Multiscale computing and homogenization

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What is multiscale computing? What is homogenization?

- Homogenization: Spatial averaging
- Periodic media; Random media
- Subspace projection formalism; Issue of oversampling
- Numerical computations using FreeFem++
- Subspace projection with limited oversampling captures homogenization

Spatial averaging

Partial differential equations with rapidly oscillating coefficients, periodic or random, may behave as if they have constant coefficients:

$$-\nabla \cdot (a(x)\nabla u(x)) = f(x) \ , \quad x \in \mathcal{D} \subset R^d \ , \quad u(x) = 0 \ , \quad x \in \partial\mathcal{D}$$

If $a(x)$ varies rapidly with respect to a typical diameter of $\mathcal{D}$ while $f(x)$ is slowly varying, then $u(x)$ behaves like $\bar{u}(x)$ that satisfies

$$-\nabla \cdot (a^H \nabla \bar{u}(x)) = f(x) \ , \quad x \in \mathcal{D} \subset R^d \ , \quad \bar{u}(x) = 0 \ , \quad x \in \partial\mathcal{D}$$

When can this approximation be done?

What is a^H? How can it be computed?

Periodic media

The origins of spatial averaging and homogenization are in the physics of mesoscopic structures and the effective properties of materials.

Homogenization of periodic structures in the seventies: Introduce explicitly the separation of scales with a parameter $\epsilon > 0$ so that $a(x) \to a(\frac{x}{\epsilon})$ and $u(x) \to u^\epsilon(x)$. Prove a theorem: $u^\epsilon(x)$ converges to $\bar{u}(x)$ in L^2 (and in other ways) and a^H can be computed by solving a periodic, "cell", problem which does not depend on $\mathcal{D}$ or f.

Approach: use correctors: $u^\epsilon(x) = \bar{u}(x) + \epsilon\chi(\frac{x}{\epsilon}) \cdot \nabla\bar{u}(x) + e^\epsilon(x)$, where the corrector $\chi(y)$ is periodic and satisfies the cell problem. Show the error $e^\epsilon(x)$ is small in H^1.

Correctors and cell problem

The cell problem is:

$$\nabla_y[a(y)(e_i + \nabla_y \chi_i(y))] = 0 \ , \quad \chi(y) \quad \text{periodic}$$

The effective coefficients a^H in the homogenized problem

$$-\nabla \cdot (a^H \nabla \bar{u}(x)) = f(x) \ , \quad x \in \mathcal{D} \subset R^d \ , \quad \bar{u}(x) = 0 \ , \quad x \in \partial\mathcal{D}$$

are given by $a^H = (a^H_{ij})$ where

$$a^H_{ij} = \left\langle a(y)(e_i + \nabla_y \chi_i(y)) \cdot e_j \right\rangle = \left\langle a(y)(e_i + \nabla_y \chi_i(y)) \cdot (e_j + \nabla_y \chi_j(y)) \right\rangle$$

Random media

Question in mid-seventies: Can homogenization be done with $a(x)$ a stationary random process?

We do not have separation of scales. Role of ϵ.

What should replace the periodic cell problem?

Represent the stationary ergodic diffusion coefficient $a(x,\omega) = \tilde{a}(\tau_x\omega)$ where $(\Omega, \mathcal{F}, P)$ is a probability space, $\omega \in \Omega$.

Assume that $\tau_x \ , \quad x \in R^d$ is a group of measure preserving transformations $\tau_x : \Omega \to \Omega$, $P(\tau_x A) = P(A)$ for $A \in \mathcal{F}$ that acts ergodically.

Assume that $0 < a_0 \leq \tilde{a}(\omega) \leq a_1 < \infty$.

Random PDE:

$$-\nabla\cdot(a(\frac{x}{\epsilon},\omega)\nabla u^\epsilon(x,\omega)) = f(x) \ , \ \ x \in \mathcal{D} \subset R^d \ , \ \ u(x,\omega) = 0 \ , \ \ x \in \partial\mathcal{D}$$

With no other hypotheses we have a homogenization theorem (Papanicolaou and Varadhan 1978; S. Kozlov 1979):

There exists a^H such that

$$\lim_{\epsilon \to 0} E\{\int_{\mathcal{D}} (u^\epsilon(x,\omega) - \bar{u}(x))^2 dx\} = 0$$

The constant, homogenized coefficients a^H solve an abstract "cell" problem now.

