbb{C}_{\mathrm{m}^i}, \kappa_{\mathrm{m}^i}, \alpha_{\mathrm{m}^i},$
    - Defined from silicon crystal properties
  - Each $\mathbb{C}_{m^i}$ is assigned a random orientation
    - Following XRD distributions



- Stochastic homogenization
  - Several SVE realizations
  - For each SVE $\omega_j = \cup_i \omega_i$

$$\mathbb{C}_{\mathrm{m}^i}, \kappa_{\mathrm{m}^i}, \alpha_{\mathrm{m}^i} \quad \forall i \quad \xrightarrow{\text{Computational homogenization}} \quad \mathbb{C}_{\mathrm{M}^j}, \kappa_{\mathrm{M}^j}, \alpha_{\mathrm{M}^j}$$

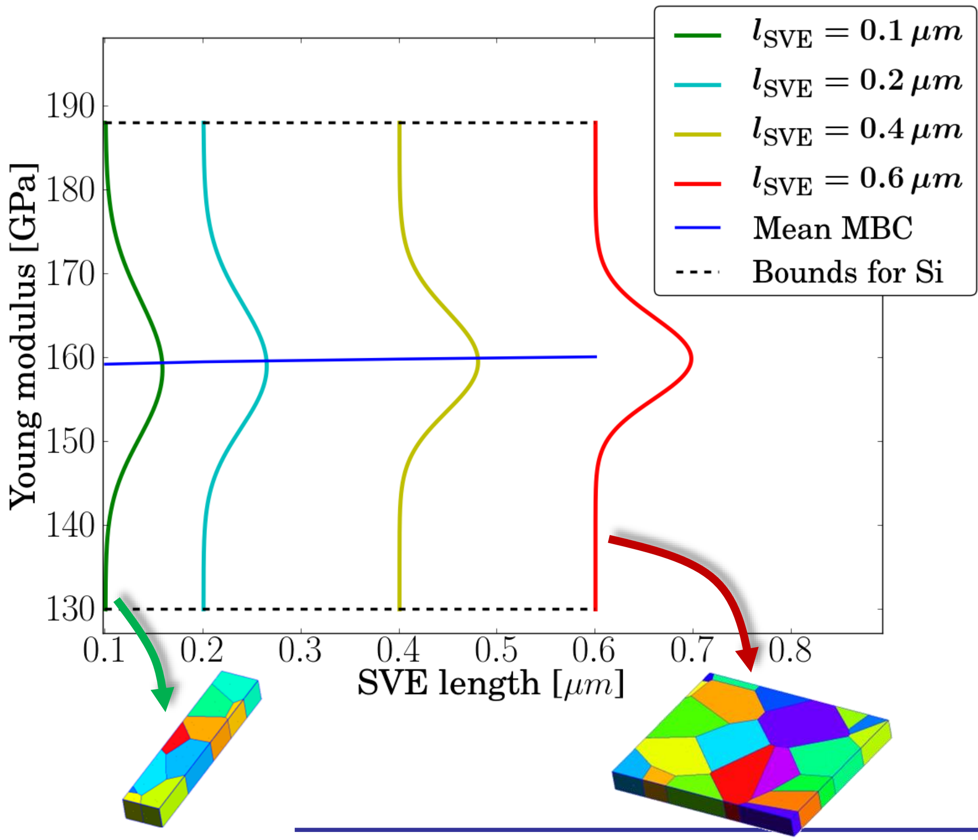
Samples of the meso-scale homogenized elasticity tensors

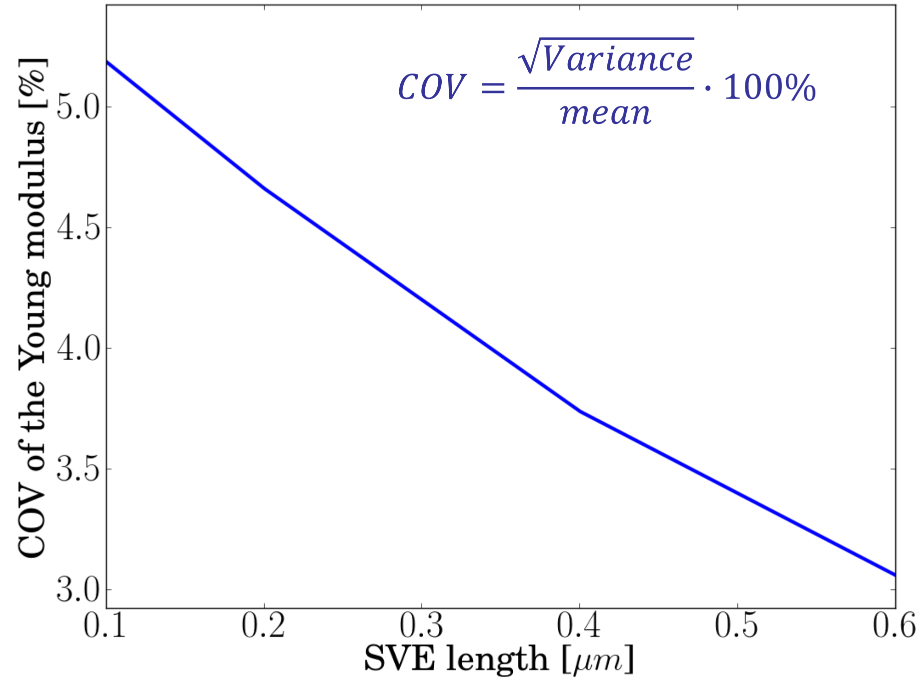
  - Homogenized material tensors not unique as statistical representativeness is lost*

*"C. Huet, 1990

From the micro-scale to the meso-scale

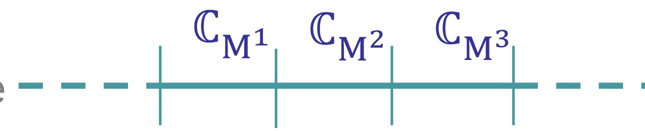
- Distribution of the apparent meso-scale elasticity tensor $\mathbb{C}_M$
  - For large SVEs, the apparent tensor tends to the effective (and unique) one

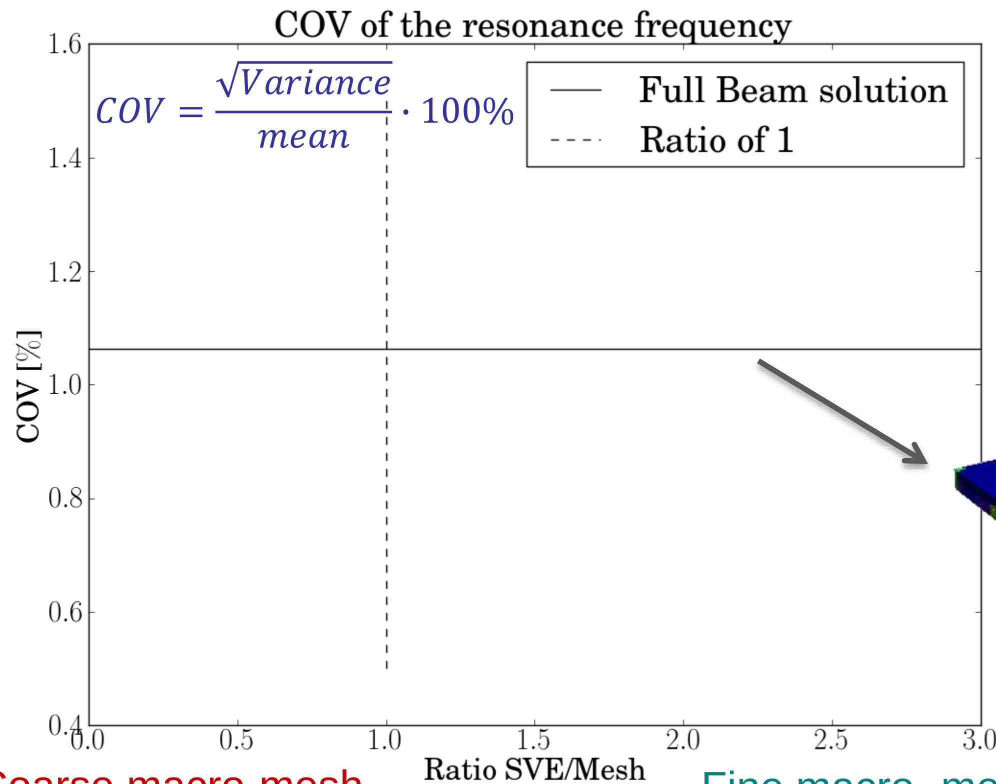




- The bounds do not depend on the SVE size but on the silicon elasticity tensor
- However, the larger the SVE, the lower the probability to be close to the bounds

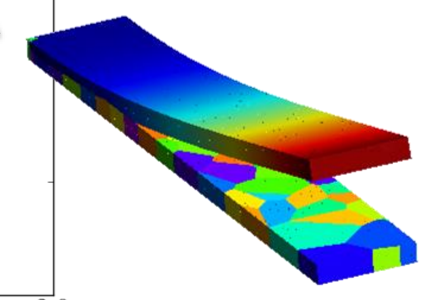
- Use of the meso-scale distribution with macro-scale finite elements
  - Beam macro-scale finite elements
  - Use of the meso-scale distribution as a random variable
  - Monte-Carlo simulations





First bending mode of

a 3.2 μm-long beam

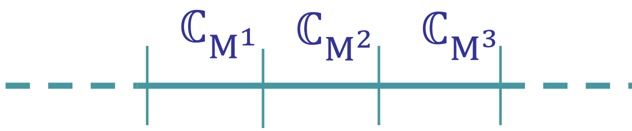


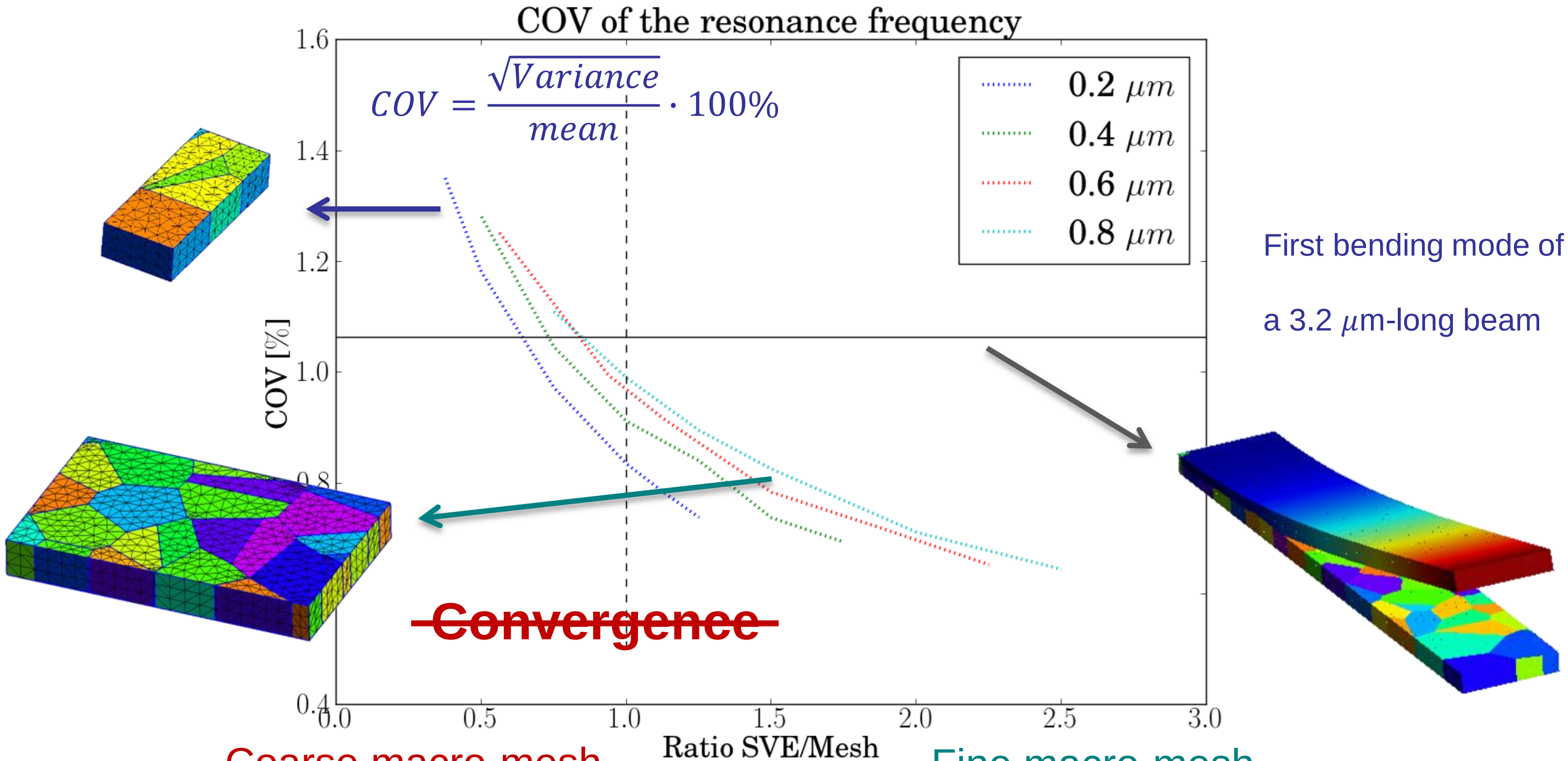
Coarse macro-mesh

Fine macro- mesh

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





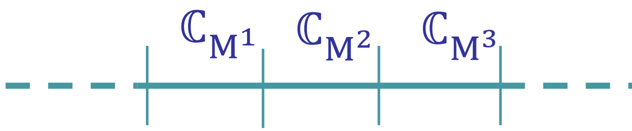
Coarse macro-mesh

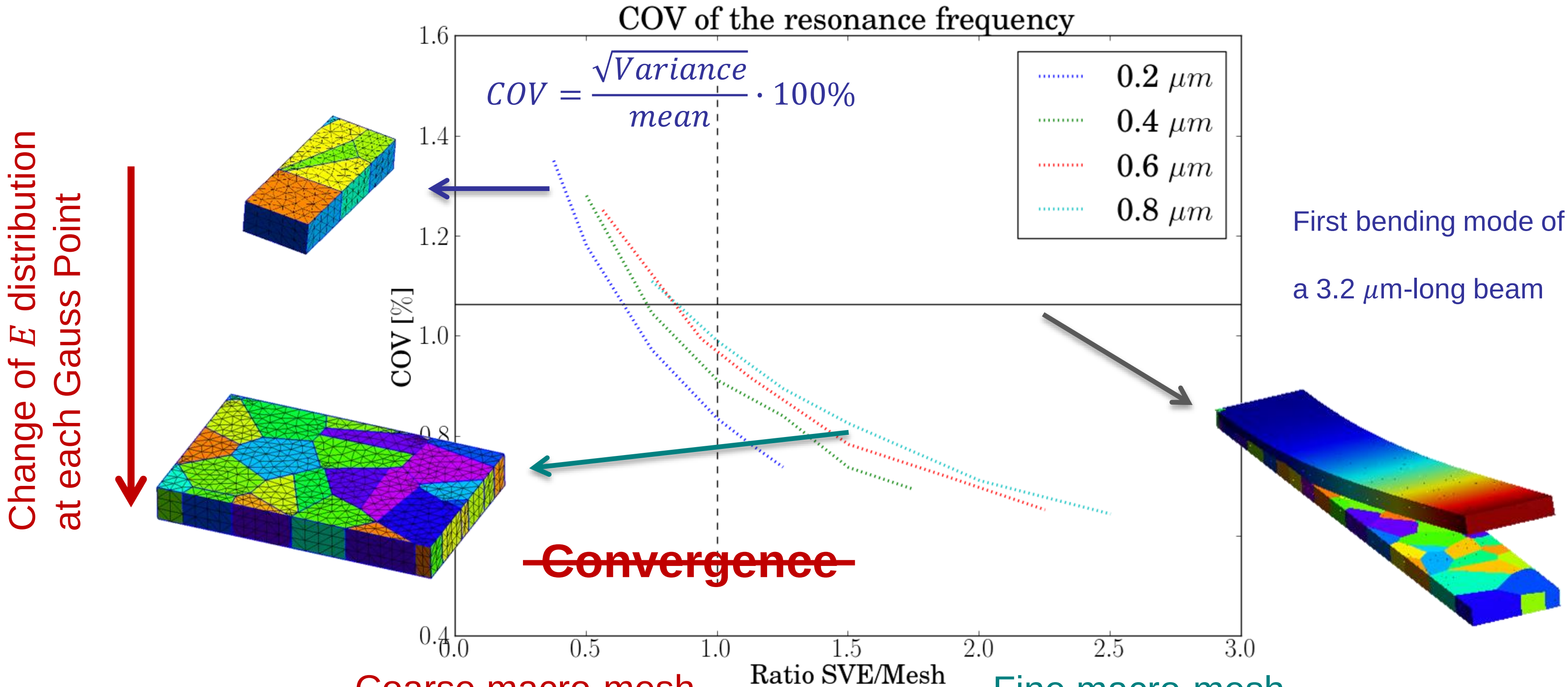
Fine macro-mesh

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





Coarse macro-mesh

Fine macro-mesh

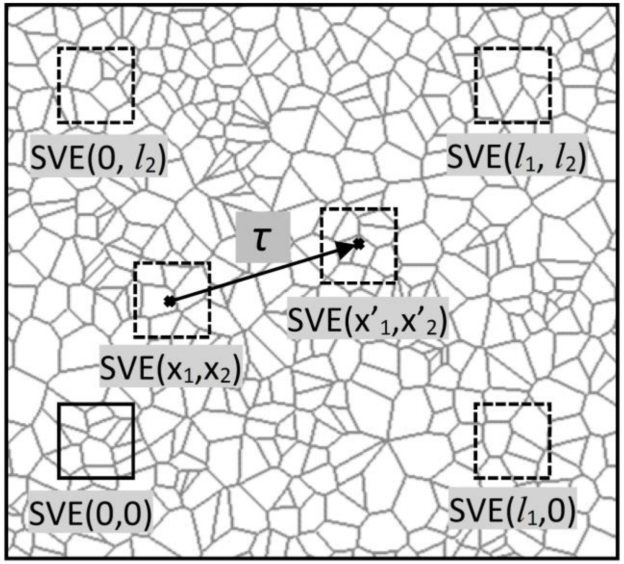
More random variables having the same distribution

