Northwestern Polytechnical University

Efficient Methods for Homogenization of Random Heterogeneous Materials

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Workshop on Modeling and Simulation of Interface-related Problems
Institute for Mathematical Sciences :: National University of Singapore

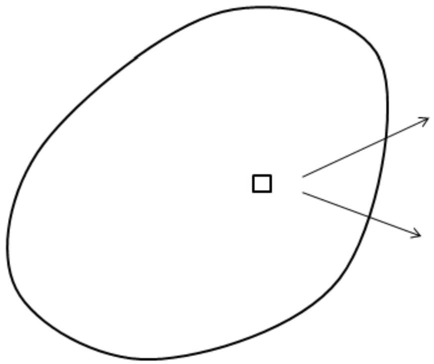
Contents

Contents

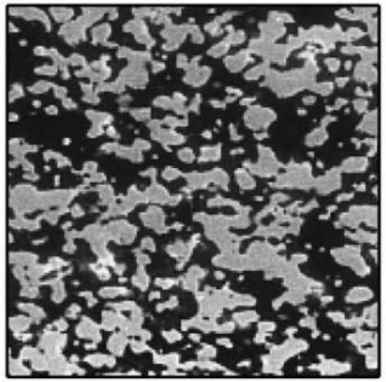
Multiscale problem

Many practical problems have multiple-scale feature.

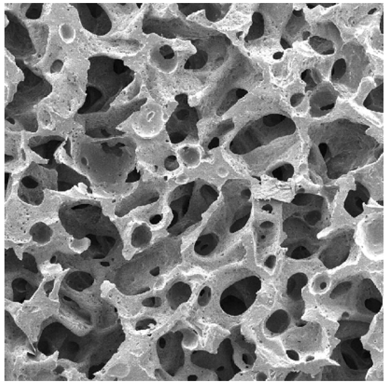
- Composite materials
- Porous media



(a) Macroscopic domain



(b) Composites at the microscale



(c) Porous media at the microscale

Multiscale problem

BVP with random rapidly oscillating coefficients

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

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

Multiscale problem

- It is difficult to solve the multiscale problem with traditional numerical methods.

  (Finite element method, Boundary element method, etc.)

  FEM $h \ll L_{\text{micro}} \ll L_{\text{macro}}$

- Macroscopic behavior of the heterogeneous material may be approximated by that of a fictitious homogeneous one.

Multiscale problem

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

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

- $\bar{a}$ is called effective (or homogeneous) coefficient tensor.
- $\bar{a}$ is a constant tensor if a^{ε} 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

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

where u is the solution of

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

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

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

- Dirichlet boundary condition (DBC)

$$u\left(y,\omega\right)=\xi_i\cdot y \quad \text{on } \partial Y_L,\ i=1,\cdots,d$$

- Neumann boundary condition (NBC)

$$a\left(y,\omega\right)\nabla u\left(y,\omega\right)\cdot n=\eta_i\cdot n \quad \text{on } \partial Y_L,\ i=1,\cdots,d$$

Homogenization

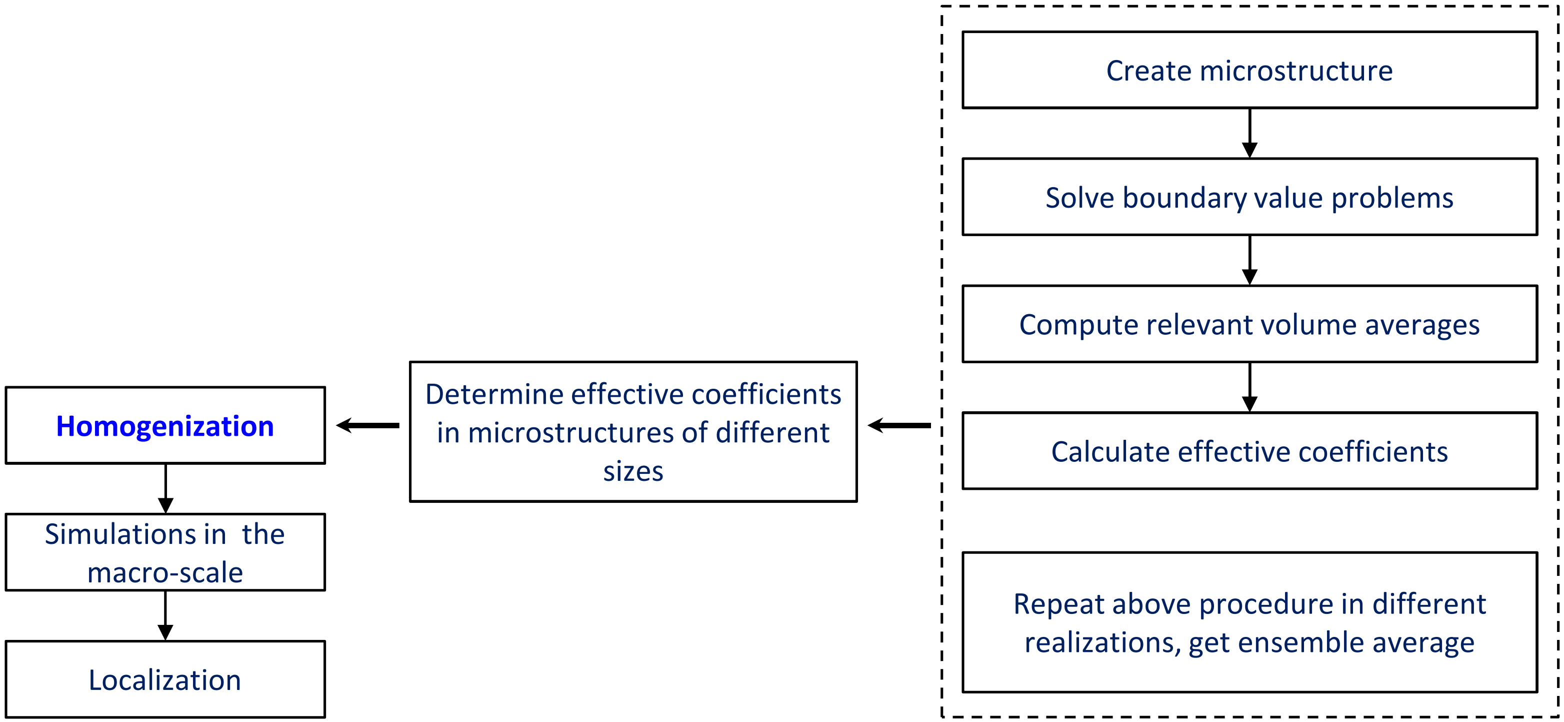


Figure: The main procedure of multiscale method for random heterogeneous materials

Contents

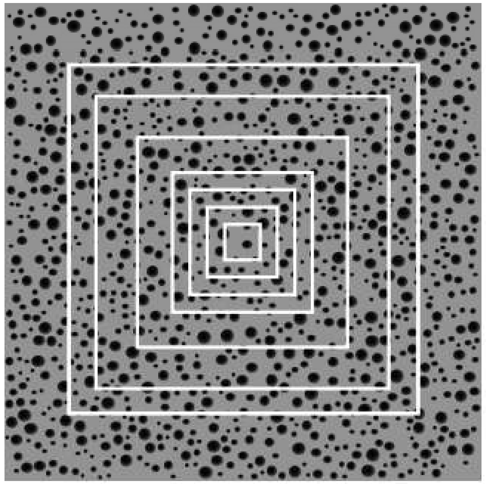
Motivation

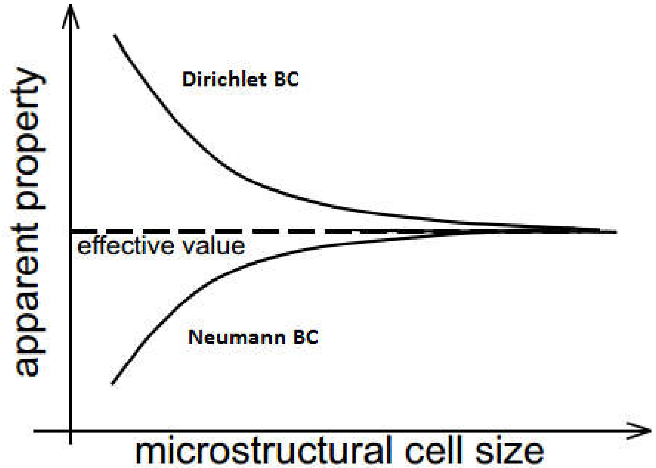
Some results

- With proper boundary condition, approximate effective coefficients converge to the true effective coefficients as $L \to \infty$. (*Bourgeat* 2004)
- (Numerical) convergence rates of DBC and NBC approximations are $\mathrm{O}(1/L)$. (*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.





