A parameter identification problem in stochastic homogenization

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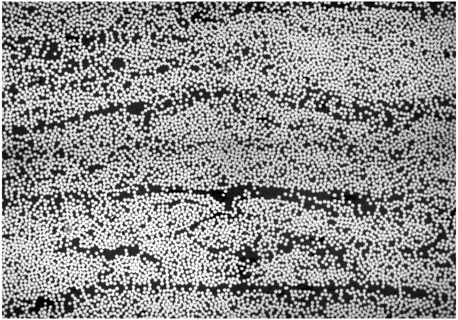
Multiscale materials often leads to very expensive computations, and practical difficulties.

We consider a simple (linear) problem for a complex materials:

$$\begin{cases} -\text{div}\ [A_\varepsilon(x)\nabla u^\varepsilon(x)] = f(x) \quad x \in \mathcal{D} \subset\subset \mathbb{R}^d, \\ u_\varepsilon = 0 \quad \partial\mathcal{D}. \end{cases}$$



Airplane wing.

Courtesy M. Thomas and EADS

$$\boxed{-\text{div}\ \left(A_{\varepsilon}(x)\nabla u^{\varepsilon}\right) = f \quad \text{in} \quad \mathcal{D}, \qquad u^{\varepsilon} = 0 \quad \text{on} \quad \partial\mathcal{D}}$$

Application	A_{ε}	u^{ε}	f
Elasticity	elastic moduli	displacement	mechanical load
Thermal conductivity	thermal conductivity	temperature	heat source
Electrostatics	permittivity	electric potential	charge density
Darcy flow	flow conductivity	pressure	sources

Consider $A(y)$ a $\mathbb{Z}^d$-periodic matrix field.

$$-\text{div}\left(A\left(\frac{x}{\varepsilon}\right)\nabla u^{\varepsilon}\right) = f \quad \text{in} \quad \mathcal{D}, \quad u^{\varepsilon} = 0 \quad \text{on} \quad \partial\mathcal{D} \tag{1}$$

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This difficult oscillatory problem homogenizes to:

$$-\text{div}\,(A^{\star}\nabla u^{\star}) = f \quad \text{in} \quad \mathcal{D}, \quad u^{\star} = 0 \quad \text{on} \quad \partial\mathcal{D}, \tag{2}$$

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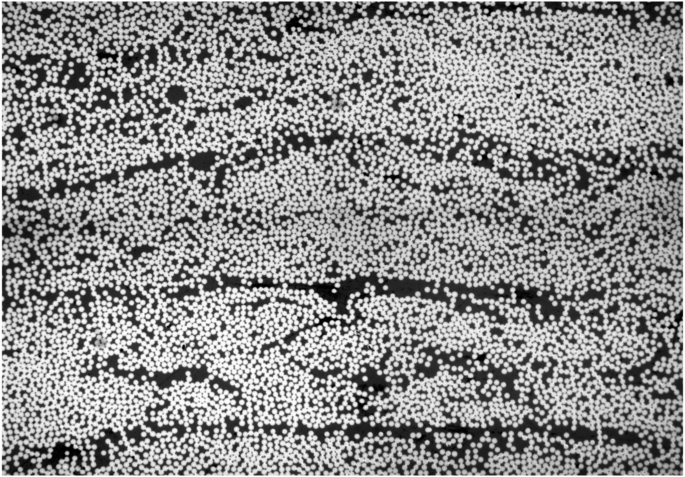
The homogenized matrix $A^\star$ is defined by an average in the unit cell $Q = (0,1)^d$ involving so-called correctors functions w:

$$\boxed{A^\star e_j = \int_Q A(x)\ \left(\nabla w_{e_j}(x) + e_j\right)\,dx,} \tag{3}$$

and the (easy) corrector equation reads:

$$\begin{cases} -\text{div}\ \left[A(\nabla w_p + p)\right] = 0 \quad \text{on } \mathbb{R}^d, \\ \nabla w_p \quad \text{periodic,} \ \displaystyle\int_Q \nabla w_p = 0. \end{cases} \tag{4}$$



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and the corrector equation, in $\mathbb{R}^d$, reads, for any $p\in\mathbb{R}^d$:

$$\begin{cases} -\operatorname{div}\ [A(\nabla w_p+p)]=0 \quad \text{in } \mathbb{R}^d \ \text{ a.s.,} \\ \nabla w_p \text{ stationary,} \ \displaystyle\int_Q \mathbb{E}[\nabla w_p]=0. \end{cases}$$

Note that $A^{\star}$ (and hence $u^{\star}$) is deterministic.

