Exponentially Convergent Multiscale Methods for solving elliptic and Helmholtz's equation

Yifan Chen

Computing and Mathematical Sciences, Caltech

May 2023

Collaborators and Related Papers [Chen, Hou, Wang 2021, 2021, 2022]





Thomas Hou Caltech Yixuan Wang Caltech

- Exponential Convergence for Multiscale Linear Elliptic PDEs via Adaptive Edge Basis Functions, SIAM-MMS, 2021
- Exponentially Convergent Multiscale Methods for 2D High Frequency Heterogeneous Helmholtz Equations, SIAM-MMS, 2022
- Exponentially Convergent Multiscale Finite Element Method, CAMC, 2022 (review paper)

Outline

1 The Problems of Heterogeneity and High Frequency

2 The Challenges in Numerical Approximation

3 The Methodology of Exponential Convergence

4 Our Contributions: Helmholtz's Equation and Nonoverlapping

Outline

1 The Problems of Heterogeneity and High Frequency

2 The Challenges in Numerical Approximation

3 The Methodology of Exponential Convergence

4 Our Contributions: Helmholtz's Equation and Nonoverlapping

Multiscale Problems: Heterogeneous Media and High Frequency Waves



Figure: Heterogeneity and high frequency

Figure credited to Google online search

Mathematical Setup

Model problem:

 $-\nabla \cdot (A \nabla u) + V u = f$, in Ω , w/ boundary conditions

(subsurface flows, diffusions, elasticity, waves)

Mathematical Setup

Model problem:

 $-\nabla \cdot (A \nabla u) + V u = f$, in Ω , w/ boundary conditions

(subsurface flows, diffusions, elasticity, waves)

Mathematical conditions:

• Heterogeneity:

 $A, V \in L^{\infty}(\Omega), \text{ and } 0 < A_{\min} \leq A(x) \leq A_{\max} < \infty$

• High frequency:

e.g.,
$$V=-k^2$$
 (Helmholtz's equation)

Outline

1 The Problems of Heterogeneity and High Frequency

2 The Challenges in Numerical Approximation

3 The Methodology of Exponential Convergence

4 Our Contributions: Helmholtz's Equation and Nonoverlapping

Literature: Scale Separation v.s. Continuum of Scales

Explicit scale parameter ϵ : $A = A(x, x/\epsilon)$

- Theory: with scale separation and periodicity assumptions \Rightarrow there is a homogenized $A_0 = A_0(x)$ when $\epsilon \to 0$
- Coarse scale behaviors of the solution are often identified using asymptotic analysis and homogenization theory

Literature: Scale Separation v.s. Continuum of Scales

Explicit scale parameter ϵ : $A = A(x, x/\epsilon)$

- Theory: with scale separation and periodicity assumptions \Rightarrow there is a homogenized $A_0 = A_0(x)$ when $\epsilon \to 0$
- Coarse scale behaviors of the solution are often identified using asymptotic analysis and homogenization theory

Continuum of scales: $A \in L^{\infty}$

- Find local basis functions that capture the fine scale information, and use them to identify the correct coarse scale behaviors of the solution
- "Coarse scale" becomes a design choice in numerical approximation

Galerkin's method:

- Construct basis functions and plug them into the variational form
- Key: Quasi-optimality, i.e.,

Galerkin solution err \sim optimal approx-err in $\|\cdot\|_{\mathcal{H}(\Omega)}$

Galerkin's method:

- Construct basis functions and plug them into the variational form
- Key: Quasi-optimality, i.e.,

Galerkin solution err \sim optimal approx-err in $\|\cdot\|_{\mathcal{H}(\Omega)}$

Challenges:

• Heterogeneity $\Rightarrow u$ or ∇u is oscillatory (!) approx-err of FEM can be arbitrarily bad [Babuška, Osborn 2000]

Galerkin's method:

- Construct basis functions and plug them into the variational form
- Key: Quasi-optimality, i.e.,