Method

Dirichlet boundary condition

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

It satisfies

$$\langle \nabla u(y,\omega)\rangle=\xi_i$$

Approximate effective coefficients are calculated by

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

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

Method

Neumann boundary condition

$$a(y,\omega)\nabla u(y,\omega)\cdot n=\eta_i\cdot n \qquad \text{on } \partial Y_L,\ i=1,\cdots,d$$

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

$$\mathbb{E}\bar{a}_{N,1} \leq \cdots \leq \mathbb{E}\bar{a}_{N,L} \leq \mathbb{E}\bar{a}_{N,2L} \leq \cdots \leq \bar{a}_{\infty}$$

Method

Assume the first-order convergence rates of DBC and NBC approximations are satisfied, then we have

$$\mathbb{E}\,\overline{a}_{BC,L} - \overline{a}_{\infty} = C\frac{1}{L} + O\left(\frac{1}{L^{\beta}}\right), \qquad \text{where } \beta > 1$$

Since

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

We get Richardson extrapolation sequence

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

Method

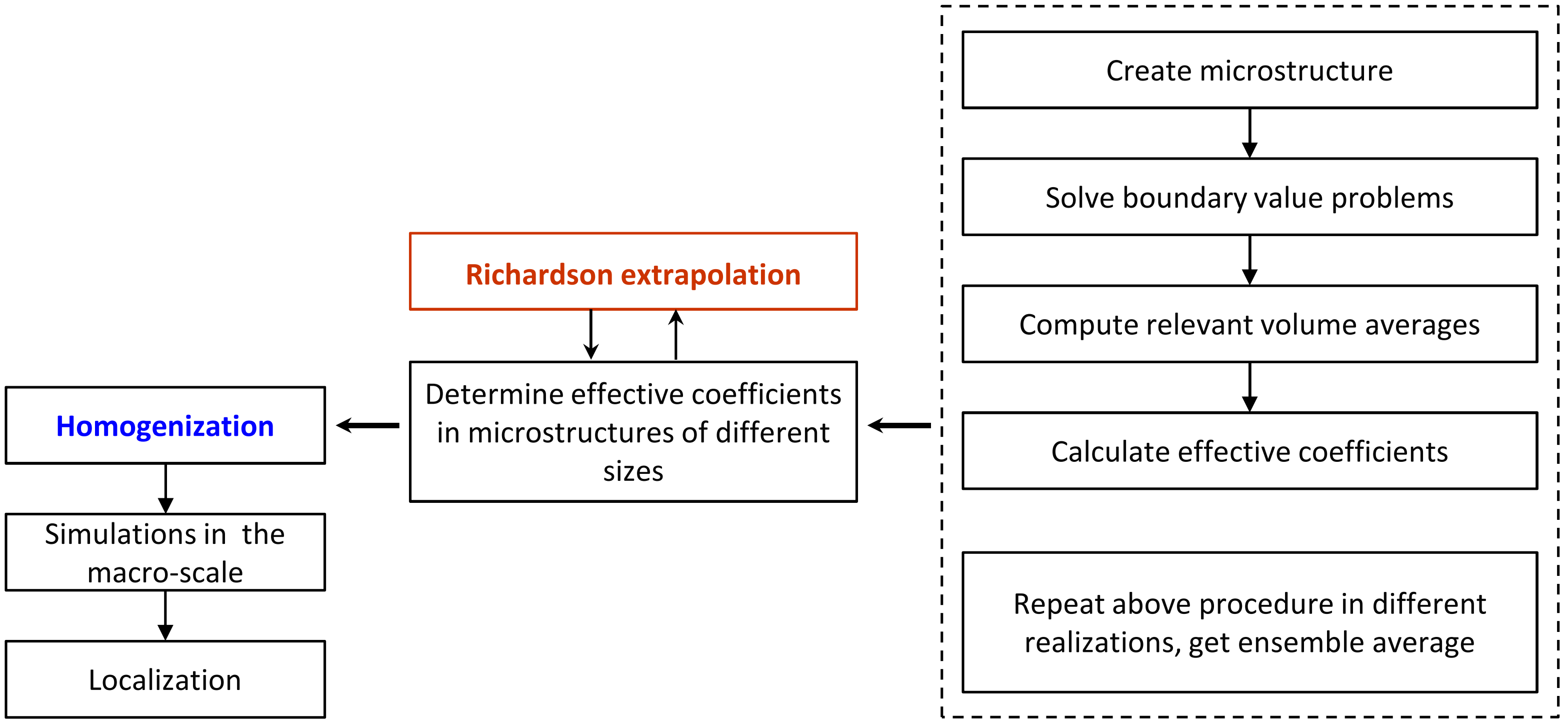
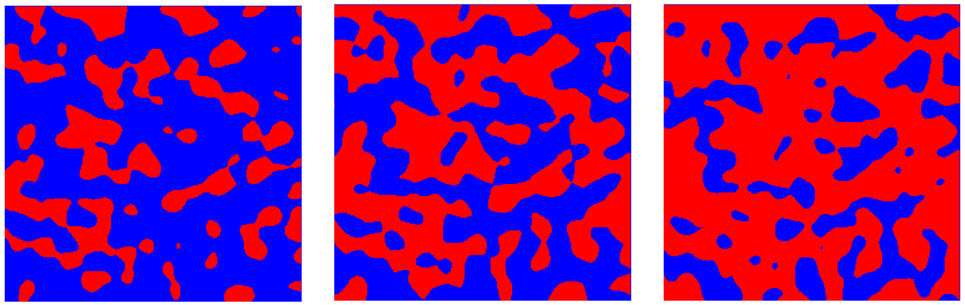


Figure: The main procedure of multiscale method combined with Richardson extrapolation technique

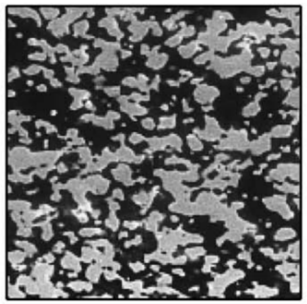
Numerics

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_2O_3 micrographs

Numerics

Example

We predict effective thermal conductivity of actual Al/Al_2O_3 with different volume fractions of Al.

