LABORATOIRE DE MODÉLISATION ET SIMULATION MULTI ÉCHELLE

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Stochastic representation of random positive-definite tensor-valued properties: application to 3D anisotropic permeability random fields

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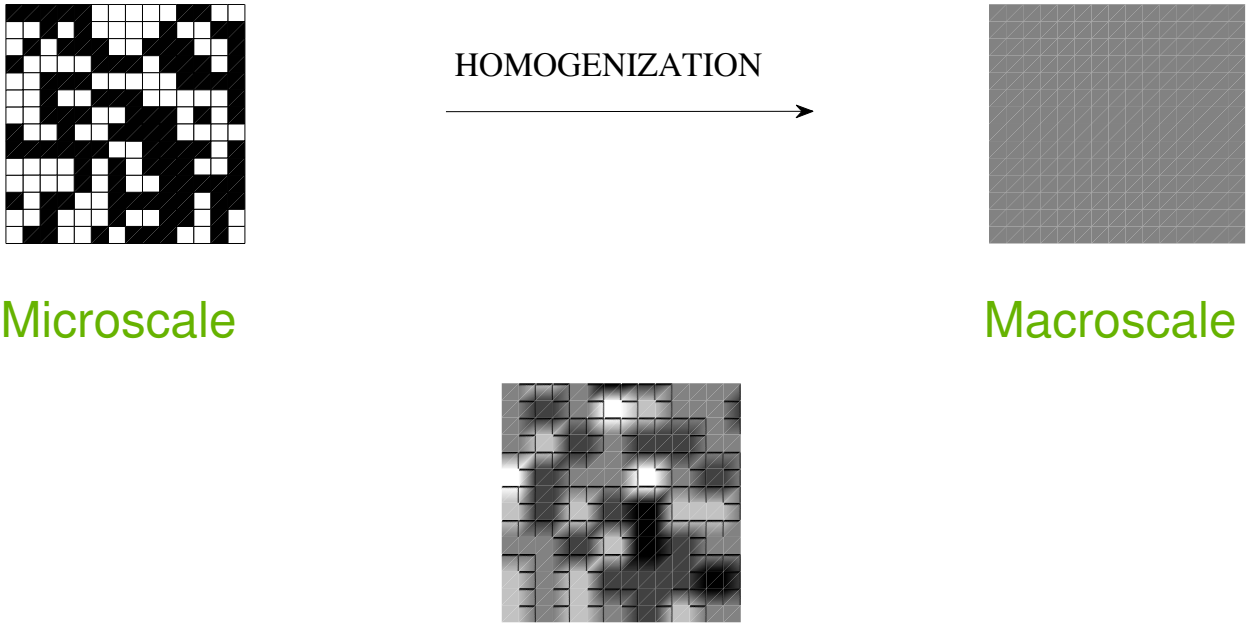
Outline

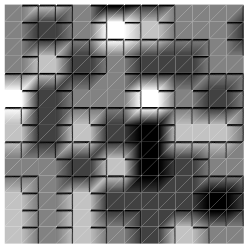
Central issue : modeling, generation and calibration of a matrix-valued random field (*e.g.* a permeability tensor field) - with various interpretations.

- Classical multiscale framework :



The medium is, hence, described through random fields of apparent properties.

- Modeling of uncertainties, and identification solving an underdetermined inverse problem :



Limited measurements are made on boundaries, and used to calibrate the model at any point.

The aim here is to derive models :

- that are consistent from a mathematical standpoint ;
- that contain as much physics as possible ;
- that do not rely on too many parameters.

Notation and overview of the construction

- Let $\{[\boldsymbol{A}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ be any $\mathbb{M}_n^+(\mathbb{R})$-valued random field, indexed by $\Omega \subset \mathbb{R}^d$.
- Methodology :
  - construct an information-theoretic stochastic model for the family of first order marginal distributions ;
  - define $\{[\boldsymbol{A}(\boldsymbol{x})], \boldsymbol{x} \in \Omega\}$ through a pointwise nonlinear mapping $\mathcal{T}$, acting on some underlying vector-valued Gaussian random field, such that it exhibits the above family of first-order marginal distributions.
- Relevant issues :
  - how to define the marginal ?
  - how to construct mapping $\mathcal{T}$?

Reminder on Information Theory

- Assume that $[\boldsymbol{A}(\boldsymbol{x})]$ ($\boldsymbol{x}$ fixed) satisfies n_c algebraic constraints :

$$\mathbb{E}\{\boldsymbol{g}^i([\boldsymbol{A}(\boldsymbol{x})])\} = \boldsymbol{f}^i(\boldsymbol{x}) \ , \quad 1 \leqslant i \leqslant n_c$$

- Information theory and Maximum entropy principle :

$$p_{[\boldsymbol{A}(\boldsymbol{x})]} = \underset{p \in \mathcal{C}_{ad}(\boldsymbol{x})}{\arg\max} \ \mathrm{S}(p)$$

with

$$\mathrm{S}(p) = -\int_{\mathbb{M}_n^+(\mathbb{R})} p([A]) \ln(p([A]))d[A]$$

- MaxEnt estimate for the probability density function :

$$p_{[\boldsymbol{A}(\boldsymbol{x})]}([A]) = \mathbb{1}_{\mathbb{M}_n^+(\mathbb{R})}([A]) \, c_0 \, \exp\left(-\sum_{i=1}^{n_c} < \boldsymbol{\mathcal{L}}_i(\boldsymbol{x}), \boldsymbol{g}^i([A]) >_{\mathbb{H}_i}\right)$$

