Computation of Eigenvalues by Upscaling

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Multiscale problems

Applications such as

- composite materials
- flow in a porous medium

require numerical solution of partial differential equations with rough data (module of elasticity, conductivity, or permeability).

Major challenge: Features on multiple non-separated scales.
Multiscale methods

Let $A$ be rapidly varying data and consider a differential equation and its corresponding numerical approximation,

$$\mathcal{L}(A)u = f \quad \mathcal{L}_h(A)u_h = f_h.$$ 

For classical methods in many situations

$$|||u - u_h||| \leq C(A, A') h^\beta.$$ 

Multiscale methods seek an upscaled representation

$$\mathcal{L}_H(A)u_H = f_H$$

fulfilling $|||u_h - u_H||| \leq C(A) H^\beta$ with $C$ independent of $A'$.

How well is the (low part of the) spectrum of $\mathcal{L}$ preserved?
Outline

1. Model problem
2. Upscaling technique and error analysis
3. Numerical experiments
4. Application to a non-linear eigenvalue problem
5. Conclusions
Model multiscale eigenvalue problem

Prototypical self-adjoint eigenvalue problem

\[- \nabla \cdot A \nabla u = \lambda u \quad \text{in } \Omega \quad u = 0 \quad \text{on } \partial \Omega\]

with data \(0 < \alpha \leq A \in L^\infty(\Omega)\)
Model multiscale eigenvalue problem

Prototypical self-adjoint eigenvalue problem (variational form): find $u \in V := H^1_0(\Omega)$ and $\lambda \in \mathbb{R}$ such that

$$a(u, v) := \int_{\Omega} (A \nabla u) \cdot \nabla v \, dx = \lambda \int_{\Omega} u \cdot v \, dx \quad \text{for all } v \in V$$

with data $0 < \alpha \leq A \in L^\infty(\Omega)$
Model multiscale eigenvalue problem

Prototypical self-adjoint eigenvalue problem (FE approximation):

\( u_h \in V_h \subset V \) and \( \lambda_h \in \mathbb{R} \) such that

\[
a(u_h, v) := \int_{\Omega} (A \nabla u_h) \cdot \nabla v \, dx = \lambda_h \int_{\Omega} u_h \cdot v \, dx \quad \text{for all } v \in V_h
\]

with data \( 0 < \alpha \leq A \in L^\infty(\Omega) \)
Model multiscale eigenvalue problem

Prototypical self-adjoint eigenvalue problem \((\text{FE approximation})\):
\(u_h \in V_h \subset V\) and \(\lambda_h \in \mathbb{R}\) such that

\[
a(u_h, v) := \int_\Omega (A \nabla u_h) \cdot \nabla v \, dx = \lambda_h \int_\Omega u_h \cdot v \, dx \quad \text{for all } v \in V_h
\]

with data \(0 < \alpha \leq A \in L^\infty(\Omega)\)

Numerical error (piecewise linear continuous FE approximation)

- For an eigenpair \((u^{(k)}, \lambda^{(k)})\) with \(u^{(k)} \subset H^2(\Omega)\) it holds

  \[
  \lambda^{(k)} \leq \lambda_h^{(k)} \leq \lambda^{(k)} + C(A, A', k)h^2,
  \]

  \[
  \|\|u^{(k)} - u_h^{(k)}\|\| := \|A^{1/2} \nabla (u^{(k)} - u_h^{(k)})\|_{L^2(\Omega)} \leq C(A, A', k)h.
  \]

- The mesh size \(h\) has to resolve the variations in \(A\), e.g. \(h < \epsilon\) if \(A\) is periodic.
Investigate how well the localized orth. decomposition technique in

A. Målqvist and D. Peterseim.

Localization of Elliptic Multiscale Problems.


preserves the (low) spectrum of \(-\nabla \cdot A \nabla\).

Without any assumptions on scales \((A')\) or regularity \((u)\):

\[
\lambda_h \leq \lambda_{ms}^{H} \leq \lambda_h + CH^4,
\]

\[
\|\|u_h - u_{ms}^{H}\|\| \leq CH^2.
\]

A. Målqvist and D. Peterseim.

Computation of eigenvalues by numerical upscaling.