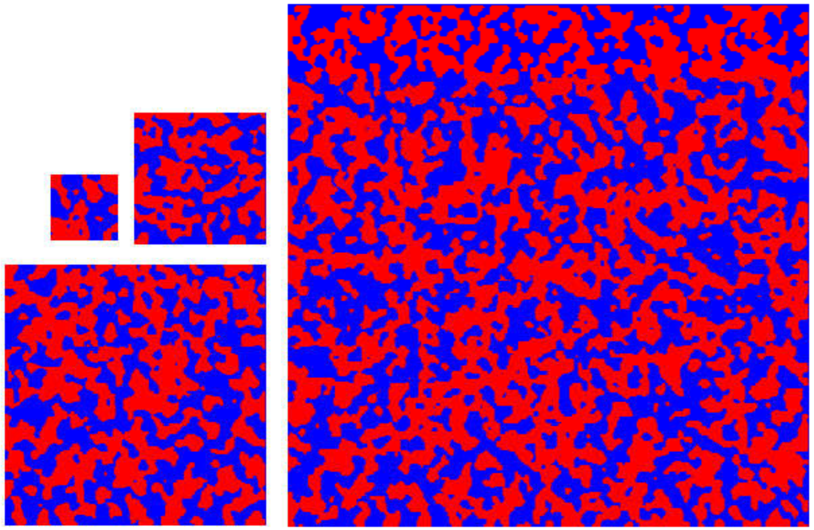


Figure: Microstructures with different sizes

Numerics

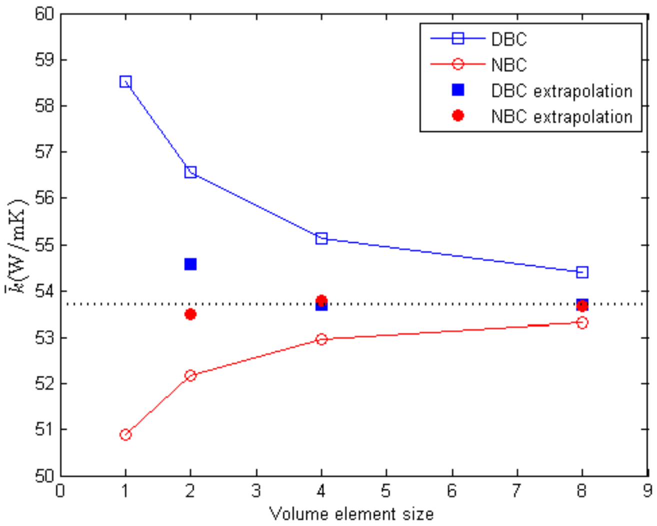
Table: Properties of constituent materials

Material	Al	Al_2O_3
k (W/mK)	233.0	30.0

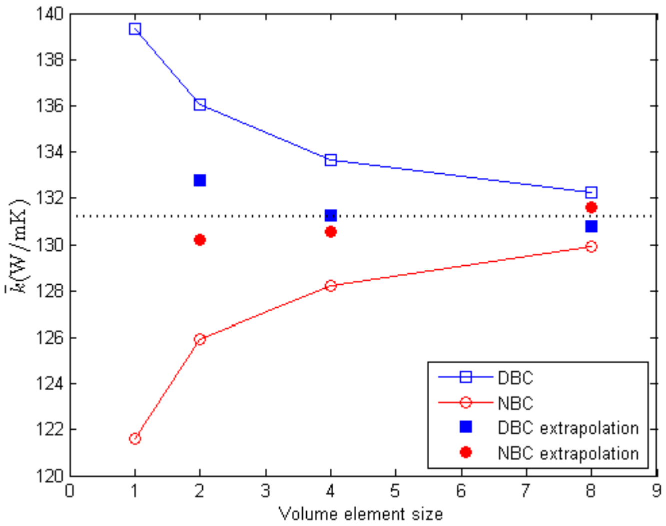
Table: Convergence rates of approximate effective coefficients

V_{Al} (%)	10	30	50	70	90
DBC	1.08	0.93	0.95	0.99	1.04
NBC	1.02	0.99	0.82	0.95	0.98

Numerics



(a) V_{Al}=30 %



(b) V_{Al}=70 %

Figure: Comparison of approximate effective coefficients by homogenization and extrapolation with increasing volume element size

Numerics

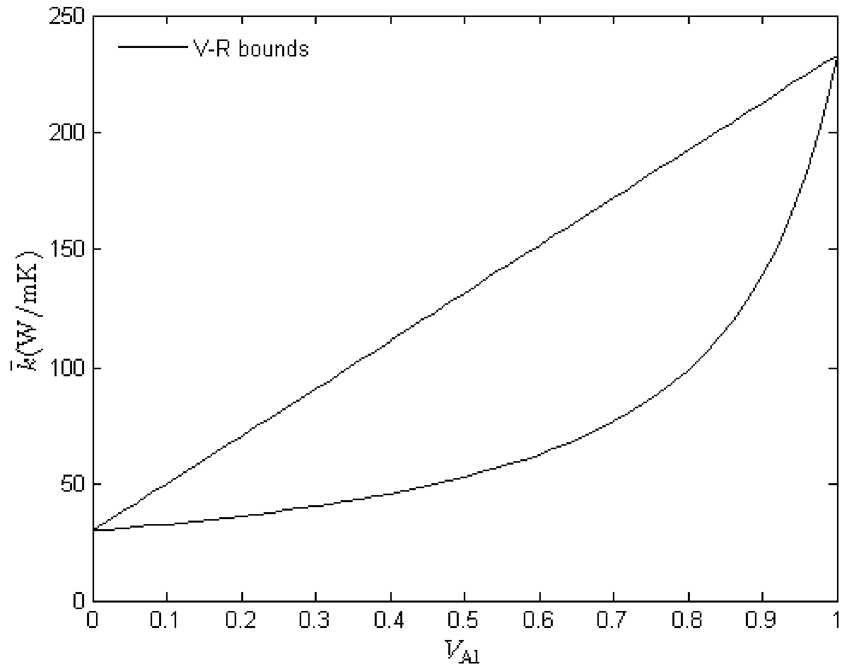
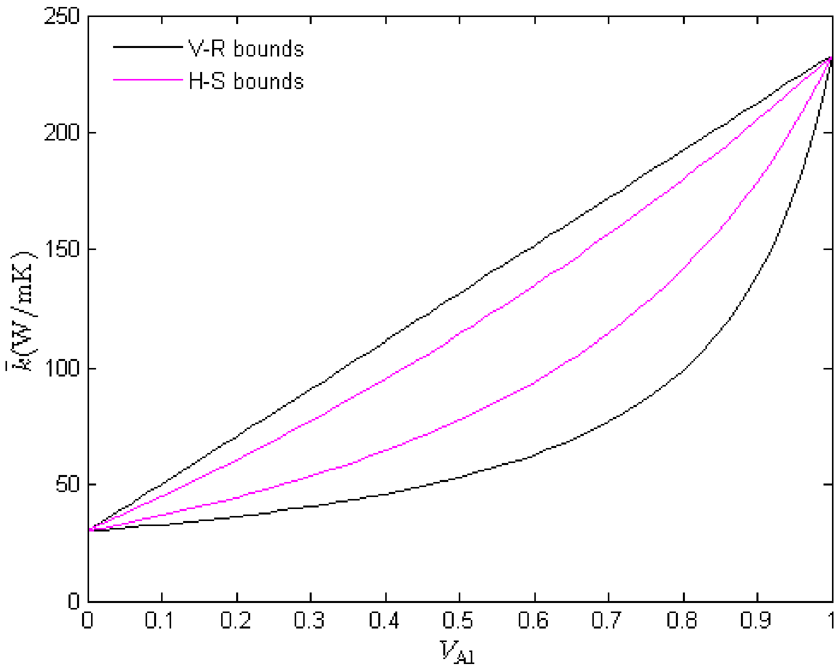


Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bounds and Hashin-Shtrikman bounds)