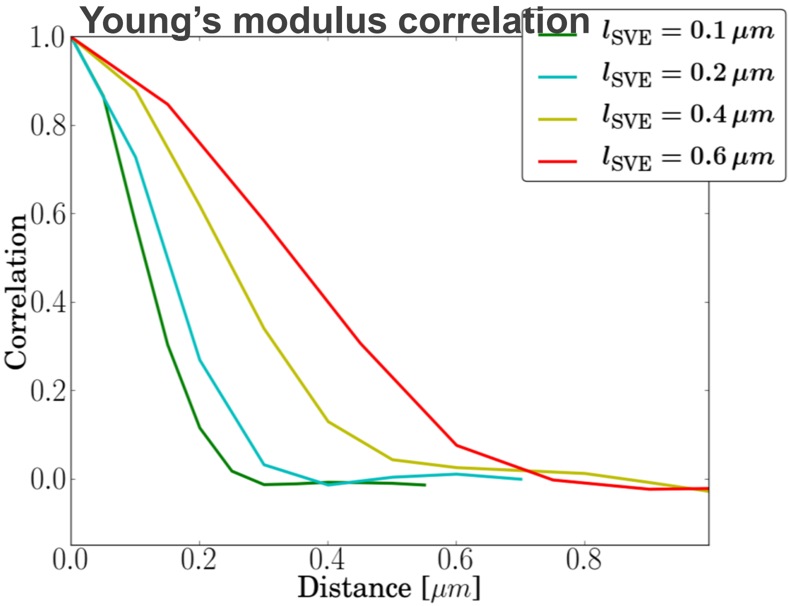
- Need for a meso-scale random field
  - Introduction of the (meso-scale) spatial correlation
    - Define large tessellations
    - SVEs extracted at different distances in each tessellation
  - Evaluate the spatial correlation between the components of the meso-scale material operators
  - For example, in 1D-elasticity
    - Young's modulus correlation

$$R_{E_x}(\boldsymbol{\tau}) = \frac{\mathbb{E}\left[\left(\boldsymbol{E_x}(\boldsymbol{x}) - \mathbb{E}(\boldsymbol{E_x})\right)\left(\boldsymbol{E_x}(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}(\boldsymbol{E_x})\right)\right]}{\mathbb{E}\left[\left(\boldsymbol{E_x} - \mathbb{E}(\boldsymbol{E_x})\right)^2\right]}$$

    - Correlation length

$$L_{E_x} = \frac{\int_{-\infty}^{\infty} R_{E_x}(\tau)d\tau}{R_{E_x}(0)}$$



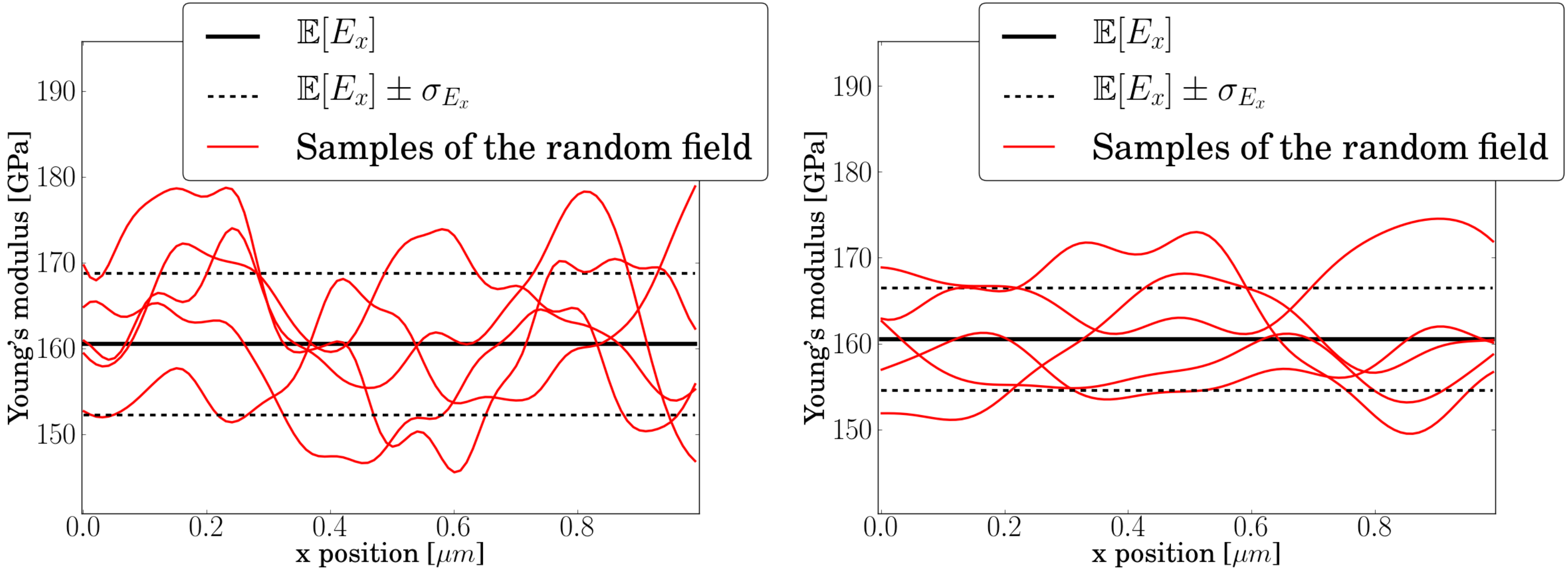


From the micro-scale to the meso-scale

- Need for a meso-scale random field (2)
  - The meso-scale random field is characterized by the correlation length L_{E_x}
  - The correlation length L_{E_x} depends on the SVE size

Random field with different SVEs sizes

$l_{\mathrm{SVE}} = 0.1\ \mu m$ $l_{\mathrm{SVE}} = 0.4\ \mu m$

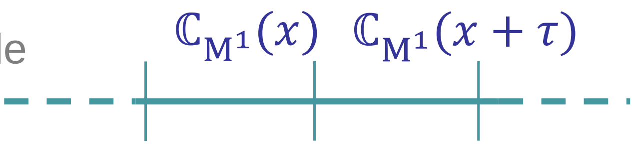


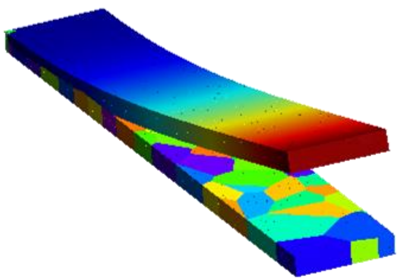
From the micro-scale to the meso-scale

- Need for a meso-scale random field (3)
  - Use of the meso-scale random field

    → Monte-Carlo simulations at the macro-scale

  - Macro-scale beam elements of size l_{mesh}
  - Convergence in terms of $\alpha = \frac{L_{E_x}}{l_{\text{mesh}}}$





First bending mode of

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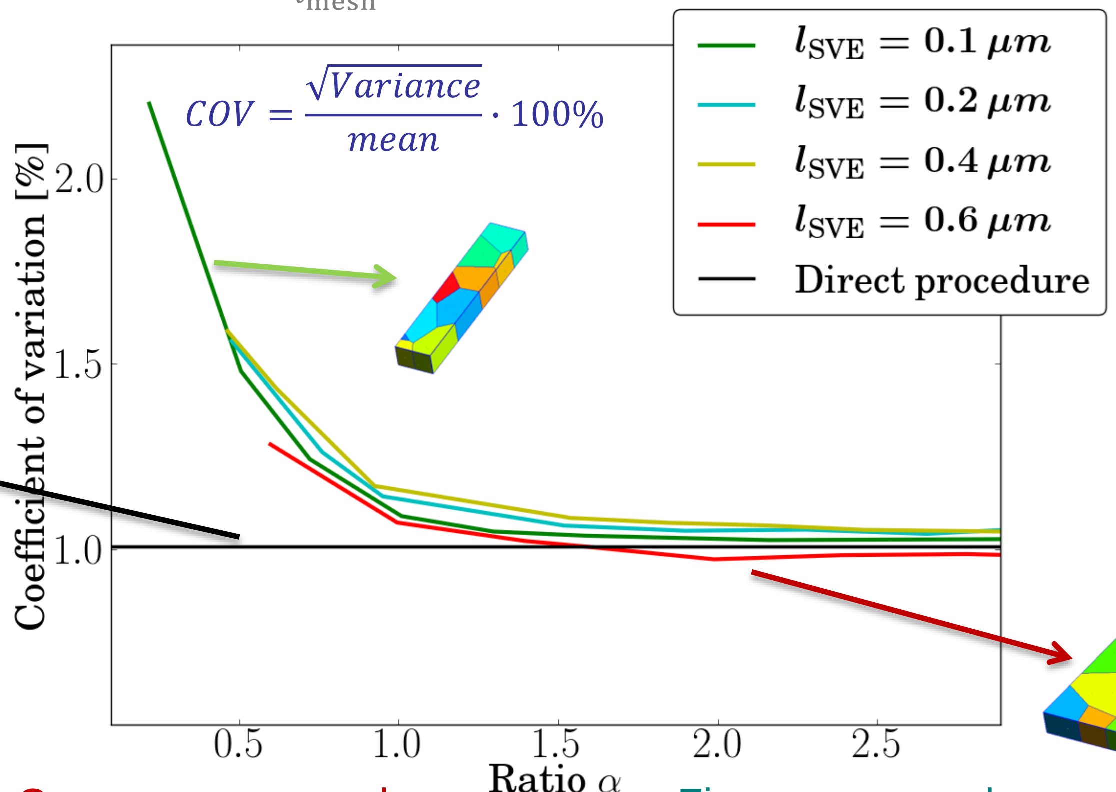
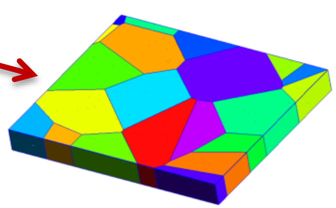




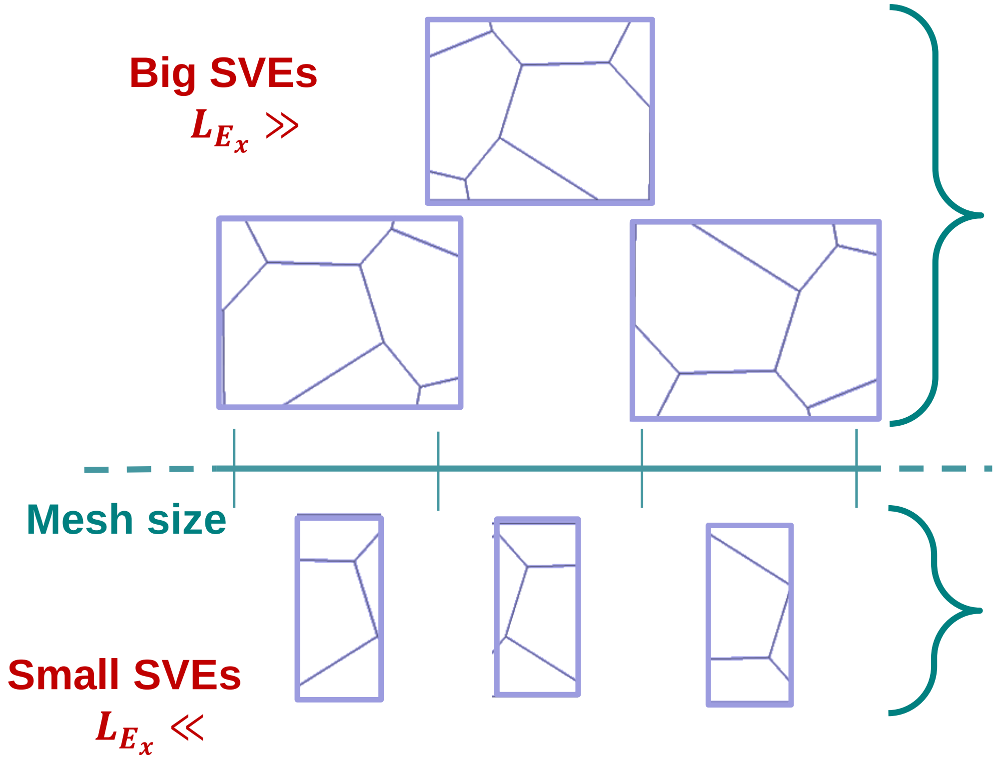
Coarse macro-mesh

Fine macro-mesh

Université de Liège

From the micro-scale to the meso-scale

- Need for a meso-scale random field (3)
  - Effect of the ratio $\alpha = \frac{L_{E_x}}{l_{\text{mesh}}}$ (Only one gauss point in one element)



$\alpha = \frac{L_{E_x}}{l_{\text{mesh}}} > 1$ → The spatial correlation is accounted for

$\alpha = \frac{L_{E_x}}{l_{\text{mesh}}} < 1$ → 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 $l_{\text{SVE}} \sim L_{\text{micro}}$

Content

- Thermo-mechanical problems
  - Governing equations
  - Macro-scale stochastic finite element
  - Meso-scale volume elements
- From the micro-scale to the meso-scale
  - Thermo-mechanical homogenization
  - Definition of Stochastic Volume Elements (SVEs) & Stochastic homogenization
  - Need for a meso-scale random field
- The meso-scale random field
  - Definition of the thermo-mechanical meso-scale random field
  - Stochastic model of the random field: Spectral generator & non-Gaussian mapping
- From the meso-scale to the macro-scale
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  - Second-order stochastic homogenization
  - Rough Stochastic Volume Elements
  - Topology uncertainties effects