1. Model problem
2. **Upscaling technique and error analysis**
3. Numerical experiments
4. Application to a non-linear eigenvalue problem
5. Conclusions
Multiscale decomposition

- (coarse) FE mesh $\mathcal{T}$ with parameter $H$
- P1-FE space $V_H := \{ v \in V \mid \forall T \in \mathcal{T}, v|_T \in P_1(T) \}$
- $\mathcal{S}_T : V \rightarrow V_H$ a Clément interpolation operator

Decomposition

\[ V = V_H \oplus V^f \quad \text{with} \quad V^f := \text{kernel} \mathcal{S}_T = \{ v \in V \mid \mathcal{S}_Tv = 0 \} \]

Example:

rough coefficient
Multiscale decomposition

- (coarse) FE mesh $\mathcal{T}$ with parameter $H$
- P1-FE space $V_H := \{ v \in V \mid \forall T \in \mathcal{T}, v|_T \in P_1(T) \}$
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**Decomposition**

$$V = V_H \oplus V^f \quad \text{with} \quad V^f := \text{kernel} \mathcal{I}_T = \{ v \in V \mid \mathcal{I}_T v = 0 \}$$

**Example:**

$$u \in V = u_H \in V_H + u^f \in V^f$$
Orthogonalization

For each \( v \in V_H \) define finescale projection \( \mathcal{F}v \in V^f \) by

\[
a(\mathcal{F}v, w) = a(v, w) \quad \text{for all } w \in V^f
\]

Orthogonal Decomposition

\[ V = V^\text{ms}_H \oplus V^f \text{ with } V^\text{ms}_H := (V_H - \mathcal{F}V_H) \]

Example:

\[ u \in V \quad = \quad u^\text{ms}_H \in V^\text{ms}_H \quad + \quad u^f \in V^f \]
Given the space $V_{ms}^H$ we construct a Galerkin approximation:

**Ideal method**

Find $u_{ms}^H \in V_{ms}^H$, $\lambda_{ms}^H \in \mathbb{R}$ such that

$$a(u_{ms}^H, v) = \lambda_{ms}^H (u_{ms}^H, v), \quad \forall v \in V_{ms}^H.$$

- We note that $\dim(V_{ms}^H) = \dim(V_H)$.
- For $V_{ms}^H$ to be useful we need a discrete localized basis.
- But first of all we need to show that $\lambda_{ms}^H$ is a good approximation of $\lambda$. 
A priori error bound (ideal case)

For the $k$:th eigenvalue it holds

**Theorem**

$$\lambda^{(k)} \leq \lambda_{H}^{ms,(k)} \leq \lambda^{(k)} + CH^4,$$

*with $C$ independent on variations in $A$ or the regularity of $u$.*

**Sketch of proof for the lowest eigenvalue:**

Let $u^{(1)} := u = u_c + u_f$ with $u_c \in V_H^{ms}$ and $u_f \in V_f$, such that $\|u\|_{L^2(\Omega)} = 1$. Then

$$\lambda_{H}^{ms,(1)} \leq \frac{a(u_c, u_c)}{(u_c, u_c)} \leq \frac{a(u, u)}{(u_c, u_c)} = \frac{a(u, u)}{(u - u_f, u - u_f)} \lambda^{(1)} \leq \frac{\lambda^{(1)}}{1 - 2(u, u_f)}.$$
A priori error bound (ideal case)

For the $k$:th eigenvalue it holds

**Theorem**

$$\lambda^{(k)} \leq \lambda_{H}^{\text{ms},(k)} \leq \lambda^{(k)} + CH^{4},$$

with $C$ independent on variations in $A$ or the regularity of $u$.

**Sketch of proof for the lowest eigenvalue:**

- Since $\mathcal{Z}_{T} u_f = 0$, $(\mathcal{Z}_{T} u, u_f) = 0$ (weighted Clement), $a(u_c, u_f) = 0$, and $\| \| u \| \|^{2} = \lambda^{(1)}$, we have

  $$\langle u, u_f \rangle = \langle u - \mathcal{Z}_{T} u, u_f - \mathcal{Z}_{T} u_f \rangle \leq CH^{2} \| u \| \cdot \| u_f \| \leq C'H^{2} \| u_f \|,$$

  $$\| u_f \|^{2} = a(u, u_f) = \lambda^{(1)}(u - \mathcal{Z}_{T} u, u_f - \mathcal{Z}_{T} u_f) \leq CH^{2} \| u_f \|.$$

- We conclude $\lambda_{H}^{\text{ms},(1)} \leq \frac{\lambda^{(1)}}{1-CH^{4}} \leq \lambda^{(1)} + 2CH^{4}$. 
A priori error bound (ideal case)

For the $k$:th eigenfunction it holds

**Theorem**

$$|||u^{(k)} - u^{ms,(k)}_H||| \leq CH^2,$$

*with $C$ independent on variations in $A$ or the regularity of $u$.*

- Similar arguments using $\mathcal{S}_T u_f = 0$ and $(\mathcal{S}_T u, u_f) = 0$.
- Only $H^1(\Omega)$ regularity is assumed.