Randomness disappears in the limit. We have a new kind of ergodic theorem for nonlinear functionals of the coefficients $\tilde{a}(\omega)$, defined by the PDE, that is, the solution $u^\epsilon(x,\omega)$.

Where is homogenization theory today?

For very few problems is it possible to go from periodic to random without any hypotheses other than stationarity and ergodicity of the coefficients. That is, without any separation of scales hypotheses.

Such problems have special, structural properties such as: divergence form equations, time-reversibility as processes, variational characterizations, etc.

What if correctors cannot be constructed? This happens with the stochastic Hamilton-Jacobi-Bellman equation:

$$u_t(t,x,\omega)+\Delta u(t,x,\omega)+H(x,\nabla u(t,x,\omega),\omega)=0\ ,\ \ t<T\ ,\ \ x\in R^d\ ,\ \ \omega\in\Omega$$

with terminal conditions $u(T,x,\omega)=f(x)$.

Cannot construct correctors. But the variational form of the solution can used for homogenization (Varadhan, Rezakhanlou, Kosygina, 2006). A long-standing problem (since 1982) is solved.

Broader, computational issues arising in multiscale PDE's

- How do we find properties of a^H? Theory of bounds (G. Milton)

- How do we compute $u^\epsilon(x,\omega)$ numerically, without knowing that it homogenizes? Construct adaptive finite element (or other) schemes that capture homogenization (T. Hou)

- How do we deal with nonlinear PDE's that generate intrinsically multiscale problems? Variational methods with applications to materials

- How do we compute numerically the probability law, or higher statistics, of $u^\epsilon(x,\omega)$? (Multiscale sampling algorithms)

Subspace projection formalism

Introduce $H_0^1(D) = X_C \oplus X_F$, a decomposition into coarse element subspace and fine element subspace.

Write the solution $u \in X_C \oplus X_F$ as

$$u = u_C + \mathcal{M}(\nabla u_C)$$

where $u_C \in X_C$ and $\mathcal{M}(\nabla u_C) \in X_F$.

They are determined by the relation

$$\mathcal{M}(\nabla v) = \mu_F + \mathcal{M}^o(\nabla v)$$

and the following three equations.

The subspace projection formalism II

Effective coarse scale equation:

$$(a(\mathcal{I} + \nabla\mathcal{M})\nabla u_C, \nabla v) = \langle\, f, v \,\rangle \quad \forall\, v \in X_C.$$

or, the equivalent symmetrized and reduced form:

$$(a(\mathcal{I} + \nabla\mathcal{M}^o)\nabla u_C, (\mathcal{I} + \nabla\mathcal{M}^o)\nabla v) = \langle\, f, v + \mathcal{M}^o\nabla v \,\rangle \quad \forall\, v \in X_C.$$

Fine scale equation defining the linear operator $\mathcal{M}^o$:

$$(a\nabla(\mathcal{M}^o\nabla w), \nabla v) = -(a\nabla w, \nabla v) \quad \forall\, v \in X_F,\ w \in X_C.$$

or, equivalently:

$$(a(\mathcal{I} + \nabla(\mathcal{M}^o\nabla w)), \nabla v) = 0 \quad \forall\, v \in X_F,\ w \in X_C.$$

Fine scale equation defining the function $\mu_F \in X_F$:

$$(a\nabla\mu_F, \nabla v) = \langle\, f, v \,\rangle \quad \forall\, v \in X_F.$$

Key step: limited oversampling

Most costly thing to compute: $\mathcal{M}^o(\nabla w)$ for $w \in X_C$.

For each coarse finite element $w \in X_C$, one needs to solve the fine scale equation (analog of cell problem) for $\mathcal{M}^o(\nabla w) \in X_F$.