Definition of $\mathcal{RM}$: available information

- Constraints (no dependence on $\boldsymbol{x}$ for notational convenience) :

$$(1) \quad \mathbb{E}\left\{[\boldsymbol{A}]\right\} = \int_{\mathbb{M}_n^+(\mathbb{R})} [A]\, p_{[\boldsymbol{A}]}\left([A]\right) \mathrm{d}[A] = [\underline{A}]$$

$$(2) \quad \int_{\mathbb{M}_n^+(\mathbb{R})} \ln\left(\det\left([A]\right)\right) p_{[\boldsymbol{A}]}\left([A]\right) \mathrm{d}[A] = \beta, \quad |\beta| < +\infty$$

$$(3) \quad \mathbb{E}\left\{\left(\underline{\boldsymbol{\varphi}}^{k^{\mathsf{T}}}\, [\boldsymbol{A}]\, \underline{\boldsymbol{\varphi}}^k\right)^2\right\} = s_k^2 \underline{\lambda}_k^2, \quad k \in \{1, \ldots, m\}$$

- (1) is related to the mean value, (2) to finiteness of second-order moments, and (3) are constraints on the spectrum.
- Let :

$$[\boldsymbol{A}(\boldsymbol{x})] = [\underline{L}(\boldsymbol{x})][\boldsymbol{G}(\boldsymbol{x})][\underline{L}(\boldsymbol{x})]^{\mathsf{T}}$$

with $[\boldsymbol{G}(\boldsymbol{x})] = [\boldsymbol{H}(\boldsymbol{x})][\boldsymbol{H}(\boldsymbol{x})]^{\mathsf{T}}$ and $[\boldsymbol{H}(\boldsymbol{x})]$ a lower triangular random matrix.

Definition of $\mathcal{RM}$: joint P.D.F.

Assume $m = n$.

- For i fixed, r.v. $\{H_{i\ell}\}_{\ell=1}^{i}$ are jointly distributed :

$$p_{H_{i1},\ldots,H_{ii}}(\boldsymbol{h}) = \mathbb{1}_{\mathcal{S}}(\boldsymbol{h})\, c_0\, {h_{ii}}^{n-1-i+2\alpha(\boldsymbol{x})}\, \varphi(\boldsymbol{h}; \mu_i(\boldsymbol{x}), \tau_i(\boldsymbol{x}))$$

  where φ is defined as :

$$\varphi(\boldsymbol{h}; \mu_i(\boldsymbol{x}), \tau_i(\boldsymbol{x})) := \exp\left(-\mu_i(\boldsymbol{x})\left(\sum_{\ell=1}^{i} {h_{i\ell}}^2\right) - \tau_i(\boldsymbol{x})\left(\sum_{\ell=1}^{i} {h_{i\ell}}^2\right)^2\right)$$

- Parameter $\mu_i(\boldsymbol{x})$ satisfies :

$$\int_{\mathbb{R}+} c_1\, g^{(n+2\alpha(\boldsymbol{x})-1)/2}\, \exp\{-\mu_i(\boldsymbol{x})g - \tau_i(\boldsymbol{x})g^2\}\, dg = 1 \tag{1}$$

- $\boldsymbol{x} \mapsto \alpha(\boldsymbol{x})$: level of fluctuations.
- $\boldsymbol{x} \mapsto \tau_i(\boldsymbol{x})$: variance of λ_i (ordered statistics).

Non linear mapping

How to define mapping $\mathcal{T}$?

- Rosenblatt transformation.
- Numerical approximation :
  - KL decomposition (PCA) :

$$\boldsymbol{H}^{(i)} \simeq \underline{\boldsymbol{h}}^{(i)} + \sum_{j=1}^{N_{KL}} \sqrt{\lambda_j}\eta_j \boldsymbol{v}^j$$

  - Polynomial chaos expansion :

$$\boldsymbol{\eta}^{pce} \simeq \sum_{\gamma=1}^{N_{pce}} \boldsymbol{z}^{\gamma} \Psi_{\gamma}(\boldsymbol{U}^{(i)})$$

- Computation of the coefficients by the maximum likelihood method (first-order m.p.d.f., joint p.d.f.).

Context

- Darcean flows through random porous media[1] :

$$\boldsymbol{v} = -\frac{1}{\mu}[K(\boldsymbol{x})]\boldsymbol{\nabla} p$$

- Various fields of applications :
  - Geomechanics : oil industry, etc.
  - Composite manufacturing : resin transfer molding, etc.
- Let

$$[\underline{K}] = \begin{bmatrix} 1.05 & 0 \\ 0 & 0.95 \end{bmatrix}$$

and

$$[\boldsymbol{H}] = \begin{pmatrix} h_{11} & 0 \\ h_{21} & h_{22} \end{pmatrix}$$

