Homogenization and Multiscale Modeling

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Homogenization is a collection of methods to approximate a heterogeneous problem by a homogeneous one.

Example (Elliptic)

\[ A^\varepsilon(u^\varepsilon) = f : - \sum (a_{ij}^\varepsilon(x)u_{xi}^\varepsilon)x_j = f, \text{ where } a_{ij}^\varepsilon(x) = a_{ij}(x/\varepsilon), \text{ and } a_{ij}(\cdot) \text{ are 1-periodic in } \mathbb{R}^n. \]

Exact model at microscale

\[ a_{ij}(x/\varepsilon) \]

replaced by homogenized model

with constant \( \tilde{a}_{ij} \)
First Issues

Question

*Can we find a limiting problem, \( Au = f \), whose solution \( u \) characterizes the limit, \( \lim_{\epsilon \to 0} u^\epsilon = u \)?*

Example (Elliptic)

\[
A(u) = f : \quad - \sum (\tilde{a}_{ij} u_x)_x = f, \text{ where } \tilde{a}_{ij} \text{ are constant.}
\]

This is the *homogenized equation* with *effective* coefficients.

Question

*Is \( A \) of the same type as \( A^\epsilon \)?*

The answer is frequently ‘No!’.
An Elliptic Problem

Let $Y$ be the unit cube in $\mathbb{R}^N$. Assume $a(\cdot)$ is $Y$-periodic. We want to approximate the solution to the *singular problem*

$$u^\epsilon \in H^1_0(\Omega) :$$

$$\int_{\Omega} a(x/\epsilon) \nabla u^\epsilon(x) \cdot \nabla \varphi(x) \, dx = \int_{\Omega} F(x) \varphi(x) \, dx \text{ for all } \varphi \in H^1_0(\Omega).$$

(1)
We seek an approximation

\[ u^\varepsilon(x) = u(x, x/\varepsilon) + \varepsilon U(x, x/\varepsilon) + \mathcal{O}(\varepsilon^2), \quad x \in \Omega, \]

in which each \( u(x, y) \) and \( U(x, y) \) is \( Y \)-periodic.

The gradient is given (formally) by

\[ \nabla u^\varepsilon(x) = \nabla_x u(x, x/\varepsilon) + \frac{1}{\varepsilon} \nabla_y u(x, x/\varepsilon) + \nabla_y U(x, x/\varepsilon) + \mathcal{O}(\varepsilon). \]
The solution $u^\epsilon$ has a bounded gradient, so $\nabla_y u(x, y) = 0$ and

$$u^\epsilon(x) = u(x) + \epsilon U(x, x/\epsilon) + O(\epsilon^2) \quad (2a)$$

$$\nabla u^\epsilon(x) = \nabla u(x) + \nabla_y U(x, x/\epsilon) + O(\epsilon) \quad (2b)$$

Substitute (2) into (1) with a test function of the same form

$$\varphi(x) + \epsilon \Phi(x, x/\epsilon)$$

where $\Phi(x, y)$ is $Y$-periodic for each $x \in \Omega$. 
Two-scale limits $\epsilon \to 0$ give the system

$$u \in H^1_0(\Omega), \quad U \in L^2(\Omega, H^1_\#(Y)):$$

$$\int_\Omega \int_Y a(y)(\nabla u(x) + \nabla_y U(x, y)) \cdot (\nabla \varphi(x) + \nabla_y \Phi(x, y)) \, dy \, dx$$

$$= \int_\Omega F(x) \varphi(x) \, dx \text{ for all } \varphi \in H^1_0(\Omega), \quad \Phi \in L^2(\Omega, H^1_\#(Y)). \quad (3)$$
The homogenized system

