Identification de paramètres dans un problème d'homogénéisation aléatoire

Frédéric Legoll

ENPC (Navier) et INRIA (équipe MATHERIALS)

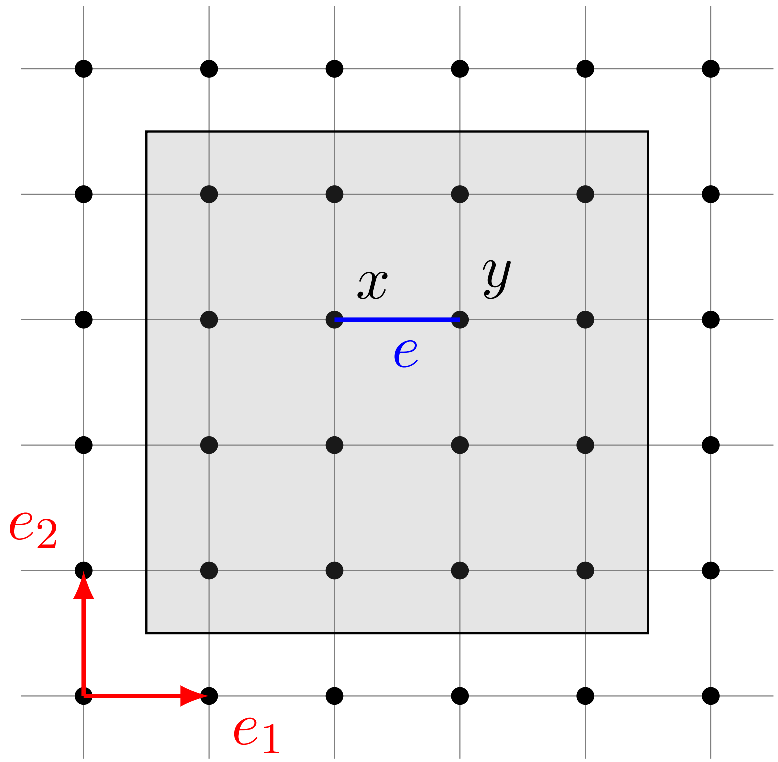
avec W. Minvielle (ENPC et INRIA),
A. Obliger (Paris 6, physique), M. Simon (ENS Lyon)
et le soutien financier de NEEDS

Journées annuelles NEEDS 2014

Nantes, 21–22 octobre 2014

Motivation: subsurface modelling (courtesy PECSA Paris 6)

Fluid and/or molecular diffusion in clay is often modelled using the so-called Pore Network Model:



Discrete elliptic equation (on $\mathbb{Z}^d$) with random coefficients:

$$-\text{div}\left[A\left(\frac{x}{\varepsilon},\omega\right)\nabla u^{\varepsilon}\right] = f \qquad \text{(Darcy law, } u^{\varepsilon} \equiv \text{pressure)}$$

Random homogenization: theory

$$-\text{div}\left[A\left(\frac{x}{\varepsilon},\omega\right)\nabla u^\varepsilon\right]=f \quad \text{in } \mathcal{D}, \qquad u^\varepsilon=0 \text{ on } \partial\mathcal{D}, \qquad A \text{ stat. homog.}$$

$u^\varepsilon(\cdot,\omega)$ converges (almost surely) to $u^\star$ solution to

$$-\text{div}\left[A^\star\nabla u^\star\right]=f \quad \text{in} \quad \mathcal{D}, \qquad u^\star=0 \text{ on } \partial\mathcal{D},$$

where the homogenized matrix $A^\star$ is

- constant, deterministic,
- theory provides a formula, but challenging to compute!

Review article: A. Anantharaman et al, in Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, volume 22, 197-272 (2011), W. Bao and Q. Du eds.

