Efficient Methods for Homogenization of Random Heterogeneous Materials

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Workshop on Modeling and Simulation of Interface-related Problems
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Contents

- Background information
- Improving convergence rate with Richardson extrapolation
- Robin boundary condition for high-contrast materials
- Conclusions
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- Background information
- Improving convergence rate with Richardson extrapolation
- Robin boundary condition for high-contrast materials
- Conclusions
Many practical problems have multiple-scale feature.

- Composite materials
- Porous media
Multiscale problem

BVP with random rapidly oscillating coefficients

\[
\begin{aligned}
-\nabla \cdot \left( a^\varepsilon(x, \omega) \nabla u^\varepsilon(x, \omega) \right) &= f(x) \quad \text{in } D \subset \mathbb{R}^d \\
u^\varepsilon(x, \omega) &= g(x) \quad \text{on } \partial D
\end{aligned}
\]

- $\varepsilon > 0$ is a parameter describing the multiscale feature.
- $\omega$ denotes a realization of the random coefficient tensor in probability space $(\Omega, \mathcal{F}, P)$.
- $f(x)$ and $g(x)$ are macroscopic functions.
Multi-scale problem

- It is difficult to solve the multi-scale problem with traditional numerical methods.
  (Finite element method, Boundary element method, etc.)
  \[ \text{FEM} \quad h \ll L_{\text{micro}} \ll L_{\text{macro}} \]

- Macroscopic behavior of the heterogeneous material may be approximated by that of a fictitious **homogeneous** one.
Typical multiscale methods for the BVP

- Asymptotic homogenization method (Lions 1978)
- Variational multiscale method (Hughes 1995)
- Multiscale finite element method (Hou & Efendiev 1997)
- Heterogeneous multiscale method (E & Engquist 2003)
Multiscale problem

Homogenized BVP

\[ \begin{cases} -\nabla \cdot (\bar{a} \nabla u^0(x)) = f(x) & \text{in } D \subset \mathbb{R}^d \\ u^0(x,\cdot) = g(x) & \text{on } \partial D \end{cases} \]

- $\bar{a}$ is called effective (or homogeneous) coefficient tensor.
- $\bar{a}$ is a constant tensor if $a^\varepsilon$ is a statistically homogeneous ergodic tensor, i.e., $a^\varepsilon(x,\omega) = a(y,\omega)$, $y = x/\varepsilon$. 
Homogenization

Effective coefficients $\bar{a}$

- Defined in the probability space $(\Omega, \mathcal{F}, P)$, which cannot be computed by numerical methods
- According to the **ergodic theorem**, $\bar{a}$ is approximated by

$$\bar{a} \cdot e_i = \lim_{L \to \infty} \langle a(y, \omega) \nabla u(y, \omega) \rangle$$

where $u$ is the solution of

$$-\nabla \cdot (a(y, \omega) \nabla u(y, \omega)) = 0 \quad \text{in} \ Y_L = [0, L]^d$$

which satisfies $\langle \nabla u \rangle = e_i$, and $e_i \ (i = 1, \cdots, d)$ are canonical bases in $\mathbb{R}^d$. 
Homogenization

Auxiliary problem in volume element

\[-\nabla \cdot \left( a(y, \omega) \nabla u(y, \omega) \right) = 0 \quad \text{in } Y_L\]

- Dirichlet boundary condition (DBC)
  \[u(y, \omega) = \xi_i \cdot y \quad \text{on } \partial Y_L, \ i = 1, \cdots, d\]

- Neumann boundary condition (NBC)
  \[a(y, \omega) \nabla u(y, \omega) \cdot n = \eta_i \cdot n \quad \text{on } \partial Y_L, \ i = 1, \cdots, d\]
Homogenization

Simulations in the macro-scale

Localization

Determine effective coefficients in microstructures of different sizes

Create microstructure

Solve boundary value problems

Compute relevant volume averages

Calculate effective coefficients

Repeat above procedure in different realizations, get ensemble average

Figure: The main procedure of multiscale method for random heterogeneous materials
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Motivation

Some results

- With proper boundary condition, approximate effective coefficients converge to the true effective coefficients as $L \rightarrow \infty$. (Bourgeat 2004)