Decouple the system:

\[ U \in L^2(\Omega, H^1_#(Y)) : \]
\[ \int_{\Omega} \int_Y a(y)(\nabla_y U(x, y) + \nabla u(x)) \cdot \nabla_y \Phi(x, y) \, dy \, dx = 0 \]

for all \( \Phi \in L^2(\Omega, H^1_#(Y)) \). \hspace{1cm} (4a)

\[ u \in H^1_0(\Omega) : \]
\[ \int_{\Omega} \int_Y a(y)(\nabla u(x) + \nabla_y U(x, y)) \, dy \cdot \nabla \varphi(x) \, dx = \int_{\Omega} F(x) \varphi(x) \, dx \]

for all \( \varphi \in H^1_0(\Omega) \). \hspace{1cm} (4b)
The local problem (4a) is equivalent to requiring

\[ U(x, \cdot) \in H^1_\#(Y) : \int_Y a(y)(\nabla_y U(x, y) + \nabla u(x)) \cdot \nabla_y \Phi(y) \, dy = 0 \text{ for all } \Phi \in H^1_\#(Y). \]

Define \( \omega_i(y) \) for each \( 1 \leq i \leq N \) to be the solution of the cell problem

\[ \omega_i \in H^1_\#(Y) : \int_Y a(y)(\nabla_y \omega_i(y) + e_i) \cdot \nabla_y \Phi(y) \, dy = 0 \text{ for all } \Phi \in H^1_\#(Y). \]

(5)

where \( e_i \) is the indicated coordinate vector in \( \mathbb{R}^N \).
The Homogenized problem

By linearity the solution is given by

\[ U(x, y) = \sum_{i=1}^{i=N} \partial_i u(x) \omega_i(y) \]

This is substituted into (4b) to obtain

\[ u \in H^1_0(\Omega) : \int_{\Omega} \tilde{a}_{ij} \partial_i u(x) \cdot \partial_j \varphi(x) \, dx = \int_{\Omega} F(x) \varphi(x) \, dx \]

for all \( \varphi \in H^1_0(\Omega) \). (6)

where the constant coefficients are given by

\[ \tilde{a}_{ij} = \int_Y a(y) \left( \delta_{ij} + \partial_j \omega_i(y) \right) \, dy \] (7)
The approximate solution

\[ u^\varepsilon(x) = u(x) + \varepsilon \nabla u(x) \cdot (\omega_1(x/\varepsilon), \omega_2(x/\varepsilon), \ldots, \omega_N(x/\varepsilon)) + \mathcal{O}(\varepsilon^2), \]

\[ \nabla u^\varepsilon(x) = \nabla u(x) + \nabla u(x) \cdot (\nabla \omega_1(x/\varepsilon), \nabla \omega_2(x/\varepsilon), \ldots, \nabla \omega_N(x/\varepsilon)) + \mathcal{O}(\varepsilon) \]

of the singular elliptic problem.
Homogenization


Homogenization and Multiscale Modeling

Multiscale Flow and Transport: The Classical Case

\[ \mathbf{u}(x) = -K(x) \nabla p(x), \quad \nabla \cdot \mathbf{u}(x) = 0 \]

\[ \phi \frac{\partial c(x, t)}{\partial t} + \nabla \cdot (\mathbf{u}(x)c(x, t) - \mathbf{D}(\mathbf{u}(x))\nabla c(x, t)) = 0 \]

\[ K_{\text{fast}}, K_{\text{slow}} \rightarrow u_{\text{fast}}, u_{\text{slow}} \rightarrow D_{\text{fast}}, D_{\text{slow}} \]
The Parabolic Equation

The Exact Model ... with fine-scale coefficients

\[ \phi(x) \frac{\partial c}{\partial t} - \nabla \cdot D(x) \nabla c = 0, \quad x \in \Omega, \]

with \( D(x) = D_{\text{slow}} \) on \( \Omega_{\text{slow}} \) and \( = D_{\text{fast}} \) on \( \Omega_{\text{fast}} \).