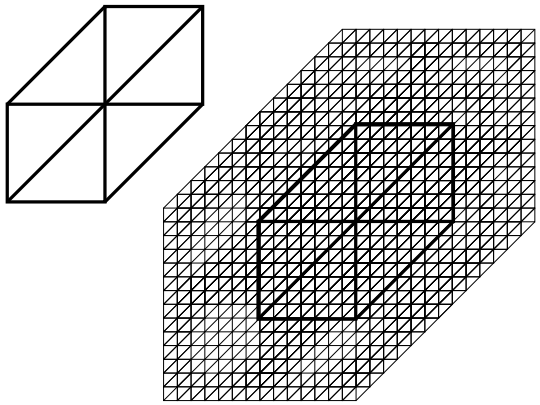
Restrict this (adaptively) to only a neighborhood of the finite element w.

In homogenization we have the equivalent of "absolute" localization.

Show that, with limited oversampling, the solution $u = u_C + \mathcal{M}(\nabla u_C)$ captures homogenization (Nolen-Papanicolaou-Pironneau, SIAM MMS 2008).

Related work: T. Hughes (1995), T. Hou++ (1997, 1999, ...), use of wavelets (Engquist++), use of harmonic coordinates, etc.

The finite elements

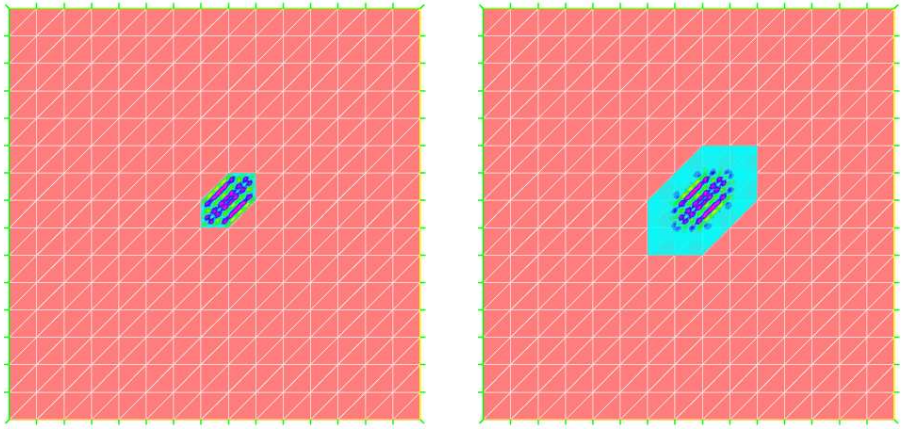


Left: The support of a coarse scale element ϕ_k^C on the coarse mesh $\mathcal{T}_C$.

Right: The coarse scale element within the refined mesh $\mathcal{T}_R$. The space Y_k^F is defined over this fine mesh. Here, one layer of oversampling is shown.

In all the numerical calculations we use FreeFem++.

Role of oversampling

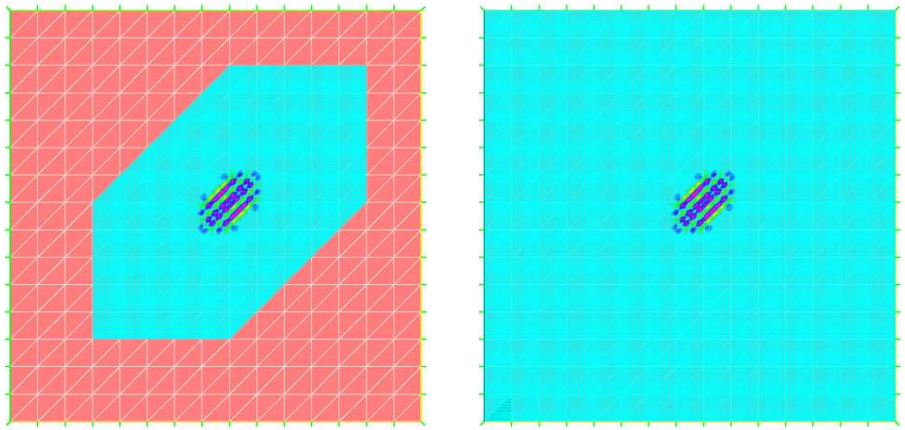


The function $\tilde{\mathcal{M}}^o(\nabla\phi_k^C)$ computed with no oversampling (left) and one layer of oversampling (right).

The projection is the H^1 projection.

The relative H^1 error between these approximations and $\mathcal{M}^o(\nabla\phi_k^C)$ computed with complete oversampling is 20% and 0.7%, respectively.