1. See Guilleminot, J., Soize, C. and Ghanem, R. G., IJNAMG, 36(13), 2012.

Influence of parametrization

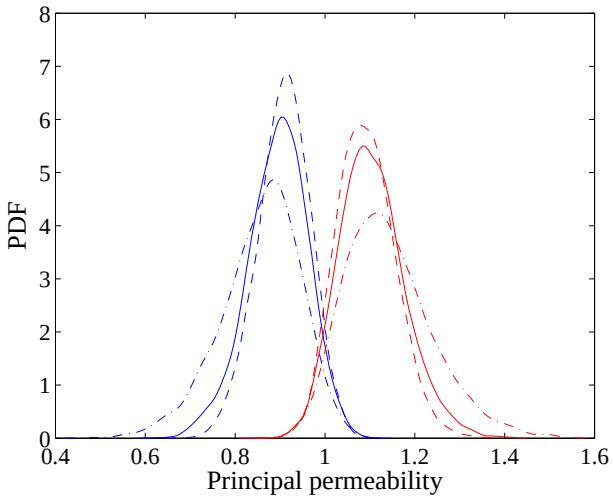


FIGURE 1: Plot of the p.d.f. of λ_x (red line) and λ_y (blue line), in 10^{-10} m^2, for $\tau_x = \tau_y = 10^2$ and $\alpha = 20$ (dash-dot line), $\alpha = 50$ (solid line) and $\alpha = 80$ (dashed line).

Influence of parametrization

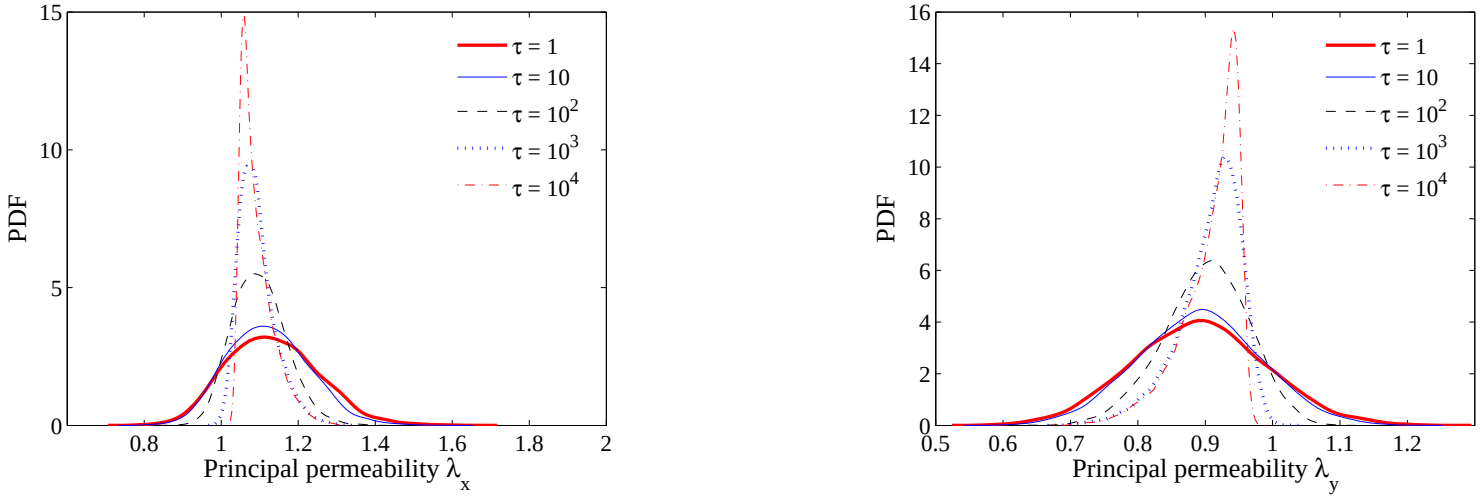


FIGURE 2: Plot of the p.d.f. of λ_x (left) and λ_y (right), for $\alpha = 60$ and different values of $\tau_x = \tau_y = \tau$.