Galerkin solution err \sim optimal approx-err in $\|\cdot\|_{\mathcal{H}(\Omega)}$

Challenges:

- Heterogeneity $\Rightarrow u$ or ∇u is oscillatory (!) approx-err of FEM can be arbitrarily bad [Babuška, Osborn 2000]
- High frequency \Rightarrow stability issues

e.g., $\|u\|_{\mathcal{H}(\Omega)} \leq C_{\mathsf{stab}}(k) \|f\|_{L^2(\Omega)}$ for $C_{\mathsf{stab}}(k) \succeq 1 + k^{\gamma}$

(!) approx-err amplified by the stability constant

- quasi-optimality also deteriorates, e.g., require $H = O(1/k^2)$
- phenomenon known as pollution effect [Babuška, Sauter, 1997]

Galerkin's method:

- Construct basis functions and plug them into the variational form
- Key: Quasi-optimality, i.e.,

Galerkin solution err \sim optimal approx-err in $\|\cdot\|_{\mathcal{H}(\Omega)}$

Challenges:

- Heterogeneity $\Rightarrow u$ or ∇u is oscillatory (!) approx-err of FEM can be arbitrarily bad [Babuška, Osborn 2000]
- High frequency \Rightarrow stability issues

e.g., $\|u\|_{\mathcal{H}(\Omega)} \leq C_{\mathsf{stab}}(k) \|f\|_{L^2(\Omega)}$ for $C_{\mathsf{stab}}(k) \succeq 1 + k^{\gamma}$

(!) approx-err amplified by the stability constant

- quasi-optimality also deteriorates, e.g., require $H = O(1/k^2)$
- phenomenon known as pollution effect [Babuška, Sauter, 1997]

(!) Need high accuracy approximation

Outline

1 The Problems of Heterogeneity and High Frequency

2 The Challenges in Numerical Approximation

3 The Methodology of Exponential Convergence

4 Our Contributions: Helmholtz's Equation and Nonoverlapping

How to Approximate A Function with High Accuracy?

When the function is smooth:

How to Approximate A Function with High Accuracy?

When the function is smooth:

• Just choose polynomial basis functions for approximation

 \Rightarrow exponential convergence of accuracy

When the function is smooth:

 ${\ensuremath{\, \bullet }}$ Just choose polynomial basis functions for approximation

 \Rightarrow exponential convergence of accuracy

- e.g., hp-FEM for solving PDEs with smooth solutions
 - provably handles pollution effects in Helmholtz's equation with $p = O(\log k)$ [Melenk, Sauter 2010, 2011]

When the function is smooth:

• Just choose polynomial basis functions for approximation

 \Rightarrow exponential convergence of accuracy

- e.g., hp-FEM for solving PDEs with smooth solutions
 - provably handles pollution effects in Helmholtz's equation with $p = O(\log k)$ [Melenk, Sauter 2010, 2011]

If the function is non-smooth?

Exponential Convergence for Approximating A-harmonic functions

Warm-up: A-harmonic functions

• Function space: assume $0 < A_{\min} \leq A(x) \leq A_{\max} < \infty$

$$U(D) := \{ v \in H^1(D), -\nabla \cdot (A\nabla v) = 0 \text{ in } D \} / \mathbb{R}$$

• Norm:

$$||v||_{H^1_A(D)} := ||A^{1/2} \nabla v||_{L^2(D)}$$

Exponential Convergence for Approximating A-harmonic functions

Warm-up: A-harmonic functions

• Function space: assume $0 < A_{\min} \le A(x) \le A_{\max} < \infty$

$$U(D) := \{ v \in H^1(D), -\nabla \cdot (A\nabla v) = 0 \text{ in } D \} / \mathbb{R}$$

• Norm:

$$||v||_{H^1_A(D)} := ||A^{1/2} \nabla v||_{L^2(D)}$$

Theorem [Babuška, Lipton 2011]