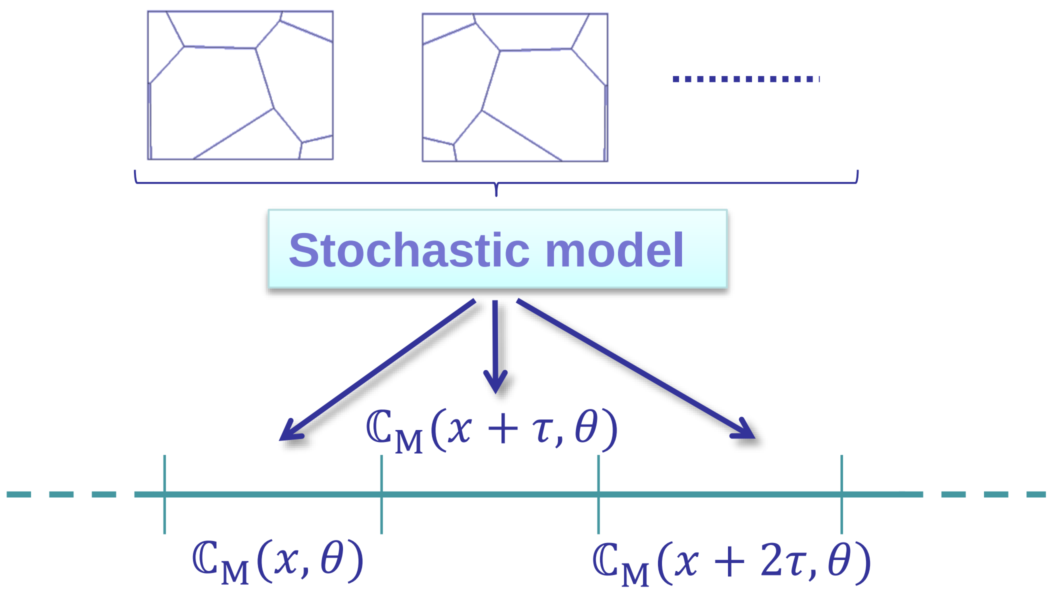
The meso-scale random field

- Use of the meso-scale distribution with stochastic (macro-scale) finite elements
  - Use of the meso-scale random field

    $\longrightarrow$ Monte-Carlo simulations at the macro-scale

  - BUT we do not want to evaluate the random field from the stochastic homogenization for each simulation $\longrightarrow$ Meso-scale random field from a generator

Stochastic model of meso-scale elasticity tensors



The meso-scale random field

- Definition of the thermo-mechanical meso-scale random field
  - Elasticity tensor $\mathbb{C}_{\mathrm{M}}(x,\theta)$ (matrix form $\boldsymbol{C}_M$) & thermal conductivity $\boldsymbol{\kappa}_{\mathrm{M}}$ are bounded
    - Ensure existence of their inverse
    - Define lower bounds $\mathbb{C}_{\mathrm{L}}$ and $\boldsymbol{\kappa}_{\mathrm{L}}$ such that

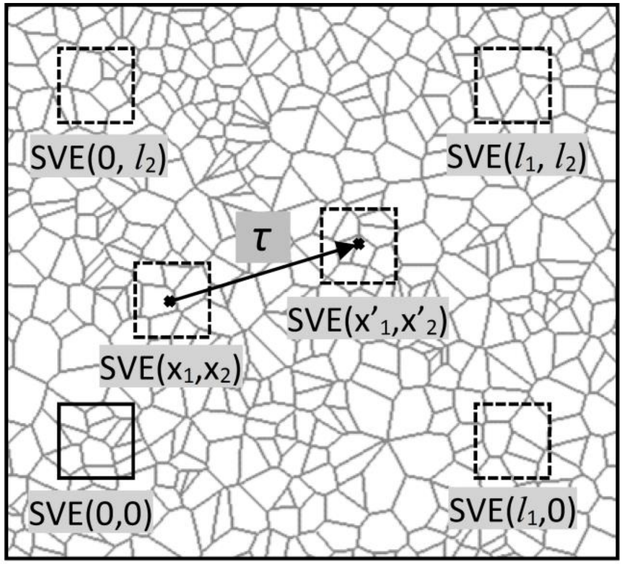
$$\begin{cases} \boldsymbol{\varepsilon} : (\mathbb{C}_{\mathrm{M}} - \mathbb{C}_{\mathrm{L}}) : \boldsymbol{\varepsilon} > 0 & \forall \boldsymbol{\varepsilon} \\ \nabla\vartheta \cdot (\boldsymbol{\kappa}_{\mathrm{M}} - \boldsymbol{\kappa}_{\mathrm{L}}) \cdot \nabla\vartheta > 0 & \forall \nabla\vartheta \end{cases}$$

  - Use a Cholesky decomposition when semi-definite tensors are required

$$\begin{cases} \boldsymbol{C}_{\mathrm{M}}(\boldsymbol{x},\boldsymbol{\theta}) = \boldsymbol{C}_{\mathrm{L}} + \left(\bar{\boldsymbol{\mathcal{A}}} + \boldsymbol{\mathcal{A}}'(\boldsymbol{x},\boldsymbol{\theta})\right)^T \left(\bar{\boldsymbol{\mathcal{A}}} + \boldsymbol{\mathcal{A}}'(\boldsymbol{x},\boldsymbol{\theta})\right) \\ \boldsymbol{\kappa}_{\mathrm{M}}(\boldsymbol{x},\boldsymbol{\theta}) = \boldsymbol{\kappa}_{\mathrm{L}} + \left(\bar{\boldsymbol{\mathcal{B}}} + \boldsymbol{\mathcal{B}}'(\boldsymbol{x},\boldsymbol{\theta})\right)^T \left(\bar{\boldsymbol{\mathcal{B}}} + \boldsymbol{\mathcal{B}}'(\boldsymbol{x},\boldsymbol{\theta})\right) \\ \boldsymbol{\alpha}_{\mathrm{M}_{ij}}(\boldsymbol{x},\boldsymbol{\theta}) = \bar{\boldsymbol{\mathcal{V}}}^{(t)} + \boldsymbol{\mathcal{V}'}^{(t)}(\boldsymbol{x},\boldsymbol{\theta}) \end{cases}$$

  - We define the homogenous zero-mean random field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x},\boldsymbol{\theta})$, with as entries
    - Elasticity tensor $\mathcal{A}'(\boldsymbol{x},\boldsymbol{\theta}) \Rightarrow \boldsymbol{\mathcal{V}'}^{(1)} \dots \boldsymbol{\mathcal{V}'}^{(21)}$,
    - Heat conductivity tensor $\mathcal{B}'(\boldsymbol{x},\boldsymbol{\theta}) \Rightarrow \boldsymbol{\mathcal{V}'}^{(22)} \dots \boldsymbol{\mathcal{V}'}^{(27)}$
    - Thermal expansion tensors $\boldsymbol{\mathcal{V}'}^{(t)} \Rightarrow \boldsymbol{\mathcal{V}'}^{(28)} \dots \boldsymbol{\mathcal{V}'}^{(33)}$

- Characterization of the meso-scale random field
  - Generate large tessellation realizations
  - For each tessellation realization
    - Extract SVEs centred on $\boldsymbol{x}+\boldsymbol{\tau}$
    - For each SVE evaluate $\mathbb{C}_{\mathrm{M}}(\boldsymbol{x}+\boldsymbol{\tau})$, $\kappa_{\mathrm{M}}(\boldsymbol{x}+\boldsymbol{\tau}), \alpha_{\mathrm{M}}(\boldsymbol{x}+\boldsymbol{\tau})$
  - From the set of realizations $\mathbb{C}_{\mathrm{M}}(\boldsymbol{x},\boldsymbol{\theta})$, $\kappa_{\mathrm{M}}(\boldsymbol{x},\boldsymbol{\theta}), \alpha_{\mathrm{M}}(\boldsymbol{x},\boldsymbol{\theta})$
    - Evaluate the bounds $\mathbb{C}_{\mathrm{L}}$ and $\boldsymbol{\kappa}_{\mathrm{L}}$
    - Apply the Cholesky decomposition ⇒ $\boldsymbol{\mathcal{A}}'(\boldsymbol{x},\boldsymbol{\theta})$, $\boldsymbol{\mathcal{B}}'(\boldsymbol{x},\boldsymbol{\theta})$
    - Fill the 33 entries of the zero-mean homogenous field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x},\boldsymbol{\theta})$
    - NB: for the thermal conductivity we use a grain-size dependent empirical relation
  - Compute the auto-/cross-correlation matrix



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

The meso-scale random field

- Stochastic model of the meso-scale random field: Spectral generator*
  - Start from the auto-/cross-covariance matrix

$$\tilde{R}^{(rs)}_{\boldsymbol{\mathcal{V}}'}(\boldsymbol{\tau}) = \sigma_{\boldsymbol{\mathcal{V}}'^{(r)}}\sigma_{\boldsymbol{\mathcal{V}}'^{(s)}} R^{(rs)}_{\boldsymbol{\mathcal{V}}'}(\boldsymbol{\tau}) = \mathbb{E}\left[\left(\boldsymbol{\mathcal{V}}'^{(r)}(\boldsymbol{x}) - \mathbb{E}\left(\boldsymbol{\mathcal{V}}'^{(r)}\right)\right)\left(\boldsymbol{\mathcal{V}}'^{(s)}(\boldsymbol{x}+\boldsymbol{\tau}) - \mathbb{E}\left(\boldsymbol{\mathcal{V}}'^{(s)}\right)\right)\right]$$

  - Evaluate the spectral density matrix from the periodized zero-padded matrix $\tilde{\boldsymbol{R}}^{\mathrm{P}}_{\boldsymbol{\mathcal{V}}'}(\boldsymbol{\tau})$

$$\boldsymbol{S}^{(rs)}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(m)}\right] = \sum_{n} \tilde{R}^{\mathrm{P}}_{\boldsymbol{\mathcal{V}}'}{}^{(rs)}\left[\boldsymbol{\tau}^{(n)}\right] e^{-2\pi i \boldsymbol{\tau}^{(n)}\cdot\boldsymbol{\omega}^{(m)}} \quad \& \quad \boldsymbol{S}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(m)}\right] = \boldsymbol{H}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(m)}\right]\boldsymbol{H}^{*}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(m)}\right]$$

    - $\boldsymbol{\omega}$ gathers the discrete frequencies
    - $\boldsymbol{\tau}$ gathers the discrete spatial locations
  - Generate a Gaussian random field $\boldsymbol{\mathcal{V}}'(\boldsymbol{x},\boldsymbol{\theta})$

$$\boldsymbol{\mathcal{V}}'^{(r)}(\boldsymbol{x},\boldsymbol{\theta}) = \sqrt{2\Delta\omega}\,\Re\left(\sum_{s}\sum_{\boldsymbol{m}} \boldsymbol{H}^{(\boldsymbol{rs})}_{\boldsymbol{\mathcal{V}}'}\left[\boldsymbol{\omega}^{(\boldsymbol{m})}\right]\eta^{(s,\boldsymbol{m})}\, e^{2\pi i\left(\boldsymbol{x}\cdot\boldsymbol{\omega}^{(\boldsymbol{m})}+\boldsymbol{\theta}^{(s,m)}\right)}\right)$$

    - $\boldsymbol{\eta}$ and $\boldsymbol{\theta}$ are independent random variables
  - Quid if a non-Gaussian distribution is sought?

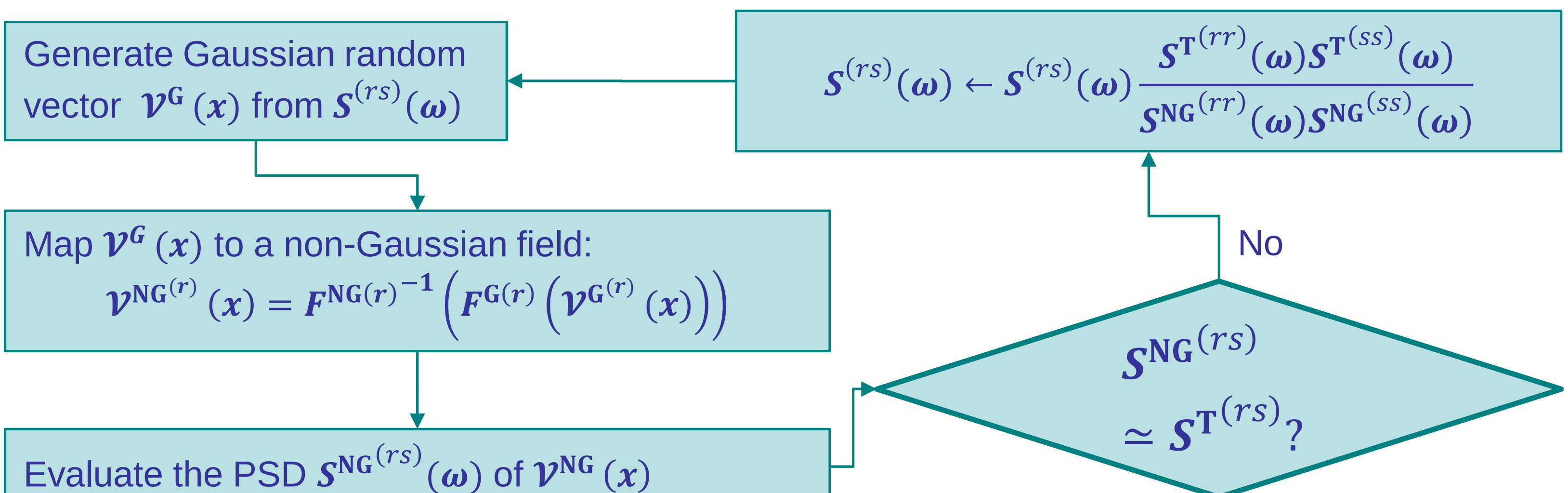
Shinozuka, M., Deodatis, G., 1988

The meso-scale random field

- Stochastic model of the meso-scale random field: non-Gaussian mapping*
  - Start from micro-sampling of the stochastic homogenization
    - The continuous form of the targeted PSD function

$$\boldsymbol{S}^{\mathrm{T}^{(rs)}}(\boldsymbol{\omega}) = \boldsymbol{\Delta\tau} \boldsymbol{S}_{\mathcal{V}'}^{(rs)}\left[\boldsymbol{\omega}^{(m)}\right] = \boldsymbol{\Delta\tau} \sum_{n} \widetilde{R}_{\mathcal{V}'}^{\mathrm{P}^{(rs)}}\left[\boldsymbol{\tau}^{(n)}\right] e^{-2\pi i \boldsymbol{\tau}^{(n)} \cdot \boldsymbol{\omega}^{(m)}}$$

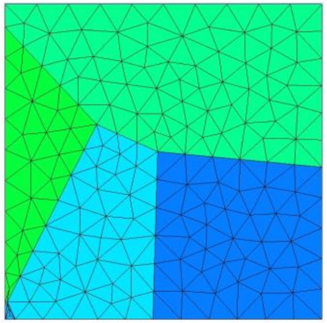
    - The targeted marginal distribution density function $\boldsymbol{F}^{\mathrm{NG}(r)}$ of the random variable $\mathcal{V}'^{(r)}$
    - A marginal Gaussian distribution $\boldsymbol{F}^{G(r)}$ of zero-mean and targeted variance $\boldsymbol{\sigma}_{\mathcal{V}'^{(r)}}$
  - Iterate

