Statistical inverse method for the multiscale identification of the apparent random elasticity field of heterogeneous microstructures

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Outline

1. Problem to be solved, difficulties and strategy

2. Prior stochastic model of the apparent elasticity random field at mesoscale


1. Problem to be solved, difficulties and strategy
1.1. Multiscale statistical inverse problem to be solved

- Material for which the elastic heterogeneous **microstructure cannot be described in terms of constituents** (example: biological tissues such as the cortical bone).

Cortical bone: photo: Julius Wolff Institute, Charité - Universitätsmedizin Berlin

- **Objective:** Identification of the tensor-valued **elasticity random field**, \( \{ C^{\text{meso}}(x), x \in \Omega^{\text{meso}} \} \) (apparent elasticity field) **at mesoscale**, \( \Omega^{\text{meso}} \), using multiscale experimental data.
1.2. Difficulties of the statistical inverse problem for the identification

- $\{C_{\text{meso}}(x), x \in \Omega_{\text{meso}}\}$ is a **second-order** random field in HD,
  - which is a **Non-Gaussian tensor-valued random field**.
  - which must verify **algebraic properties**: deterministic or random bounds; positive-definite symmetric tensor-valued random field with invariance properties (induced by material symmetries); etc.

- A methodology has recently been proposed for the experimental identification (through a stochastic BVP) of a general parametric representation of $C_{\text{meso}}$ in HD, based on the use of its **polynomial chaos expansion (PCE)**.

- This is a very challenging problem due to HD, and due to the fact that the PCE coefficients belong to a **manifold** that is very complicated to describe and to explore for computing the coefficients from experimental data.


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1.3. Strategy proposed for the identification of $C_{meso}$

Present work limited to the first two steps of the general methodology:

- **Step 1: Constructing a prior stochastic model for $C_{meso}$.**

  Introducing an adapted **prior stochastic model** $\{C_{meso}(x; b), x \in \Omega_{meso}\}$ on $(\Theta, I, P)$, depending on a vector-valued hyperparameter $b \in B_{ad}$ in low dimension (statistical mean tensor, dispersion parameters, spatial correlation lengths, etc).

**Comment:** In HD, the real possibility to correctly identify random field $C_{meso}$, through a **stochastic BVP**, is directly related to the **capability** of the constructed prior stochastic model for **representing fundamental properties** such as lower bound, positiveness, invariance related to material symmetry, mean value, support of the spectrum, spatial correlation lengths, level of statistical fluctuations, etc.
Step 2: Identifying hyperparameter $b$ of the prior stochastic model
\[ \{C_{\text{meso}}(x; b), \ x \in \Omega_{\text{meso}} \} \]

- Identification of $b$ performed in the framework of a **multiscale identification** of random field $C_{\text{meso}}$ at mesoscale;
- Using a **multiscale experimental digital image correlation** at macroscale and at mesoscale.

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2. Prior stochastic model of the apparent elasticity random field at mesoscale
2.1. Family \( \{ C_{\text{meso}}(x; b) \}, x \in \Omega_{\text{meso}} \} \) of prior stochastic models for the non-Gaussian tensor-valued random field at mesoscale, and its generator

- **Framework:**
  - 3D linear elasticity of microstructures
  - \( (6 \times 6) \)-matrix notation of the 4th-order tensor: \( [A_{\text{meso}}(x; b)]_{IJ} = C_{\text{meso}}^{ijkh}(x; b) \).
  - \( \{[A_{\text{meso}}(x; b)], x \in \Omega_{\text{meso}} \} \): apparent elasticity field of microstructure \( \Omega_{\text{meso}} \) at mesoscale, depending on a hyperparameter \( b \) (that will be defined later and that is removed below for simplifying notation).

For all \( x \) fixed in \( \Omega_{\text{meso}} \), random elasticity matrix \( [A_{\text{meso}}(x)] \):

(i) is, in mean, close to a given symmetry class (independent of \( x \)), induced by a material symmetry;

(ii) exhibits more or less anisotropic fluctuations around this symmetry class;

(iii) exhibits a level of statistical fluctuations in the symmetry class, which must be controlled independently of the level of statistical anisotropic fluctuations.
• Notation and properties for positive matrices with symmetry classes

\( \mathbb{M}_n^+(\mathbb{R}) \subset \mathbb{M}_n^S(\mathbb{R}) \subset \mathbb{M}_n(\mathbb{R}) \) (positive-definite, symmetric, all).

