Computation of eigenvalues using multiscale techniques

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Multiscale eigenvalue problems

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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,

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

Classical finite element methods typically give

$$||u-u_h|| \leq C(\mathbf{A}, \mathbf{A}')h^{\gamma}.$$

Multiscale methods seek an upscaled representation

$$\mathcal{L}_{H}(A)u_{H} = f_{H}$$

fulfilling $||u_h - u_H|| \le C(A)H^{\gamma}$ with C independent of A'.

How well is the spectrum of \mathcal{L} preserved?

Model problem

- Opscaling technique and error analysis
- Numerical experiments
- Applications to non-linear eigenvalue problems

Conclusions

Prototypical self-adjoint eigenvalue problem

$$-\nabla \cdot \mathbf{A} \nabla u = \lambda u$$
 in Ω $u = 0$ on $\partial \Omega$

with data $0 < \alpha \le A \le \beta < \infty$



Prototypical self-adjoint eigenvalue problem (variational form): find $u \in V := H_0^1(\Omega)$ and $\lambda \in \mathbb{R}$ such that

$$\mathsf{a}(u,v) := \int_{\Omega} (\mathsf{A}
abla u) \cdot
abla v \, \mathsf{d} x = \lambda \int_{\Omega} u \cdot v \, \mathsf{d} x \; ext{ for all } v \in V$$

with data $0 < \alpha \le A \le \beta < \infty$



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

$$a(u_h, v) := \int_{\Omega} (\mathbf{A} \nabla u_h) \cdot \nabla v \, dx = \lambda_h \int_{\Omega} u_h \cdot v \, dx$$
 for all $v \in V_h$

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 for all $v \in V_h$

with data $0 < \alpha \le A \le \beta < \infty$

Numerical error (piecewise linear continuous FE approximation)

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

$$\begin{split} \lambda^{(k)} &\leq \lambda_h^{(k)} \leq \lambda^{(k)} + C(A, A', k)h^2, \\ \|\|u^{(k)} - u_h^{(k)}\|\| &:= \|A^{1/2} \nabla (u^{(k)} - u_h^{(k)})\|_{L^2(\Omega)} \leq C(A, A', k)h. \end{split}$$

The mesh size *h* has to resolve the variations in *A*, e.g. *h* < *ϵ* if *A* is periodic.

Objectives

Investigate how the Localized Orth. Decomposition (LOD) in



A. Målqvist and D. Peterseim.

Localization of Elliptic Multiscale Problems. Mathematics of Computation 2014 preserves the (low part of the) spectrum of $-\nabla \cdot A\nabla$.

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

$$\lambda_h \le \lambda_H^{\rm ms} \le \lambda_h + CH^4,$$

$$|||u_h - u_H^{\rm ms}||| \le CH^2.$$



Computation of eigenvalues by numerical upscaling. *arXiv*, submitted for publication

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Opscaling technique and error analysis

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Multiscale decomposition

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



Decomposition

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

Example:



rough coefficient

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Multiscale decomposition

- (coarse) FE mesh \mathcal{T} with parameter H
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Example:



Orthogonalization

• For each $v \in V_H$ define finescale projection $\mathfrak{F} v \in V^{\mathsf{f}}$ by

$$a(\mathfrak{F}v,w)=a(v,w)$$
 for all $w\in V^{\mathsf{f}}$

Orthogonal Decomposition

$$V = V_H^{ms} \oplus V^{f}$$
 with $V_H^{ms} := (V_H - \mathfrak{F} V_H)$

Example:



Ideal multiscale representation

Given the space V_{H}^{ms} we construct a Galerkin approximation:

Ideal method
Find
$$u_{H}^{ms} \in V_{H}^{ms}$$
, $\lambda_{H}^{ms} \in \mathbb{R}$ such that
 $a(u_{H}^{ms}, v) = \lambda_{H}^{ms}(u_{H}^{ms}, v)$, $\forall v \in V_{H}^{ms}$.

- We note that $\dim(V_H^{ms}) = \dim(V_H)$.
- For V_{H}^{ms} to be useful we need a discrete localized basis.
- But first of all we need to show that λ^{ms}_H is a good approximation of λ.