In practice, truncate over $Q_N := (0, N)^d$:

$$- \operatorname{div} \left[A(\nabla w_p^N + p) \right] = 0 \quad \text{in } Q_N \quad \text{a.s.}, \qquad w_p^N \quad Q_N - \text{periodic}.$$

$$A_N^\star(\omega) e_j := \frac{1}{|Q_N|} \int_{Q_N} A(y,\omega)(e_j + \nabla w_{e_j}^N(y,\omega))\, dy.$$

For that reason alone, randomness comes again in the picture.

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In the sequel, we focus on computing $\mathbb{E}[A_N^\star]$.

Introduce the estimator $\mathcal{I}_M^{MC} := \frac{1}{M}\sum_{m=1}^{M} A_N^\star(\omega_m)$, where (ω_m) are i.i.d.

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$$\boxed{A^\star - \mathcal{I}_M^{MC} = A^\star - \mathbb{E}[A_N^\star] + \mathbb{E}[A_N^\star] - \mathcal{I}_M^{MC}} \tag{5}$$

The bias error is often small. The statistical error is *controlled by the variance*. Variance reduction approaches are useful to reduce the error.

$$\boxed{\left|\mathbb{E}[A_N^\star] - \mathcal{I}_M^{MC}\right| \leq 1.96 \frac{\sqrt{\mathbb{V}\text{ar}[A_N^\star]}}{\sqrt{M}}}$$

F. Legoll and WM *A control variate approach based on a defect-type theory for variance reduction in stochastic homogenization*, 2014, Submitted. ArXiv 1407.8029

An inverse problem in stochastic homogenization

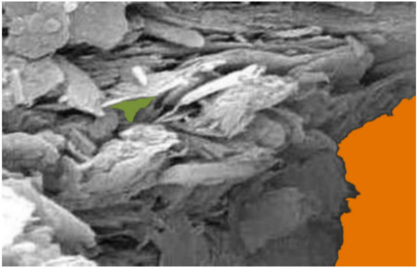
joint work with

F. Legoll, A. Obliger, M. Simon.

F. Legoll, W.M., A. Obliger, M. Simon. A parameter identification problem in stochastic homogenization, 2014, arXiv 1402.0982. Accepted in ESAIM:ProcS.

Subsurface modeling (Courtesy PECSA, Paris VI)

Diffusion in clay modeled by the so-called Pore Network Model.



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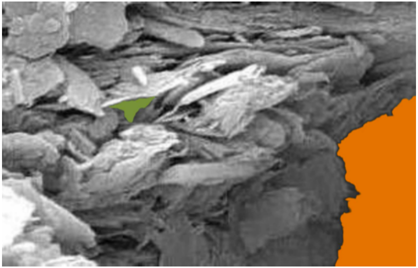

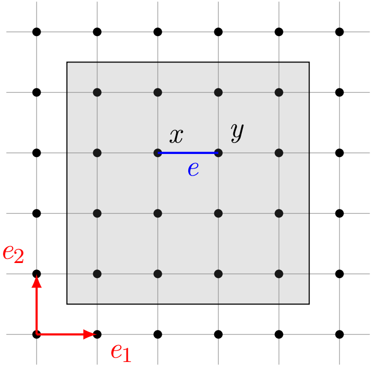

Discrete elliptic equation $\quad -\mathrm{div}\left[A(\frac{x}{\varepsilon},\omega)\nabla u_\varepsilon\right] = f$

Can we recover some microscopic quantities

on the basis of

a few macroscopic quantities?

