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:

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

Airplane wing. 

Courtesy M. Thomas and EADS
An introduction to homogenization

Setting

Least square formulation

Multiscale materials

Truncation

\[-\text{div} \left( A_\varepsilon(x) \nabla u_\varepsilon \right) = f \text{ in } \mathcal{D}, \quad u_\varepsilon = 0 \text{ on } \partial \mathcal{D}\]

<table>
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<th>Application</th>
<th>$A_\varepsilon$</th>
<th>$u_\varepsilon$</th>
<th>$f$</th>
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<td>flow conductivity</td>
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Consider $A(y)$ a $\mathbb{Z}^d$-periodic matrix field.

$$-\text{div} \left( A \left( \frac{x}{\varepsilon} \right) \nabla u^\varepsilon \right) = f \quad \text{in} \quad D, \quad u^\varepsilon = 0 \quad \text{on} \quad \partial D \quad (1)$$
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This difficult oscillatory problem homogenizes to:

\[-\text{div} \left( A^* \nabla u^* \right) = f \quad \text{in} \quad D, \quad u^* = 0 \quad \text{on} \quad \partial D, \quad (2)\]
Consider \( A(y) \) a \( \mathbb{Z}^d \)-periodic matrix field.

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(1)

This difficult oscillatory problem homogenizes to:

\[
- \text{div} \ (A^* \nabla u^*) = f \quad \text{in} \ D, \quad u^* = 0 \quad \text{on} \ \partial D, 
\]  

(2)

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

\[
A^* e_j = \int_Q A(x) \left( \nabla w_{e_j}(x) + e_j \right) dx, 
\]  

(3)

and the (easy) corrector equation reads:

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

(4)
An introduction to homogenization

Setting

Least square formulation

Multiscale materials

Truncation

Courtesy M. Thomas and EADS
Consider $A(y, \omega)$ a stationary matrix field.

$$- \text{div} \left( A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^{\varepsilon} \right) = f \text{ in } \mathcal{D}, \quad u^{\varepsilon} = 0 \text{ on } \partial \mathcal{D}.$$
Consider \( A(y, \omega) \) a stationary matrix field.

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- \text{div} \left( A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u^\varepsilon \right) = f \quad \text{in} \quad \mathcal{D}, \quad u^\varepsilon = 0 \quad \text{on} \quad \partial \mathcal{D}.
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where $A^*$ is defined by:

$$A^* e_j = \int_Q \mathbb{E} \left[ A(y, \cdot) \left( \nabla w_{e_j}(y, \cdot) + e_j \right) \right] \, dy,$$
Consider $A(y, \omega)$ a stationary matrix field.

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

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$$A^* e_j = \int_Q \mathbb{E} \left[ A(y, \cdot) \left( \nabla w_{e_j}(y, \cdot) + e_j \right) \right] \, dy,$$

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

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

Note that $A^*$ (and hence $u^*$) is deterministic.
In practice, truncate over $Q_N := (0, N)^d$:

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

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

For that reason alone, randomness comes again in the picture.
In practice, truncate over $Q_N := (0, N)^d$:

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

Introduce the estimator $\mathcal{I}_M^{MC} := \frac{1}{M} \sum_{m=1}^{M} A_N^*(\omega_m)$, where $(\omega_m)$ are i.i.d.
In practice, truncate over \( Q_N := (0, N)^d \):

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\[
A^*_N(\omega) e_j := \frac{1}{|Q_N|} \int_{Q_N} A(y, \omega)(e_j + \nabla w^N_{e_j}(y, \omega)) dy.
\]

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In the sequel, we focus on computing \( \mathbb{E}[A^*_N] \).

Introduce the estimator \( I^{MC}_M := \frac{1}{M} \sum_{m=1}^M A^*_N(\omega_m) \), where \( (\omega_m) \) are i.i.d.

\[
A^* - I^{MC}_M = A^* - \mathbb{E}[A^*_N] + \mathbb{E}[A^*_N] - I^{MC}_M
\]

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

\[
|\mathbb{E}[A^*_N] - I^{MC}_M| \leq 1.96 \frac{\sqrt{\text{Var}[A^*_N]}}{\sqrt{M}}
\]

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


Subsurface modeling (Courtesy PECSA, Paris VI)

**Diffusion** in *clay* modeled by the so-called Pore Network Model.
Subsurface modeling (Courtesy PECSA, Paris VI)

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

Discrete elliptic equation

\[-\text{div} \left[ A \left( \frac{x}{\varepsilon}, \omega \right) \nabla u_\varepsilon \right] = f\]
Can we recover some \textit{microscopic quantities} on the basis of a few \textit{macroscopic quantities}?
Modelling:

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

Figure 1 : Weibull distributions.
Modelling:

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

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

- Macroscopic permeability $A_N^*(\omega)$.
- Macroscopic variance $\text{Var}[A_N^*]$. 
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Forward problem: given $A(\cdot, \omega)$, compute
- Macroscopic permeability $A_N^*(\omega)$.
- Macroscopic variance $\text{Var}[A_N^*]$.