Influence of parametrization

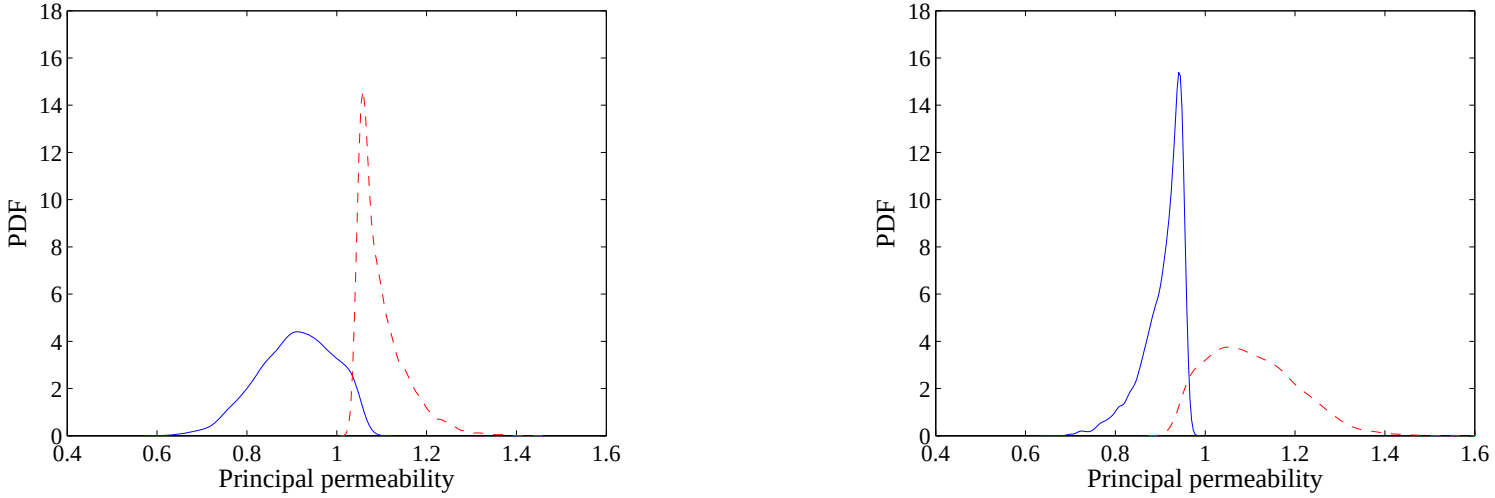


FIGURE 3: Plot of the p.d.f. of the first (red dashed line) and second (blue solid line) stochastic principal permeability (in 10^{-10} m^2). Left : $\alpha = 80$, $\tau_x = 10^4$ and $\tau_y = 1$. Right : $\alpha = 80$, $\tau_x = 1$ and $\tau_y = 10^4$.

Defining $\mathcal{T}$ with the chaos expansion

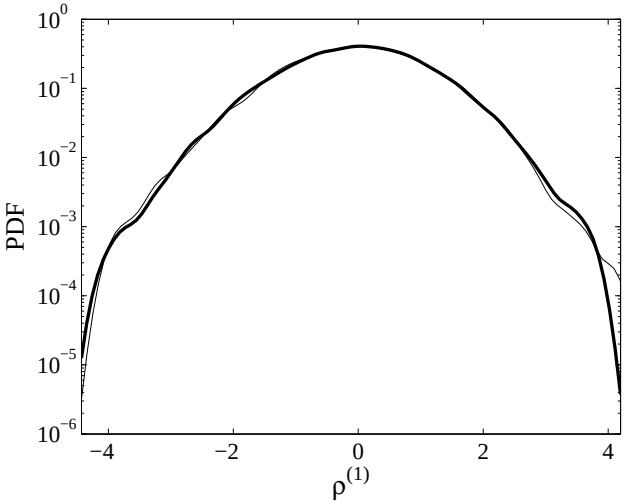


FIGURE 4: Plot (in semi-log scale) of the p.d.f. of random variable $\rho^{(1)}$: target (thin solid line) and $10th$-order chaos projection (thick solid line).

Defining $\mathcal{T}$ with the chaos expansion

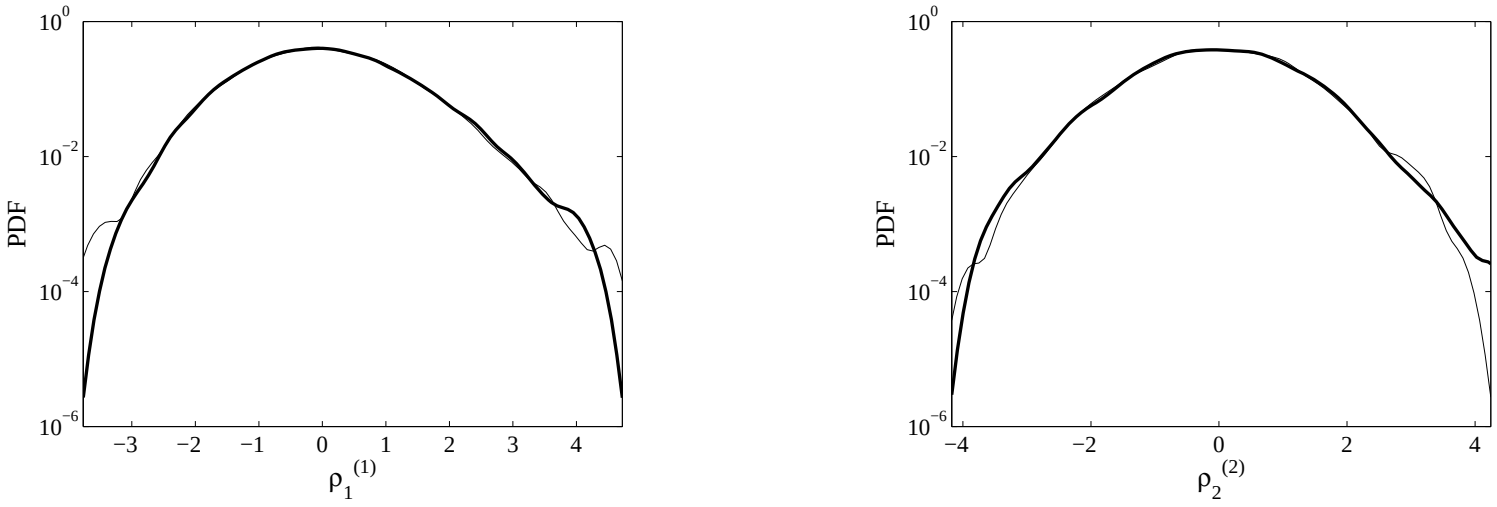


FIGURE 5: Plot (in semi-log scale) of the p.d.f. $p_{\eta_j^{(2)}}$. Reference : thin solid line ; Estimation based on chaos expansion ($4th$-order expansion) : thick solid line. Left : $j = 1$; Right : $j = 2$.