Numerics



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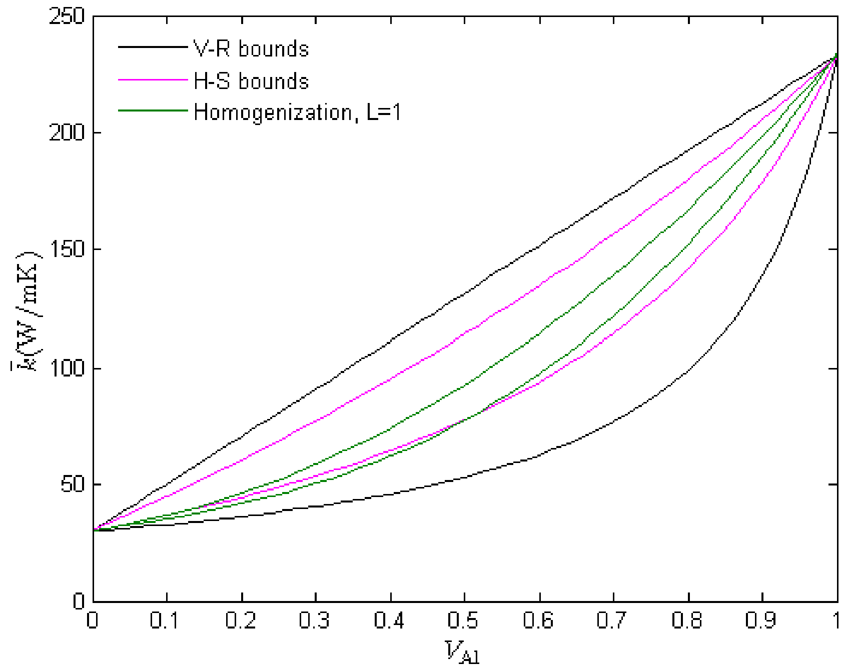
Numerics



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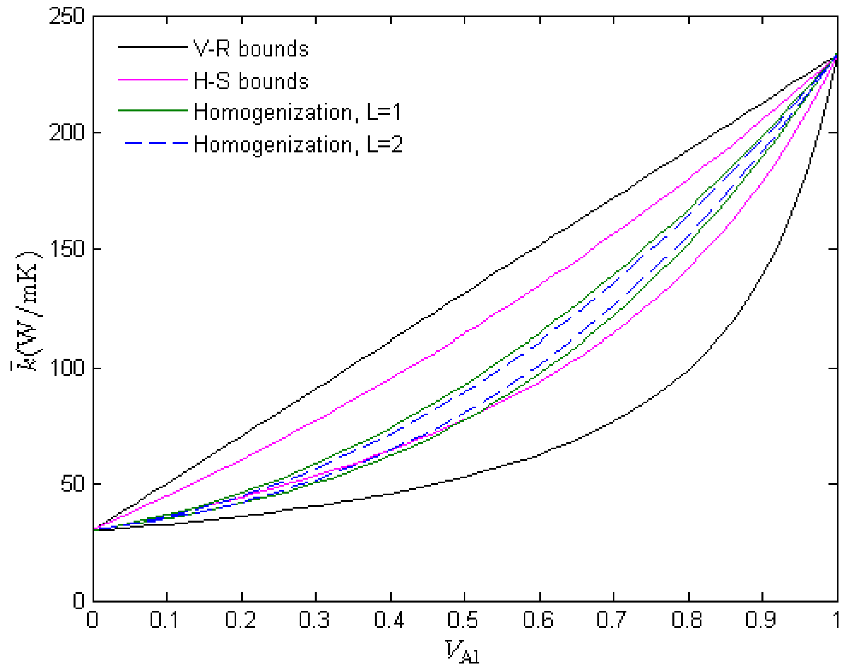

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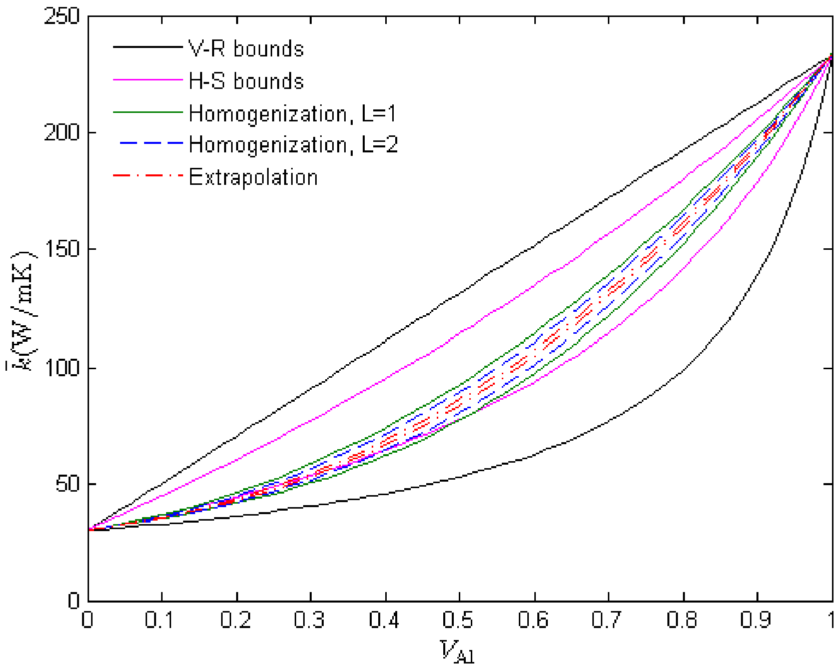


Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bounds and Hashin-Shtrikman bounds)

Numerics

Example

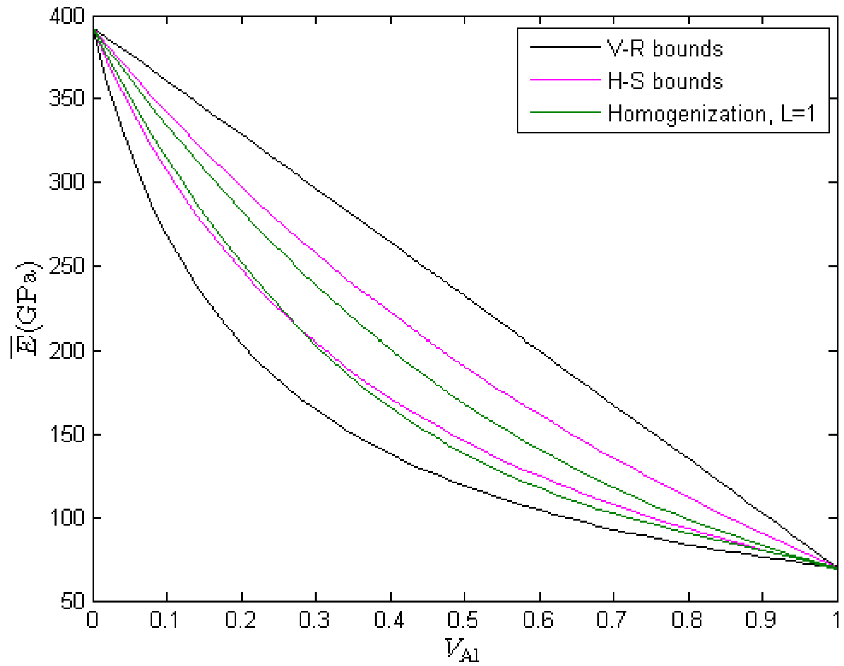
We predict effective mechanical properties of actual Al/Al_2O_3 with different volume fractions of Al.

The contrast ratio between the elastic modulus of Al_2O_3 and Al is 5.6.

Table: Properties of constituent materials

Material	Al	Al_2O_3
E (GPa)	70	393
ν	0.30	0.22

Numerics



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Numerics

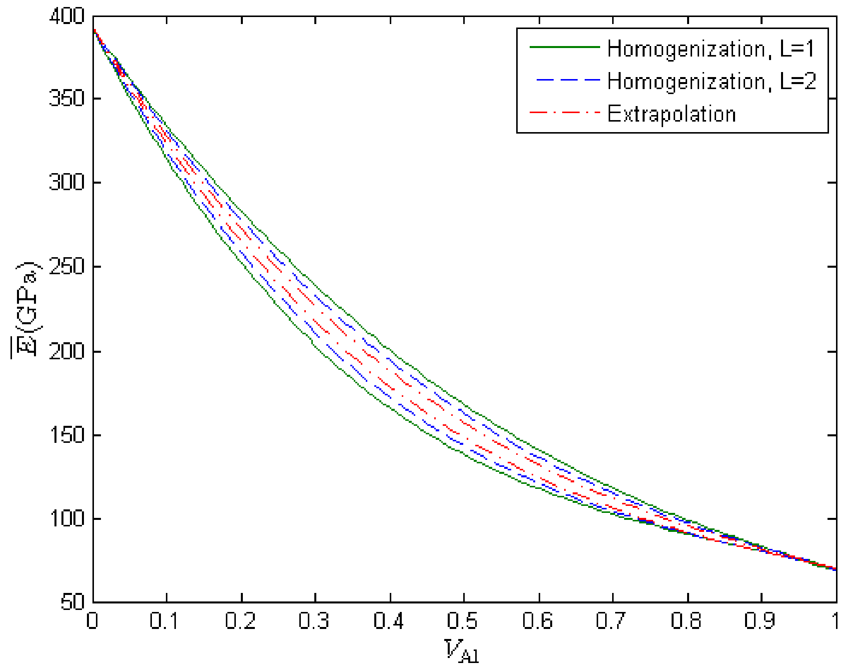


Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bounds and Hashin-Shtrikman bounds)