A given symmetry class is defined by the subset \( \mathbb{M}_n^{\text{sym}}(\mathbb{R}) \subset \mathbb{M}_n^+(\mathbb{R}) \) such that,

\[
[M] = \sum_{i=1}^{n_s} m_i [E_i^{\text{sym}}] , \quad m = (m_1, \ldots, m_{n_s}) \in \mathcal{C} , \quad [E_i^{\text{sym}}] \in \mathbb{M}_n^S(\mathbb{R})
\]

\( \mathcal{C} = \{ m \in \mathbb{R}^{n_s} \mid \sum_{i=1}^{n_s} m_i [E_i^{\text{sym}}] \in \mathbb{M}_n^+(\mathbb{R}) \} \)

\( \{ [E_i^{\text{sym}}], i = 1, \ldots, n_s \} \) is a matrix basis (Walpole’s tensor basis).

Examples of usual symmetry classes for \( n = 6 \) (3D elasticity),

- \( n_s = 2 \): isotropic symmetry
- \( n_s = 5 \): transverse isotropic symmetry
- \( n_s = 9 \): orthotropic symmetry

etc... and, \( n_s = 21 \): anisotropy

Properties: if \( [M] \) and \( [M'] \) \( \in \mathbb{M}_n^{\text{sym}}(\mathbb{R}) \), then

\[
[M][M'] \in \mathbb{M}_n^{\text{sym}}(\mathbb{R}) , \quad [M]^{-1} \in \mathbb{M}_n^{\text{sym}}(\mathbb{R}) , \quad [M]^{1/2} \in \mathbb{M}_n^{\text{sym}}(\mathbb{R})
\]
2.2. An advanced prior stochastic model for \( \{A^{\text{meso}}(x), x \in \Omega^{\text{meso}} \} \)


**Prior algebraic representation** *(Guilleninot & Soize SIAM MMS 2013)*:

\[
\forall x \in \Omega^{\text{meso}}, \quad [A^{\text{meso}}(x)] = [C_\ell(x)] + [A(x)]
\]

\( \{[C_\ell(x)], x \in \Omega \} \): \( \mathbb{M}_n^+(\mathbb{R}) \)-valued deterministic field (lower-bound)

\( \{[A(x)], x \in \Omega \} \): \( \mathbb{M}_n^+(\mathbb{R}) \)-valued random field

\[
[A(x)] = [S(x)]^T [M(x)]^{1/2} [G(x)] [M(x)]^{1/2} [S(x)]
\]

\( \{[G(x)], x \in \Omega \} \): \( \mathbb{M}_n^+(\mathbb{R}) \)-valued random field.

\( \{[M(x)], x \in \Omega \} \): \( \mathbb{M}^{\text{sym}}(\mathbb{R}) \)-valued random field independent of \( \{[G(x)], x \in \Omega \} \).

\( \{[S(x)], x \in \Omega \} \): \( \mathbb{M}_n(\mathbb{R}) \)-valued deterministic field.

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Anisotropic statistical fluctuations: \{[G(x)], x \in \Omega\} which is a non-Gaussian \(\mathbb{M}^+_n(\mathbb{R})\)-valued random field (MaxEnt construction and generator are given in Soize, CMAME 2006), for which \(E\{[G(x)]\} = [I_n]\).

The hyperparameters of \{[G(x)], x \in \Omega\} are: \(d \times n(n + 1)/2\) spatial correlation lengths and a scalar dispersion parameter \(\delta_G\) controlling the anisotropic statistical fluctuations.

**Statistical fluctuations in the given symmetry class:** \{[M(x)], x \in \Omega\} (independent of \([G]\)), which is a non-Gaussian \(\mathbb{M}_{n}^{\text{sym}}(\mathbb{R})\)-valued random field (algebraic representation, MaxEnt construction and generator using an ISDE are given in Guilleminot & Soize, SIAM MMS 2013), for which

\[
E\{[M(x)]\} = [M(x)] = \mathcal{P}^{\text{sym}}([a(x)]),
\]

with \(\mathcal{P}^{\text{sym}}\) the projection operator from \(\mathbb{M}^+_n(\mathbb{R})\) on \(\mathbb{M}^{\text{sym}}_n(\mathbb{R})\), and

\[
[a(x)] = E\{[A(x)]\} = E\{[A^{\text{meso}}(x)]\} - [C_\ell(x)] \in \mathbb{M}^+_n(\mathbb{R}),
\]