Example

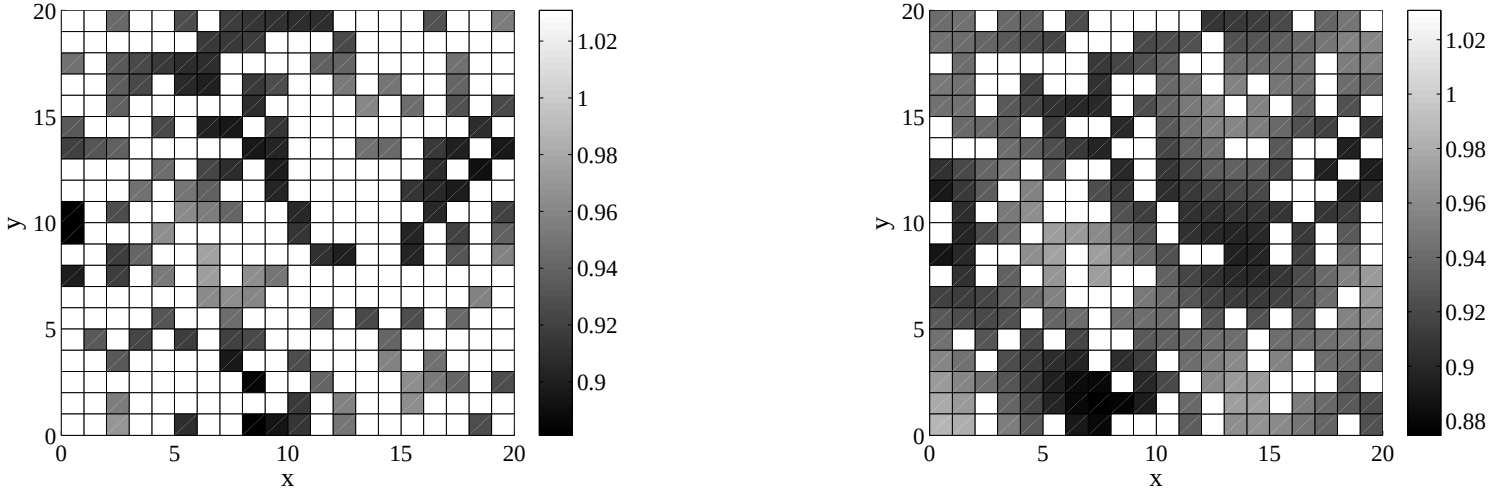


FIGURE 6: Plot of a realisation of random fields $\boldsymbol{x} \mapsto \lambda_x(\boldsymbol{x})$ (left) and $\boldsymbol{x} \mapsto \lambda_y(\boldsymbol{x})$ (right).

Two important applications :

- in geomechanics : orientation of cracks ;
- in composite manufacturing : local architecture of the preform (racetracking channels, etc.).

Revisiting the initial formulation

The previous derivations involve PCEs, and require a reference generator to be available : can we circumvent these drawbacks ?

Let $\widetilde{p}$ be the target marginal p.d.f., and let :

$$\widetilde{p}(\boldsymbol{u}) := c \, \exp\left(-\Phi(\boldsymbol{u})\right) \ , \quad \forall \boldsymbol{u} \in \mathcal{S} \subseteq \mathbb{R}^q \ , \tag{2}$$

with Φ the potential. In our case, for the i-th row ($q = i$) :

$$\Phi(\boldsymbol{u}) = -\log\left(\mathbb{1}_{\mathcal{S}}(\boldsymbol{u})\right) - \beta(\boldsymbol{x}) \log\left(u_i\right) + \mu_i(\boldsymbol{x}) \left(\sum_{\ell=1}^{i} {u_\ell}^2\right) + \tau_i(\boldsymbol{x}) \left(\sum_{\ell=1}^{i} {u_\ell}^2\right)^2$$

with $\beta(\boldsymbol{x}) := n - 1 - i + 2\alpha(\boldsymbol{x})$. Two cases of practical interest :

- unconstrained case, $\mathcal{S} = \mathbb{R}^q$;
- constrained case, $\mathcal{S} \subset \mathbb{R}^q$ (recall that $H_{ii} > 0$ a.s.).

The sampling scheme in a nutshell ($\mathcal{S} = \mathbb{R}^q$)

Let $\{\boldsymbol{W}(r,\boldsymbol{x}), r \in \mathbb{R}^+, \boldsymbol{x} \in \Omega\}$ be a Gaussian random field, with values in $\mathbb{R}^q$, such that :

- for $\boldsymbol{x}$ fixed in $\mathbb{R}^d$, $\{\boldsymbol{W}(r,\boldsymbol{x}), r \in \mathbb{R}^+\}$ is a normalized Wiener process ;
- for r fixed $\mathbb{R}^+$, $\{\boldsymbol{W}(r,\boldsymbol{x}), \boldsymbol{x} \in \mathbb{R}^d\}$ is a colored Gaussian field.