Numerics

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

Material	Stainless Steel (SS)	Resin
E (GPa)	193.8	1.31
ν	0.29	0.40

Numerics

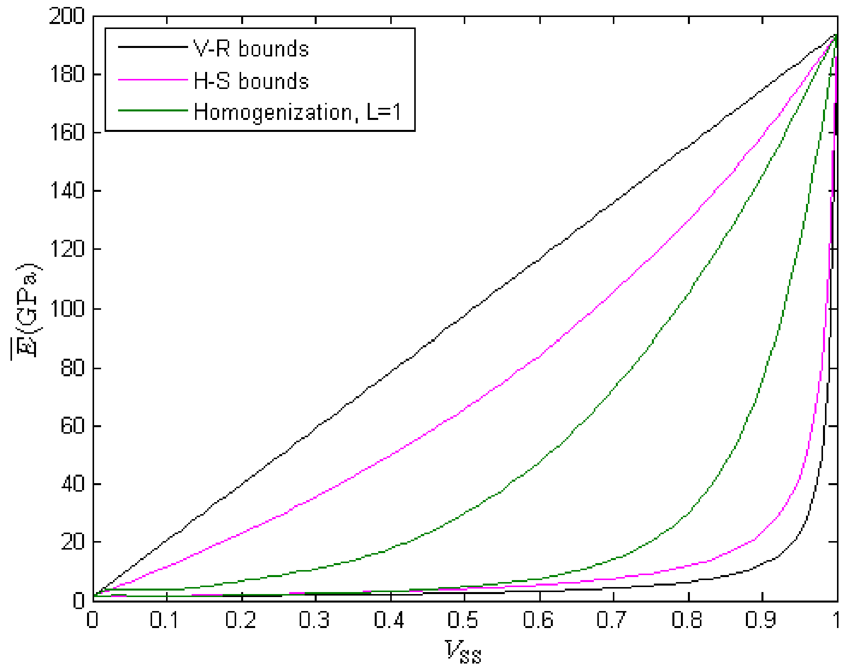


Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bounds and Hashin-Shtrikman bounds)

Numerics

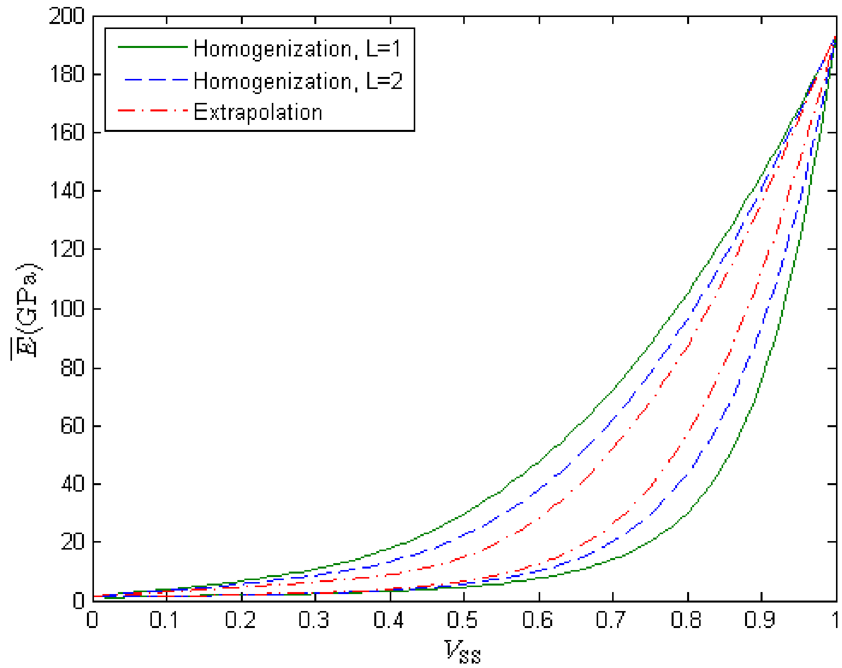


Figure: Comparison of Homogenization, Extrapolation and Variational bounds (Voigt-Reuss bonds and Hashin-Shtrikman bounds)

Contents

Motivation

- Many random heterogeneous materials have a high contrast of constituent properties.

  a. Composite materials (e.g., CNT-reinforced polymers)

  b. Porous media

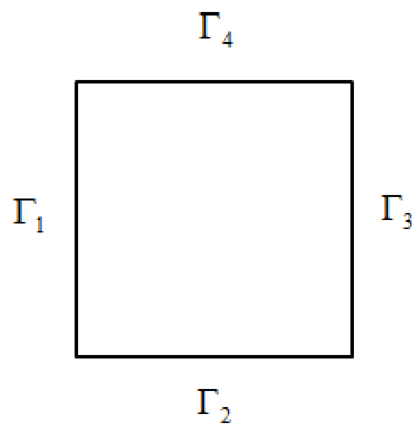
- The high contrast leads to very broad Dirichlet-Neumann upper and lower bounds.

Motivation

Mixed Dirichlet-Neumann boundary condition (DNBC)

approximations lie within the Dirichlet-Neumann bounds. (*Yue* 2007)

$$
\begin{aligned}
u(y,\omega) &= \xi_i \cdot y \quad && \text{on } \partial_1 Y_L \\
a(y,\omega)\nabla u(y,\omega)\cdot n &= 0 && \text{on } \partial_2 Y_L
\end{aligned}
$$



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

And $i = 1, \cdots, d$.

Method

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

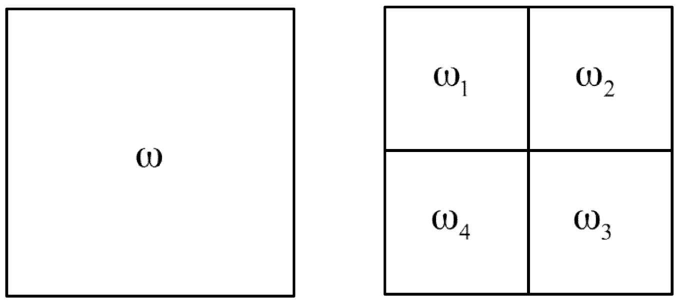


Figure: Volume elements with different sizes

Continuous properties

$$u_{\omega_1} = u_{\omega_2}$$
$$a\nabla u_{\omega_1} \cdot n_{\omega_1} = -a\nabla u_{\omega_2} \cdot n_{\omega_2}$$

Method

Robin boundary condition (RBC)