Can we find a localized discrete basis that approximates $V^{ms}_H$?
Modified nodal basis

- $\mathcal{N}$ denotes set of interior vertices of $\mathcal{T}$
- $\phi_x \in V_H$ denotes classical nodal basis function ($x \in \mathcal{N}$)
- $\mathcal{F}\phi_x \in V^f$ denotes finescale correction of $\phi_x$ ($x \in \mathcal{N}$)

Ideal multiscale FE space

$$V^{ms}_H = \text{span} \{ \phi_x - \mathcal{F}\phi_x \mid x \in \mathcal{N} \}$$

Example

$$\phi_x - \mathcal{F}\phi_x \in V^{ms}_H = \phi_x \in V_H - \mathcal{F}\phi_x \in V^f$$
Modified nodal basis

- $\mathcal{N}$ denotes set of interior vertices of $\mathcal{T}$
- $\phi_x \in V_H$ denotes classical nodal basis function ($x \in \mathcal{N}$)
- $\mathcal{G}\phi_x \in V^f$ denotes finescale correction of $\phi_x$ ($x \in \mathcal{N}$)

Ideal multiscale FE space

$$V_{ms}^H = \text{span} \{ \phi_x - \mathcal{G}\phi_x \mid x \in \mathcal{N} \}$$

Example
Assuming more regularity on $A$ we have $\phi_x - \bar{\phi}_x \in H^2(\Omega) \cap H^1_0(\Omega)$. 
Define nodal patches of $\ell$-th order $\omega_{x,\ell}$ about $x \in \mathcal{N}$

Localized corrections $\mathcal{F}\phi_{x,\ell} \in V^f(\omega_{x,\ell}) := \{ v \in V^f \mid v|_{\Omega \setminus \omega_{x,\ell}} = 0 \}$

solve

$$a(\mathcal{F}\phi_{x,\ell}, w) = a(\phi_x, w) \quad \text{for all} \ w \in V^f(\omega_{x,\ell})$$

Localized multiscale FE spaces

$$V_{ms}^{H,\ell} = \text{span}\{ \phi_x - \mathcal{F}\phi_{x,\ell} \mid x \in \mathcal{N} \}$$
Fine scale discretization

- Finescale mesh

\[ \mathcal{T} \sim \mathcal{T}_h \text{ with } h \leq H \]

- Reference FE space

\[ V_h := \{ v \in V \mid \forall T \in \mathcal{T}(\Omega), v|_T \in P_1(T) \} \]

- Reference FE solution \( u_h \in V_h \) and \( \lambda_h \in \mathbb{R} \) solves

\[ a(u_h, v) = \lambda_h (u_h, v) \quad \text{for all } v \in V_h \]

- Fully discrete corrections \( \mathcal{S}_h \phi_{x,\ell} \in V^f_h(\omega_{x,\ell}) := V^f(\omega_{x,\ell}) \cap V_h : \)

\[ a(\mathcal{S}_h \phi_{x,\ell}, w) = a(\phi_{x}, w) \quad \text{for all } w \in V^f_h(\omega_{x,\ell}) \]
Localized Orthogonal Decomposition (LOD)

Fully discrete multiscale FE spaces

\[ V_{H,\ell}^{\text{ms},h} = \text{span}\{\phi_x - \mathcal{G}\phi_{x,\ell} \mid x \in \mathcal{N}\} \]

Fully discrete multiscale approximation \( u_{H,\ell}^{\text{ms},h} \in V_{H,\ell}^{\text{ms},h}, \lambda_{H,\ell}^{\text{ms},h} \in \mathbb{R} \)

\[ a(u_{H,\ell}^{\text{ms},h}, v) = \lambda_{H,\ell}^{\text{ms},h}(u_{H,\ell}^{\text{ms},h}, v) \text{ for all } v \in V_{H,\ell}^{\text{ms},h} \]

Remarks:

- \( \dim V_{H,\ell}^{\text{ms},h} = |\mathcal{N}| = \dim V_H \)
- The basis functions have local support, with overlap depending on \( \ell \approx \log \frac{1}{H} \), and are independent.
Lemma (Truncation error)

There exist $C_1 < \infty$ and $\gamma < 1$ independent of $x, \ell, H$ such that

$$\|\mathcal{F}_x^h - \mathcal{F}_{x,\ell}^h\| \leq C_1 \gamma^\ell \|\mathcal{F}_x^h\|.$$ 