More on oversampling

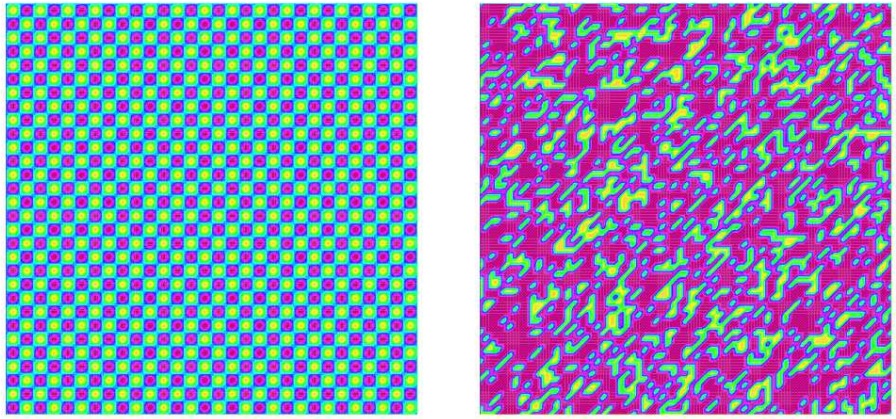


The function $\tilde{\mathcal{M}}^o(\nabla\phi_k^C)$ computed with four layers of oversampling (left) and complete oversampling (right).

The projection is the H^1 projection.

The relative H^1 error between the function shown in the left plot and $\mathcal{M}^o(\nabla\phi_k^C)$ computed with complete oversampling is 0.07%

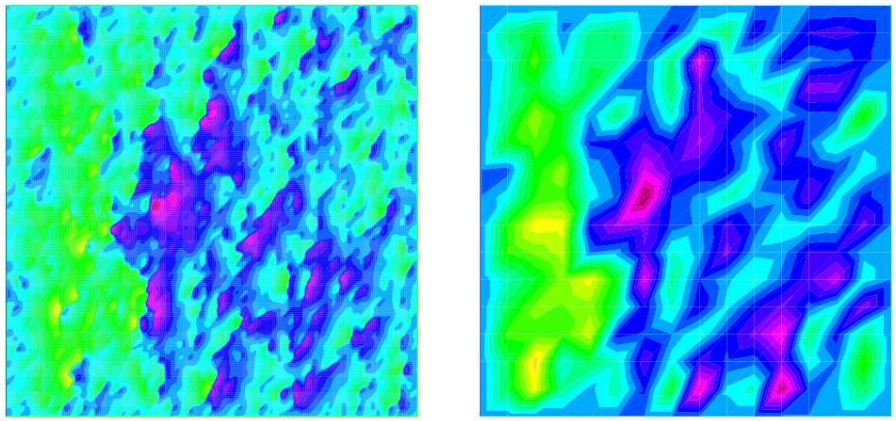
The oscillating coefficients



Left: The periodic function $a(x)$. Here the ratio of domain width to period size is $n = 15$.

Right: The randomly generated function $a(x) = 1.0$ (purple) or $a(x) = 0.01$ (yellow).

Numerical results

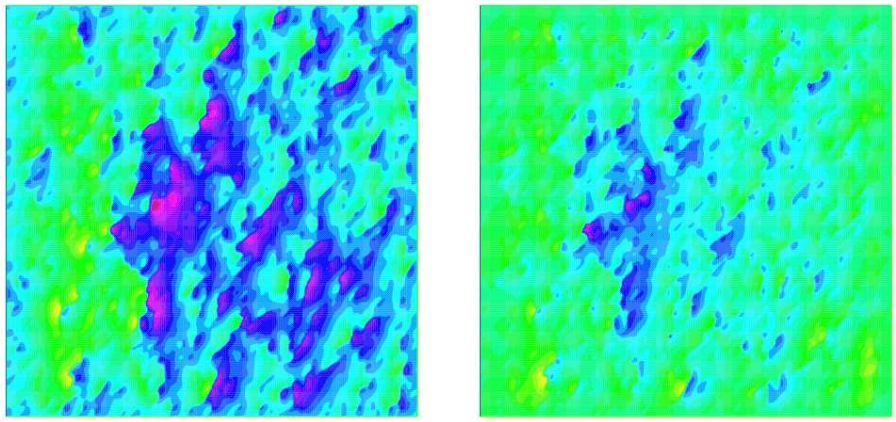


Random coefficients with pressure gradient

Left: High resolution Galerkin solution. Right: Low resolution Galerkin solution.