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

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

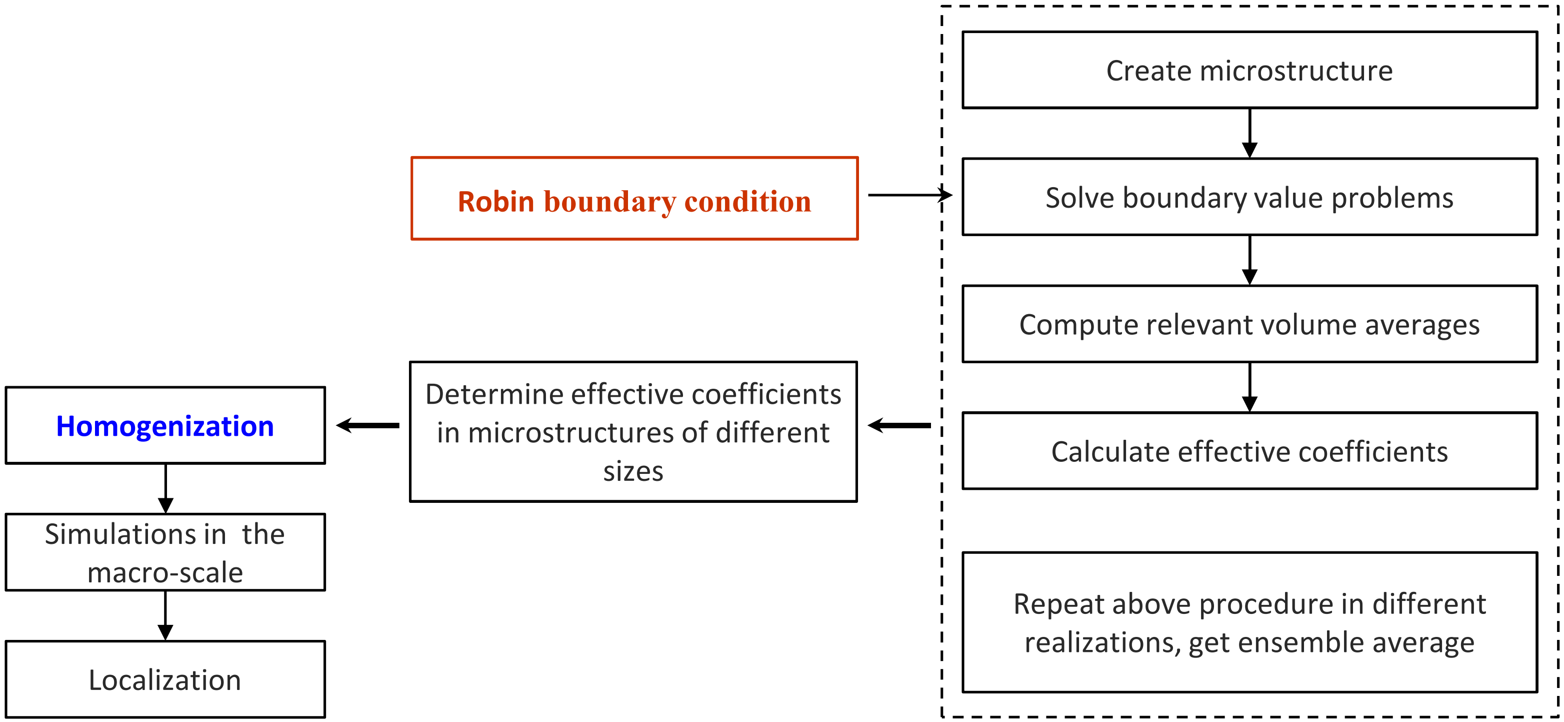
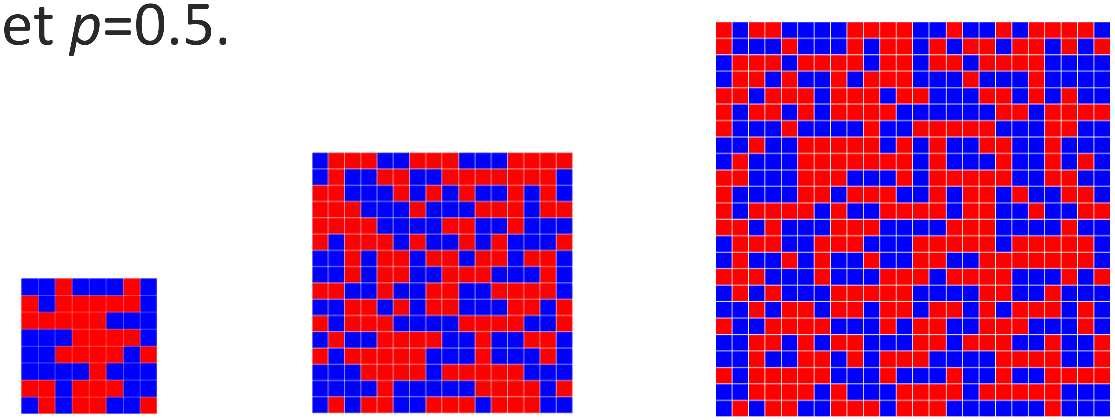


Figure: The main procedure of multiscale method combined with Robin boundary condition

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 $p=0.5$.



(a) $L=8$ (b) $L=16$ (c) $L=24$

Figure: Random checker-board microstructures with different sizes

Numerics

For two-phase random heterogeneous materials,

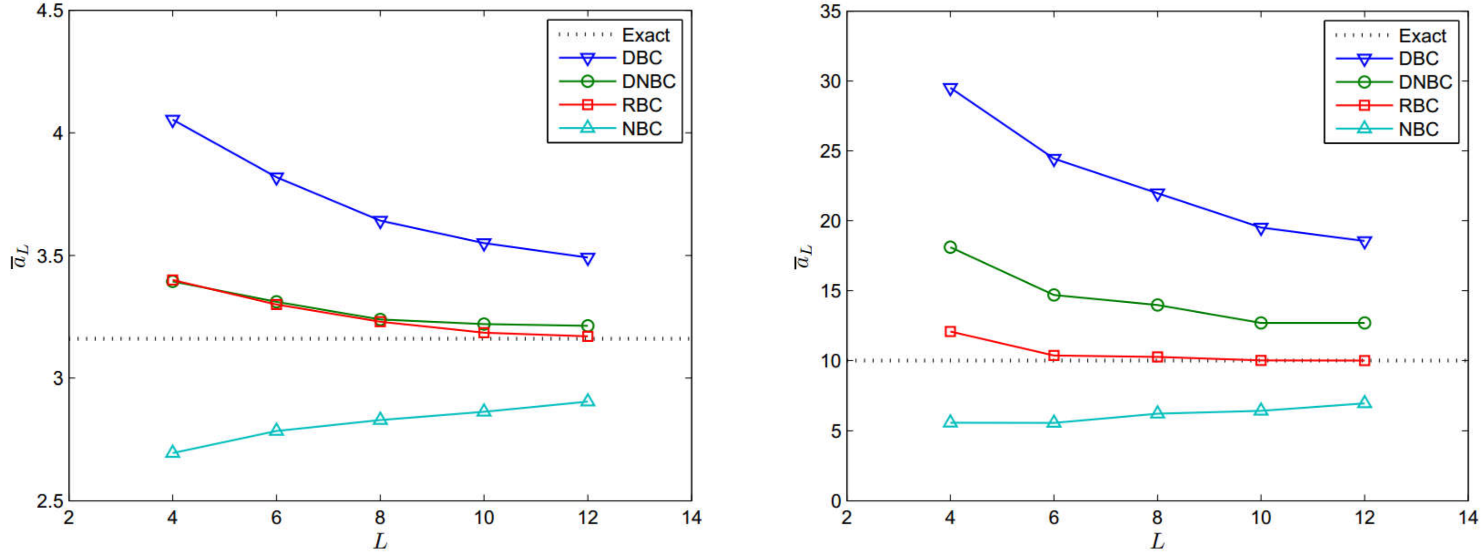
$$a(y,\omega) = \begin{cases} a_1 \cdot I, & y \in Y_L^m \\ a_2 \cdot I, & y \in Y_L^r \end{cases}$$

has a high contrast, i.e.,

$$r = \frac{a_2}{a_1} \gg 1$$

Here, I is the identity matrix.