- (Numerical) convergence rates of DBC and NBC approximations are $O(1/L)$. (Yue 2007)

- DBC overestimates the true effective coefficients, while NBC underestimate the true effective coefficients. (Dirichlet-Neumann bounds)
Motivation

- Sufficiently large volume elements are always needed, which is time-consuming and high-demanding for computer memory.
Dirichlet boundary condition

\[ u(y, \omega) = \xi_i \cdot y \quad \text{on } \partial Y_L, \ i = 1, \ldots, d \]

It satisfies

\[ \left\langle \nabla u \left( y, \omega \right) \right\rangle = \xi_i \]

Approximate effective coefficients are calculated by

\[ \bar{a}_{D,L} \left( \omega \right) \cdot \xi_i = \left\langle a \left( y, \omega \right) \nabla u \left( y, \omega \right) \right\rangle \]

Mathematical expectation \( \mathbb{E} \bar{a}_{D,L} \) is then computed.
Method

Neumann boundary condition

\[ a(y, \omega) \nabla u(y, \omega) \cdot n = \eta_i \cdot n \quad \text{on } \partial Y_L, \quad i = 1, \ldots, d \]

It satisfies

\[ \langle a(y, \omega) \nabla u(y, \omega) \rangle = \eta_i \]

Approximate effective coefficients are calculated by

\[ \bar{a}_{N,L}(\omega) \cdot \langle \nabla u(y, \omega) \rangle = \eta_i \]

Mathematical expectation \( \mathbb{E} \bar{a}_{N,L} \) is then computed.
Method

Theorem (Wu, Nie, Yang 2014)

Let $\mathbb{E}\bar{a}_{D,L}$ and $\mathbb{E}\bar{a}_{N,L}$ be the approximate effective coefficients under DBC and NBC respectively, and let $\bar{a}_\infty$ be the true effective coefficients, then we have

$$\mathbb{E}\bar{a}_{D,1} \geq \cdots \geq \mathbb{E}\bar{a}_{D,L} \geq \mathbb{E}\bar{a}_{D,2L} \geq \cdots \geq \bar{a}_\infty$$

and

$$\mathbb{E}\bar{a}_{N,1} \leq \cdots \leq \mathbb{E}\bar{a}_{N,L} \leq \mathbb{E}\bar{a}_{N,2L} \leq \cdots \leq \bar{a}_\infty$$
Assume the first-order convergence rates of DBC and NBC approximations are satisfied, then we have

\[
\mathbb{E} \bar{a}_{BC,L} - \bar{a}_\infty = C \frac{1}{L} + O\left( \frac{1}{L^\beta} \right), \quad \text{where } \beta > 1
\]

Since

\[
\mathbb{E} \bar{a}_{BC,2L} - \bar{a}_\infty = C \frac{1}{2L} + O\left( \frac{1}{2^\beta L^\beta} \right)
\]

We get Richardson extrapolation sequence

\[
R_{BC,L} - \bar{a}_\infty = \left[ 2\mathbb{E} \bar{a}_{BC,2L} - \mathbb{E} \bar{a}_{BC,L} \right] - \bar{a}_\infty = O\left( \frac{1}{L^\beta} \right)
\]
Methods for Homogenization of RHMs

**Method**

- **Determine effective coefficients**
- **Create microstructure**
- **Solve boundary value problems**
- **Compute relevant volume averages**
- **Richardson extrapolation**

**Figure:** The main procedure of multiscale method combined with Richardson extrapolation technique.
Microstructure

- (RMDF) random morphology description function, proposed by Vel et al. in 2010.
- Closely resemble actual micrographs manufactured by techniques including plasma spraying and powder processing.

(a) Microstructures generated by computer with different volume fractions of Al

(b) Actual Al/Al$_2$O$_3$ micrographs
Example
We predict effective thermal conductivity of actual Al/Al$_2$O$_3$ with different volume fractions of Al.