The color yellow corresponds to the lowest value; purple corresponds to the highest value.

Numerical results II

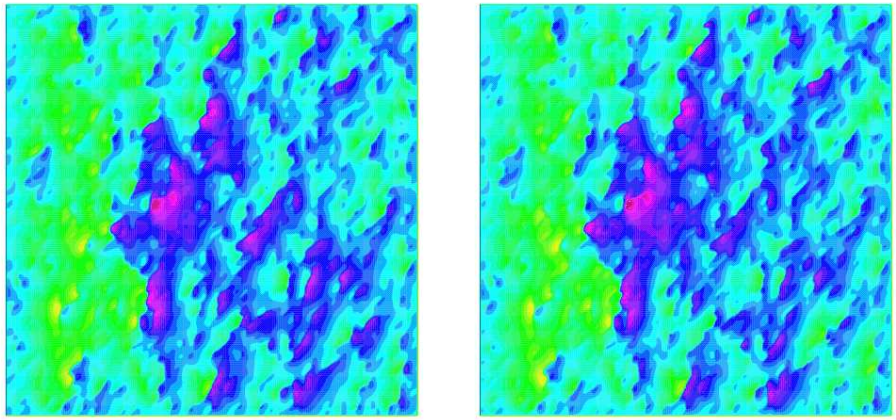


Random coefficients with pressure gradient

Left: High resolution Galerkin solution. Right: The multiscale solution u_C **with reconstruction** of fine scales using **no oversampling**.

The fine scale features in the solution are reproduced somewhat, but not as well as in the case when oversampling is used (next figure). Note: we have subtracted off the linear part of the solution.

Numerical results III

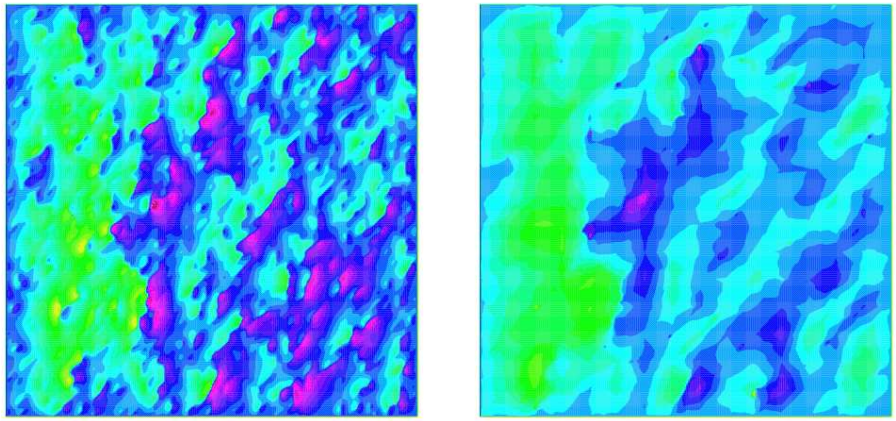


Random coefficients with pressure gradient

Left: High resolution Galerkin solution. Right: The multiscale solution u_C **with reconstruction** of fine scales using **one layer of oversampling**.

The fine scale features in the solution are reproduced well. Note: we have subtracted off the linear part of the solution.

Numerical results IV



Random coefficients with pressure gradient

Left: High resolution Galerkin solution. Right: The multi-scale solution reconstructed solution **without the μ_F correction**: $u_C + \tilde{\mathcal{M}}^o(\nabla u_C)$.

Two layers of oversampling are used. This example shows the importance of computing the term μ_F in reconstructing the fine scales of the solution.

Summary and conclusions

- The projection formalism with adaptive oversampling captures homogenization

- The computational advantage of the projection formalism with limited oversampling improves dramatically over direct Galerkin as the complexity of the problem increases

- The theory and the detailed implementation of adaptive oversampling, including error tracking, need much further study