Random homogenization: standard approximation procedure

- Solve the corrector problem on a large but finite domain (RVE):

$$\begin{cases} -\text{div}\left[A(y,\omega)\left(p + \nabla w_p^N(y,\omega)\right)\right] = 0, \\ w_p^N \quad \text{is } Q_N\text{-periodic}, \quad Q_N = (-N,N)^d. \end{cases}$$

- Approximate (apparent) homogenized matrix:

$$\forall p \in \mathbb{R}^d, \quad A_N^\star(\omega)p = \frac{1}{|Q_N|}\int_{Q_N} A(y,\omega)\,\left(p + \nabla w_p^N(y,\omega)\right)\,dy$$

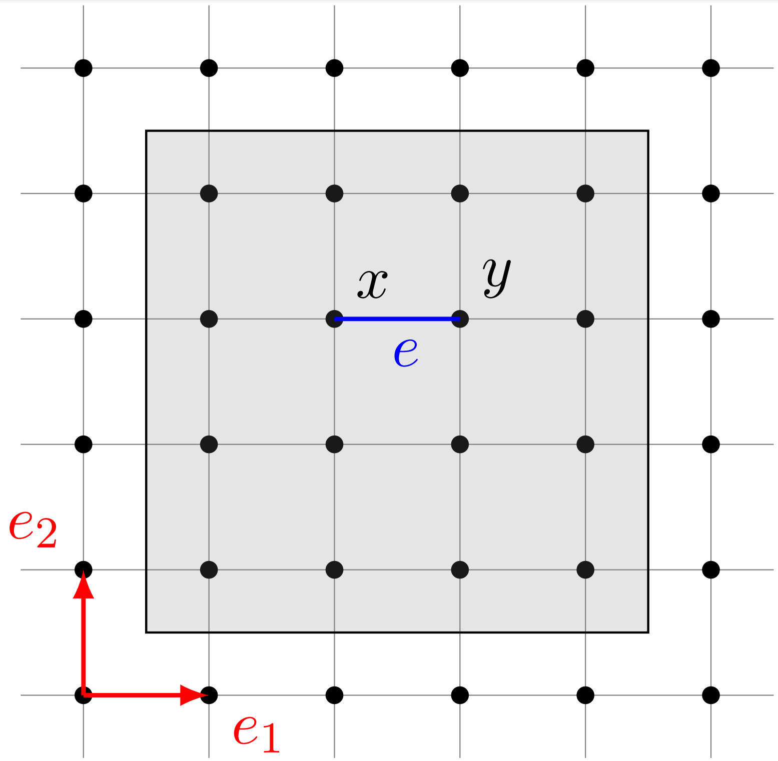
With mechanics notation: $A_N^\star \langle \text{Strain} \rangle_N = \langle \text{Stress} \rangle_N$.

- Due to numerical truncation, $A_N^\star$ is random! Hence Monte Carlo approaches . . .

Bourgeat & Piatnitski, 2004: $\lim_{N\to\infty} A_N^\star(\omega) \to A^\star$ a.s.

A parameter fitting problem in random homogenization

F.L., W. Minvielle, A. Obliger and M. Simon, to appear in ESAIM Proceedings (arxiv 1402.0982)



Darcy law: discrete elliptic equation with random coefficients:

$$\nabla_\varepsilon^\star \left[A\left(\frac{x}{\varepsilon}, \omega\right) \nabla_\varepsilon u^\varepsilon \right] = f \text{ in } \mathcal{D} \cap \varepsilon \mathbb{Z}^d \quad \to \quad -\text{div}\left[A^\star \nabla u^\star\right] = f \text{ in } \mathcal{D}$$