The singular values $\sigma_m(R)$ of the restriction operator

$$R: (U(\omega^*), \|\cdot\|_{H^1_A(\omega^*)}) \to (U(\omega), \|\cdot\|_{H^1_A(\omega)})$$

decays nearly exponentially fast:

$$\sigma_m(R) \le C_\epsilon \exp\left(-m^{\frac{1}{d+1}-\epsilon}\right)$$

for some C_ϵ independent of H and m



Approximating A-harmonic functions can be exponentially convergent

• For any $u \in H^1_A(\omega^*)$, there are m functions $v_j, 1 \leq j \leq m$

$$\|u - \sum_{j=1}^{m} c_j v_j\|_{H^1_A(\omega)} \le C_{\epsilon} \exp\left(-m^{\frac{1}{d+1}-\epsilon}\right) \|u\|_{H^1_A(\omega^*)}$$

• v_j are left singular vectors of the restriction operator R

Approximating A-harmonic functions can be exponentially convergent

• For any $u \in H^1_A(\omega^*)$, there are m functions $v_j, 1 \leq j \leq m$

$$\|u - \sum_{j=1}^{m} c_j v_j\|_{H^1_A(\omega)} \le C_{\epsilon} \exp\left(-m^{\frac{1}{d+1}-\epsilon}\right) \|u\|_{H^1_A(\omega^*)}$$

• v_j are left singular vectors of the restriction operator R

Summarize the property: Restrictions of *A*-harmonic functions are of low approximation complexity

[Babuška, Lipton 2011], [Babuška, Lipton, Sinz, Stuebner 2020], [Ma, Scheichl, Dodwell 2021]

For elliptic equations with rough coefficients

 $-\nabla\cdot (A\nabla u)=f, \ \text{in} \ \Omega, \ \ \text{w/ boundary conditions}$

[Babuška, Lipton 2011], [Babuška, Lipton, Sinz, Stuebner 2020], [Ma, Scheichl, Dodwell 2021]

For elliptic equations with rough coefficients

 $-\nabla \cdot (A \nabla u) = f$, in Ω , w/ boundary conditions

Decompose the solution to local components:

$$u = \sum_i \eta_i u = \sum_i \eta_i u^{\mathsf{h}}_{\omega_i} + \sum_i \eta_i u^{\mathsf{b}}_{\omega_i}$$

• Overlapped domain decomp. ω_i is of size O(H)



- Partition of unity functions $\sum_i \eta_i = 1$, supp $\eta_i = \omega_i$, η_i smooth
- Harmonic-bubble splitting

$$\begin{cases} -\nabla \cdot (A\nabla u_{\omega_i}^{\mathsf{h}}) = 0, & \text{in } \omega_i \\ u_{\omega_i}^{\mathsf{h}} = u, & \text{on } \partial \omega_i \\ \int -\nabla \cdot (A\nabla u_{\omega_i}^{\mathsf{b}}) = f, & \text{in } \omega_i \\ u_{\omega_i}^{\mathsf{b}} = 0, & \text{on } \partial \omega_i \end{cases}$$

11/20

[Babuška, Lipton 2011], [Babuška, Lipton, Sinz, Stuebner 2020], [Ma, Scheichl, Dodwell 2021]

$$u = \sum_{i} \eta_{i} u = \sum_{i} \eta_{i} u_{\omega_{i}}^{\mathsf{h}} + \sum_{i} \eta_{i} u_{\omega_{i}}^{\mathsf{b}}$$

 η_iu^h_{ωi} is a restriction of an A-harmonic function, so can be approximated by basis functions with nearly exponential accuracy

[Babuška, Lipton 2011], [Babuška, Lipton, Sinz, Stuebner 2020], [Ma, Scheichl, Dodwell 2021]

$$u = \sum_{i} \eta_{i} u = \sum_{i} \eta_{i} u_{\omega_{i}}^{\mathsf{h}} + \sum_{i} \eta_{i} u_{\omega_{i}}^{\mathsf{b}}$$