Figure: Microstructures with different sizes
**Numerics**

**Table:** Properties of constituent materials

<table>
<thead>
<tr>
<th>Material</th>
<th>Al</th>
<th>Al₂O₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$ (W/mK)</td>
<td>233.0</td>
<td>30.0</td>
</tr>
</tbody>
</table>

**Table:** Convergence rates of approximate effective coefficients

<table>
<thead>
<tr>
<th>$V_{Al}$ (%)</th>
<th>10</th>
<th>30</th>
<th>50</th>
<th>70</th>
<th>90</th>
</tr>
</thead>
<tbody>
<tr>
<td>DBC</td>
<td>1.08</td>
<td>0.93</td>
<td>0.95</td>
<td>0.99</td>
<td>1.04</td>
</tr>
<tr>
<td>NBC</td>
<td>1.02</td>
<td>0.99</td>
<td>0.82</td>
<td>0.95</td>
<td>0.98</td>
</tr>
</tbody>
</table>
Figure: Comparison of approximate effective coefficients by homogenization and extrapolation with increasing volume element size

(a) $V_{Al} = 30\%$

(b) $V_{Al} = 70\%$
Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bounds and Hashin-Shtrikman bounds)
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Example

We predict effective mechanical properties of actual Al/Al$_2$O$_3$ with different volume fractions of Al.

The contrast ratio between the elastic modulus of Al$_2$O$_3$ and Al is 5.6.

Table: Properties of constituent materials

<table>
<thead>
<tr>
<th>Material</th>
<th>Al</th>
<th>Al$_2$O$_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>70</td>
<td>393</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.30</td>
<td>0.22</td>
</tr>
</tbody>
</table>
Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bounds and Hashin-Shtrikman bounds)
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Example

We predict effective mechanical properties of actual stainless steel/epoxy with different volume fractions of stainless steel. The contrast ratio between the elastic modulus of stainless steel and epoxy is high (more than 100).

Table: Properties of constituent materials

<table>
<thead>
<tr>
<th>Material</th>
<th>Stainless Steel (SS)</th>
<th>Resin</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ (GPa)</td>
<td>193.8</td>
<td>1.31</td>
</tr>
<tr>
<td>$\nu$</td>
<td>0.29</td>
<td>0.40</td>
</tr>
</tbody>
</table>
Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bounds and Hashin-Shtrikman bounds)
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Motivation

- Many random heterogeneous materials have a high contrast of constituent properties.
  a. Composite materials (e.g., CNT-reinforced polymers)
  b. Porous media

- The high contrast leads to very broad Dirichlet-Neumann upper and lower bounds.
Motivation

Mixed Dirichlet-Neumann boundary condition (DNBC) approximations lie within the Dirichlet-Neumann bounds. (Yue 2007)

\[
\begin{align*}
    u(y, \omega) &= \xi_i \cdot y & \text{on } \partial_1 Y_L \\
    a(y, \omega) \nabla u(y, \omega) \cdot n &= 0 & \text{on } \partial_2 Y_L
\end{align*}
\]

Where \( \partial Y_L = \overline{\partial_1 Y_L} \cup \overline{\partial_2 Y_L} \),

And \( i = 1, \ldots, d \).
Method

- Boundary conditions destroy the ergodicity of solutions to the auxiliary problem.
- When the ergodicity can be satisfied, we have $E\bar{a}_L = \bar{a}_\infty$ for any $L$.

**Continuous properties**

\[
\begin{align*}
    u_{\omega_1} &= u_{\omega_2} \\
    a_\omega \nabla u_{\omega_1} \cdot n_{\omega_1} &= -a_\omega \nabla u_{\omega_2} \cdot n_{\omega_2}
\end{align*}
\]

**Figure:** Volume elements with different sizes
Method

Robin boundary condition (RBC)

\[ a(y, \omega) \nabla u(y, \omega) \cdot n + \lambda u(y, \omega) = \eta_i \cdot n + \lambda \xi_i \cdot y \quad \text{on } \partial Y_L \]

where \( \lambda \in (0, \infty) \) is the adjusting factor, and \( i = 1, \cdots, d \).