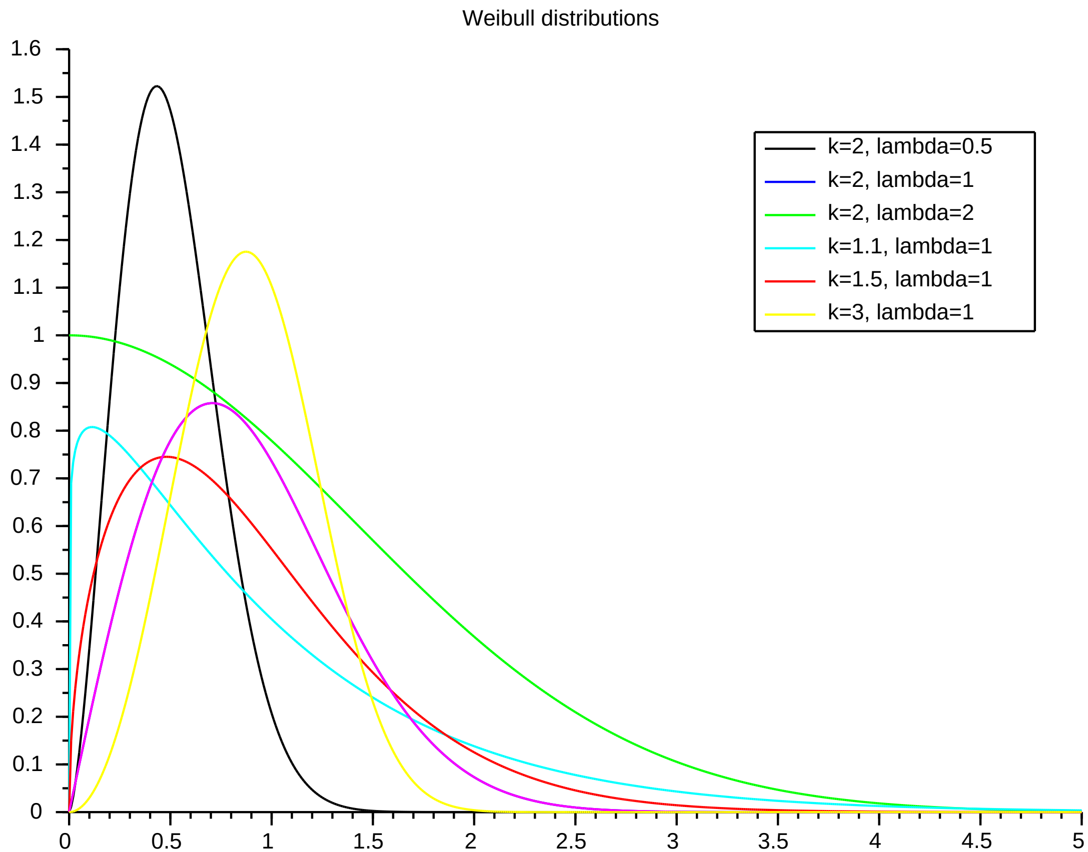
The permeability A is defined on each edge.

∇_ε: discrete gradient

Modelling - 1

Diameters d of channels are random, i.i.d., and distributed according to a Weibull law: $d \sim W(\lambda, k)$, i.e.

$$d(\omega) = \lambda\Big(-\ln(1 - u(\omega))\Big)^{1/k}, \quad u(\omega) \sim \mathcal{U}(0,1)$$



Modelling - 2

- On each edge e, permeability
  $A(e,\omega) = (d_e(\omega))^4 = (\text{edge diameter})^4$,
  $$d(\omega) = \lambda\Big(-\ln(1-u(\omega))\Big)^{1/k}, \quad u(\omega) \sim \mathcal{U}(0,1)$$
- On $\mathbb{Z}^d$, the permeability is given by
  $$A(\cdot,\omega) = \mathcal{A}\Big(\lambda, k, \{u_k(\omega)\}_{k\in\mathbb{Z}^d}\Big), \qquad u_k(\omega) \text{ i.i.d. and } \sim \mathcal{U}(0,1)$$

