Practical computation of homogenized coefficients

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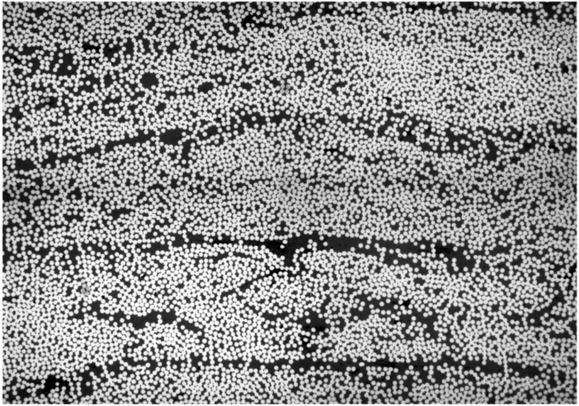
Outline

- Homogenization problem
- Alternative approach: Arlequin method
- Alternative approach: Minimization problem
- Analysis of the approach
- Conclusions

Motivation

How to compute very complex composite materials?



A composite material used in the aeronautics industry, reproduced from Anantharaman, A., Costaouec, R., Bris, C. L., Legoll, F., Thomines, F. (2012)

Homogenization problem

Consider the linear, elliptic problem

$$-\mathrm{div}(A_\varepsilon \nabla u_\varepsilon) = f,$$

where $A_\varepsilon(x)$ is a symmetric definite positive oscillatory matrix-valued coefficient that varies at the characteristic scale ε (and may be random).

We have a sequence of similar problems parametrized by a lengthsclae ε.

Homogenization amounts to perform an asymptotic analysis when $\varepsilon \to 0$:

$$\lim_{\varepsilon \to 0} u_\varepsilon = u^\star.$$

Homogenization problem

If ε is asymptotically small, the solution u_ε can be accurately approximated by the solution to the homogenized problem

$$-\mathrm{div}(A^\star \nabla u^\star) = f.$$

TWO CONNECTED BUT DIFFERENT QUESTIONS:

How to find $u^\star$? How to find $A^\star$?

We know that if A is periodic, then $A\left(\frac{x}{\varepsilon}\right) \xrightarrow[\varepsilon \to 0]{} \langle A \rangle = \frac{1}{|Y|}\int_Y A$ weakly.

First naive idea: $A^\star = \langle A \rangle$?

[1] see, for instance, Anantharaman, A., Costaouec, R., Bris, C. L., Legoll, F., Thomines, F. (2012)

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For convenient A_ε the homogenized coefficient $A^\star$ can be evaluated beforehand by solving the corrector problem (we will see now 2 different examples). However, computing the corrector function (and hence $A^\star$) can be expensive and difficult.

[1] see, for instance, Anantharaman, A., Costaouec, R., Bris, C. L., Legoll, F., Thomines, F. (2012)

Homogenization problem: periodic example

$$\begin{cases} -\operatorname{div}\left(A_{per}\left(\frac{x}{\varepsilon}\right)\nabla u_\varepsilon\right) = f & \text{in } \Omega, \\ u_\varepsilon = 0, & \text{on } \partial\Omega, \end{cases}$$

where a coefficient $A_{per}(y)$ is Y-periodic and satisfies the classical boundedness and coercivity conditions: $\forall \xi \in \mathbb{R}^n$ and for two constants $c_1 > 0$, $c_2 > 0$

$$A_{per}(y)\xi\cdot\xi \geq c_1|\xi|^2, \quad \left|A_{per}(y)\xi\right| \leq c_2|\xi| \qquad \text{a.e. on } \Omega.$$

Corresponding homogenized equation:

$$\begin{cases} -\operatorname{div}(A^\star\nabla u^\star) = f & \text{in } \Omega, \\ u^\star = 0, & \text{on } \partial\Omega, \end{cases}$$