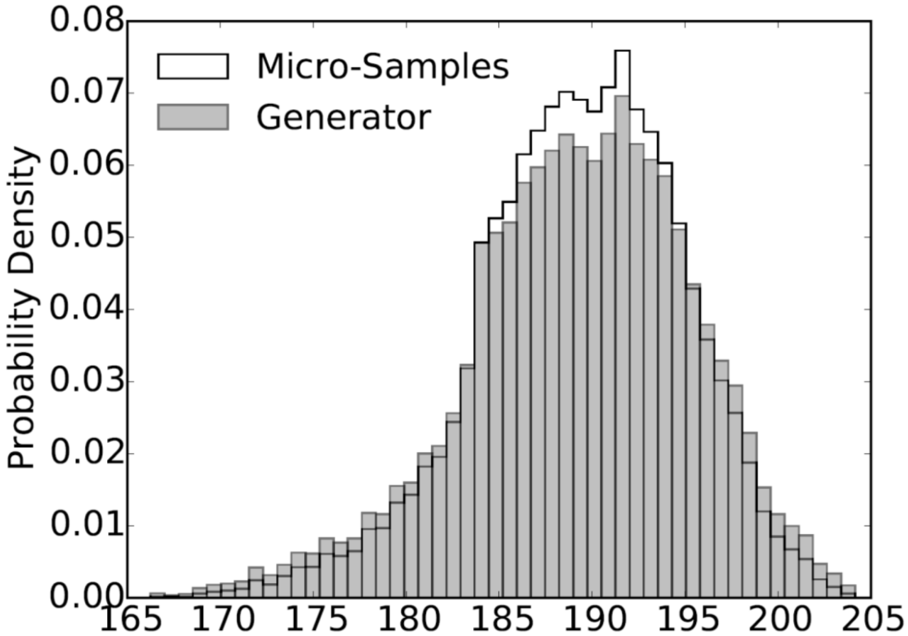


*"*Deodatis, G., Micaletti, R., 2001*

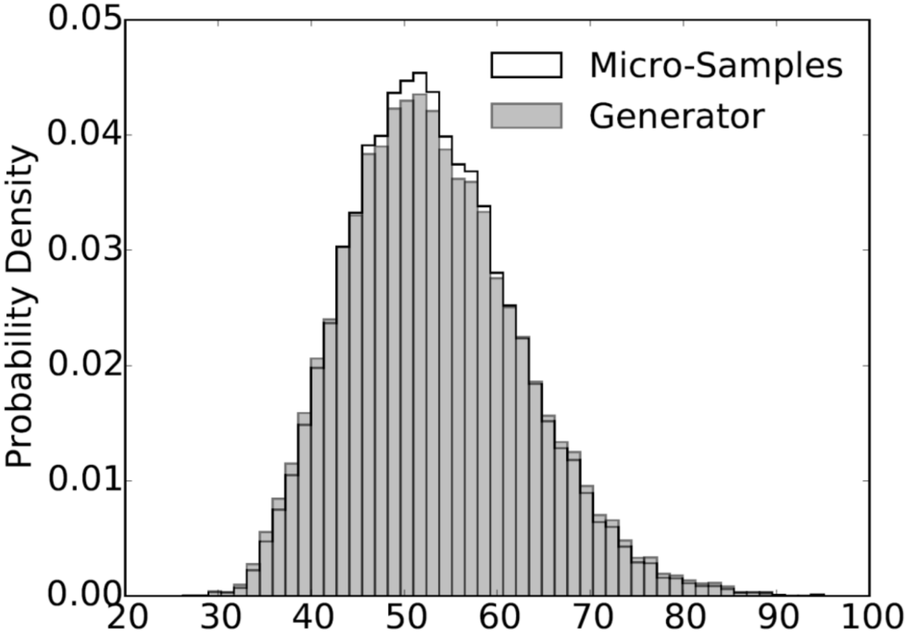
The meso-scale random field

- Polysilicon film deposited at 610 ºC
  - SVE size of 0.5 x 0.5 $\mu\mathrm{m}^2$
  - Comparison between micro-samples and generated field PDF





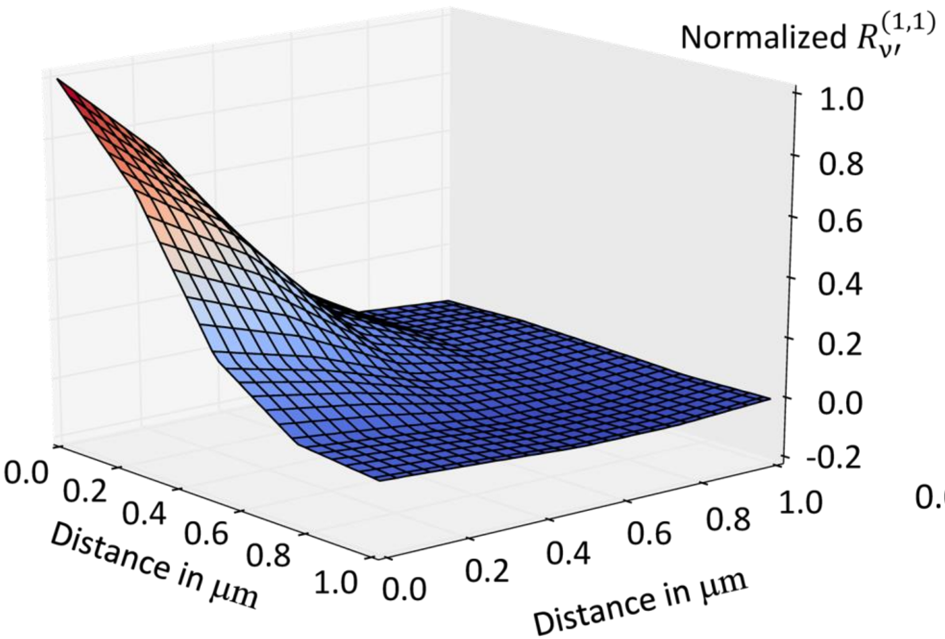
$\boldsymbol{C}_{\mathrm{M}_{11}}$ [GPa]



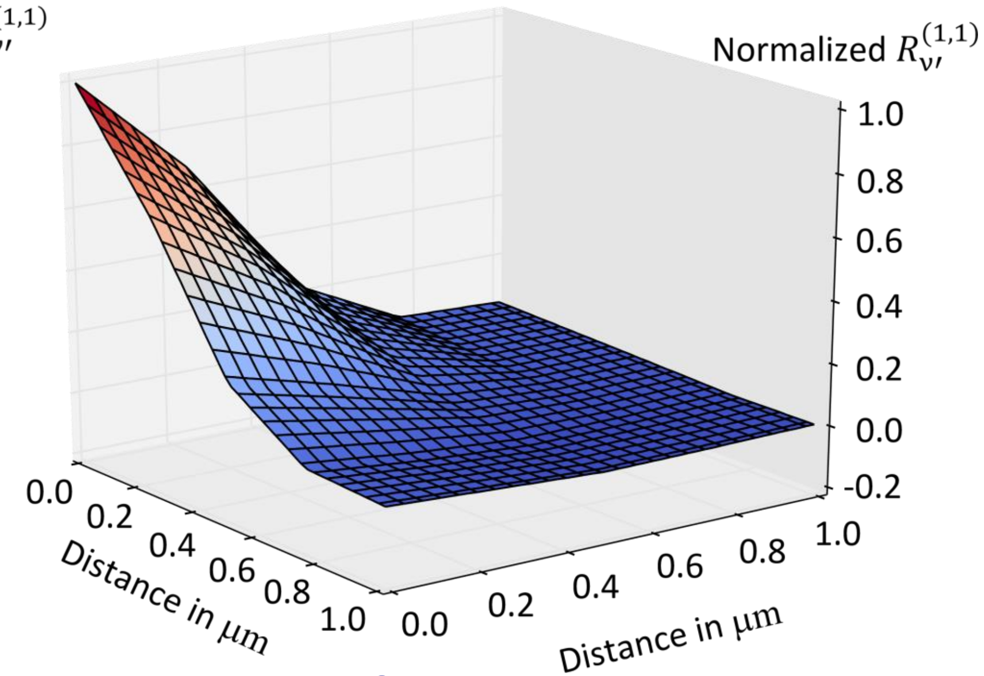
$\kappa_{\mathrm{M}_{33}}$ $[\mathrm{W}/(\mathrm{m}\cdot K)]$

The meso-scale random field

- Polysilicon film deposited at 610 ºC (2)
  - Comparison between micro-samples and generated field cross-correlations



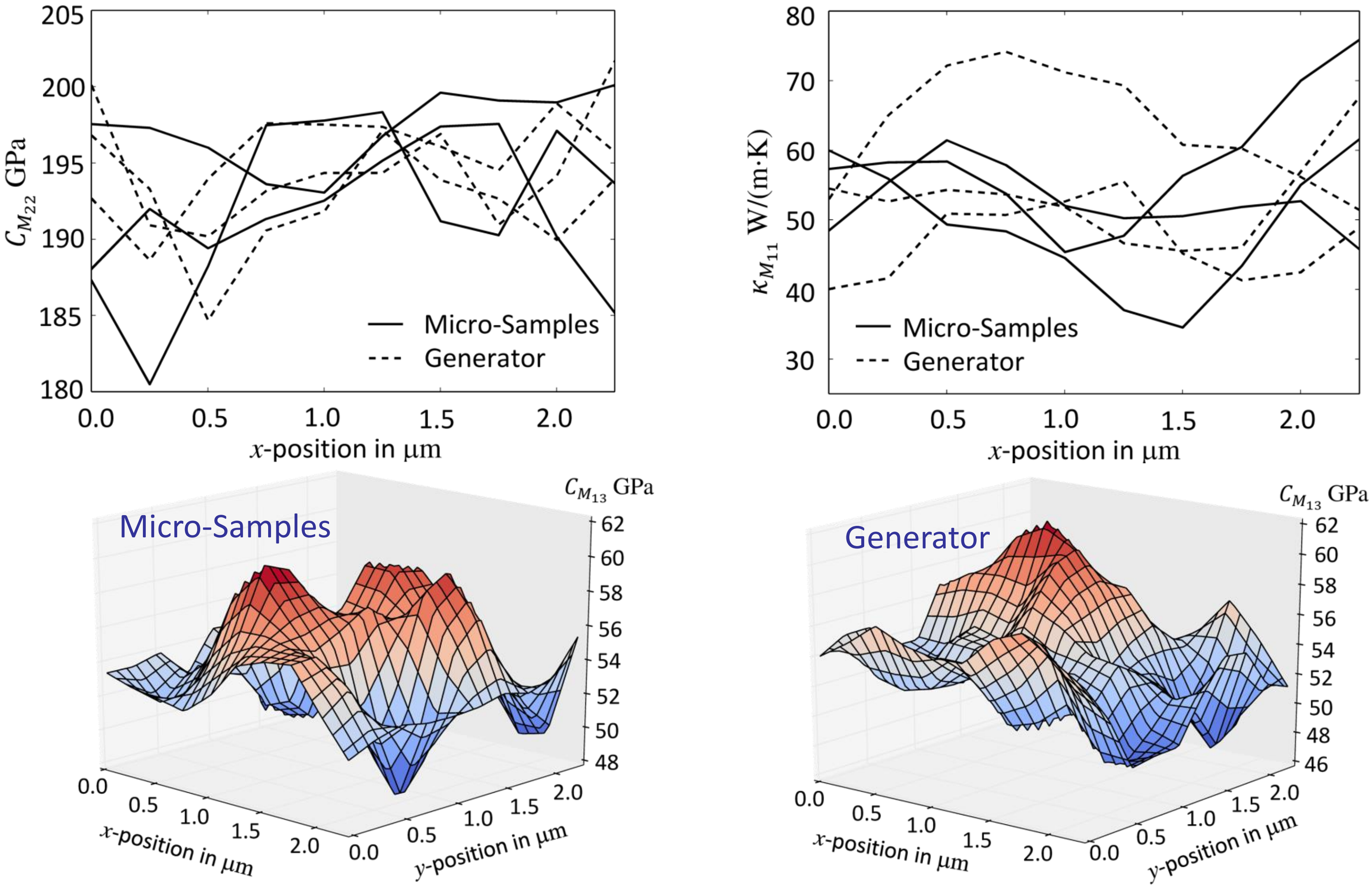
Micro-Samples



Generator

The meso-scale random field

- Polysilicon film deposited at 610 ºC (3)
  - Comparison between micro-samples and generated random field realizations



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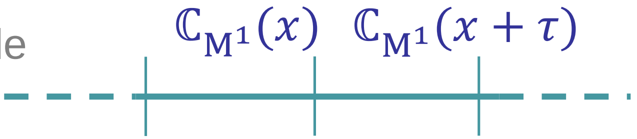
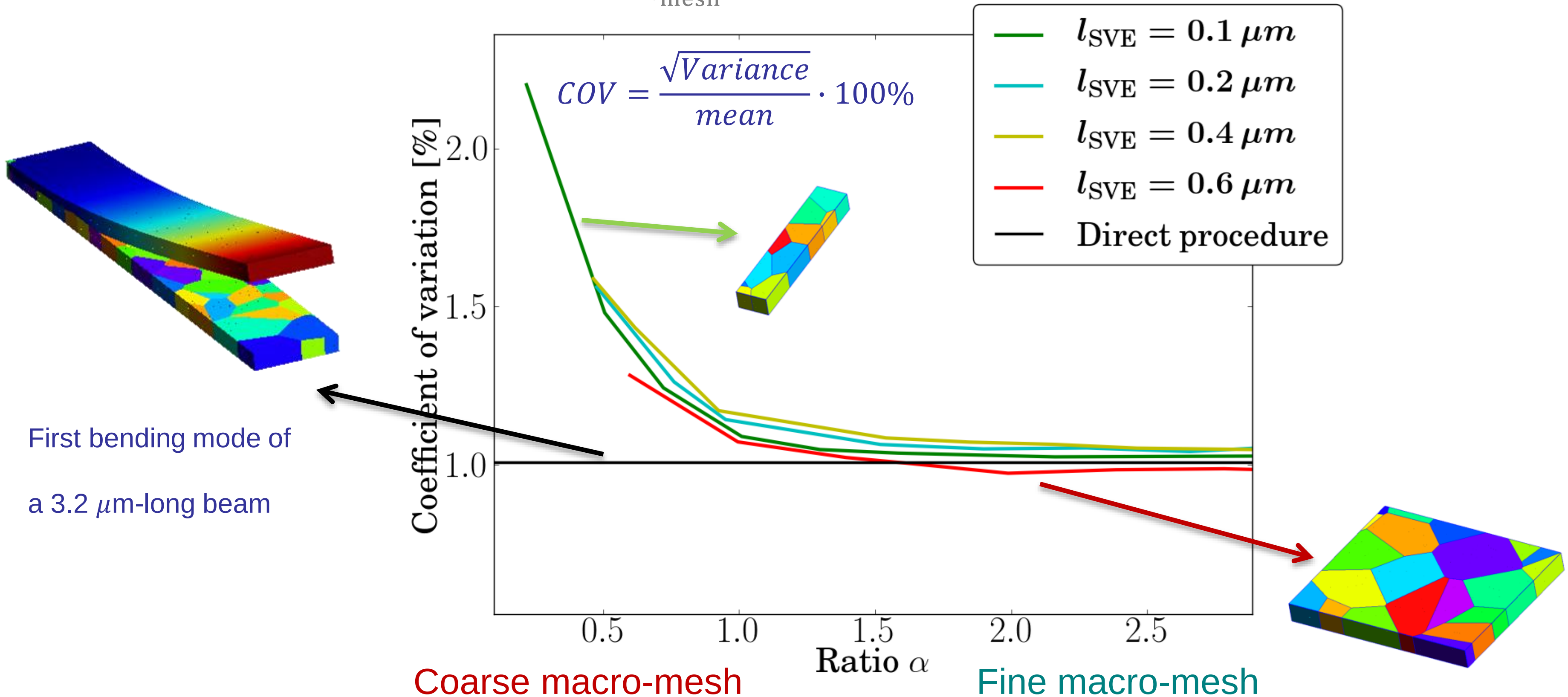
- 3-Scale approach verification with direct Monte-Carlo simulations
  - Use of the meso-scale random field

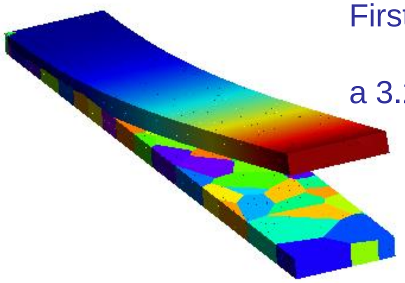
    → Monte-Carlo simulations at the macro-scale
  - Macro-scale beam elements of size l_{mesh}
  - Convergence in terms of $\alpha = \frac{l_{E_x}}{l_{\text{mesh}}}$