... or in transmission form

\[ \phi_\alpha \frac{\partial c_\alpha}{\partial t} - \nabla \cdot D_\alpha \nabla c_\alpha = 0, \quad x \in \Omega_\alpha, \quad \alpha = \text{fast, slow} \]

with the interface conditions on \( \partial \Omega_{\text{slow}} \cap \partial \Omega_{\text{fast}} \):

\[ c_{\text{fast}} = c_{\text{slow}}, \quad D_{\text{fast}} \nabla c_{\text{fast}} \cdot \nu = D_{\text{slow}} \nabla c_{\text{slow}} \cdot \nu \]
The classical case

The coefficients are $D = [D_{\text{fast}}, D_{\text{slow}}]$:

$$\tilde{\phi} \frac{\partial \tilde{c}}{\partial t} - \nabla \cdot \tilde{\mathbf{D}} \nabla \tilde{c} = 0$$

- The fine-scale geometry is eliminated . . .
- . . . replaced by the constant effective coefficient $\tilde{\mathbf{D}}$.
- The upscaled limit is of the same type . . . a single equation.
- The fast and slow regions are coupled by gradients of the solution (flux).
- Accurate only in this low contrast case.
... the algorithm

Exact model at microscale

\[ D(x) = D_{\text{slow}}, D_{\text{fast}} \]

replaced by homogenized model

with constant \( \tilde{D} \)

Compute homogenized coefficient \( \tilde{D} = \tilde{D}(D_{\text{fast}}, D_{\text{slow}}) \)

\[ \tilde{D}_{jk} = \frac{1}{|\Omega_0|} \int_{\Omega_0} D_{jk}(y)(\delta_{jk} + \partial_k \omega_j(y))dA \]

\[ \begin{cases} -\nabla \cdot D(y) \nabla \omega_j(y) = \nabla \cdot (D(y)e_j), \\ \omega_j(y) \text{ is periodic,} \end{cases} \]

\( \Omega_0 \)
Homogenization and Multiscale Modeling

... the algorithm

Exact model at microscale

$D(x) = D_{\text{slow}}, D_{\text{fast}}$

replaced by homogenized model

with constant $\tilde{D}$

Compute homogenized coefficient $\tilde{D} = \tilde{D}(D_{\text{fast}}, D_{\text{slow}})$

$\tilde{D}_{jk} = \frac{1}{|\Omega_0|} \int_{\Omega_0} D_{jk}(y)(\delta_{jk} + \partial_k \omega_j(y))dA$

$$\begin{cases} -\nabla \cdot D(y) \nabla \omega_j(y) &= \nabla \cdot (D(y)e_j), \\ \omega_j(y) &\text{is periodic.} \end{cases}$$

It works well for problems with low contrast $D_{\text{fast}}/D_{\text{slow}}$.
The **Obstacle** Problem . . . a special case

The coefficients are $D = [D_{fast}, 0]$:

$$
\tilde{\phi}^0 \frac{\partial \tilde{c}^0}{\partial t} - \nabla \cdot \tilde{D}^0 \nabla \tilde{c}^0 = 0
$$

- The slow region $\Omega_{slow}$ is impervious.
Classical homogenization is not adequate for time-dependent problems with large contrast $\frac{D_{\text{fast}}}{D_{\text{slow}}}$

Low contrast: classical homogenization

$$\| u_\epsilon \|_0 + \| \nabla u_\epsilon \|_0 \leq C$$
local averages

High contrast: double porosity models

$$\| u_\epsilon \|_0 + \epsilon \| \nabla u_\epsilon \| \leq C$$
local averages versus special averages
The Double-porosity model

The coefficients are \( D = [D_{fast}, \epsilon_0^2 D_{slow}] \):

\[
\tilde{\phi}^0 \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{D}^0 \nabla \tilde{c} = 0, \quad q_i(t) = \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} D_{slow} \nabla c_i \cdot \nu ds,
\]

\[
\phi_{slow} \frac{\partial c_i}{\partial t} - \nabla \cdot D_{slow} \nabla c_i = 0, \quad c_i|_{\Gamma_i} = \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \tilde{c}(x) dA.
\]

- The upscaled model is a system, highly parallel.
- The coupling from the cell to global equation is via gradients.
- The coupling from the global equation to the cell is via the values.
- The contribution of the cells is a secondary storage.
- Accurate only in this high contrast case.
- It will not couple any advective effects to the local cell.
Double-porosity Micro-structure Model

**Exact model**

Global equation, \( x \in \Omega \)

\[
\phi^0 \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{D}^0 \nabla \tilde{c} = 0
\]

\[
q_i(t) = \Pi_{0,i}^* (D_{\text{slow}} \nabla c_i(\cdot, t) \cdot \nu)
\]