Homogenization problem: periodic example

Periodic checkerboard geometry

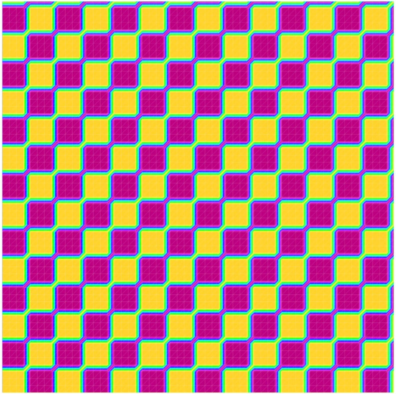


Figure 1: Periodic coefficient A_{per}. Each square is of size $\varepsilon \times \varepsilon$. On the red squares, $A_{per}(x) = 1$. On the yellow squares, $A_{per}(x) = 100$.

Homogenization problem: periodic example

Effective coefficient

$$A^{\star}{}_{ij} = \int_Y [(A_{per}(y)\nabla_y w_i)\cdot e_j + A_{per\,ij}(y)]dy,$$

where w_i is the corrector function that we obtain from the microscopic problem (called the corrector problem in the terminology of homogenization theory):

$$\begin{cases} -\mathrm{div}_y\left(A_{per}(y)\left(e_i + \nabla_y w_i(y)\right)\right) = 0 & \text{in } Y, \\ y \to w_i(y), & Y-\text{periodic}, \end{cases}$$

Homogenization: random problem example

$$\begin{cases} -\mathrm{div}\left(A\left(\frac{x}{\varepsilon},\omega\right)\nabla u_\varepsilon(x,\omega)\right) = f & \text{in } \Omega, \\ u_\varepsilon(x,\omega) = 0, & \text{on } \partial\Omega, \end{cases}$$

where the coefficient A now is random (and as before bounded and coercive).

+ Stationarity: For any $k \in \mathbb{Z}^d$, $A(x,\cdot)$ and $A(x+k,\cdot)$ share the same probability distribution.
+ Ergodic property: space average $\simeq$ average over realizations.

Homogenized problem

$$\begin{cases} -\mathrm{div}(A^\star \nabla u^\star) = f & \text{in } \Omega, \\ u^\star = 0, & \text{on } \partial\Omega, \end{cases}$$

where $A^\star$ is the deterministic and constant homogenized coefficient.

Homogenization: random checkerboard

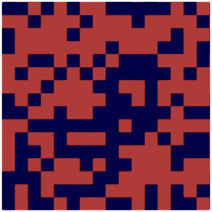


Figure 2: Random coefficient A. Each square is of size $\varepsilon \times \varepsilon$. On the red squares, $a_j(x) = 1$. On the blue squares, $a_j(x) = 100$.

$$A(x,\omega) = \sum_{j \in \mathbb{Z}^2} a_j(\omega)\ 1_{j+Q}(x), \tag{1}$$

where $Q = (0,1)^2$ is the unit square, and where a_j are i.i.d. random variables.

Homogenization: random problem example

Effective coefficient

$$A^{\star}{}_{ij} = \mathbb{E}\left(\int_Q [(A(y,\cdot)\nabla_y w_i(y,\cdot))\cdot e_j + A_{ij}(y,\cdot)]dy\right),$$

where for any $p \in \mathbb{R}^d$ the corrector function w_p is obtained from the microscopic problem:

$$\begin{cases} -\mathrm{div}\left(A(y,\omega)\left(e_i + \nabla w_i(y,\omega)\right)\right) = 0 \quad \text{a.s. in } \mathbb{R}^d, \\ \nabla w_p \text{ is stationary }, \\ \mathbb{E}\left(\int_Q \nabla w_p(y,\cdot)dy\right). \end{cases}$$

$\Rightarrow$ computing the corrector function (and hence $A^{\star}$) can be expensive and difficult.

Motivation for an alternative approach

It is possible to determine $A^\star$ upon solving a minimization problem of the type

$$I_\varepsilon = \inf_{\overline{A} \text{ constant matrix}} \ \sup_{f \text{ of unit norm}} \left\| u(A_\varepsilon, f) - u(\overline{A}, f) \right\|_{L^2}$$

where $u(A_\varepsilon, f)$ and $u(\overline{A}, f)$ respectively denote the solution of the diffusion problem with coefficient matrix A_ε and $\overline{A}$, for the same right-hand side f.