\[
[M(x)] = [M(x)]^{1/2}[N(x)][M(x)]^{1/2} \quad \text{with} \quad E\{[N(x)]\} = [I_n].
\]
\{[ N(x) ], x \in \Omega \} is a non-Gaussian \( M_{n}^\text{sym}(\mathbb{R}) \)-valued random field written as 

\[ [ N(x) ] = \expm([ N'(x) ]) \] in which 

\[ [ N'(x) ] = \sum_{i=1}^{n_s} \nu_i(x)[ E^\text{sym}_i ] \] with \{ \nu(x), x \in \Omega \} is a \( \mathbb{R}^{n_s} \)-valued random process.

The hyperparameters of \{ [ M(x) ], x \in \Omega \} are: \( d \times n_s \) spatial correlation lengths and a scalar dispersion parameter \( \delta_M \) controlling the statistical fluctuations in the symmetry class.

**Construction of the \( M_n(\mathbb{R}) \)-valued deterministic field \{ [S(x) ], x \in \Omega \}:**

The Cholesky factorizations of 

\[ [ a(x) ] = E\{[ A^{\text{meso}}(x) ] \} - [ C_\ell(x) ] \in M_{n}^+(\mathbb{R}) \] yields the upper matrix \( [ L_a(x) ] \), and 

\[ [ M(x) ] = \mathcal{P}^\text{sym}( [ a(x) ] ) \in M_{n}^\text{sym}(\mathbb{R}) \] yields the upper matrix \( [ L_M(x) ] \). Since 

\[ [ a(x) ] = [ S(x) ]^T [ M(x) ] [ S(x) ] \], it can be deduced that 

\[ [ S(x) ] = [ L_M(x) ]^{-1} [ L_a(x) ] \]
2.3. Fully anisotropic case

The "sym class" is chosen as the "anisotropic class" with \( n_s = 21 \) and \( \delta_M \) is taken as 0; then

\[
[A(x)] = [a(x)]^{1/2}[G(x)][a(x)]^{1/2}.
\]

Consequently:

\[
\forall x \in \Omega^{\text{meso}}, \quad [A^{\text{meso}}(x)] = [C_\ell(x)] + [a(x)]^{1/2}[G(x)][a(x)]^{1/2}
\]

**Particular choice:**

\[
[C_\ell(x)] = \frac{\varepsilon}{1 + \varepsilon} E\{[A^{\text{meso}}(x)]\} \quad \text{with} \quad 0 < \varepsilon \ll 1
\]

**Hyperparameter \( b \):** for a homogeneous mean value, \( [\varrho] = E\{[A^{\text{meso}}(x)]\} \),
b is of dimension 10 and is written as,

\[
b = (\{[\varrho]_{ij}\}_{i \geq j}, (L_1, L_2, L_3), \delta_G)
\]
3. Multiscale identification of the prior stochastic model using a multiscale experimental digital image correlation, at macroscale and at mesoscale
3.1. Difficulties and multiscale identification

- Problem consists of the experimental identification of hyperparameter \( b \) of the prior stochastic model of the apparent elasticity random field \( \{ C_{\text{meso}}(x; b), x \in \Omega^{\text{meso}} \} \)

- \( b \) is made up of the statistical mean tensor, \( \mathbb{E}\{ C_{\text{meso}}(x) \} \), and other parameters that control the statistical fluctuations.

- Difficulty: \( \mathbb{E}\{ C_{\text{meso}}(x) \} \) cannot directly be identified using only the measurements of the displacement field \( u_{\text{exp}}^{\text{meso}} \) at mesoscale in \( \Omega^{\text{meso}} \), and requires macroscale measurements.

\[ \Rightarrow \] Experimental multiscale measurements are required and must be made simultaneously at macroscale and at mesoscale.
3.2. Hypotheses concerning experimental digital image correlation at macroscale and at mesoscale

Only a single specimen, submitted to a given load applied at macroscale, is tested.

▷ A measurement of the strain field at macroscale is carried out in $\Omega^\text{macro}$ (spatial resolution $10^{-3} \, m$, for instance);

▷ Simultaneously, the measurement of the strain field at mesoscale is carried out in $\Omega^\text{meso}$ (spatial resolution $10^{-5} \, m$, for instance)
3.3. Hypotheses and strategy for solving the statistical inverse problem

- Hypotheses used for the statistical inverse problem:
  - Separation of macroscale $\Omega^{\text{macro}}$ from mesoscale $\Omega^{\text{meso}}$ that is thus a RVE.
  - At macroscale, the elasticity tensor is constant (independent of $x$).
  - At mesoscale, the apparent elasticity random field is homogeneous.