Numerics



(a) r = 10 (b) r = 100

Figure: Approximate effective coefficients with different boundary conditions and different contrast ratios ($\lambda = 40$ in RBC)

Numerics

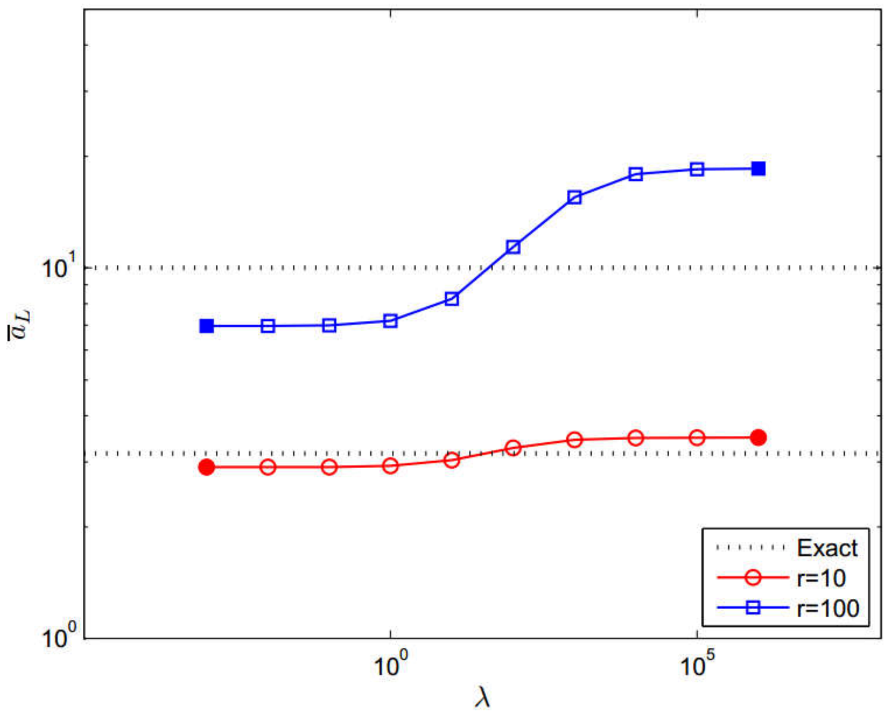
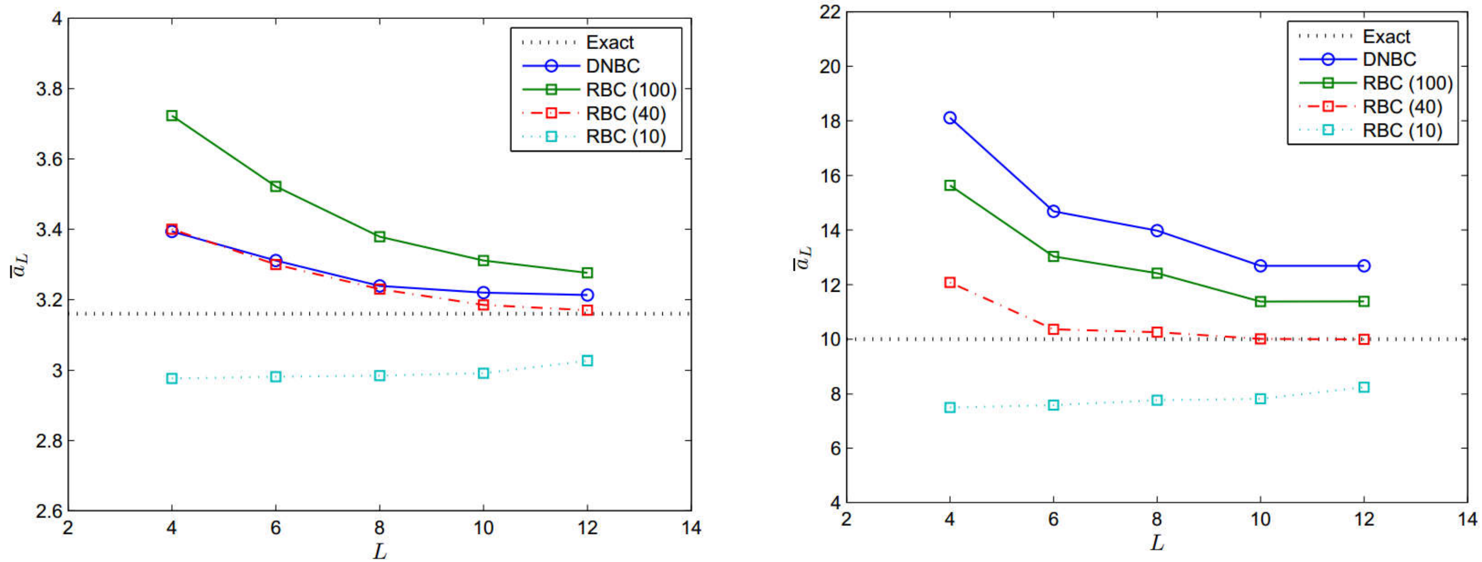


Figure: Effect of adjusting factor in RBC on the accuracy of approximate effective coefficients

Numerics



(a) r = 10

(b) r = 100

Figure: Approximate effective coefficients with different adjusting factor in RBC

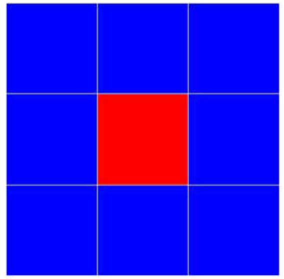
More Discussion

- 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

$$\begin{cases} -\nabla \cdot \left(a\left(y,\omega\right)\nabla u\left(y,\omega\right)\right)=0 & \text{in } Y_L \\ u\left(y,\omega\right)=\xi_i \cdot y & \text{on } \partial Y_L,\ i=1,\cdots,d \end{cases}$$

More Discussion



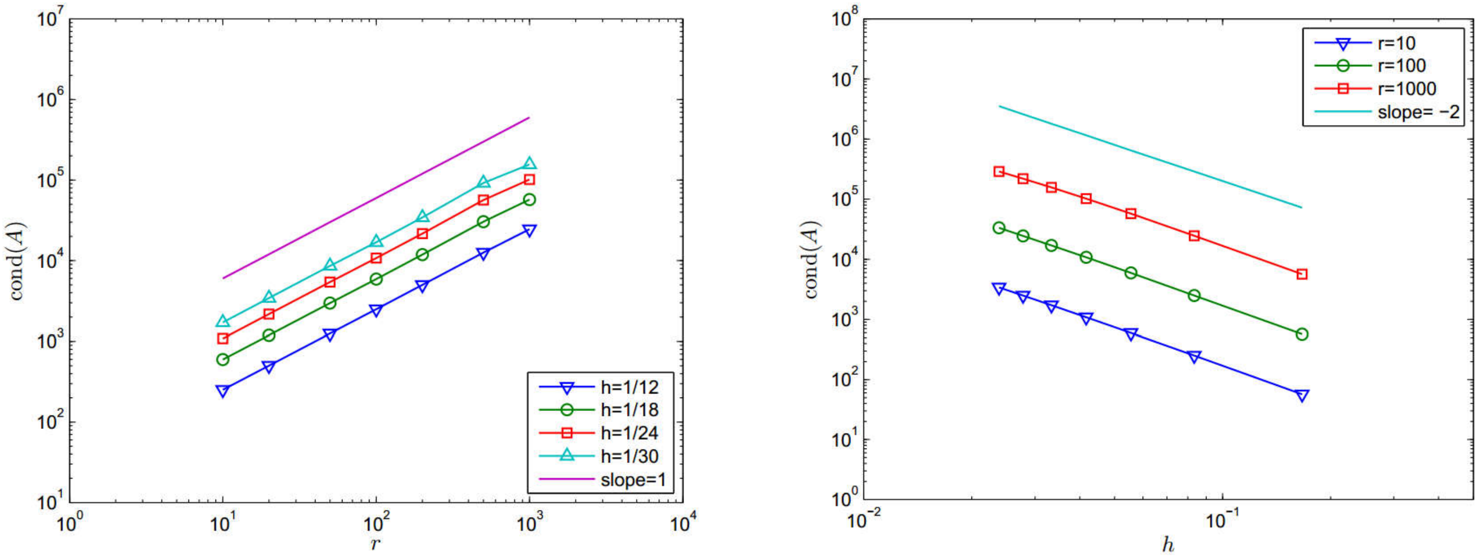
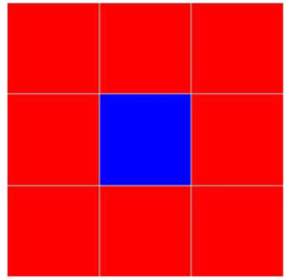
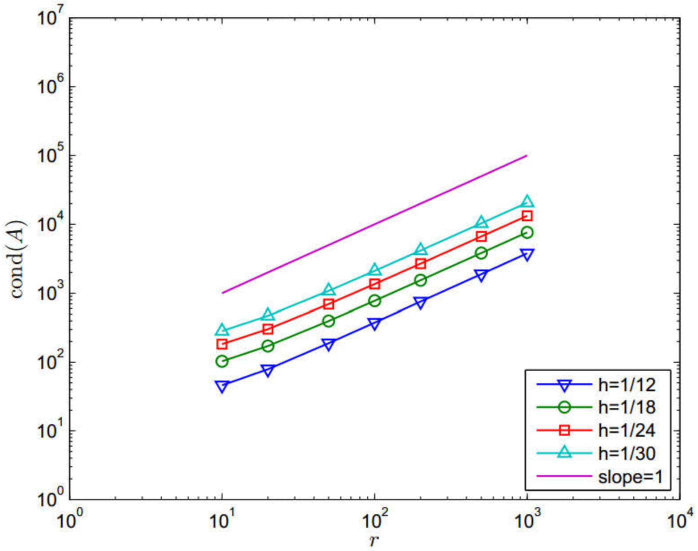