Inverse problem: given observed $A_N^*$ and $\text{Var}[A_N^*]$, find $\lambda, k$. 
An introduction to homogenization

Setting

Least square formulation

Physics

Forward problem

Figure 1: For two choices of \((\lambda, k)\), convergence of \(\mathbb{E}[A^*_N]\) wrt \(|Q_N|\).

Continuous line: empirical mean.
Dashed line: confidence intervals.

\[
\left| \mathbb{E}[A^*_N] - \mathcal{I}_{MC}^M \right| \leq 1.96 \frac{\sqrt{\text{Var}[A^*_N]}}{\sqrt{M}}
\]
A minimization problem

\( A_{\text{obs}} \): observed macroscopic permeability.
\( V_{\text{obs}} \): observed relative variance \( \Rightarrow \) \( \text{Var}R[X] := \text{Var}[X]/\mathbb{E}[X]^2 \)
A minimization problem

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Fix \( M \) realizations \( \omega = (\omega_m)_{m \in \{1, \ldots, M\}} \).

Problem: Find \( (\lambda, k) \) which minimizes \( F_M \):

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

where \( \mathcal{I}_M^{MC}(\omega) := \frac{1}{M} \sum_{m=1}^{M} A_N^*(\omega_m), \ V_M^{MC}(\omega) := \text{Var}R^M[A_N^*](\omega) \).

with \( \text{Var}R^M[A_N^*](\omega) := \frac{1}{M} \sum_{m=1}^{M} \left( A_N^*(\omega_m) - \mathcal{I}_M^{MC}(\omega) \right)^2 \frac{\mathcal{I}_M^{MC}(\omega)^2}{\mathcal{I}_M^{MC}(\omega)} \).
A minimization problem

$A_{obs}$: observed macroscopic permeability.
$V_{obs}$: observed relative variance $\Rightarrow \text{Var}_R[X] := \text{Var}[X]/\mathbb{E}[X]^2$

Fix $M$ realizations $\omega = (\omega_m)_{m \in \{1,\ldots,M\}}$.

Problem: Find $(\lambda, k)$ which minimizes $F_M$:

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

where $\mathcal{I}^{MC}_M(\omega) := \frac{1}{M} \sum_{m=1}^M A^*_N(\omega_m), \ V^{MC}_M(\omega) := \text{Var}_R^M[A^*_N](\omega)$.

Newton algorithm (Derivatives of $F_M \Rightarrow$ OK!)
1D

- Homogenization $\Rightarrow$ OK!
- Minimization problem $\Rightarrow$ Well posed!
- Numerics $\Rightarrow$ Easy!
1D

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

2D

- Homogenization ⇒ OK.
- Minimization problem ⇒ Theoretically unknown
- Numerics ⇒ More difficult
Figure 2: $F(\lambda, k)$ for $\lambda \in [1 \pm 50\%], k \in [15 \pm 50\%]$. 

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An inverse problem in stochastic homogenization
An introduction to homogenization

Setting

Least square formulation

Minimization formulation

Numerical results

Landscape - Close-up

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

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An inverse problem in stochastic homogenization
Forward problem: statistical error

Figure 4: Left: $A_N^*$, right: $\text{Var}R[A_N^*]$ ($k^* = 15; \lambda^* = 1$).
Random environment

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

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

Figure 5: Absolute error ($k^* = 15; \lambda^* = 1$).
Forward problem statistical error:

$$\text{Var}_R[A_N^*(\lambda^*, k^*)] \approx 1.4 \times 10^{-6} \quad \text{Var}_R[\mathcal{V}_{MC}^M(\lambda^*, k^*)] \approx 10^{-3},$$

Inverse problem error:

$$\text{Var}_R[\lambda_{\text{opt}}] \approx 7.9 \times 10^{-7} \quad \text{Var}_R[k_{\text{opt}}] \approx 1.7 \times 10^{-4}.$$
2D Preliminary results

Figure 6: Relative error \((k^* = 15; \lambda^* = 1)\).
2D Preliminary results

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

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

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Conclusion

**Future work:** extension to the 2D case

- Homogenization with unbounded coefficients: 
  \[ c \leq A(x, \omega) \leq C \quad \forall x, \omega. \]
- Numerical computations.
Conclusion

Future work: extension to the 2D case

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Modeling issues

- Robustness of the best \((\lambda, k)\) with respect to the observed values \(A_{obs}, V_{obs}\) ?
Conclusion

Future work: extension to the 2D case

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- Numerical computations.

Modeling issues

- Robustness of the best \((\lambda, k)\) with respect to the observed values \(A_{\text{obs}}, V_{\text{obs}}\) ?

Numerical issues

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