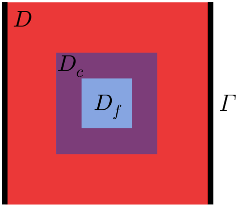
- Le Bris, C.; Legoll F.; Lemaire, S., ESAIM: Control, Optimisation and Calculus of Variations, 24(4), 1345-1380 (2018)

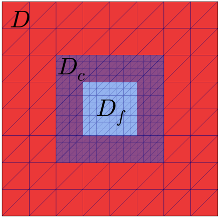
The approach is based upon the theoretical result that as $\varepsilon \to 0$, the minimum of I_ε is achieved at the homogenized matrix $A^\star$. The approach does not require to solve a corrector problem !
A similar idea, based on a minimization problem to capture $A^\star$ is described now.

The Arlequin method

We choose a specific minimization problem based on the Arlequin coupling method:

- Cottereau, R., Int. J. Numer. Methods Eng. 95, No. 1, 71-90 (2013)

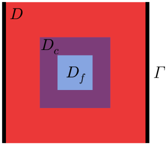




2 models + 3 domains

We have a part of the domain D where only the effective model ($\overline{k}$) is defined, a part of the domain D_f where only the fine model (k_ε) is defined and a part of the domain D_c where both models are defined and over which they are coupled.

Arlequin problem



Consists in considering the following minimization problem:

$$\inf \left\{ \begin{array}{c} \mathscr{E}(\overline{u}, u_\varepsilon), \quad \overline{u} \in H^1(D \cup D_c), \quad \overline{u}(x) = x_1 \text{ on } \Gamma, \\ u_\varepsilon \in H^1(D_c \cup D_f), \quad C(\overline{u} - u_\varepsilon, \phi) = 0 \text{ for any } \phi \in H^1(D_c) \end{array} \right\}, \tag{2}$$

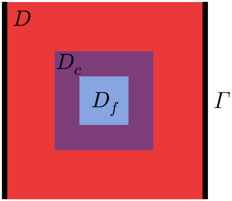
where the energy $\mathscr{E}$ is the sum of the contributions of each of the three subdomains:

$$\begin{aligned} \mathscr{E}(\overline{u}, u) = \frac{1}{2} \int_D \overline{k} \, |\nabla \overline{u}(x)|^2 + \frac{1}{2} \int_{D_f} k_\varepsilon(x) \, |\nabla u_(x)|^2 \\ + \frac{1}{2} \int_{D_c} \Big(\frac{1}{2} \overline{k} \, |\nabla \overline{u}(x)|^2 + \frac{1}{2} k_\varepsilon(x) \, |\nabla u_\varepsilon(x)|^2 \Big). \end{aligned} \tag{3}$$

Arlequin problem

Find $\overline{u} \in V$, $u_\varepsilon \in W$, $\psi \in W^c$ such that

$$\begin{cases} \overline{A}_{\overline{k}}(\overline{u},\overline{v}) + C(\boldsymbol{\psi},\overline{v}) = 0, & \forall \overline{v} \in V|_{\overline{v}(\Gamma)=0}, \\ A_{k_\varepsilon}(\boldsymbol{u}_\varepsilon,\boldsymbol{v}_\varepsilon) - C(\boldsymbol{\psi},\boldsymbol{v}_\varepsilon) = 0, & \forall \boldsymbol{v}_\varepsilon \in W, \\ C(\boldsymbol{\phi},\boldsymbol{u}_\varepsilon - \overline{u}) = 0, & \forall \boldsymbol{\phi} \in W^c. \end{cases} \qquad (*)$$



with $\underline{\overline{u}|_\Gamma = x_1}$ and $V = H^1(D \cup D_c)$, $W = H^1(D_c \cup D_f)$, $W^c = H^1(D_c)$,