Let $\mathcal{F}$ be the family of ISDEs, indexed by $\boldsymbol{x}$, such that :

$$\forall r \geqslant 0 \ , \quad \left\{ \begin{array}{l} \mathrm{d}\boldsymbol{U}(r,\boldsymbol{x}) = \boldsymbol{V}(r,\boldsymbol{x}) \ \mathrm{d}r \\ \mathrm{d}\boldsymbol{V}(r,\boldsymbol{x}) = \left(-\nabla_{\boldsymbol{u}} \Phi(\boldsymbol{U}(r,\boldsymbol{x})) - \dfrac{\eta}{2} \boldsymbol{V}(r,\boldsymbol{x}) \right) \mathrm{d}r + \sqrt{\eta} \, \mathrm{d}\boldsymbol{W}(r,\boldsymbol{x}) \end{array} \right. \tag{3}$$

with given initial conditions. Under some assumptions on Φ :

$$\lim_{r \to +\infty} \boldsymbol{U}(r,\boldsymbol{x}) \overset{law}{=} \boldsymbol{A}(\boldsymbol{x}) \ . \tag{4}$$

Summary [2] :

- family of ergodic homogeneous diffusion processes ;
- definition of the associated family of invariant measures.

2. See Guilleminot, J., Soize, C., SIAM MULTISCALE MODEL. SIMUL., 11(3), 2013.

Tackling the constrained case : $\mathcal{S} \subset \mathbb{R}^q$ [3]

Let Ψ be the target potential :

$$\Psi(\boldsymbol{u}) := -\log(\mathbb{1}_{\mathcal{S}}(\boldsymbol{u})) + \mathcal{Z}(\boldsymbol{u}) \ , \quad \forall \boldsymbol{u} \in \mathcal{S} \ . \tag{5}$$

Step 1 : define the potential Ψ_ϵ, $0 < \epsilon \ll 1$, through

$$\Psi_\epsilon(\boldsymbol{u}) := -\log\left(\mathbb{1}^\epsilon_{\mathcal{S}}(\boldsymbol{u})\right) + \mathcal{Z}(\boldsymbol{u}) \ , \quad \forall \boldsymbol{u} \in \mathbb{V} \supseteq \mathcal{S} \ , \tag{6}$$

with $\mathbb{1}^\epsilon_{\mathcal{S}}$ the regularized indicator function ($\lim_{\epsilon \downarrow 0} \mathbb{1}^\epsilon_{\mathcal{S}} = \mathbb{1}_{\mathcal{S}}$), $\mathcal{S} \subseteq \mathbb{V} \subset \mathbb{R}^q$, such that

- Ψ_ϵ satisfies all the assumptions related to the SDE analysis ;
- $\lim_{\epsilon \downarrow 0} \Psi_\epsilon = \Psi$ in $\overset{\circ}{\mathcal{S}}$.

For all $\boldsymbol{x}$ in Ω :

$$\lim_{r \to +\infty} \boldsymbol{U}_\epsilon(r, \boldsymbol{x}) \overset{law}{=} \boldsymbol{A}_\epsilon(\boldsymbol{x}) \tag{7}$$

Then consider the asymptotic case $\epsilon \downarrow 0$.

3. See Guilleminot, J., Soize, C., SIAM J. SCI. COMPUT., 36(6), 2014.

Step 2 : definition of an adaptive scheme (adapted from Lamberton & Lemaire (2005))

- Let $(\gamma_k)_{k\geq 1}$ be the sequence :

$$\gamma_k := \gamma_0\, k^{-1/\tau}\ , \quad \forall k \geqslant 1\ , \tag{8}$$

with $\gamma_0 > 0$ and $\tau \in \mathbb{N}_*$. Let $\left\{\{\chi_{\boldsymbol{x}}^k, k \geqslant 1\}\right\}_{\boldsymbol{x}\in\Omega}$ be the family of processes defined as :

$$\chi_{\boldsymbol{x}}^k := \frac{2\,\mathcal{V}(\boldsymbol{U}_\epsilon^k(\boldsymbol{x}), \boldsymbol{V}_\epsilon^k(\boldsymbol{x}))}{\|\boldsymbol{b}(\boldsymbol{U}_\epsilon^k(\boldsymbol{x}), \boldsymbol{V}_\epsilon^k(\boldsymbol{x})\|^2 \vee 1}\ , \quad \forall k \geqslant 0\ , \quad \forall \boldsymbol{x} \in \Omega\ . \tag{9}$$

Define the step sequence $(\widetilde{\gamma}_{k+1})_{k\geqslant 0}$ as :

$$\widetilde{\gamma}_{k+1} := \min_{\boldsymbol{x}\,\in\,\Omega} \left(\gamma_{k+1} \wedge \chi_{\boldsymbol{x}}^k\right)\ , \quad \forall k \geqslant 0\ , \tag{10}$$

with $\widetilde{\gamma}_0 = \gamma_0$.

- Scheme :

$$\boldsymbol{X}_\epsilon^{k+1}(\boldsymbol{x}) = \mathfrak{D}_{\mathsf{SV}}\left(\boldsymbol{X}_\epsilon^k(\boldsymbol{x}), \Delta\boldsymbol{W}^{k+1}(\boldsymbol{x}), \widetilde{\gamma}_{k+1}\right)\ , \quad k \geqslant 0\ . \tag{11}$$

with $\boldsymbol{X}_\epsilon^0(\boldsymbol{x}) = \boldsymbol{x}_0$ a.s. for all $\boldsymbol{x}$ in Ω ($\boldsymbol{x}_0 = (\boldsymbol{u}_0, \boldsymbol{v}_0) \in \mathcal{S} \times \mathbb{R}^q$).

The computational cost is essentially governed by :

- the rate of convergence towards the stationary solution ;
- the gradient computation ;
- the sampling algorithm for the underlying Gaussians.

Current applications deal with more than 100,000 points (100,000 SDEs are integrated simultaneously).