By choosing $\ell = C \log(H^{-1})$ with appropriate $C$ we guarantee that the truncation leads to a higher order perturbation:

Theorem

$$\lambda_h^{(k)} \leq \lambda_{H,\ell}^{ms,(k)} \leq \lambda_h^{(k)} + CH^4,$$

$$\|u_h^{(k)} - u_{H,\ell}^{ms,(k)}\| \leq CH^2,$$

with $C$ independent on variations in $A$ or the regularity of $u$. 
A priori error analysis (discrete case)

The result can be improved using a postprocessing technique:

J. Xu and A. Zhou.
A two-grid discretization scheme for eigenvalue problems.

Find $u^p_h \in V_h$ s.t.

$$a(u^p_h, v) = \lambda^{ms}_{H,\ell}(u^{ms}_{H,\ell}, v), \quad v \in V_h,$$

and letting $\lambda^p_h = a(u^p_h, u^p_h)/(u^p_h, u^p_h)$.

**Theorem**

$$\lambda^{(k)}_h \leq \lambda^{p,(k)}_h \leq \lambda^{(k)}_h + CH^8,$$

$$\|\|u^{(k)}_h - u^{p,(k)}_h\|\| \leq CH^4.$$
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**Eigenvalue Problem**

\[ \lambda_h^{(k)} = e^{(k)}(1/2 \sqrt{2}) \]

\[ e^{(k)}(1/4 \sqrt{2}) = e^{(k)}(1/8 \sqrt{2}) = e^{(k)}(1/16 \sqrt{2}) \]

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**Table:** Errors \( e^{(k)}(H) = \frac{\lambda_{ms}^{(k)} - \lambda_h^{(k)}}{\lambda_h^{(k)}} \) and \( h = 2^{-7} \sqrt{2} \).
### Eigenvalue Problem

\[
0.01 \quad 1 \quad 100 \quad 10000
\]

\[
k \quad \lambda_h^{(k)} \quad e_h^{(k)}(1/2 \sqrt{2}) \quad e_h^{(k)}(1/4 \sqrt{2}) \quad e_h^{(k)}(1/8 \sqrt{2}) \quad e_h^{(k)}(1/16 \sqrt{2})
\]

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**Table**: Errors $e_h^{(k)}(H) =: \frac{\lambda_{\text{ms},(k)} - \lambda_h^{(k)}}{\lambda_h^{(k)}}$ and $h = 2^{-7} \sqrt{2}$. 

Målvist (Uppsala)  
Computation of Eigenvalues by Upscaling  
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1 Model problem
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Consider the Gross-Pitaevskii equation: find \( u \in V, \|u\|_{L^2(\Omega)} = 1 \), and \( \lambda \in \mathbb{R} \) such that

\[
(A \nabla u, \nabla v) + (bu, v) + (u^3, v) = \lambda(u, v), \quad \forall v \in V.
\]

The equation describes the quantum states of a boson gas cooled down to an ultra-low temperature.

- We reuse the same discrete space \( V_{H,\ell}^{ms,h} \) i.e. we ignore the low order non-linearity on the fine scale.
- We then solve the upscaled non-linear eigenvalue problem on the coarse scale.

Consider the Gross-Pitaevskii equation: find $u \in V$, $\|u\|_{L^2(\Omega)} = 1$, and $\lambda \in \mathbb{R}$ such that

$$(A \nabla u, \nabla v) + (bu, v) + (u^3, v) = \lambda (u, v), \quad \forall v \in V.$$ 

The equation describes the quantum states of a boson gas cooled down to an ultra-low temperature.

**Theorem**

$$\lambda \leq \lambda_h^p \leq \lambda + CH^2 \|u - u_h\|_{H^1(\Omega)} + CH^4,$$

$$\|u - u_h^p\|_{H^1(\Omega)} \leq C\|u - u_h\|_{H^1(\Omega)} + CH^3.$$ 

for the ground state, with $C$ independent on the regularity of $u$ and variations in $A$. 

Outline

1. Model problem
2. Upscaling technique and error analysis
3. Numerical experiments
4. Application to a non-linear eigenvalue problem
5. Conclusions
Conclusion

- The Localized Orthogonal Decomposition (LOD) technique preserves the low spectrum of the operator. In particular the eigenvalue error is proportional to $H^4$ after postprocessing $H^8$.
- Numerical experiments indicates even higher rates possibly due to additional regularity in the solution that is not taken advantage of in the analysis.
- The technique is applicable also for non-linear eigenvalue problems again with very impressive convergence rates.

Thank you for your attention!