Modelling:

- Diameters of channel: Weibull law $d_e \sim W(\lambda, k)$ i.i.d.
- Conductance: $A(x,\omega) = diag((d^4_{x,x+e_j}(\omega))_{j\in\{1,\dots,d\}})$.

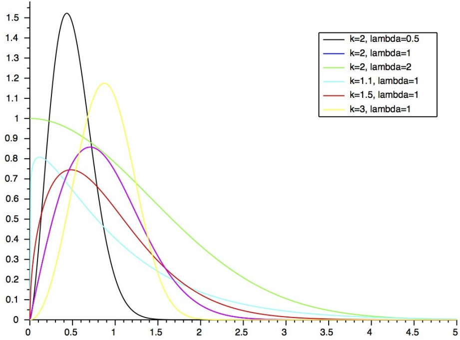

Figure 1 : Weibull distributions.

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Forward problem: given $A(\cdot,\omega)$, compute

- Macroscopic permeability $A^\star_N(\omega)$.
- Macroscopic variance $\mathbb{V}\mathrm{ar}[A^\star_N]$.

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Inverse problem: given observed $A^\star_N$ and $\mathbb{V}\mathrm{ar}[A^\star_N]$, find λ, k.

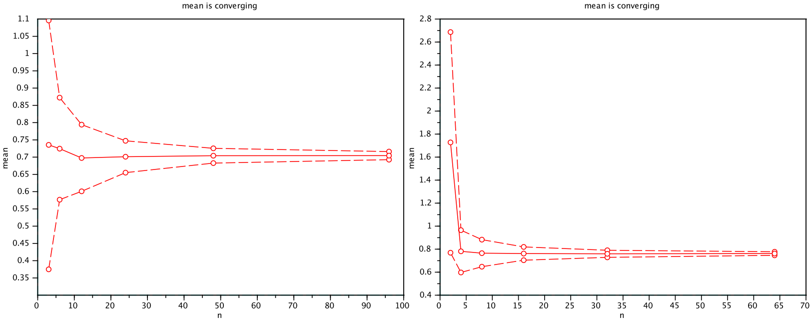

Figure 1 : For two choices of (λ, k), convergence of $\mathbb{E}[A_N^\star]$ wrt $|Q_N|$
Continuous line: empirical mean.
Dashed line: confidence intervals.

$$\left|\mathbb{E}[A_N^\star] - \mathcal{I}_M^{MC}\right| \leq 1.96 \frac{\sqrt{\mathbb{V}\mathrm{ar}[A_N^\star]}}{\sqrt{M}}$$

A minimization problem

A_{obs}: observed macroscopic *permeability*.
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Fix M realizations $\omega = (\omega_m)_{m \in \{1,\dots,M\}}$.

Problem: Find (λ, k) which minimizes F_M:

$$\boxed{F_M(\lambda, k; \omega) := \left(\frac{\mathcal{I}_M^{MC}(\omega)}{A_{obs}} - 1 \right)^2 + \left(\frac{V_M^{MC}(\omega)}{V_{obs}} - 1 \right)^2,}$$

where $\mathcal{I}_M^{MC}(\omega) := \frac{1}{M} \sum_{m=1}^{M} A_N^\star(\omega_m)$, $V_M^{MC}(\omega) := \mathbb{V}\mathrm{arR}^M[A_N^\star](\omega)$.

with $\quad \mathbb{V}\mathrm{arR}^M[A_N^\star](\omega) := \dfrac{\frac{1}{M}\sum_{m=1}^{M}\left(A_N^\star(\omega_m) - \mathcal{I}_M^{MC}(\omega)\right)^2}{\mathcal{I}_M^{MC}(\omega)^2}$

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Newton algorithm (Derivatives of $F_M \Rightarrow$ OK!)

1D

- Homogenization ⇒ OK!
- Minimization problem ⇒ Well posed!
- Numerics ⇒ Easy!