Figure: Effect of contrast ratio and mesh size on the condition number of stiffness matrix (constituent with high property in the center)

More Discussion





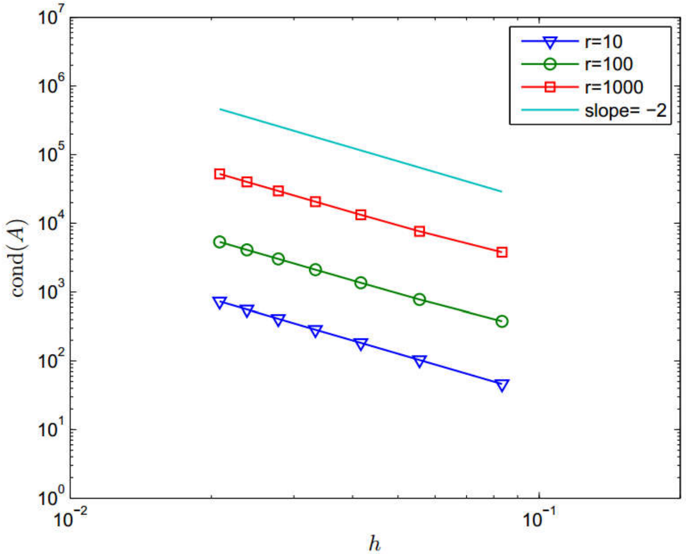


Figure: Effect of contrast ratio and mesh size on the condition number of stiffness matrix (constituent with low property in the center)

More Discussion

$$\boxed{\mathrm{cond}(A) = Crh^{-2}}$$

		$h = 1/36$ cond	N_{ite}	$h = 1/42$ cond	N_{ite}	$h = 1/48$ cond	N_{ite}
$r = 100$	CGM ICCGM	24472 1168	293 25	33306 1590	366 29	43106 2076	440 33
$r = 1000$	CGM ICCGM	218510 10325	474 29	289075 13517	612 33	**363644** 16902	768 37

- 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.

Contents

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.

Reference

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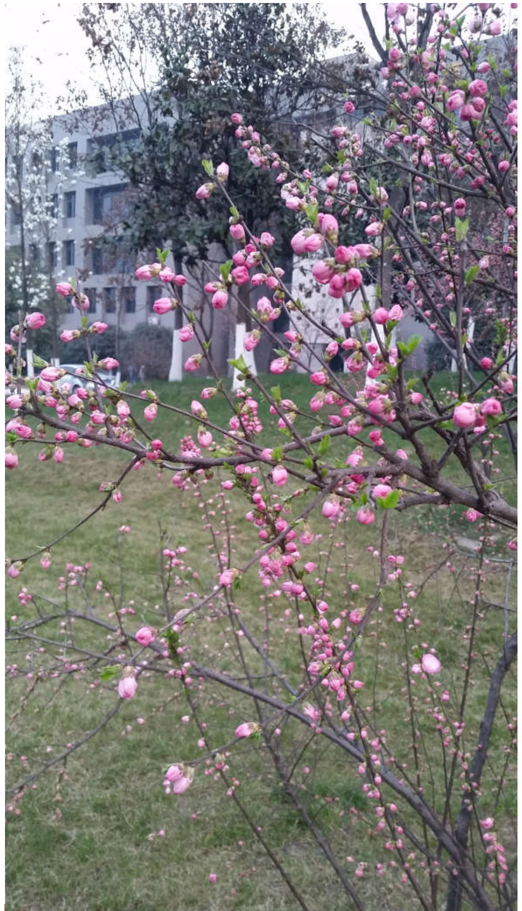

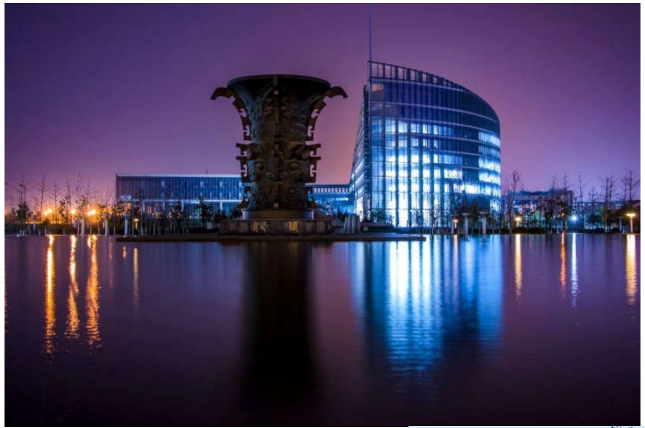

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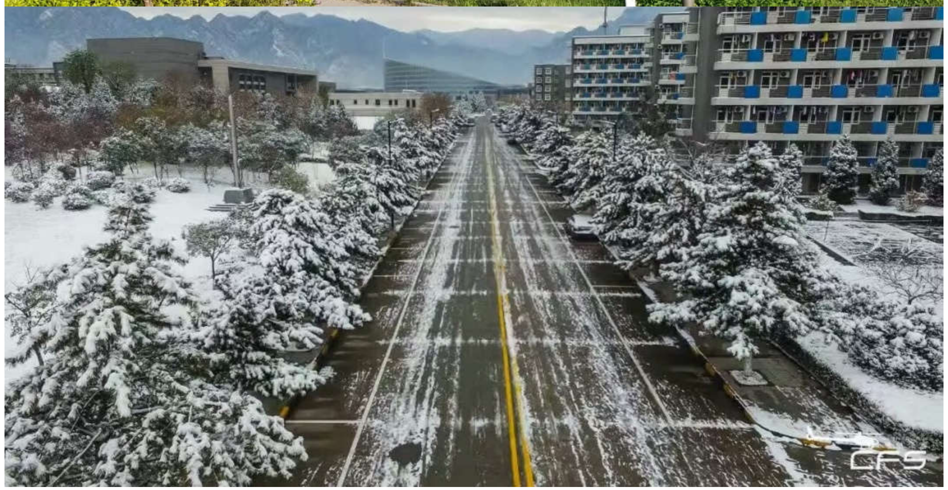

Thank you for your attention !