• $\eta_i u_{\omega_i}^{\mathsf{h}}$ is a restriction of an *A*-harmonic function, so can be approximated by basis functions with nearly exponential accuracy $\Rightarrow u = \sum_{i} \sum_{k=1}^{m} c_{i,k} v_{i,k} + O\left(\exp\left(-m^{\frac{1}{d+1}-\epsilon}\right) \|u\|_{H^1_A(\Omega)}\right) + \sum_{i} \eta_i u_{\omega_i}^{\mathsf{b}}$

(II)

[Babuška, Lipton 2011], [Babuška, Lipton, Sinz, Stuebner 2020], [Ma, Scheichl, Dodwell 2021]

$$u = \sum_i \eta_i u = \sum_i \eta_i u^{\mathsf{h}}_{\omega_i} + \sum_i \eta_i u^{\mathsf{b}}_{\omega_i}$$

• $\eta_i u_{\omega_i}^{\mathsf{h}}$ is a restriction of an *A*-harmonic function, so can be approximated by basis functions with nearly exponential accuracy $\Rightarrow u = \underbrace{\sum_{i} \sum_{k=1}^{m} c_{i,k} v_{i,k}}_{(\mathsf{I})} + O\left(\exp\left(-m^{\frac{1}{d+1}-\epsilon}\right) \|u\|_{H^1_A(\Omega)}\right) + \underbrace{\sum_{i} \eta_i u_{\omega_i}^{\mathsf{b}}}_{(\mathsf{I})}$

Offline: for a given A, one constructs local basis functions

- Compute $v_{i,k}$ in (I) by solving local spectral problems Online: given any source term f, one solves u
 - Compute (II) by solving local equations
 - Compute (I) by Galerkin's method with offline basis functions

Note: Local problems are solved on a fine mesh h < H

Outline

1 The Problems of Heterogeneity and High Frequency

2 The Challenges in Numerical Approximation

3 The Methodology of Exponential Convergence

4 Our Contributions: Helmholtz's Equation and Nonoverlapping

Our Contributions: New Local Structures and Global Coupling

Multiscale methods for Helmholtz's equation

[Peterseim 2017], [Peterseim, Verfürth 2020], [Fu, Li, Craster, Guenneau 2021]

 $- \nabla \cdot (A \nabla u) - k^2 u = f$, in Ω , w/ boundary conditions

- No pre-existing results on achieving exponential convergence
- Question: What is the structure of low approximation complexity?
- Difficulty: Indefiniteness of the operator

Non-overlapped domain decomposition [Hou, Wu 1997], [Hou, Liu 2015]



- Advantage: More localized domains, local functions less overlapped (more efficient in stiffness matrix assembly)
- Difficulty: Non-overlapping, interaction through edges

Helmholtz-harmonic functions

• Function space:

$$U_k(D) := \{ v \in H^1(D), -\nabla \cdot (A\nabla v) - k^2 v = 0 \text{ in } D \} / \mathbb{R}$$

• Energy norm:

$$\|v\|_{\mathcal{H}(D)}^2 := \|A^{1/2}\nabla v\|_{L^2(D)}^2 + \|kv\|_{L^2(D)}^2$$

Helmholtz-harmonic functions

Function space:

$$U_k(D) := \{ v \in H^1(D), -\nabla \cdot (A\nabla v) - k^2 v = 0 \text{ in } D \} / \mathbb{R}$$

Energy norm:

$$\|v\|_{\mathcal{H}(D)}^2 := \|A^{1/2}\nabla v\|_{L^2(D)}^2 + \|kv\|_{L^2(D)}^2$$