A priori error bound (ideal case)

For the k:th eigenvalue it holds

Theorem

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

C independent of A' and only H^1 -regularity of the eigenfunctions.

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

$$\lambda_{H}^{ms,(1)} \leq \frac{a(u_{c}, u_{c})}{(u_{c}, u_{c})} \leq \frac{a(u, u)}{(u_{c}, u_{c})} = \frac{a(u, u)}{(u - u_{f}, u - u_{f})}$$
$$= \frac{\lambda^{(1)}}{(u, u) - 2(u, u_{f}) + (u_{f}, u_{f})} \leq \frac{\lambda^{(1)}}{1 - 2(u, u_{f})}.$$

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Sketch of proof for the lowest eigenvalue:

• Since $\Im_{\mathcal{T}} u_f = 0$, $(\Im_{\mathcal{T}} u, u_f) = 0$ (weighted Clement, CV99), $a(u_c, u_f) = 0$, and $|||u|||^2 = \lambda^{(1)}$, we have

$$\begin{aligned} & (u, u_f) = (u - \Im_{\mathcal{T}} u, u_f - \Im_{\mathcal{T}} u_f) \le CH^2 |||u||| \cdot |||u_f||| \le C'H^2 |||u_f|||, \\ & |||u_f|||^2 = a(u, u_f) = \lambda^{(1)} (u - \Im_{\mathcal{T}} u, u_f - \Im_{\mathcal{T}} u_f) \le CH^2 |||u_f|||. \end{aligned}$$

• 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

$$|||u^{(k)} - u_H^{ms,(k)}||| \le CH^2,$$

C independent of A' and only H^1 -regularity of the eigenfunctions.

• Similar arguments using $\Im_{\mathcal{T}} u_f = 0$ and $(\Im_{\mathcal{T}} u, u_f) = 0$.

• Only $H^1(\Omega)$ regularity is assumed.

Can we find a localized discrete basis that approximates V_H^{ms} ?

Modified nodal basis

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

Ideal multiscale FE space

$$V_{H}^{ms} = \operatorname{span} \left\{ \phi_{x} - \mathfrak{F} \phi_{x} \mid x \in \mathcal{N} \right\}$$



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Modified nodal basis



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Localization

• Define nodal patches of ℓ -th order $\omega_{x,\ell}$ about $x \in \mathcal{N}$



Localized corrections δφ_{x,ℓ} ∈ V^f(ω_{x,ℓ}) := {v ∈ V^f | v|_{Ω\ω_{x,ℓ}} = 0} solve

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

Localized multiscale FE spaces

$$V_{H,\ell}^{ms} = \operatorname{span}\{\phi_x - \Im\phi_{x,\ell} \mid x \in \mathcal{N}\}$$

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Fine scale discretization

• Finescale mesh





 \mathcal{T}_h with $h \leq H$

• Reference FE space

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

mesh refinement

• Reference FE solution $u_h \in V_h$ and $\lambda_h \in \mathbb{R}$ solves $a(u_h, v) = \lambda_h(u_h, v)$ for all $v \in V_h$

• Fully discrete corrections $\Im \phi_{x,\ell}^h \in V_h^f(\omega_{x,\ell}) := V^f(\omega_{x,\ell}) \cap V_h$: $a(\Im \phi_{x,\ell}^h, w) = a(\phi_x, w) \text{ for all } w \in V_h^f(\omega_{x,\ell})$

Localized Orthogonal Decomposition (LOD)

Fully discrete multiscale FE spaces

$$V_{H,\ell}^{\mathsf{ms},h} = \mathsf{span}\{\phi_x - \mathfrak{F}\phi_{x,\ell}^h \mid x \in \mathcal{N}\}$$

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

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

Remarks:

• dim
$$V_{H,\ell}^{\mathsf{ms},h} = |\mathcal{N}| = \mathsf{dim} V_H$$

 The basis functions have local support, with overlap depending on *l*, and are independent.