Modelling - 2

- On each edge e, permeability
  $A(e,\omega) = (d_e(\omega))^4 = (\text{edge diameter})^4$,

$$d(\omega) = \lambda \Big(-\ln(1-u(\omega)) \Big)^{1/k}, \quad u(\omega) \sim \mathcal{U}(0,1)$$

- On $\mathbb{Z}^d$, the permeability is given by

$$A(\cdot,\omega) = \mathcal{A}\Big(\lambda, k, \{u_k(\omega)\}_{k\in\mathbb{Z}^d}\Big), \qquad u_k(\omega) \text{ i.i.d. and } \sim \mathcal{U}(0,1)$$

- Forward problem: given (λ, k), and hence the microscopic permeability $A(\cdot,\omega)$, compute
  - the macroscopic (homogenized) permeability $\mathbb{E}\left[A_N^\star\right]$
  - its relative variance

$$\mathbb{V}\mathrm{arR}[A_N^\star] = \frac{\mathbb{V}\mathrm{ar}[A_N^\star]}{(\mathbb{E}[A_N^\star])^2}$$

Choice of observed quantities

- Forward problem: given (λ, k), compute
  - the macroscopic (homogenized) permeability $\mathbb{E}\left[A_N^\star\right]$
  - its relative variance
$$\mathbb{V}\mathrm{arR}[A_N^\star] = \frac{\mathbb{V}\mathrm{ar}[A_N^\star]}{(\mathbb{E}[A_N^\star])^2}$$
- Inverse problem: given observed $\mathbb{E}\left[A_N^\star\right]$ and $\mathbb{V}\mathrm{arR}[A_N^\star]$, find the parameters (λ, k).

Choice of observed quantities

- Forward problem: given (λ, k), compute
  - the macroscopic (homogenized) permeability $\mathbb{E}\left[A_N^\star\right]$
  - its relative variance

$$\mathbb{V}\mathrm{arR}[A_N^\star] = \frac{\mathbb{V}\mathrm{ar}[A_N^\star]}{(\mathbb{E}[A_N^\star])^2}$$

- Inverse problem: given observed $\mathbb{E}\left[A_N^\star\right]$ and $\mathbb{V}\mathrm{arR}[A_N^\star]$, find the parameters (λ, k).

- It turns out that knowing $\mathbb{E}\left[A_N^\star\right]$ and $\mathbb{V}\mathrm{arR}[A_N^\star]$ uniquely determine (λ, k), at least in 1D, in the limit $N \to \infty$:

$$A^\star = \lambda\, \Gamma_1(k), \quad \mathbb{V}\mathrm{arR}[A_N^\star] \sim \frac{1}{N}\Gamma_2(k)$$

Formulation of the problem - ideal case

Ideal functional:

$$F_N(\lambda,k) = \left(\frac{\mathbb{E}\left[A_N^\star(\lambda,k)\right]}{A^\star_{\text{obs}}} - 1\right)^2 + \left(\frac{\mathbb{V}\text{arR}[A_N^\star(\lambda,k)]}{V_{\text{obs}}} - 1\right)^2$$