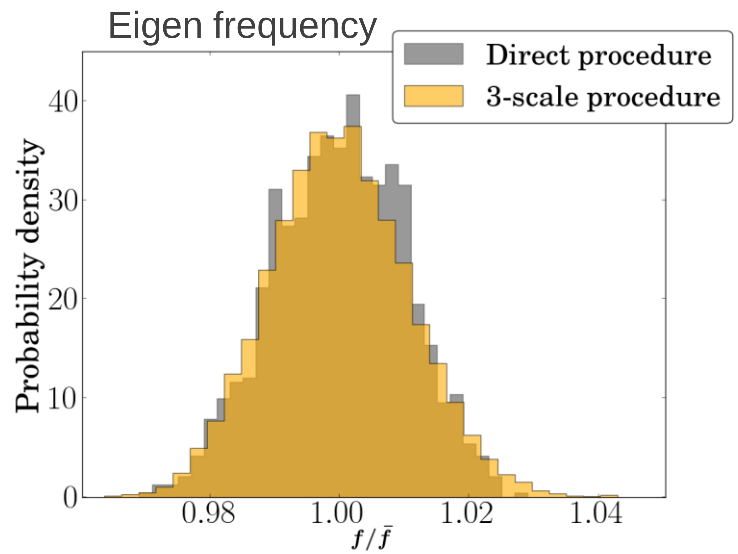
From the meso-scale to the macro-scale

- 3-Scale approach verification ($\alpha \sim 2$) with direct Monte-Carlo simulations
  - First bending mode

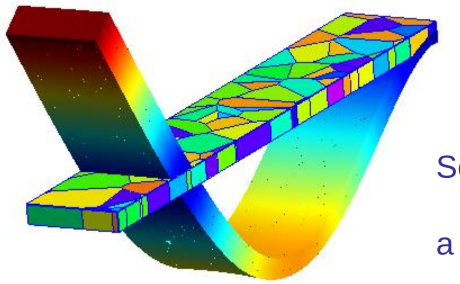


First bending mode of

a 3.2 μm-long beam



  - Second bending mode



Second bending mode of

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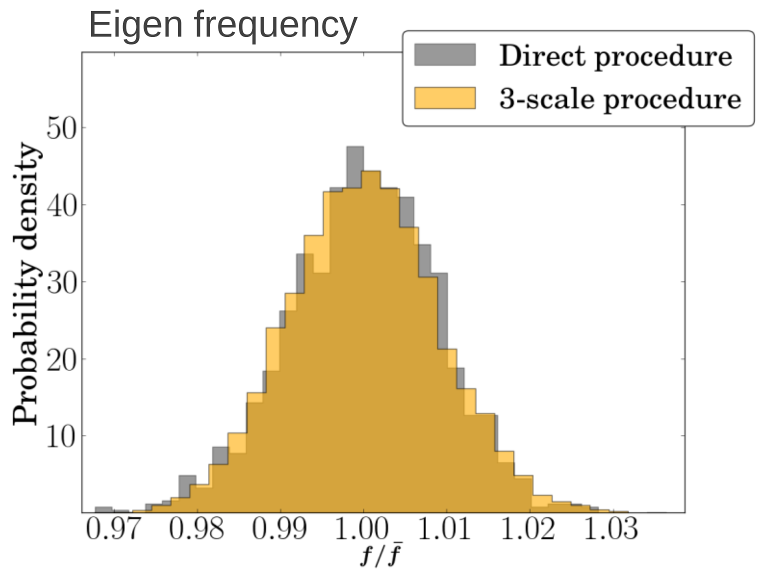
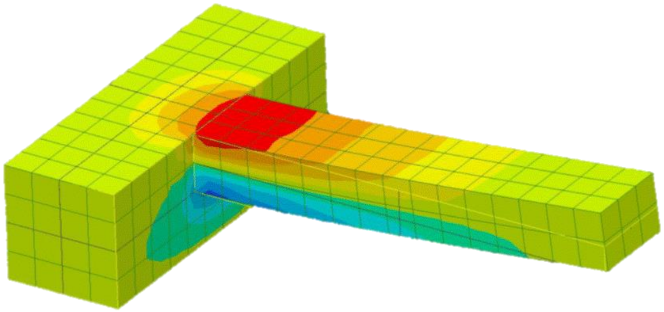


- Quality factor
  - Micro-resonators
    - Temperature changes with compression/traction
    - Energy dissipation



  - Eigen values problem
    - Governing equations

$$\begin{bmatrix}\mathbf{M} & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\ddot{\mathbf{u}}\\ \ddot{\boldsymbol{\vartheta}}\end{bmatrix}+\begin{bmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{D}_{\mathrm{u}\vartheta}(\boldsymbol{\theta}) & \mathbf{D}_{\vartheta\vartheta}\end{bmatrix}\begin{bmatrix}\dot{\mathbf{u}}\\ \dot{\boldsymbol{\vartheta}}\end{bmatrix}+\begin{bmatrix}\mathbf{K}_{\mathrm{uu}}(\boldsymbol{\theta}) & \mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\theta})\\ \mathbf{0} & \mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\theta})\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \boldsymbol{\vartheta}\end{bmatrix}=\begin{bmatrix}\boldsymbol{F}_{\mathrm{u}}\\ \boldsymbol{F}_{\vartheta}\end{bmatrix}$$

    - Free vibrating problem

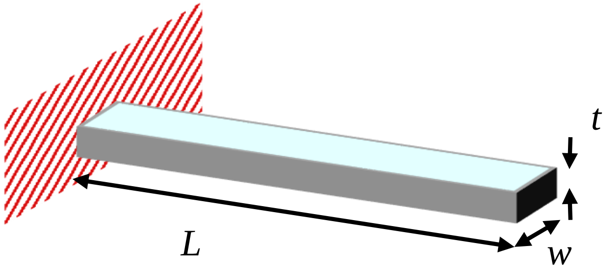
$$\begin{bmatrix}\mathbf{u}(t)\\ \boldsymbol{\vartheta}(t)\end{bmatrix}=\begin{bmatrix}\mathbf{u}_0\\ \boldsymbol{\vartheta}_0\end{bmatrix}e^{i\omega t}$$

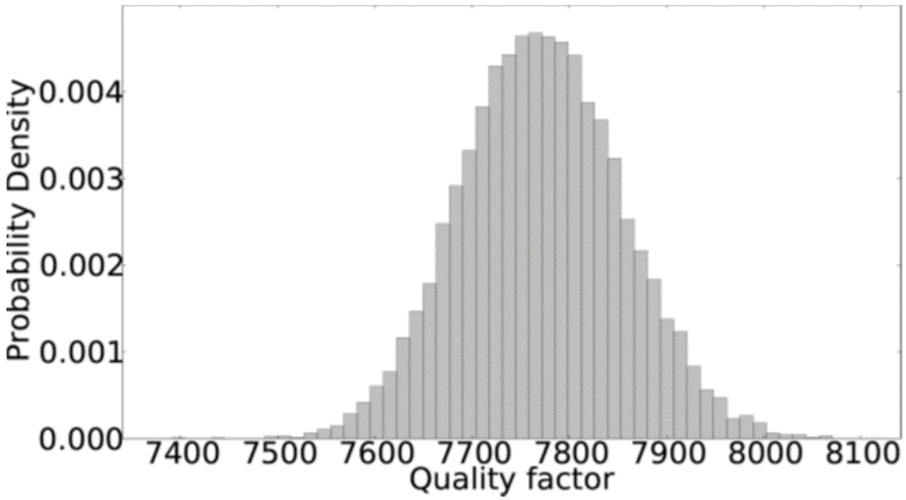
$$\begin{bmatrix}-\mathbf{K}_{\mathrm{uu}}(\boldsymbol{\theta}) & -\mathbf{K}_{\mathrm{u}\vartheta}(\boldsymbol{\theta}) & \mathbf{0}\\ \mathbf{0} & -\mathbf{K}_{\vartheta\vartheta}(\boldsymbol{\theta}) & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{I}\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \boldsymbol{\vartheta}\\ \dot{\mathbf{u}}\end{bmatrix}=i\omega\begin{bmatrix}\mathbf{0} & \mathbf{0} & \mathbf{M}\\ \mathbf{D}_{\vartheta\mathrm{u}}(\boldsymbol{\theta}) & \mathbf{D}_{\vartheta\vartheta} & \mathbf{0}\\ \mathbf{I} & \mathbf{0} & \mathbf{0}\end{bmatrix}\begin{bmatrix}\mathbf{u}\\ \boldsymbol{\vartheta}\\ \dot{\mathbf{u}}\end{bmatrix}$$

  - Quality factor
    - From the dissipated energy per cycle
    - $Q^{-1}=\dfrac{2|\Im\omega\ |}{\sqrt{(\Im\omega)^2+(\Re\omega)^2}}$

From the meso-scale to the macro-scale

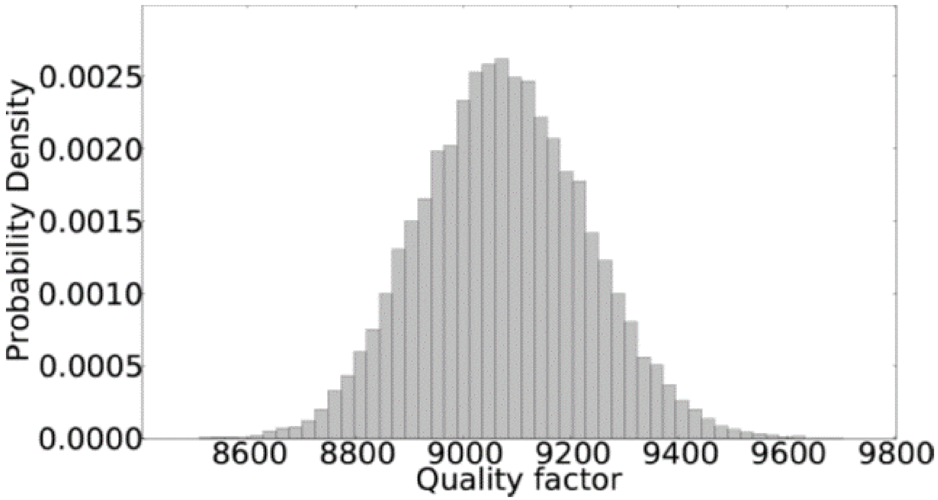
- Application of the 3-Scale method to extract the quality factor distribution
  - Perfectly clamped micro-resonator
    - Different sizes easily considered
  - Meso-scale random fields
    - From stochastic homogenization
    - Generated for different deposition temperatures
  - Effect of the deposition temperature





15 x 3 x 2 μm^3-beam,

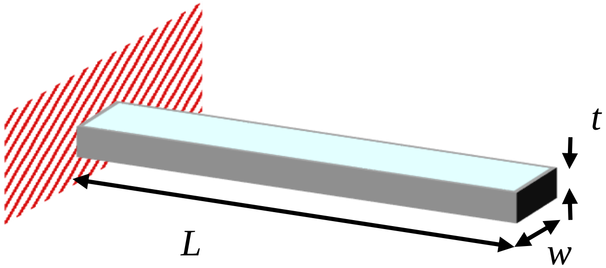
deposited at 610 ºC

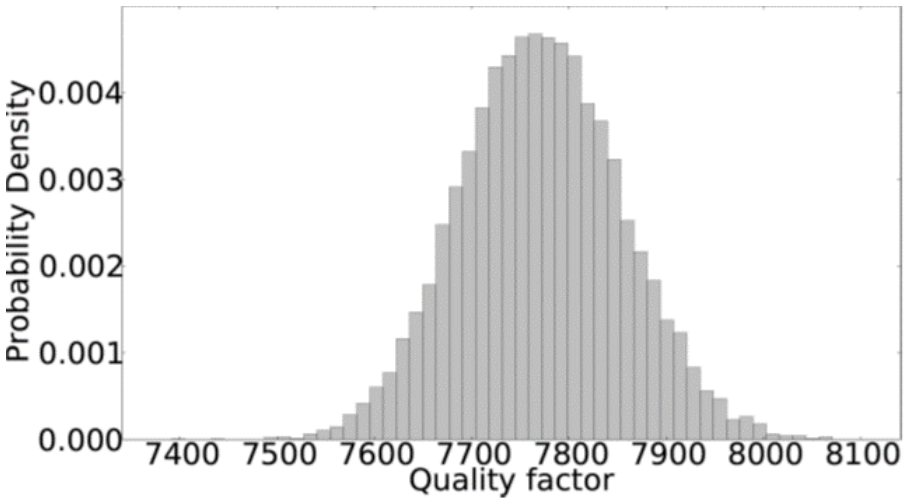


15 x 3 x 2 μm^3-beam,

deposited at 630 ºC

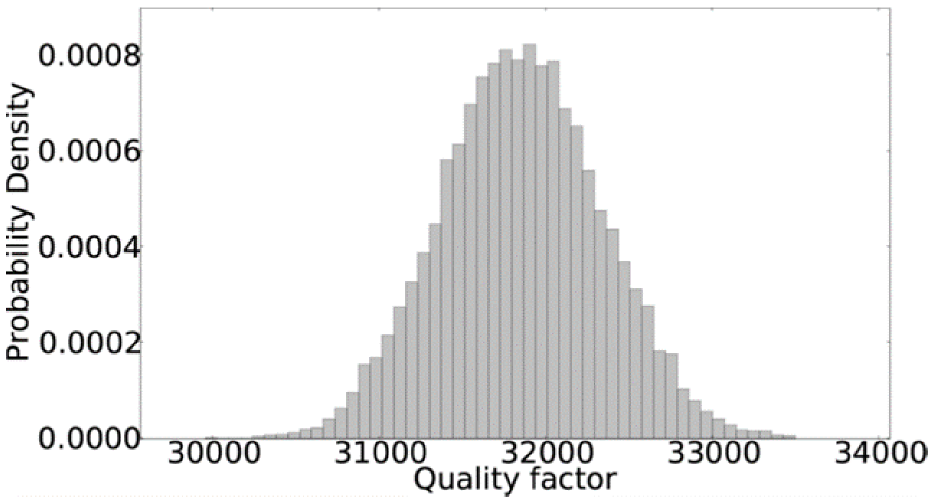
- Application of the 3-Scale method to extract the quality factor distribution (2)
  - Perfectly clamped micro-resonator
  - Effect of the geometry





15 x 3 x 2 μm^3-beam,

deposited at 610 ºC

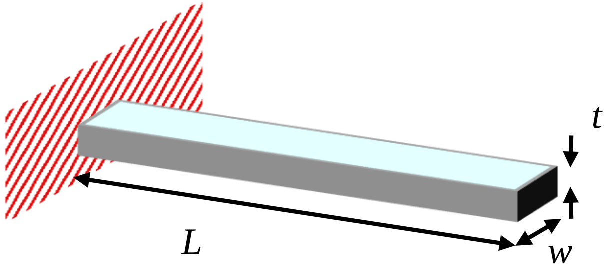


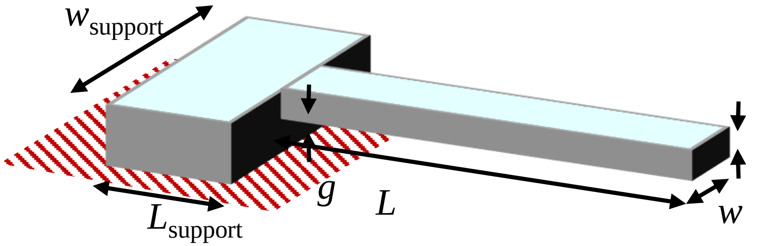
15 x 3 x 1 μm^3-beam,

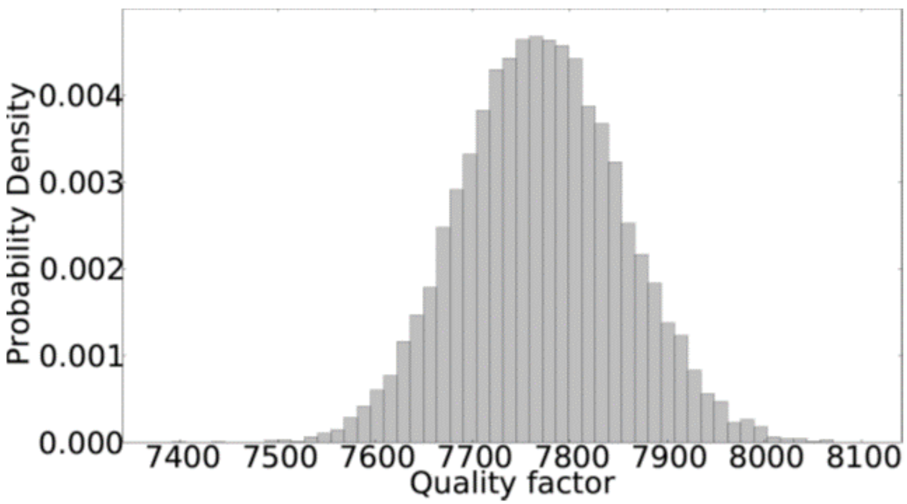
deposited at 610 ºC

From the meso-scale to the macro-scale

- Application of the 3-Scale method to extract the quality factor distribution (3)
  - 3D models readily available
  - The effect of the anchor can be studied