- Constructing:
  - A prior deterministic model of the macro elasticity tensor $C^{\text{macro}}(a)$ at macroscale, depending on a vector-valued parameter $a \in A^{\text{macro}}$.
  - A prior stochastic model of the apparent elasticity random field $\{C^{\text{meso}}(x;b), x \in \Omega^{\text{meso}}\}$ at mesoscale, depending on a vector-valued hyperparameter $b \in B^{\text{meso}}$. 

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3.4. Numerical indicators for the multiscale identification

- **Macroscopic numerical indicator**, $J_1(a)$, minimizes the distance between the experimental strain deformation at macroscale and the computed strain deformation at macroscale:

$$J_1(a) = \int_{\Omega_{\text{macro}}} \| \varepsilon_{\exp}^{\text{macro}}(x) - \varepsilon^{\text{macro}}(x; a) \|^2_F \, dx$$

$$-\text{div} \sigma^{\text{macro}} = 0 \quad \text{in} \quad \Omega^{\text{macro}}$$

$$\sigma^{\text{macro}} n^{\text{macro}} = f^{\text{macro}} \quad \text{on} \quad \Sigma^{\text{macro}}$$

$$u^{\text{macro}} = 0 \quad \text{on} \quad \Gamma^{\text{macro}}$$

$$\sigma^{\text{macro}} = C^{\text{macro}}(a) : \varepsilon^{\text{macro}}, \quad a \in \mathcal{A}^{\text{macro}}$$
• **Mesoscopic numerical indicator**, $J_2(b)$, minimizes the distance between the normalized dispersion coefficient, $\delta_{\text{meso}}(x; b)$, characterizing the statistical fluctuations of the computed random strain deformation at mesoscale, and the corresponding normalized dispersion coefficient, $\delta_{\text{exp}}^{\text{meso}}$, for the experimental strain deformation at mesoscale:

$$J_2(b) = \int_{\Omega_{\text{meso}}} \left( \delta_{\text{meso}}(x; b) - \delta_{\text{exp}}^{\text{meso}} \right)^2 \, dx$$

$$-\text{div} \sigma^{\text{meso}} = 0 \quad \text{in} \quad \Omega_{\text{meso}}$$

$$\mathbf{U}^{\text{meso}} = \mathbf{u}_{\text{exp}}^{\text{meso}} \quad \text{on} \quad \partial\Omega_{\text{meso}}$$

$$\sigma^{\text{meso}} = \mathcal{C}^{\text{meso}}(b) : \varepsilon^{\text{meso}}, \quad b \in \mathcal{B}^{\text{meso}}$$
• **Macroscopic-mesoscopic numerical indicator**, $J_3(a, b)$, minimizes the distance between the macro elasticity tensor $C^{\text{macro}}(a)$ at macroscale and the effective elasticity tensor $C^{\text{eff}}(b)$ constructed by a stochastic homogenization using the RVE $\Omega^{\text{meso}}$:

$$J_3(a, b) = \| C^{\text{macro}}(a) - E\{ C^{\text{eff}}(b) \} \|_F^2$$

The stochastic homogenization (from meso to macro) is formulated in homogeneous constraints (that is better adapted for the 2D plane stresses) with $\sigma^{\text{meso}} = C^{\text{meso}}(b) : \varepsilon^{\text{meso}}$. 
3.5. Statistical inverse problem formulated as a multi-objective optimization problem

\[(a_{\text{macro}}, b_{\text{meso}}) = \arg \min_{a \in A_{\text{macro}}, b \in B_{\text{meso}}} J(a, b)\]

\[\min J(a, b) = (\min J_1(a), \min J_2(b), \min J_3(a, b))\]
3.6. Solving the multi-objective optimization problem

- The deterministic BVP at macroscale is discretized using the FEM.

- The stochastic BVP at mesoscale
  - is discretized using the FEM,
  - is solved using the Monte Carlo method.