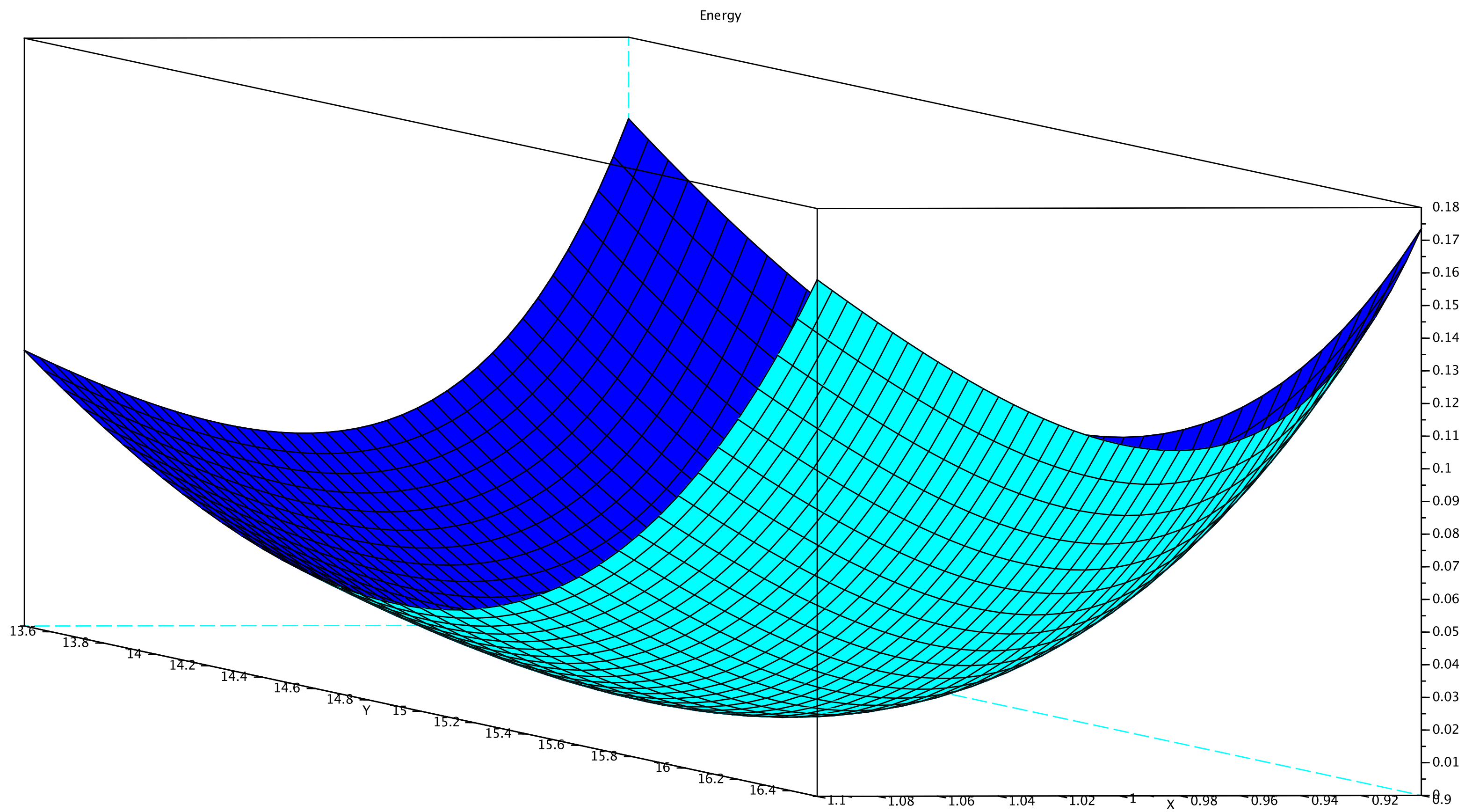
- $A^\star_{\text{obs}}$ is the observed macro permeability, i.e. $\mathbb{E}\left[A_N^\star(\lambda_{\text{obs}},k_{\text{obs}})\right]$
- V_{obs} is the observed relative variance, i.e. $\mathbb{V}\text{arR}[A_N^\star(\lambda_{\text{obs}},k_{\text{obs}})]$

Remark: we assume to know N!

We are looking for global / local minimizers of F_N.

- $F_\infty(\lambda,k) := \lim_{N\to\infty} F_N(\lambda,k)$
- Lemma: in 1D, $F_\infty(\lambda,k)$ has a unique minimizer, $(\lambda_{\text{obs}},k_{\text{obs}})$.

Functional F_∞ *to minimize with* $(\lambda_{\text{obs}}, k_{\text{obs}}) = (1; 15)$



$F_\infty(\lambda, k)$ for $\lambda \in [1 \pm 10\%]$, $k \in [15 \pm 10\%]$.