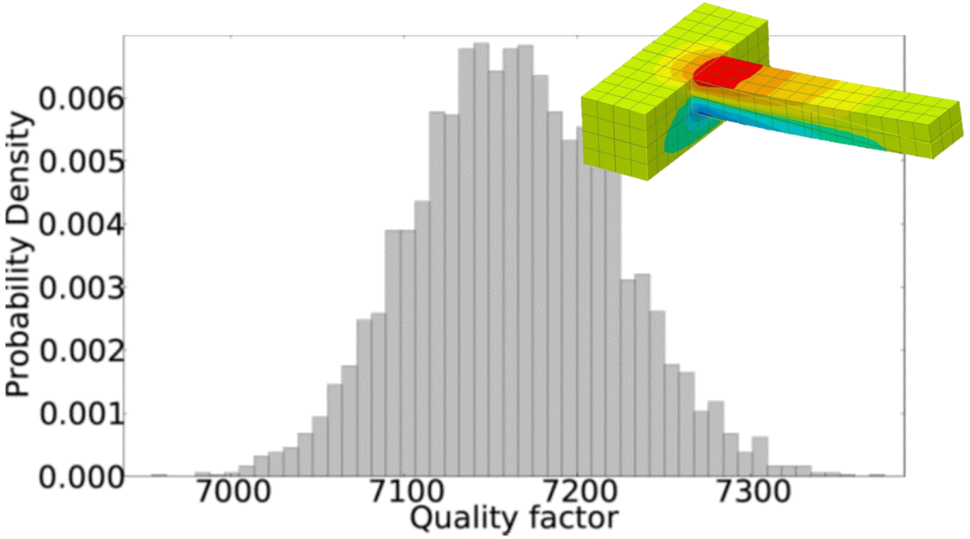






15 x 3 x 2 μm^3-beam,

deposited at 610 ºC



15 x 3 x 2 μm^3-beam & anchor,

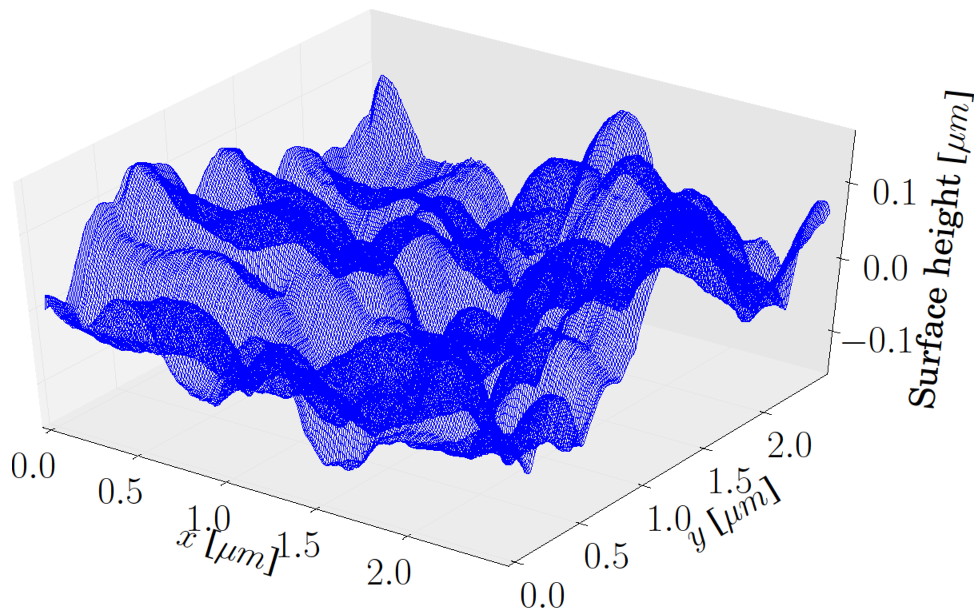
deposited at 610 ºC

Content

- Thermo-mechanical problems
  - Governing equations
  - Macro-scale stochastic finite element
  - Meso-scale volume elements
- From the micro-scale to the meso-scale
  - Thermo-mechanical homogenization
  - Definition of Stochastic Volume Elements (SVEs) & Stochastic homogenization
  - Need for a meso-scale random field
- The meso-scale random field
  - Definition of the thermo-mechanical meso-scale random field
  - Stochastic model of the random field: Spectral generator & non-Gaussian mapping
- From the meso-scale to the macro-scale
  - 3-Scale approach verification
  - Application to extract the quality factor
- Extension to stochastic-plate finite elements
  - Second-order stochastic homogenization
  - Rough Stochastic Volume Elements
  - Topology uncertainties effects

Extension to stochastic-plate finite elements

- How to account for the surface topology uncertainties?
  - Upper surface topology by AFM measurements on 2 µm-thick poly-silicon films



Temperature [ºC]	580	610	630	650
Std deviation [nm]	35.6	60.3	90.7	88.3

AFM data provided by IMT Bucharest, Rodica Voicu, Angela Baracu, Raluca Muller

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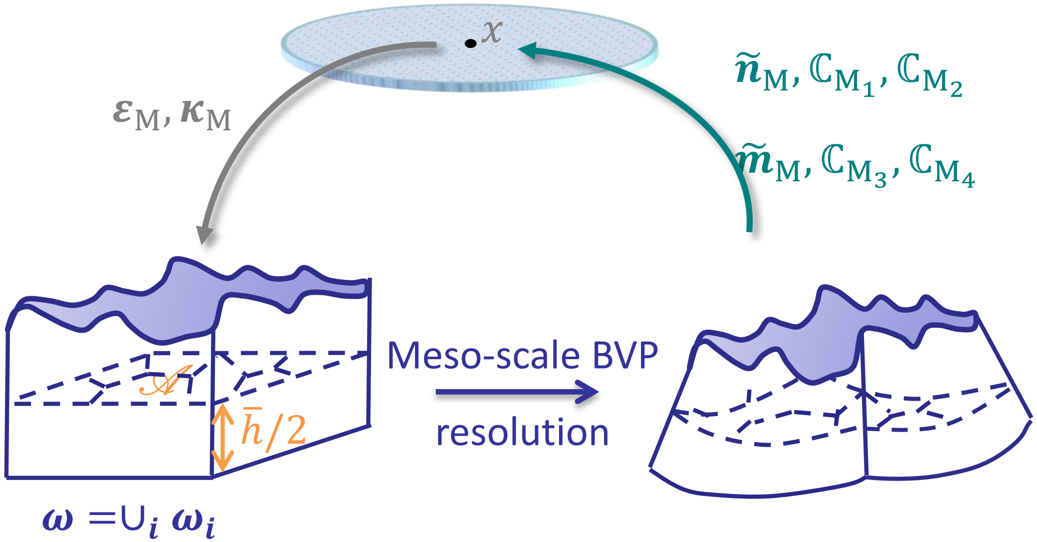
Stochastic multi-scale method for Kirchhoff-Love (KL) plates

- Macro-scale
  - Stochastic Kirchhoff-Love plates
- Meso-scale
  - Rough Stochastic Volume Elements (RSVEs)
  - Profiles from AFM
- Scale transition
  - Downscaling
    - In plane deformation $\boldsymbol{\varepsilon}_{\mathrm{M}}$
    - Curvature/torsion $\boldsymbol{\kappa}_{\mathrm{M}}$
  - Upscaling
    - In-plane stress per unit length $\tilde{\boldsymbol{n}}_{\mathrm{M}}$
    - Bending moment/torque per unit length $\tilde{\boldsymbol{m}}_{\mathrm{M}}$
- Micro-scale
  - Grain size/orientation distributions
  - From SEM/XRD measurements



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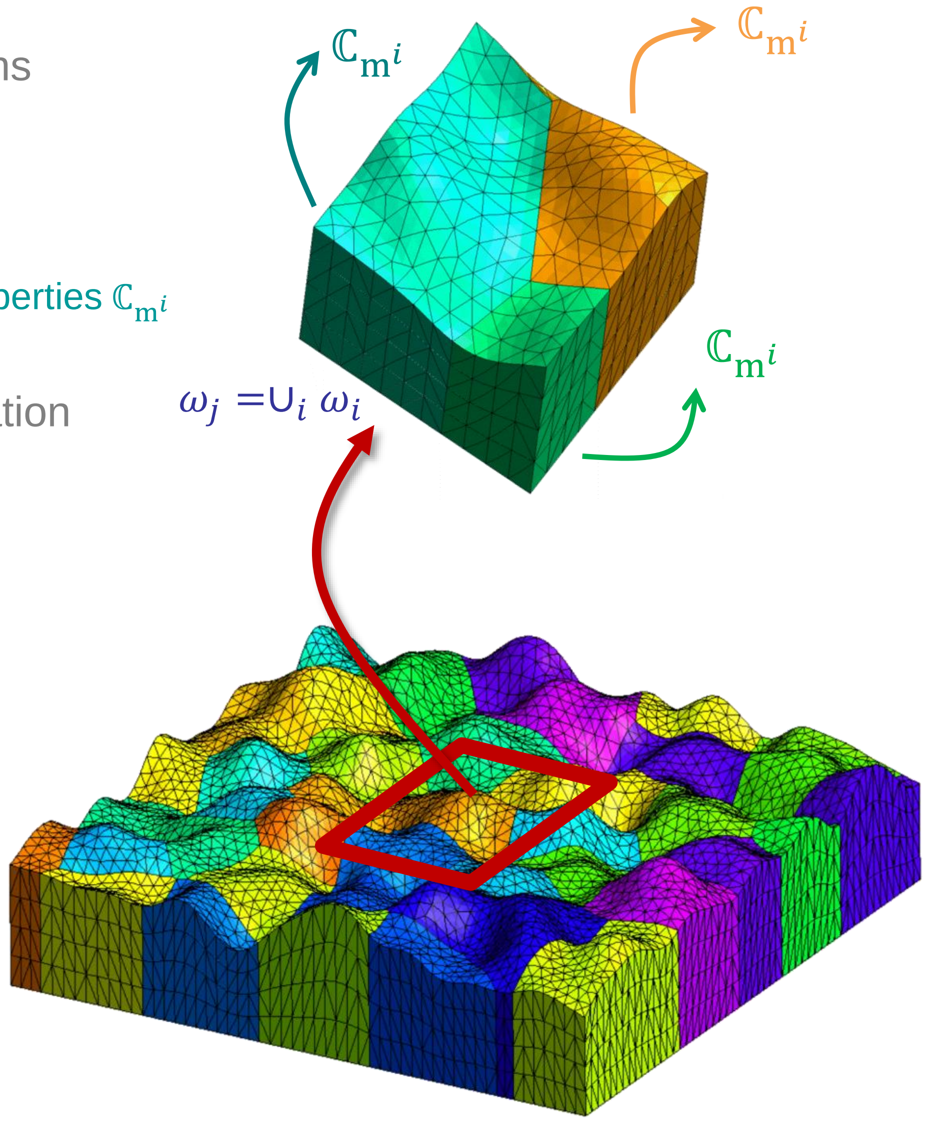
Stochastic multi-scale method for Kirchhoff-Love (KL) plates

- Rough Stochastic Volume Element
  - Poisson Voronoï tessellation realizations
    - From topology generator
    - Use of AFM measurements
  - Extraction of volume elements ω_j
    - Each grain ω_i is assigned material properties $\mathbb{C}_{\mathrm{m}^i}$
    - Defined from silicon crystal properties
  - Each $\mathbb{C}_{m^i}$ is assigned a random orientation
    - Uniformly distributed
    - Following XRD distributions
  - Governing equations
    - Classical continuum mechanics

$$\begin{cases} \nabla \cdot \boldsymbol{\sigma}_{\mathbf{m}} = 0 \\ \boldsymbol{\varepsilon}_{\mathrm{m}_{ij}} = \dfrac{\boldsymbol{u}_{\mathrm{m}_{i,j}} + \boldsymbol{u}_{\mathrm{m}_{i,j}}}{2} \end{cases}$$

    - Anisotropic grains

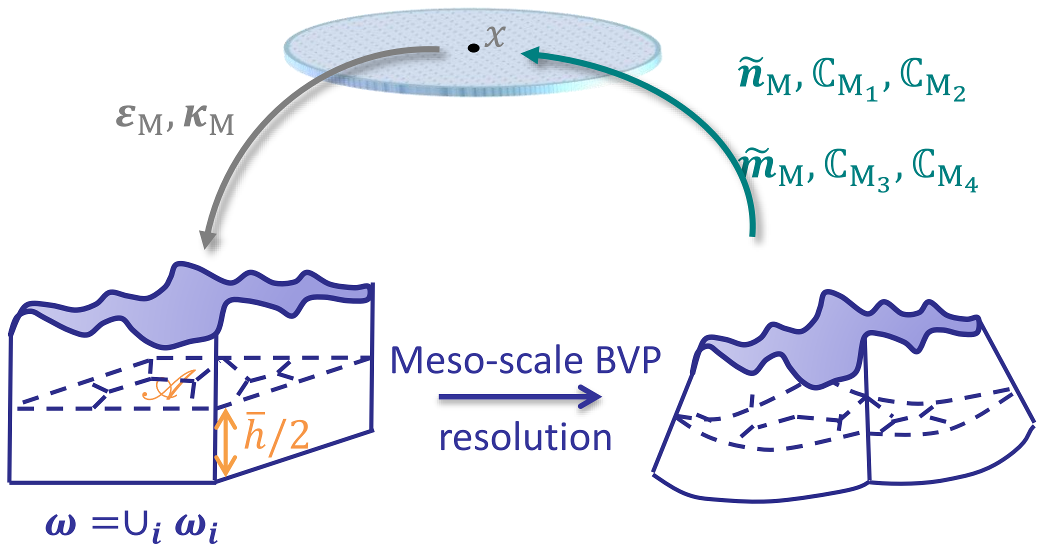
$$\boldsymbol{\sigma}_{\mathrm{m}}^{\boldsymbol{i}} = \mathbb{C}_{\mathrm{m}^i} : \boldsymbol{\varepsilon}_{\mathrm{m}}^{i}$$



Stochastic multi-scale method for Kirchhoff-Love (KL) plates

- Second-order homogenization
  - Upscaling

$$
\begin{cases}
\tilde{\boldsymbol{n}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_1} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_2} : \boldsymbol{\kappa}_{\mathrm{M}} \\
\tilde{\boldsymbol{m}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_3} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_4} : \boldsymbol{\kappa}_{\mathrm{M}}
\end{cases}
$$



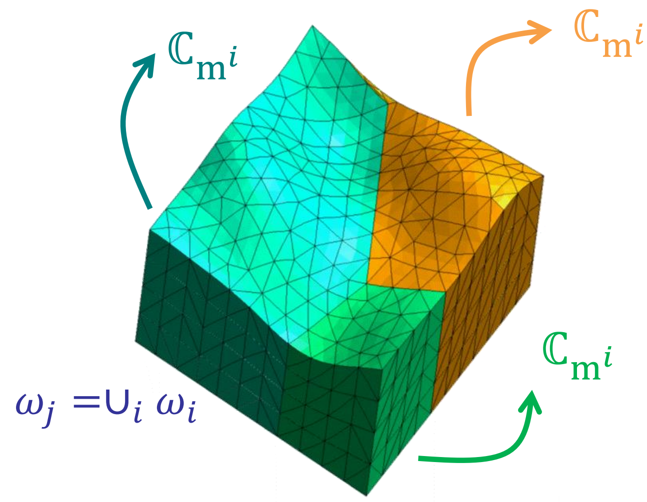
- Stochastic homogenization
  - Several SVE realizations
  - For each SVE $\omega_j = \cup_i \omega_i$

$\mathbb{C}_{\mathrm{m}^i}\ \forall i \longrightarrow \mathbb{C}_{\mathrm{M}_1^j}, \mathbb{C}_{\mathrm{M}_2^j}, \mathbb{C}_{\mathrm{M}_3^j}, \mathbb{C}_{\mathrm{M}_4^j}$