- The multi-objective optimization problem
  - is solved using the genetic algorithm, and the Pareto front is iteratively constructed at each generation of the genetic algorithm,
  - the initial value $a^{(0)}$ of $a \in A^{\text{macro}}$ is computed solving (using the simplex algorithm) the optimization problem:

$$a^{(0)} = \arg \min_{a \in A^{\text{macro}}} J_1(a),$$

- $b^{\text{meso}} \in B^{\text{meso}}$ is then chosen as the point on the Pareto front that minimizes the distance between the Pareto front and the origin.
4. Application of the method for multiscale experimental measurements of cortical bone in 2D plane stresses
4.1. Multiscale experimental measurements

  Left: Specimen of cortical bone (cube with dimensions $0.01 \times 0.01 \times 0.01 \text{ m}^3$).
  Right: Measuring bench.

- Comparison between a reference image (left) and a deformed image (right) at macroscale for a cubic cortical bovine bone sample.

- Dimensions and spatial resolution of the multiscale measurements.

\[ \Omega_{\text{macro}} : 0.01 \times 0.01 \, m^2 \text{ meshed with a } 10 \times 10 \text{-points grid yielding a spatial resolution of } 10^{-3} \times 10^{-3} \, m^2. \]

\[ \Omega_{\text{meso}} : 0.001 \times 0.001 \, m^2 \text{ meshed with a } 100 \times 100 \text{-points grid yielding a spatial resolution of } 10^{-5} \times 10^{-5} \, m^2. \]

Applied force: 9,000 N
• Experimental displacement at macroscale:
  
  Component $\{u_{\text{macro}}^{\text{exp}}\}_1$ in direction $x_1$ (horizontal) (left figure),
  Component $\{u_{\text{macro}}^{\text{exp}}\}_2$ in direction $x_2$ (vertical) (right figure).

• Experimental displacement at mesoscale:
  
  Component $\{u_{\text{meso}}^{\text{exp}}\}_1$ in direction $x_1$ (horizontal) (left figure),
  Component $\{u_{\text{meso}}^{\text{exp}}\}_2$ in direction $x_2$ (vertical) (right figure).
4.2. Hypotheses for the stochastic computational model

- 2D-plane-stresses modeling is used.

- At macroscale, the material is assumed to be **homogeneous**, transverse isotropic, and linear elastic.

  **Parameter** \( a = (E^\text{macro}_T, \nu^\text{macro}_T) \)  (transverse Young mod. and Poisson coeff.).

- At mesoscale, the material is assumed to be **heterogeneous**, anisotropic, and linear elastic. The **stochastic model** of the apparent elasticity field is deduced from the full anisotropic stochastic case, for which the statistical mean value is assumed to be transverse isotropic (Section 2.3).

  **Hyperparameter** \( b = (E_T, \nu_T, L, \delta) \):
  
  \((E_T, \nu_T)\) = statistical mean values (transverse Young mod. and Poisson coeff.).
  
  \((L, \delta)\) = spatial correlation length and dispersion parameter of the statistical fluctuations of the apparent elasticity field.

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4.3. Results obtained by the multiscale identification procedure

▷ The optimal value of $\mathbf{a} = (E^\text{macro}_T, \nu^\text{macro}_T)$ is $(6.74 \times 10^9 \, Pa, 0.32)$.

▷ The optimal values of the components of $\mathbf{b} = (L^\text{meso}, \delta^\text{meso}, E^\text{meso}_T, \nu^\text{meso}_T)$ are $L^\text{meso} = 5.06 \times 10^{-5} \, m$, $\delta^\text{meso} = 0.28$, $E^\text{meso}_T = 6.96 \times 10^9 \, Pa$, $\nu^\text{meso}_T = 0.37$.

- The identified spatial correlation length:
  - is in agreement with the assumption introduced concerning the separation of the scales,
  - is of the same order of magnitude than the distance between adjacent lamellae or osteons in cortical bovine femur.

- The identified values of $\mathbf{a}$ and $\mathbf{b}$ are coherent with the values published in literature.


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Conclusion

• In the framework of the linear elasticity, a multiscale inverse statistical method has been presented for the identification of a stochastic model of the apparent elasticity random field at mesoscale for a heterogeneous microstructure using experimental measurements at macroscale and at mesoscale.

• The proposed statistical inverse method has been validated with a simulated experimental database (not presented in the present lecture)

• The method has been applied and presented for multiscale experimental measurements obtained by the digital-image-correlation method on one sample of cortical bone observed by a CCD camera at both macroscale and mesoscale.

• Future works:
  - posterior stochastic identification of the prior stochastic model in 2D.
  - multiscale experimental identification in 3D