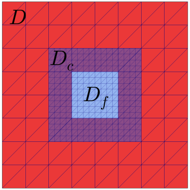
$$\overline{A}_{\overline{k}}(u,v) = \int_D \overline{k} \nabla u \nabla v + \int_{D_c} \frac{1}{2} \alpha_2(x) \overline{k} \nabla u \nabla v,$$

$$A_{k_\varepsilon}(\boldsymbol{u},\boldsymbol{v}) = \int_{D_c} \frac{1}{2} \boldsymbol{k}_\varepsilon \nabla \boldsymbol{u} \nabla \boldsymbol{v} + \int_{D_f} \boldsymbol{k}_\varepsilon \nabla \boldsymbol{u} \nabla \boldsymbol{v},$$

$$C(\boldsymbol{u},\boldsymbol{v}) = \int_{D_c} \nabla \boldsymbol{u} \nabla \boldsymbol{v} + \int_{D_c} \boldsymbol{u}\boldsymbol{v}.$$

Finite element approximation of the Arlequin problem

Find $\overline{u}^H \in V_H$, $u_\varepsilon^h \in W_h$ and $\psi^H \in W_H^c$ such that



$$\begin{cases} \overline{A}_{\overline{k}}(\overline{u}^H, \overline{v}^H) + C(\psi^H, \overline{v}^H) = 0, & \forall \overline{v}^H \in V_H|_{\overline{v}^H(\Gamma)=0}, \\ A_{k_\varepsilon}(u_\varepsilon^h, v_\varepsilon^h) - C(\psi^H, v_\varepsilon^h) = 0, & \forall v_\varepsilon^h \in W_h, \quad (**) \\ C(\phi^H, u_\varepsilon^h - \overline{u}^H) = 0, & \forall \phi^H \in W_H^c. \end{cases},$$

with $\overline{u}^H|_\Gamma = x_1$ and $V_H = \mathbb{P}_H^1(D \cup D_c)$, $W_h = \mathbb{P}_h^1(D_c \cup D_f)$, $W_H^c = \mathbb{P}_H^1(D_c)$. This corresponds to the following linear system:

$$\begin{bmatrix} \overline{A} & 0 & C_M \\ 0 & A_\varepsilon & -C_\varepsilon \\ C_M^T & -C_\varepsilon^T & 0 \end{bmatrix} \begin{bmatrix} \overline{u} \\ u_\varepsilon \\ \psi \end{bmatrix} = \begin{bmatrix} f_M \\ 0 \\ 0 \end{bmatrix}. \tag{4}$$

Minimization problem

Key idea

The solution of the coupled Arlequin problem with the homogenized model ($k^\star$) and the heterogeneous model (k_ε) "=" the solution of the homogenized model ($k^\star$) alone.

Stated otherwise, we consider the minimization problem

$$I_{\varepsilon,H,h} = \inf \left\{ J_{\varepsilon,H,h}(\overline{k}), \quad \overline{k} \in (0,\infty) \right\}, \tag{5}$$

with

$$J_{\varepsilon,H,h}(\overline{k}) = \int_{D \cup D_c} \left| \nabla \overline{u}^H_{\overline{k},k_\varepsilon} - \nabla u_{\text{ref}} \right|^2 = \int_{D \cup D_c} \left| \nabla \overline{u}^H_{\overline{k},k_\varepsilon} - e_1 \right|^2, \tag{6}$$

where we impose $\overline{u}^H_{\overline{k},k_\varepsilon} = x_1$ at the boundary of the "effective" domain D.

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Lemma

If $\overline{k} = k^\star$, then the solution to Arlequin system is $\overline{u}(x) = x_1$ in $D \cup D_c$ and $u_0(x) = x_1$ in $D_c \cup D_f$.
Conversely, if $(\overline{u}, u_0)$ is a solution to Arlequin system with $\overline{u}(x) = x_1$ in $D \cup D_c$, then $u_0(x) = x_1$ in $D_c \cup D_f$ and $\overline{k} = k^\star$.