F_∞ is not convex on $(0, \infty)^2$, but α-convex close to $(\lambda_{\text{obs}}, k_{\text{obs}})$

Formulation of the problem - practical case

In practice, noise:

$$\mathbb{E}\left[A_N^\star(\lambda,k)\right] \approx A_{N,M}^\star(\lambda,k;\omega) := \frac{1}{M}\sum_{m=1}^{M} A_N^\star(\omega_m,\lambda,k)$$

and likewise for $\mathbb{V}\mathrm{arR}[A_N^\star(\lambda,k)]$, approximated by $V_{N,M}(\lambda,k;\omega)$.

Practical formulation: Find (λ,k) minimizing

$$F_{N,M}(\lambda,k;\omega) = \left(\frac{A_{N,M}^\star(\lambda,k;\omega)}{A_{\mathrm{obs}}^\star} - 1\right)^2 + \left(\frac{V_{N,M}(\lambda,k;\omega)}{V_{\mathrm{obs}}} - 1\right)^2$$

For the numerical tests: $A_{\mathrm{obs}}^\star = A_{N,M}^\star(\lambda_{\mathrm{obs}},k_{\mathrm{obs}};\overline{\omega})$ and likewise for V_{obs}.

Optimization algorithm

Recall that

$$d(\omega) = \lambda\Big(- \ln(1 - u(\omega))\Big)^{1/k}, \quad u(\omega) \sim \mathcal{U}(0,1)$$

and $A(e,\omega) = d_e(\omega) =$ edge diameter. Therefore, on $\mathbb{Z}^d$,

$$A(\cdot,\omega) = \mathcal{A}\Big(\lambda, k, \{u_k(\omega)\}_{k\in\mathbb{Z}^d}\Big), \qquad u_k(\omega) \text{ i.i.d. and } \sim \mathcal{U}(0,1)$$

where $\mathcal{A}$ is deterministic and its derivatives wrt λ, k are easy to compute.

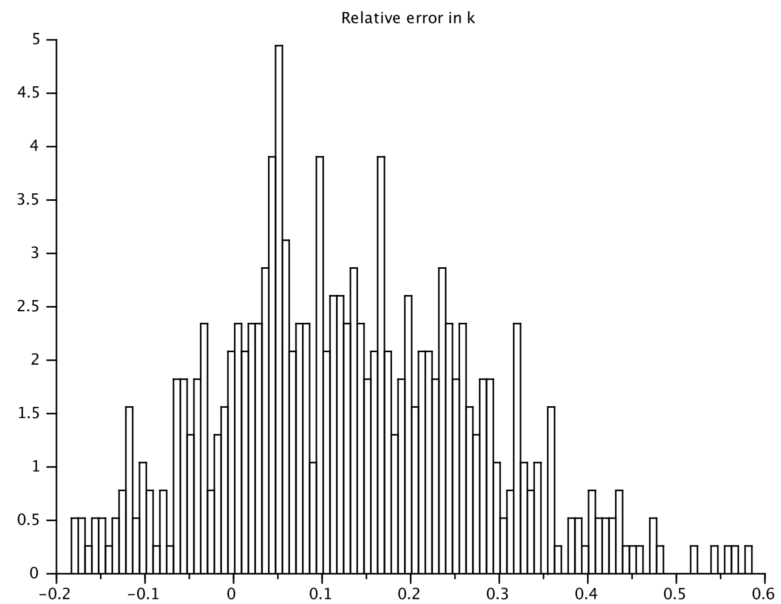
- To compute the first derivative of $A_N^\star(\lambda,k;\omega)$, only w_p^N is needed (Hellmann-Feynman type result)
- Newton algorithm: to compute the second derivatives of $A_N^\star(\lambda,k;\omega)$, we need $\dfrac{\partial w_p^N}{\partial \lambda}$ and $\dfrac{\partial w_p^N}{\partial k}$, that solve auxiliary PDEs.