Computational homogenization

Samples of the meso-scale homogenized elasticity tensors

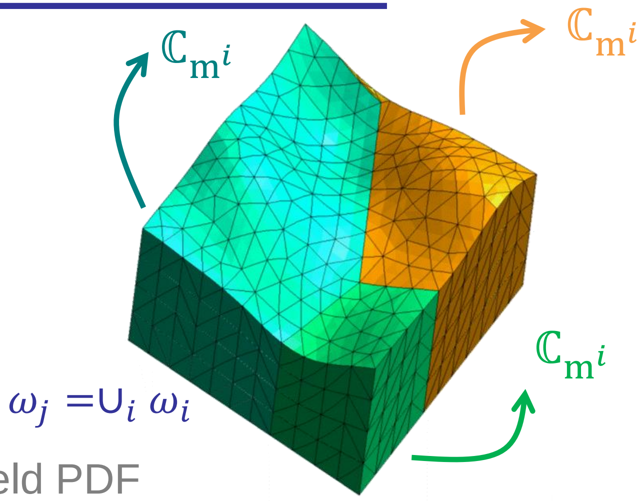
$\bar{\boldsymbol{\rho}}_{\mathrm{M}^j}$

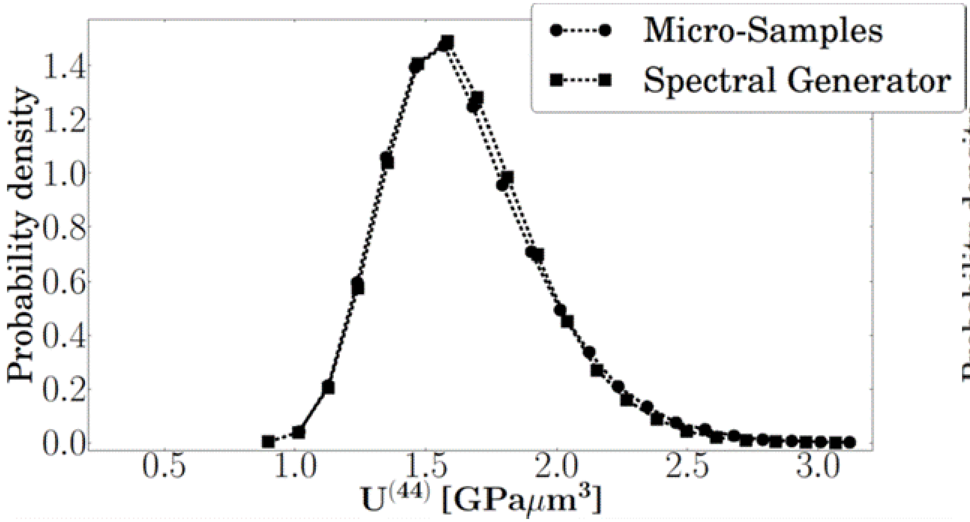


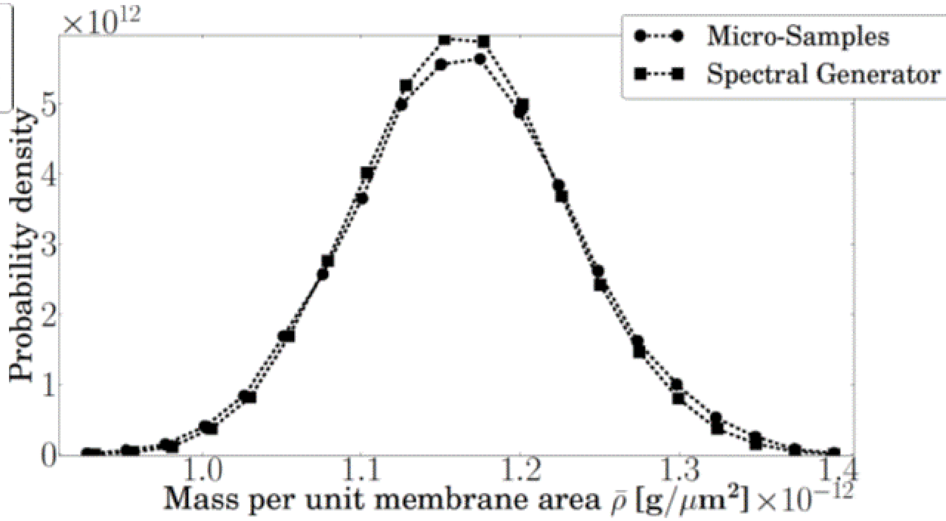
  - The density per unit area is now non-constant

The meso-scale random field

- Generator of meso-scale random fields
  - Spectral generator &
  - Non-Gaussian mapping
- Polysilicon film deposited at 610 ºC
  - SVE size of 0.5 x 0.5 x 0.5 μm^3
  - Comparison between micro-samples and generated field PDF

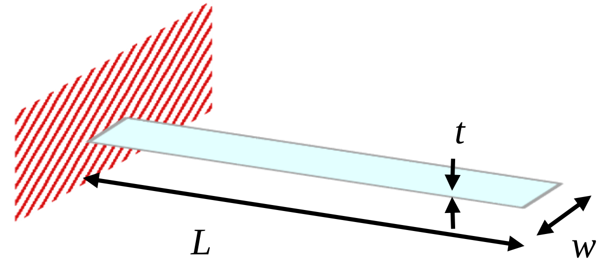


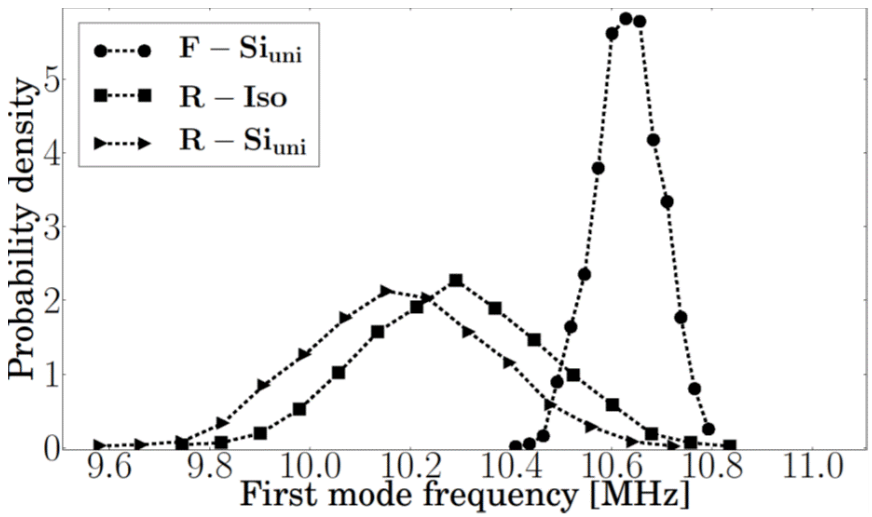


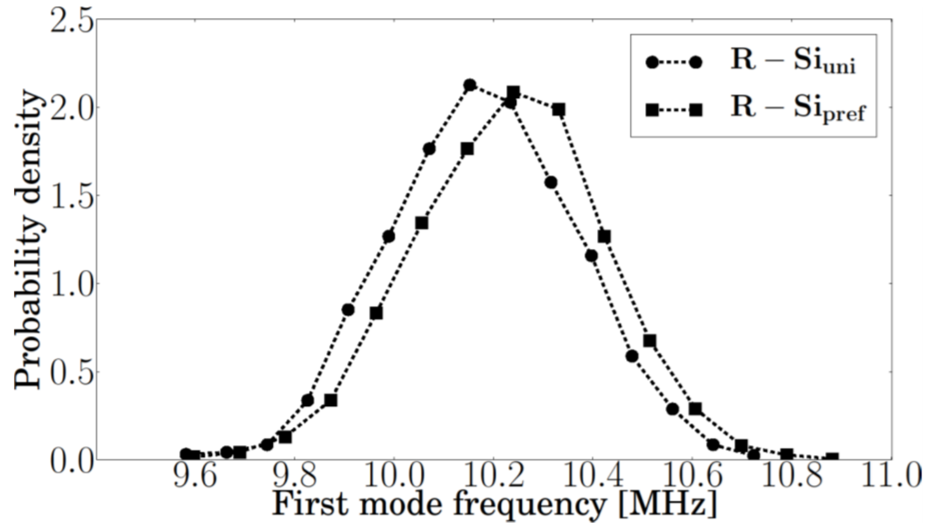


Topology uncertainties effects

- Polysilicon film deposited at 610 ºC
  - Cantilever of 8 x 3 x 0.5 μm^3
  - SVE size of 0.5 x 0.5 x 0.5 μm^3





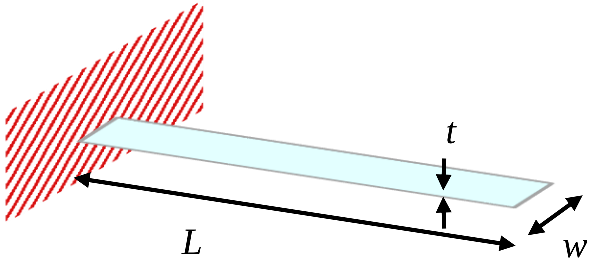


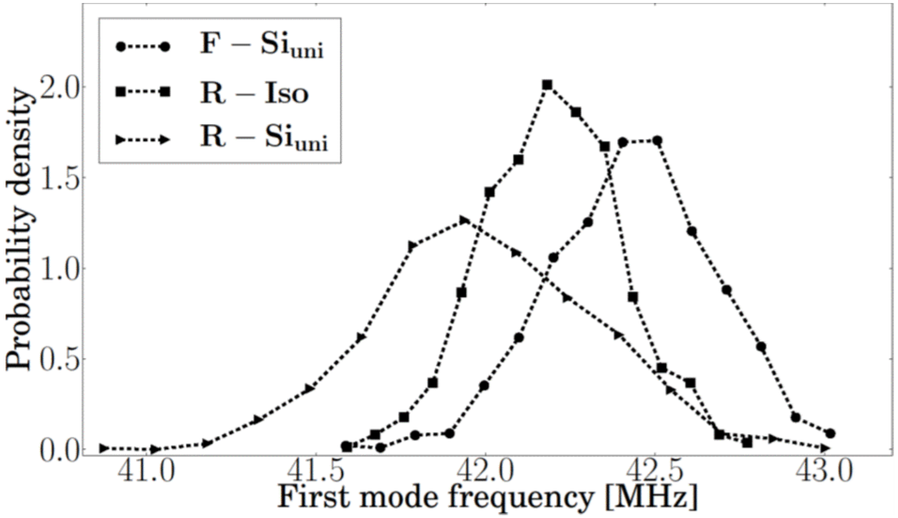
Roughness effect is the most important for 8 x 3 x 0.5 μm^3 cantilevers

Grain orientation distribution effect for 8 x 3 x 0.5 μm^3 cantilevers

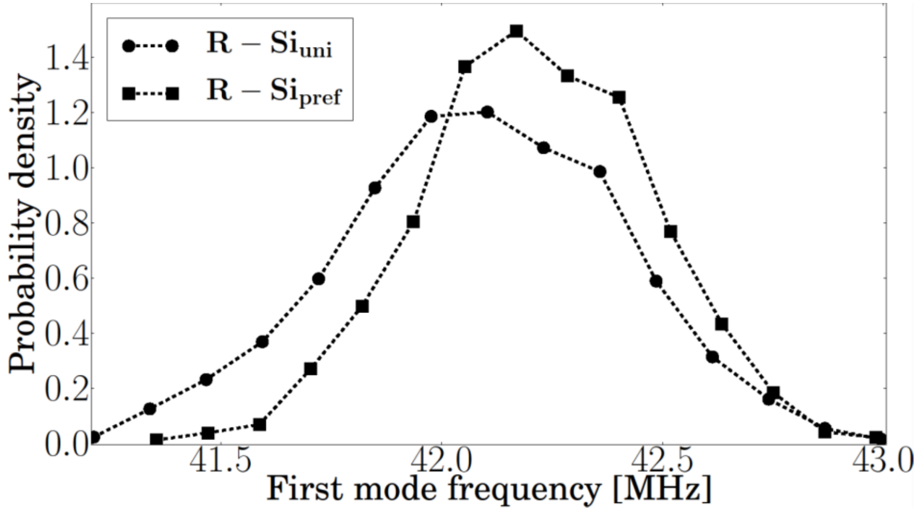
- Flat SVEs (no roughness) - F
- Rough SVEs (Polysilicon film deposited at 610 ºC) - R
- Grain orientation following XRD measurements – Si_{pref}
- Grain orientation uniformly distributed – Si_{uni}
- Reference isotropic material – Iso

- Polysilicon film deposited at 610 ºC
  - Cantilever of 8 x 3 x 2 μm^3
  - SVE size of 0.5 x 0.5 x 2 μm^3





Roughness effect is of same importance as orientation for 8 x 3 x 2 μm^3 cantilevers



Grain orientation distribution effect for 8 x 3 x 2 μm^3 cantilevers

Conclusions & Perspectives

- Efficient stochastic multi-scale method
  - Micro-structure based on experimental measurements
  - Computational efficiency rely on the meso-scale random field generator
  - Used to study probabilistic behaviors

- Perspectives
  - Other material systems
  - Non-linear behaviors
  - Non-homogenous random fields

Thank you for your attention !

Extension to stochastic-plate finite elements

- Macro-scale Kirchhoff-Love plates
  - Displacement fields
    - Displacement $\boldsymbol{u}$ of Cosserat plane, and
    - Cross section direction $\boldsymbol{t}$ with

$$\Delta \boldsymbol{t}_{\alpha} = -\boldsymbol{u}_{z,\alpha}$$

  - Kinematics: in-plane strain and curvature

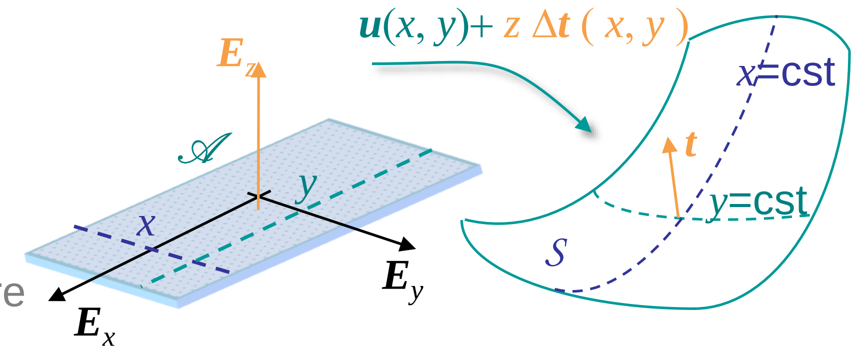
$$\begin{cases} \boldsymbol{\varepsilon}_{\mathrm{M}\alpha\beta} = \dfrac{\boldsymbol{u}_{\beta,\alpha} + \boldsymbol{u}_{\alpha,\beta}}{2} \\ \boldsymbol{\kappa}_{\mathrm{M}\alpha\beta} = \dfrac{\Delta\boldsymbol{t}_{\beta,\alpha} + \Delta\boldsymbol{t}_{\alpha,\beta}}{2} = -\boldsymbol{u}_{z,\alpha\beta} \end{cases}$$