Various techniques were benchmarked for the sampling of Gaussians, such as

- circular embedding ;
- direct factorization-based methods (Cholesky) ;
- Krylov subspace methods ;
- spectral methods.

However, it is still an open issue for large-scale simulations and for arbitrary covariance kernels.

Application 1

Let $\widetilde{p}$ be defined as :

$$\widetilde{p}(\boldsymbol{u}) := c \, \exp\{-\Psi(\boldsymbol{u})\} \ , \quad \forall \boldsymbol{u} \in \mathcal{S} \ , \tag{12}$$

where

$$\Psi(\boldsymbol{u}) := -\log\left(\mathbb{1}_{\mathcal{S}}(\boldsymbol{u})\right) + \frac{1}{2}\langle [K]\boldsymbol{u}, \boldsymbol{u}\rangle \ , \quad \forall \boldsymbol{u} \in \mathcal{S} \ , \tag{13}$$

with $\mathcal{S} := [-0.5, 0.5] \times [-0.5, 0.5]$ and $[K] := \text{diag}(1, 1)$.

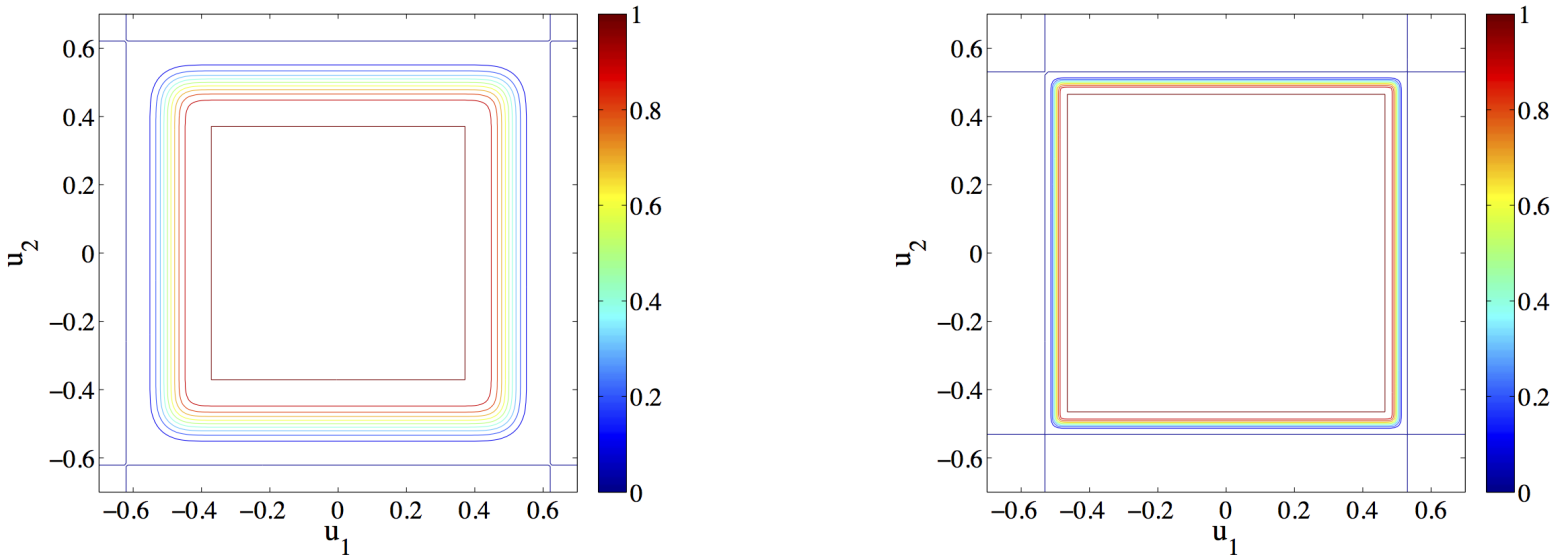


FIGURE 7: Graph of the indicator function $\mathbb{1}_{\mathcal{S}}^{\epsilon}$ for $\epsilon = 0.04$ (left) and $\epsilon = 0.01$ (right).

Sample paths of $\{(U_1^k, U_2^k), k \geqslant k_{stat}\}$:

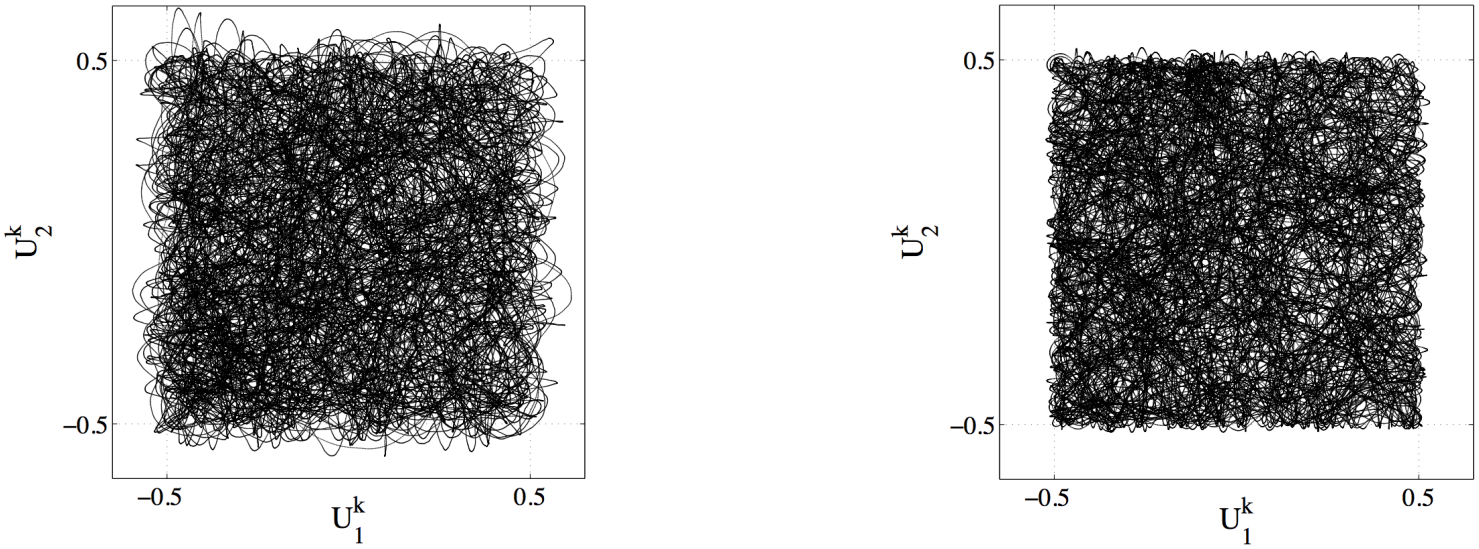


FIGURE 8: Sample paths for $\epsilon = 0.04$ (left) and $\epsilon = 0.01$ (right).

Application 2

Let the target potential be defined as (nonlinear term) :

$$\Psi(\boldsymbol{u}) := -\log\left(\mathbb{1}_{\mathcal{S}}(\boldsymbol{u})\right) - (\lambda - 1)\log\left(\det([\mathsf{Mat}(\boldsymbol{u})])\right) + \frac{q-1+2\lambda}{2}\sum_{k=1}^{q} u_{k(k+1)/2}\ , \tag{14}$$

with

$$\mathcal{S} := \left\{\boldsymbol{u} \in \mathbb{R}^n \mid [\mathsf{Mat}(\boldsymbol{u})] \in \mathbb{M}_q^+(\mathbb{R})\right\}\ . \tag{15}$$

Let ρ^k be the r.v. with values in $\mathbb{R}_+^*$ defined as :

$$\rho^k := \min\ \mathfrak{S}\left([\mathsf{Mat}(\boldsymbol{U}^k)]\right)\ , \tag{16}$$

with $\mathfrak{S}([A])$ the spectrum of $[A] \in \mathbb{M}_q^S(\mathbb{R})$ ($q = 2$ hereinafter).

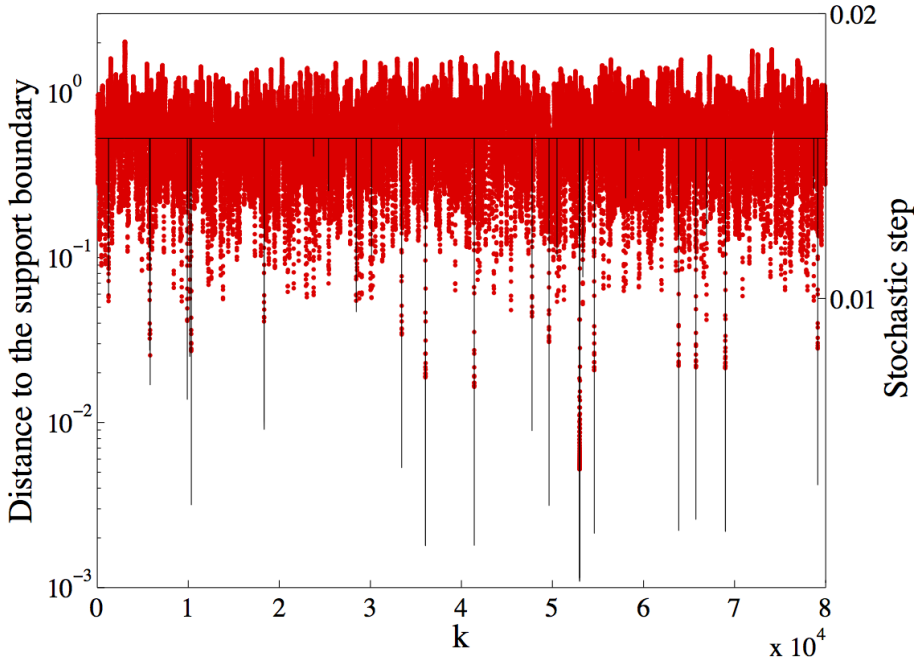


FIGURE 9: Sample paths of $\{\rho^k, k \geqslant k_{stat}\}$ (red circles, left axis) and $\{\widetilde{\gamma}^k, k \geqslant k_{stat}\}$ (black line, right axis), obtained for $\epsilon = 0.01$, $\gamma^0 = 2^{-6}$ and $\tau = 10^6$.

Concluding comments

Construction of random field models that are consistent with mathematics and physics :

- based on Information Theory ;
- for Darcean flows through porous media, it allows for the local architecture of the pore space to be accounted for (at least to some extent).

Some parts of the model

- were revisited using a transformation with memory,
- and involve an adaptive procedure.

Numerical investigations on permeability fields are currently under progress.

– Thank You –