Theorem [Chen, Hou, Wang 2021], [Ma, Alber, Scheichl 2021] Let $H^* = O(1/k)$, then singular values $\sigma_m(R)$ of the restriction operator for Helmholtz-harmonic functions

$$R: (U_k(\omega^*), \|\cdot\|_{\mathcal{H}(\omega^*)}) \to (U_k(\omega), \|\cdot\|_{\mathcal{H}(\omega)})$$

decays nearly exponentially fast:

$$\sigma_m(R) \le C_\epsilon \exp\left(-m^{\frac{1}{d+1}-\epsilon}\right)$$

for some C_ϵ independent of k,H and m

Key: $H^{\star} = O(1/k) \Rightarrow$ the Helmholtz operator is locally positive definite



Our Contributions: New Local Structures and Global Coupling

Multiscale methods for Helmholtz's equation

[Peterseim 2017], [Peterseim, Verfürth 2020], [Fu, Li, Craster, Guenneau 2021]

 $-\nabla \cdot (A \nabla u) - k^2 u = f$, in Ω , w/ boundary conditions

- No pre-existing results on achieving exponential convergence
- Question: What is the structure of low approximation complexity?
- Difficulty: Indefiniteness of the operator

Non-overlapped domain decomposition [Hou, Wu 1997], [Hou, Liu 2015]



- Advantage: More localized domains, local functions less overlapped (more efficient in stiffness matrix assembly)
- Difficulty: Non-overlapping, interaction through edges





2. Focus on edge functions

$$\sum_{i} \mathbb{1}_{T_i} u_{T_i}^{\mathsf{h}} = Q\tilde{u}^{\mathsf{h}} \in H^{1/2}(E_H)$$

• where $Q: H^{1/2}(E_H) \to H^1(\Omega)$ is the Helmholtz-harmonic extension operator







3. Edge localization $\tilde{u}^{h} = \underbrace{I_{H}\tilde{u}^{h}}_{\text{Nodal interp.}} + \underbrace{(\tilde{u}^{h} - I_{H}\tilde{u}^{h})}_{\text{Decoupled to each edges}}$ • $I_{H}\tilde{u}^{h} = \sum_{n} u(x_{n})\psi_{n}$ spanned by nodal basis funcs









Exponentially Convergent Multiscale Finite Element Method

Theorem [Chen, Hou, Wang 2021]

The following holds for the solution u of Helmholtz's equation

$$u = \left(\sum_{n} b_{n}\psi_{n} + \sum_{e} \sum_{j=1}^{m} c_{j,e}v_{j,e}\right)$$
$$+ \left(\sum_{i} \mathbb{1}_{T_{i}}u_{T_{i}}^{\mathsf{b}} + \sum_{e} Q(u_{\omega_{e}}^{\mathsf{b}} - I_{H}u_{\omega_{e}}^{\mathsf{b}})|_{e}\right)$$
$$+ O\left(\exp\left(-m^{\frac{1}{d+1}-\epsilon}\right)(\|u\|_{\mathcal{H}(\Omega)} + \|f\|_{L^{2}(\Omega)})\right)$$

Numerical Experiments: Helmholtz's Equation

The problem set-up

equation

$$-\nabla\cdot(A\nabla u)+Vu=f, \text{ in } \Omega=[0,1]^2$$

- boundary condition: mixed (Dirichlet + Neumann + Robin)
- $A(x) = |\xi(x)| + 0.5$ where $\xi(x)$ is piecewise linear functions with values as unit Gaussians r.v.; piecewise scale: 2^{-7}
- $-V/k^2$ draws from the same random field; $k=2^5$
- $f(x_1, x_2) = x_1^4 x_2^3 + 1$

Visualization of the Field



Numerical Experiments: Helmholtz's Equation

The mesh

- quadrilateral mesh
- fine mesh size $h = 2^{-10}$, coarse mesh size $H = 2^{-5}$

The accuracy of ExpMsFEM's solution compared to fine mesh solution



Figure: Numerical results for the mixed boundary and rough field example. Left: $e_{\mathcal{H}}$ versus m; right: e_{L^2} versus m. Number of basis functions $(2m + 1)/H^2$