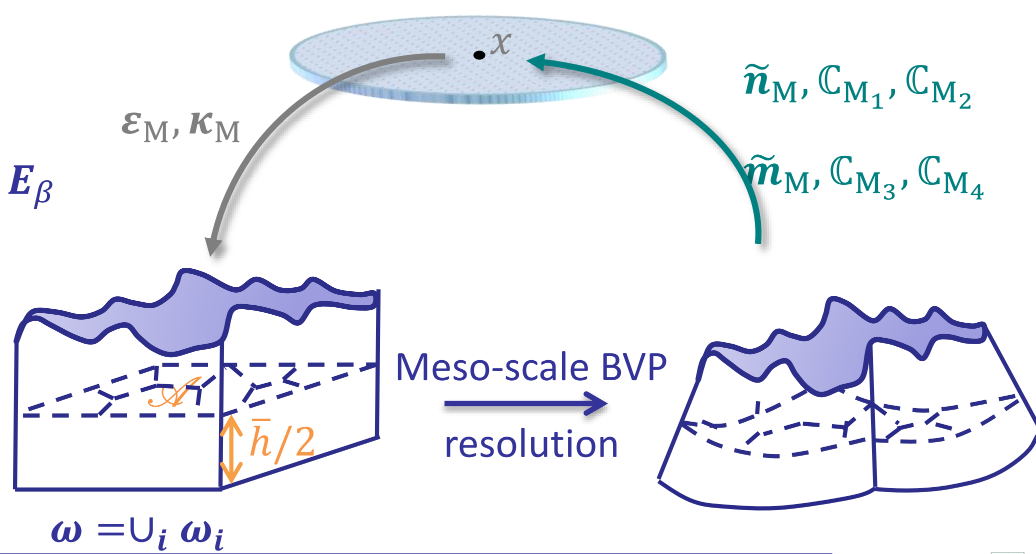
  - Resultant in-plane & bending stresses

$$\begin{cases} \boldsymbol{n}^{\alpha}_{\mathrm{M}} = \tilde{n}^{\alpha\beta}_{\mathrm{M}} \boldsymbol{E}_{\beta} = \displaystyle\int_{h} \boldsymbol{\sigma}^{\alpha\beta}_{\mathrm{M}} \, dz \, \boldsymbol{E}_{\beta} \\ \tilde{\boldsymbol{m}}^{\alpha}_{\mathrm{M}} = \tilde{m}^{\alpha\beta}_{\mathrm{M}} \boldsymbol{E}_{\beta} = \displaystyle\int_{h} \boldsymbol{\sigma}^{\alpha\beta}_{\mathrm{M}} \, z \, dz \, \boldsymbol{E}_{\beta} \end{cases}$$

  - Constitutive laws

$$\begin{cases} \tilde{\boldsymbol{n}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_1} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_2} : \boldsymbol{\kappa}_{\mathrm{M}} \\ \tilde{\boldsymbol{m}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_3} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_4} : \boldsymbol{\kappa}_{\mathrm{M}} \end{cases}$$

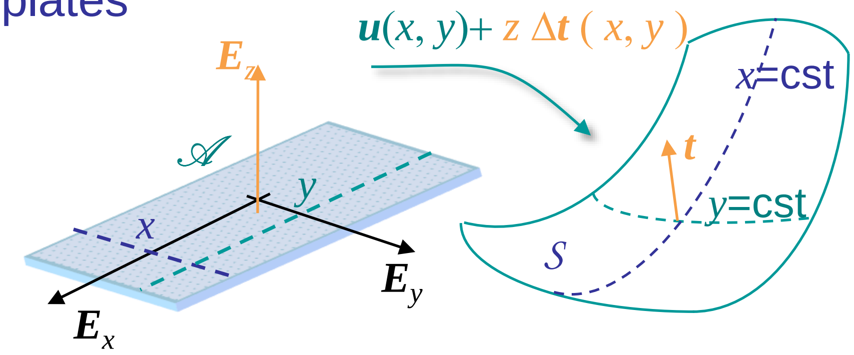




- Stochastic macro-scale Kirchhoff-Love plates
  - Strong form:

$$\begin{cases} \bar{\rho}_{\mathrm{M}} \ddot{\boldsymbol{u}} + (\boldsymbol{n}_{\mathrm{M}}^{\alpha})_{,\alpha} = 0 \\ I_{P_{\mathrm{M}}} \ddot{\boldsymbol{t}} + (-\lambda \boldsymbol{E}_z) + (\widetilde{\boldsymbol{m}}_{\mathrm{M}}^{\alpha})_{,\alpha} = 0 \end{cases}$$

with $\Delta \boldsymbol{t}_{\alpha} = -\boldsymbol{u}_{z,\alpha}$



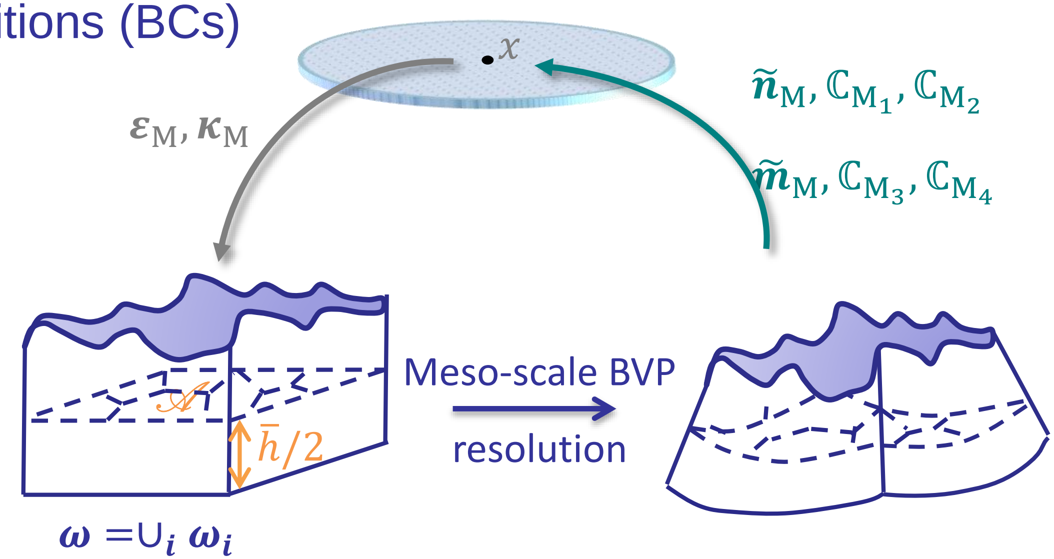
  - Constitutive equations & density per unit area from stochastic homogenization

$$\begin{cases} \widetilde{\boldsymbol{n}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_1}(\boldsymbol{x}, \boldsymbol{\theta}) : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_2}(\boldsymbol{x}, \boldsymbol{\theta}) : \boldsymbol{\kappa}_{\mathrm{M}} \\ \widetilde{\boldsymbol{m}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_3}(\boldsymbol{x}, \boldsymbol{\theta}) : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_4}(\boldsymbol{x}, \boldsymbol{\theta}) : \boldsymbol{\kappa}_{\mathrm{M}} \\ \bar{\boldsymbol{\rho}}_{\mathrm{M}}(\boldsymbol{x}, \boldsymbol{\theta}) \end{cases} \quad \text{with} \quad \begin{cases} \boldsymbol{\varepsilon}_{\mathrm{M}_{\alpha\beta}} = \dfrac{\boldsymbol{u}_{\beta,\alpha} + \boldsymbol{u}_{\alpha,\beta}}{2} \\ \boldsymbol{\kappa}_{\mathrm{M}_{\alpha\beta}} = \dfrac{\Delta \boldsymbol{t}_{\beta,\alpha} + \Delta \boldsymbol{t}_{\alpha,\beta}}{2} = -\boldsymbol{u}_{z,\alpha\beta} \end{cases}$$

  - Stochastic (Discontinuous Galerkin) finite elements

$$\rightarrow \quad \mathbf{M}(\boldsymbol{\theta})\ddot{\mathbf{u}} + \mathbf{K}_{\mathrm{uu}}(\boldsymbol{\theta})\mathbf{u} = \mathbf{F}$$

- Meso-scale BVP boundary conditions (BCs)
  - Downscaling



$$\begin{cases} \boldsymbol{\varepsilon}_{\mathrm{M}} = \dfrac{1}{V(\omega)} \displaystyle\int_{\omega} \boldsymbol{\varepsilon}_{\mathrm{m}} d\omega \\ \boldsymbol{\eta}_{\mathrm{M}} \text{ independant of BC} \end{cases}$$

  - Meso-scale BVP fluctuation field

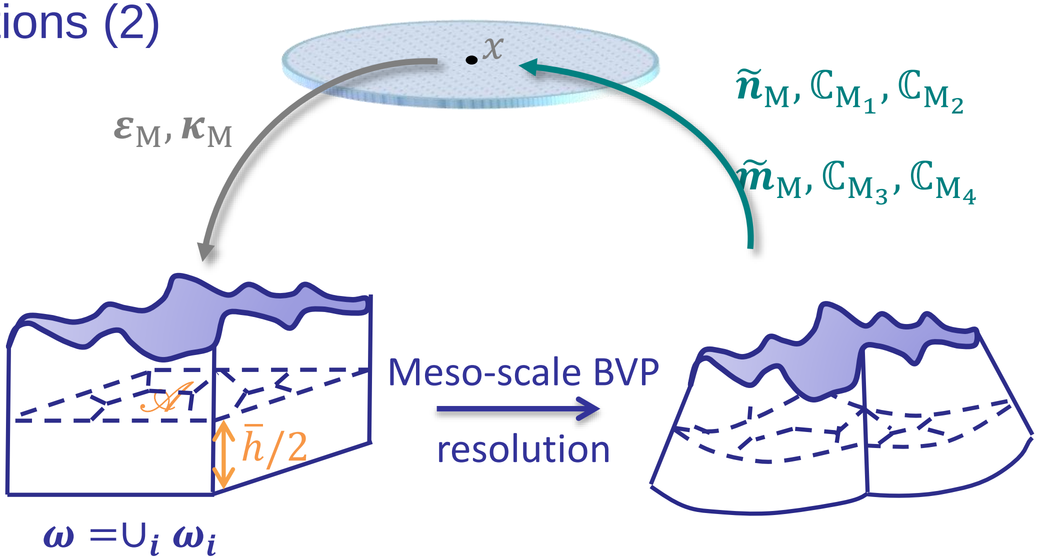
$$\boldsymbol{u}_{\mathrm{m}} = \boldsymbol{\epsilon}_{\mathrm{M}} \otimes \boldsymbol{x} + \frac{\mathbf{1}}{\mathbf{2}} \boldsymbol{\eta}_{\mathrm{M}} : (\boldsymbol{x} \otimes \boldsymbol{x}) + \boldsymbol{u}' \longrightarrow \begin{cases} 0 = \displaystyle\int_{\partial\omega} \boldsymbol{u}' \otimes \boldsymbol{n} \, d\partial\omega \\ 0 = \displaystyle\int_{\partial\omega} \boldsymbol{u}' \otimes \boldsymbol{n} \otimes \boldsymbol{x} \, d\partial\omega \end{cases}$$

$\longrightarrow$ {
Satisfied by periodic and kinematic boundary conditions
First equation satisfied by static boundary conditions

Second-order stochastic homogenization

- Meso-scale BVP boundary conditions (2)
  - Upscaling

$$\begin{cases} \boldsymbol{n}_{\mathrm{M}} = \frac{1}{S}\int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} d\omega \\ \boldsymbol{m}_{\mathrm{M}} = \frac{1}{S}\int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} \otimes \boldsymbol{x} \; d\omega \end{cases}$$



  - Consistency

$$\boldsymbol{n}_{\mathrm{M}}: \delta\boldsymbol{\varepsilon}_{\mathrm{M}} + \boldsymbol{m}_{\mathrm{M}}: \delta\boldsymbol{\eta}_{\mathrm{M}} = \frac{1}{S}\int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}}: \delta\boldsymbol{\varepsilon}_{\mathrm{m}} d\omega \longrightarrow 0 = \int_{\partial\omega} (\boldsymbol{\sigma}_{\mathrm{m}} \cdot \boldsymbol{n}) \cdot \boldsymbol{u}' \; d\partial\omega$$

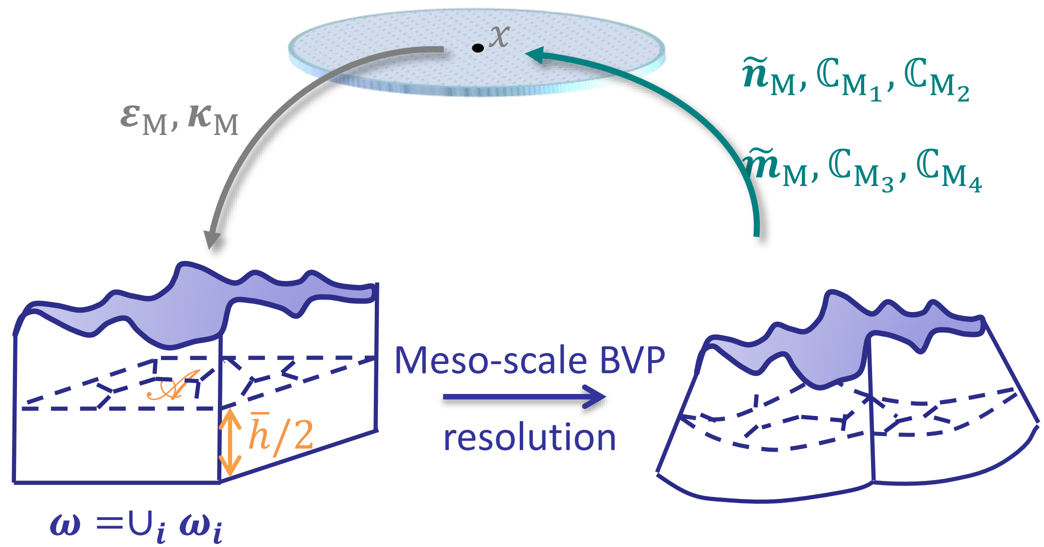
$\longrightarrow$ Satisfied by periodic, kinematic, static boundary conditions

  - Top and bottom surfaces
    - Stress free $\longrightarrow$ plane stress is naturally ensured
  - Side surfaces
    - Mixed boundary conditions

- Second-order homogenization
  - Downscaling

$$\begin{cases} \boldsymbol{\epsilon}_{\mathrm{M}} = \boldsymbol{u}_{\boldsymbol{M}} \otimes \boldsymbol{\nabla} \\ \qquad = \boldsymbol{\varepsilon}_{\mathrm{M}}^{\alpha\beta} \boldsymbol{E}_{\alpha} \otimes \boldsymbol{E}_{\beta} + \hat{\boldsymbol{\epsilon}}_{\mathrm{M}} \\ \boldsymbol{\eta}_{\mathrm{M}} = \boldsymbol{u}_{\boldsymbol{M}} \otimes \boldsymbol{\nabla} \otimes \boldsymbol{\nabla} \\ \qquad = \boldsymbol{\kappa}_{\mathrm{M}}^{\alpha\beta} \boldsymbol{E}_{\alpha} \otimes \boldsymbol{E}_{\beta} \otimes \boldsymbol{E}_{z} + \hat{\boldsymbol{\eta}}_{\mathrm{M}} \end{cases}$$

    - $\hat{\boldsymbol{\epsilon}}_{\mathrm{M}}$ & $\hat{\boldsymbol{\eta}}_{\mathrm{M}}$ undefined for KL plates



  - Upscaling

$$\begin{cases} \boldsymbol{n}_{\mathrm{M}} = \frac{1}{S} \int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} d\omega = \tilde{\boldsymbol{n}}_{\mathrm{M}}^{\alpha\beta} \boldsymbol{E}_{\beta} \otimes \boldsymbol{E}_{\beta} + \hat{\boldsymbol{n}}_{\mathrm{M}} \\ \boldsymbol{m}_{\mathrm{M}} = \frac{1}{S} \int_{\omega} \boldsymbol{\sigma}_{\mathrm{m}} \otimes \boldsymbol{x} \; d\omega = \tilde{\boldsymbol{m}}_{\mathrm{M}}^{\alpha\beta} \boldsymbol{E}_{\beta} \otimes \boldsymbol{E}_{\beta} \otimes \boldsymbol{E}_{z} + \hat{\boldsymbol{m}}_{\mathrm{M}} \end{cases}$$

    - $\hat{\boldsymbol{n}}_{\mathrm{M}} = 0$ & $\hat{\boldsymbol{m}}_{\mathrm{M}} = 0$ for KL plates

$\hookrightarrow$ $\hat{\boldsymbol{\epsilon}}_{\mathrm{M}}$ & $\hat{\boldsymbol{\eta}}_{\mathrm{M}}$ eliminated $\longrightarrow$

$$\begin{cases} \tilde{\boldsymbol{n}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_1} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_2} : \boldsymbol{\kappa}_{\mathrm{M}} \\ \tilde{\boldsymbol{m}}_{\mathrm{M}} = \mathbb{C}_{\mathrm{M}_3} : \boldsymbol{\varepsilon}_{\mathrm{M}} + \mathbb{C}_{\mathrm{M}_4} : \boldsymbol{\kappa}_{\mathrm{M}} \end{cases}$$