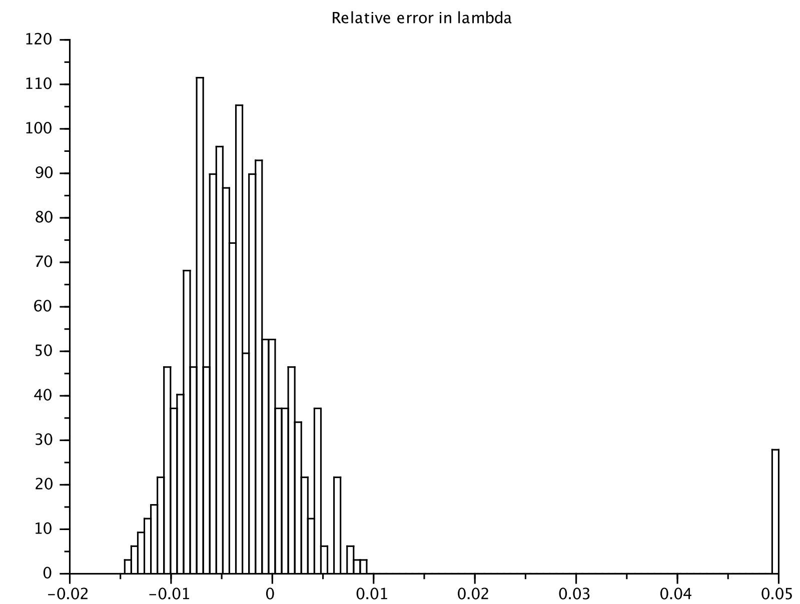
Numerical results

- Set $(\lambda_{\rm obs}, k_{\rm obs}) = (1; 15)$
- Set $A^\star_{\rm obs} = A^\star_{N,M}(\lambda_{\rm obs}, k_{\rm obs}; \overline{\omega}) \approx \mathbb{E}\left[A^\star_N(\lambda_{\rm obs}, k_{\rm obs})\right]$
- Run a Newton algorithm on $F_{N,M}(\lambda, k; \omega)$,
  - starting from an initial guess 10% off $(\lambda_{\rm obs}, k_{\rm obs})$,
  - using a realization ω different from $\overline{\omega}$.
  - we hence obtain $\lambda_{\rm opt}(\omega)$ and $k_{\rm opt}(\omega)$.
- Start again with other realizations ω to obtain histograms

2D numerical simulations, with the limited values $N = 10$ (RVE size is 10×10) and $M = 30$ Monte Carlo realizations.

Numerical results (2D: $N = 10$ and $M = 30$)





Despite the limited values of N and M,
we obtain meaningful values of $(\lambda_{\text{opt}}, k_{\text{opt}})$.

Results $(\lambda_{\text{opt}}, k_{\text{opt}})$ are noisy because M is finite.

Noise in ($\sim \mathbb{V}\text{arR}\left[A^{\star}_{N,M}\right]$) $\approx$ Noise out ($\sim \mathbb{V}\text{arR}\left[\lambda_{\text{opt}}\right]$)

Conclusions

- Observing several realizations of $A_N^\star$, we can estimate its expectation $\mathbb{E}\left[A_N^\star\right]$ and its relative variance
- Using these two macro observables, possible to identify the micro parameters (λ, k) by a least-square procedure
- Can be generalized to continuous (i.e. not discrete) PDEs

- Use better (low variance) estimators of $\mathbb{E}\left[A_N^\star\right]$?
- Knowing several realizations of $A_N^\star$, is it possible to use more than the first two moments (expectations and variance)?
- Robustness wrt observed values $A_{\text{obs}}^\star$ and V_{obs}?

F.L., W. Minvielle, A. Obliger and M. Simon, ESAIM Proc. (arxiv 1402.0982)