1D

- Homogenization $\Rightarrow$ OK!
- Minimization problem $\Rightarrow$ Well posed!
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2D

- Homogenization $\Rightarrow$ OK.
- Minimization problem $\Rightarrow$ Theoretically unknown
- Numerics $\Rightarrow$ More difficult

Landscape - Overview

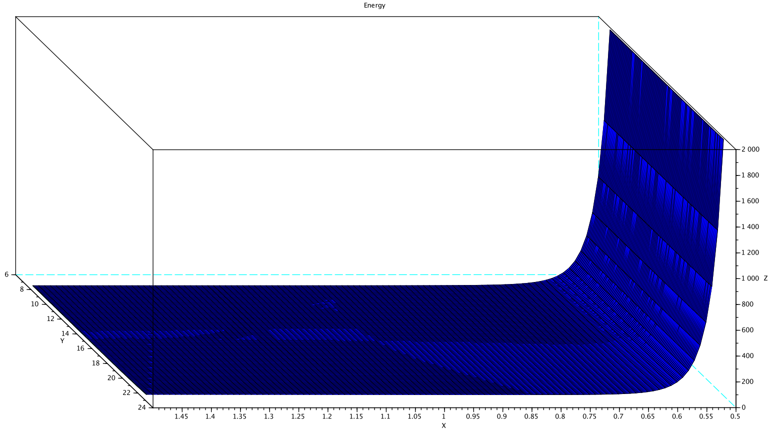

Figure 2 : $F(\lambda, k)$ for $\lambda \in [1 \pm 50\%]$, $k \in [15 \pm 50\%]$.

Landscape - Close-up

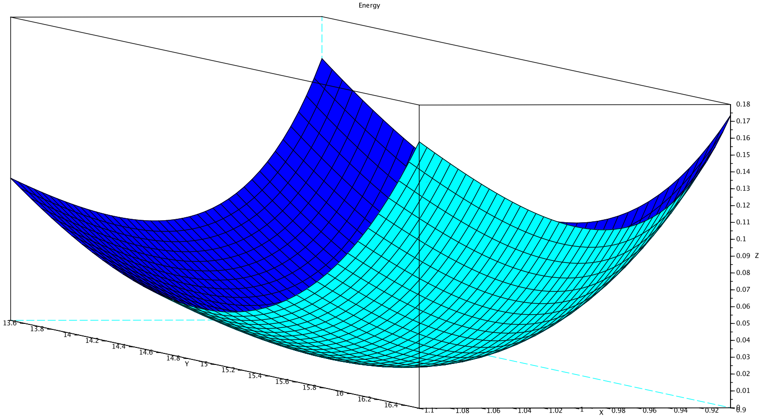

Figure 3 : $F(\lambda, k)$ for $\lambda \in [1 \pm 10\%]$, $k \in [15 \pm 10\%]$.

Forward problem: statistical error

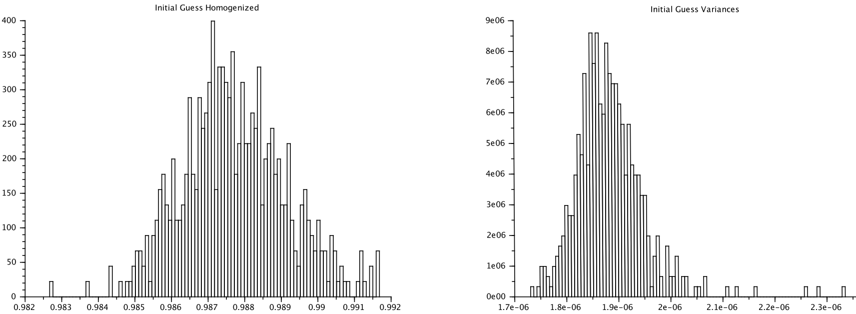

Figure 4 : Left: $A_N^\star$, right: $\mathbb{V}\mathrm{arR}[A_N^\star]$ $(k^\star = 15;\ \lambda^\star = 1)$.