Consistency

Assume that we are in 1D, $\varepsilon = 0$ and $\overline{k} = k_\varepsilon = k^\star$. If $\overline{u} = x_1$, $u_\varepsilon = x_1$ then the second line of the Arlequin system can be simplified as follows:

$$\frac{1}{2}\int_{D_c} k^\star (v_\varepsilon^h)' + \int_{D_f} k^\star (v_\varepsilon^h)' - \int_{D_c} (\psi^H)'(v_\varepsilon^h)' - \int_{D_c} \psi^H v_\varepsilon^h = 0, \quad \forall v_\varepsilon^h \in W_h.$$

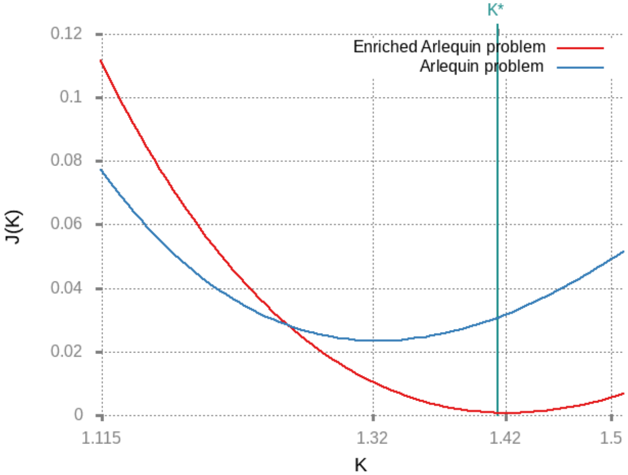
Whence we obtain that ψ^H is the solution of the exact lagrange multiplier problem:

$$\begin{cases} -\Delta\psi + \psi = 0, & \text{in } D_c, \\ \nabla\psi \cdot n = \dfrac{1}{2} k^\star, & \text{on } \partial D_c. \end{cases}$$

Remedy

Insert exact lagrange multiplier in W_H^C space = $\mathrm{W}_H^{enriched}$.

Consistency



Inserting LM in FEM space improves accuracy at no extra cost.

Variational formulation + minimization problem

Find $\overline{u}^H \in V_H^{DirBC}$, $u_\varepsilon^h \in W_h$ and $\psi^H \in W_H^{enrich}$ such that

$$\begin{cases} \forall \overline{v}^H \in V_H^0, & \overline{A}_{\overline{k}}(\overline{u}^H, \overline{v}^H) + C(\overline{v}^H, \psi^H) = 0, \\ \forall v^h \in V_h, & A_{k_\varepsilon}(u_\varepsilon^h, v^h) - C(v^h, \psi^H) = 0, \\ \forall \phi^H \in W_H^{enrich}, & C(\overline{u}^H - u_\varepsilon^h, \phi^H) = 0. \end{cases} \tag{7}$$

+ the minimization problem

$$I_{\varepsilon,H,h} = \inf \left\{ J_{\varepsilon,H,h}(\overline{k}), \quad \overline{k} \in (0,\infty) \right\}, \tag{8}$$

with

$$J_{\varepsilon,H,h}(\overline{k}) = \int_{D \cup D_c} \left| \nabla \overline{u}^H_{\overline{k},k_\varepsilon} - \nabla u_{\mathrm{ref}} \right|^2 = \int_{D \cup D_c} \left| \nabla \overline{u}^H_{\overline{k},k_\varepsilon} - e_1 \right|^2, \tag{9}$$

here e_1 is the first canonical vector.

Mathematical analysis

Following properties of the approach:

(i) for a fixed value of ε, there exists an optimized value of $\overline{k}$, denoted by k_ε^{opt}, where the cost function (3) attains its minimum.

(ii) as $\varepsilon \to 0$, the optimal value k_ε^{opt} converges to the homogenized coefficient $k^\star$.

Conclusions

- Detailed numerical and mathematical analysis of the approach
- Various improvements of the algorithm: post treatment to recover corrector function, selection approach for random realizations, good choice of initial guess [see GLL, 2020].
- More difficult matrix case (in progress)

References

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