**Cell problem at each \( x \in \Omega_i \)**

\[
\phi_{\text{slow}} \frac{\partial c_i}{\partial t} - \nabla \cdot D_{\text{slow}} \nabla c_i = 0
\]

\[
c_i|_{\Gamma_i} = \Pi_{0,i}(\tilde{c})(t)
\]
Notes

- The coefficients in the global equation are precisely those of the obstacle problem.
- The cell input to the global equation is

\[
q_i(t) = \frac{1}{|\hat{\Omega}_i|} \frac{\partial}{\partial t} \int_{\Omega_i} \phi_{\text{slow}} c_i(x, t) \, dx
\]

...the rate of secondary storage.
- The spatially-constant input to the cell problem will *not* transmit any advective transport.

We shall more tightly couple the cell by replacing the constant coupling with an affine coupling to the surrounding fast medium. This will provide a gradient coupling.
Affine approximations $\Pi_1$

AVERAGE: $\Pi_0 f = \frac{1}{|\Omega_0|} \int_{\Omega_0} f(x) dA$; assume here $|\Omega_0| = 1$.

Denote $x^C$ - center of mass of $\Omega_0$.

General affine approximation $f(x) \approx \Pi_1 f := m + n \cdot x$, $x \in \Omega_0$

Choice of $m, n$

- Taylor ($f \in C^1(\Omega_0)$) about midpoint $f(x) \approx f(x^C) + \nabla f(x^C)(x - x^C)$
- $L_2(\Omega_0)$-projection onto affines that is: $(f, v)_{\Omega_0} = (m + n \cdot x, v)_{\Omega_0}, \forall$ affine $v$
- $H^1(\Omega_0)$ projection: $f(x) \approx \Pi_1 f := \Pi_0 f + \Pi_0 \nabla f \cdot (x - x^C)$
Affine coupling $\Pi_i : H^1(\Omega) \mapsto H^1(\hat{\Omega}_i)$

$$\Pi_i(\mathbf{w})(\mathbf{x}) \equiv \Pi_0 \mathbf{w} + \Pi_0(\nabla \mathbf{w}) \cdot (\mathbf{x} - \mathbf{x}^C)$$

Its dual $\Pi_i^* : H^1(\hat{\Omega}_i)^* \mapsto H^1(\Omega)^*$ pointwise

$$\Pi_i^*(q)(\mathbf{x}) = \bar{\chi}_i(\mathbf{x}) M_i^0(q) - \nabla \cdot \bar{\chi}_i(\mathbf{x}) M_i^1(q)$$
Double-porosity Model with secondary flux

\[ \tilde{\phi}^0 \frac{\partial \tilde{c}}{\partial t} + \sum_i \chi_i q_i(t) - \nabla \cdot \tilde{D}^0 \nabla \tilde{c} = 0, \]

\[ \phi_{\text{slow}} \frac{\partial c_i}{\partial t} - \nabla \cdot D_{\text{slow}} \nabla c_i = 0, \]

\[ c_i|_{\Gamma_i} = \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \tilde{c} dA + \frac{1}{|\hat{\Omega}_i|} \int_{\hat{\Omega}_i} \nabla \tilde{c} dA \cdot (x - x^C). \]

\[ q_i(t) = \frac{1}{|\hat{\Omega}_i|} \int_{\Gamma_i} D_{\text{slow}} \nabla c_i \cdot \nu ds - \nabla \cdot \frac{\bar{\chi}_i(x)}{|\hat{\Omega}_i|} \int_{\Gamma_i} D_{\text{slow}} \nabla c_i \cdot \nu (x - x^C) dS. \]

This is \( \frac{\partial}{\partial t} \) (secondary storage) \(-\nabla \cdot \) (secondary flux) from the local cells.
Computational experiments at microscale

GOAL: reproduce qualitatively experimental results

Row-20-3-5 breakthrough curves

breakthrough curve data

ratio 1/6
ratio 1/10
ratio 1/30
ratio 1/100
ratio 1/300
ratio 1/1800
ratio 1/3000
Porous Media

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