Random environment

- Compute a numerical target A_{obs}, V_{obs} with $\lambda = 1$, $k = 15$
- Run Newton
  - Starting from an initial guess 10% off,
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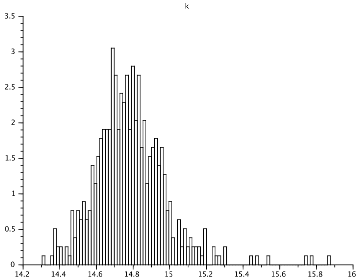

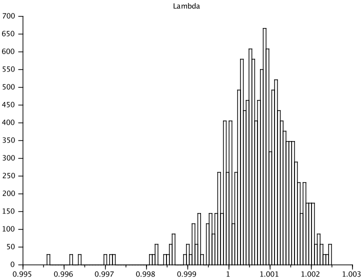

Figure 5 : Absolute error ($k^{\star} = 15$; $\lambda^{\star} = 1$).

- Forward problem statistical error:

$$\mathbb{V}\mathrm{arR}\left[A_N^\star(\lambda^\star, k^\star)\right] \approx 1.4\, 10^{-6} \qquad \mathbb{V}\mathrm{arR}\left[V_M^{MC}(\lambda^\star, k^\star)\right] \approx 10^{-3},$$

- Inverse problem error:

$$\mathbb{V}\mathrm{arR}[\lambda_{\mathrm{opt}}] \approx 7.9\ 10^{-7} \quad \mathbb{V}\mathrm{arR}[k_{\mathrm{opt}}] \approx 1.7\ 10^{-4}.$$

Accurate determination of the best λ, k.

2D Preliminary results

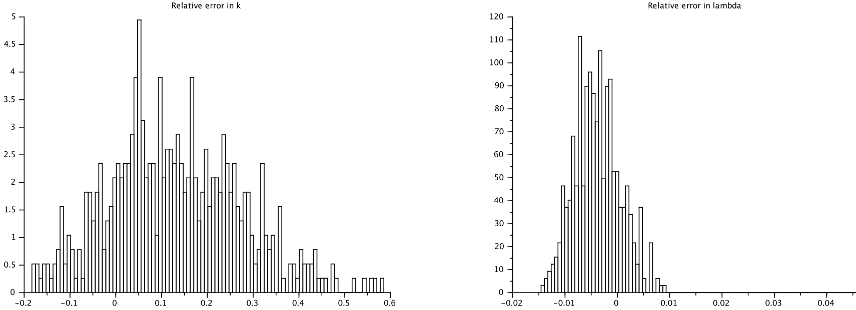

Figure 6 : Relative error ($k^\star = 15$; $\lambda^\star = 1$).

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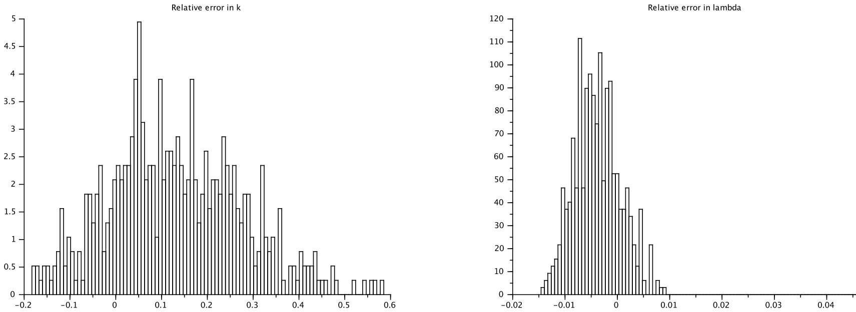

Figure 6 : Relative error ($k^\star = 15$; $\lambda^\star = 1$).

With low values of N, M ($N = 10,\ M = 30$!) we still get meaningful values of λ, k.

Conclusion

Future work: extension to the 2D case

- Homogenization with unbounded coefficients:
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Numerical issues

- Tradeoff between N (RVE size) and M (# realizations)?