Theorem (Convergence)

Let \( \mathbb{E} \bar{a}_{R,L} \) be the approximate effective coefficient tensor computed by the auxiliary problem with Robin boundary condition. Then

\[ \lim_{L \to \infty} \bar{a}_{R,L}(\omega) = \bar{a}_\infty \quad \text{a.s.} \]
Method

Determine effective coefficients
Create microstructure
Solve boundary value problems
Compute relevant volume averages
Calculate effective coefficients
Repeat above procedure in different realizations, get ensemble average

Homogenization
Simulations in the macro-scale
Localization

Robin boundary condition

Figure: The main procedure of multiscale method combined with Robin boundary condition
Numerics

Example

We consider effective coefficients of random checker-board microstructures. Each unit cell is occupied by matrix material or reinforcement material with probability $p$ and $1-p$ ($(0<p<1)$). Here we set $p=0.5$.

Figure: Random checker-board microstructures with different sizes
For two-phase random heterogeneous materials, 

\[ a(y, \omega) = \begin{cases} 
  a_1 \cdot I, & y \in Y_L^m \\
  a_2 \cdot I, & y \in Y_L^r 
\end{cases} \]

has a high contrast, i.e.,

\[ r = \frac{a_2}{a_1} \gg 1 \]

Here, \( I \) is the identity matrix.
Figure: Approximate effective coefficients with different boundary conditions and different contrast ratios ($\lambda = 40$ in RBC)
Figure: Effect of adjusting factor in RBC on the accuracy of approximate effective coefficients
Figure: Approximate effective coefficients with different adjusting factor in RBC
More Discussion

- High contrast leads to large condition number of stiffness matrix, which may reduce the numerical accuracy of approximate effective coefficients.
- We discuss the effect of condition number on the accuracy of approximate effective coefficients.

Auxiliary problem with DBC

\[ \begin{aligned}
- \nabla \cdot \left( a(y, \omega) \nabla u(y, \omega) \right) &= 0 \quad \text{in } Y_L \\
\nabla u(y, \omega) &= \xi_i \cdot y \quad \text{on } \partial Y_L, \ i = 1, \ldots, d
\end{aligned} \]
More Discussion

**Figure**: Effect of contrast ratio and mesh size on the condition number of stiffness matrix (constituent with high property in the center)
More Discussion

Figure: Effect of contrast ratio and mesh size on the condition number of stiffness matrix (constituent with low property in the center)
More Discussion

\[
\text{cond}(A) = Ch^{-2}
\]

<table>
<thead>
<tr>
<th>$r = 100$</th>
<th>$h = 1/36$</th>
<th>$h = 1/42$</th>
<th>$h = 1/48$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{CGM}$</td>
<td>$\text{ICCG}$</td>
<td>$\text{M}$</td>
</tr>
<tr>
<td>$\text{cond}$</td>
<td>24472</td>
<td>293</td>
<td>33306</td>
</tr>
<tr>
<td>$N_{\text{ite}}$</td>
<td>1168</td>
<td>25</td>
<td>1590</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$r = 1000$</th>
<th>$h = 1/36$</th>
<th>$h = 1/42$</th>
<th>$h = 1/48$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\text{CGM}$</td>
<td>$\text{ICCG}$</td>
<td>$\text{M}$</td>
</tr>
<tr>
<td>$\text{cond}$</td>
<td>218510</td>
<td>474</td>
<td>289075</td>
</tr>
<tr>
<td>$N_{\text{ite}}$</td>
<td>10325</td>
<td>29</td>
<td>13517</td>
</tr>
</tbody>
</table>

- Largest condition number is no more that $10^6$, while double-precision floating-point system guarantees more than 15 significant digits of freedom.
- Condition number has little effect on the accuracy of approximate effective coefficients.
Background information

Improving convergence rate with Richardson extrapolation

Robin boundary condition for high-contrast materials

Conclusions
Conclusion

Richardson extrapolation is an effective technique for predicting effective coefficients of random heterogeneous materials.

- Since smaller volume elements are used, a lot of computation time and computer memory could be saved.
Conclusion

Robin boundary condition is proposed for predicting effective coefficients of random heterogeneous materials.

- It provides much better approximate effective coefficients than other boundary conditions.
- It is more flexible than other boundary conditions because of the adjusting factor.
- It is more suitable for random heterogeneous materials with high contrast.


Thank you for your attention!