A priori error analysis (discrete case)

Lemma (Truncation error)

$$|||\mathfrak{F}\phi^h_x - \mathfrak{F}\phi^h_{x,\ell}||| \le C_1 \gamma^\ell |||\mathfrak{F}\phi^h_x|||.$$

 $C_1 < \infty$ and $\gamma < 1$ depends on β/α , not A'.

By choosing $\ell = C_2 \log(H^{-1})$ with appropriate C_2 we guarantee that the truncation leads to a higher order perturbation:

Theorem

$$\begin{split} \lambda_h^{(k)} &\leq \lambda_{H,\ell}^{\text{ms},h,(k)} \leq \lambda_h^{(k)} + CH^4, \\ & |||u_h^{(k)} - u_{H,\ell}^{\text{ms},h,(k)}||| \leq CH^2, \end{split}$$

with C independent of A' and the regularity of the eigenfunctions.

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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. Mathematics of Computation 2001.

Find $u_h^p \in V_h$ s.t.

$$a(u_h^p,v)=\lambda_{H,\ell}^{\mathrm{ms},h}(u_{H,\ell}^{\mathrm{ms},h},v), \quad v\in V_h,$$

and letting $\lambda_h^p = a(u_h^p, u_h^p)/(u_h^p, u_h^p)$.

Theorem

$$\begin{split} \lambda_h^{(k)} &\leq \lambda_h^{p,(k)} \leq \lambda_h^{(k)} + CH^6, \\ & |||u_h^{(k)} - u_h^{p,(k)}||| \leq CH^4. \end{split}$$

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Eigenvalue Problem



k	$\lambda_h^{(k)}$	$e^{(k)}(1/2\sqrt{2})$	$e^{(k)}(1/4\sqrt{2})$	$e^{(k)}(1/8\sqrt{2})$	$e^{(k)}(1/16\sqrt{2})$
1	9.6436869	0.003494567	0.000034466	0.000000546	0.000000010
2	15.1989274	0.009621397	0.000079887	0.00000845	0.00000010
3	19.7421815	0.023813222	0.000213097	0.000002073	0.00000023
4	29.5281571	0.096910157	0.000724615	0.000006574	0.00000076
5	31.9265496	0.094454625	0.000874659	0.000009627	0.00000138
6	41.4922250	-	0.002395227	0.000019934	0.00000254
7	44.9604884	-	0.002443271	0.000019683	0.00000223
8	49.3631826	-	0.003651870	0.000028869	0.000000308
9	49.3655623	-	0.004266472	0.000032835	0.00000355
10	56.7389993	-	0.006863742	0.000055219	0.00000618
11	65.4085991	-	0.011534878	0.000082414	0.00000856
12	71.0947630	-	0.012596114	0.000090083	0.000001002
13	71.6064671	-	0.014249938	0.000098736	0.000001006
14	79.0043994	-	0.021801461	0.000164436	0.000001605
15	89.3706421	-	0.033550079	0.000211985	0.000002296
16	92.3648207	-	0.040060692	0.000239441	0.000002295
17	97.4459210	-	0.037438984	0.000284936	0.000002724
18	98.7545147	-	0.044544409	0.000269854	0.000002559
19	98.7545639	-	0.047835987	0.000276139	0.000002539
20	101.6755971	-	0.038203654	0.000297356	0.000002909

Table : Errors
$$e^{(k)}(H) =: \frac{\lambda_H^{\mathrm{ms},(k)} - \lambda_h^{(k)}}{\lambda_h^{(k)}}$$
 and $h = 2^{-7}\sqrt{2}$.

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Eigenvalue Problem



k	$\lambda_h^{(k)}$	$e^{(k)}(1/2\sqrt{2})$	$e^{(k)}(1/4\sqrt{2})$	$e^{(k)}(1/8\sqrt{2})$	$e^{(k)}(1/16\sqrt{2})$
1	21.4144522	5.472755371	0.237181706	0.010328293	0.000781683
2	40.9134676	-	0.649080539	0.032761482	0.002447049
3	44.1561133	-	1.687388874	0.097540102	0.004131422
4	60.8278691	-	1.648439518	0.028076168	0.002079812
5	65.6962136	-	2.071005692	0.247424446	0.006569640
6	70.1273082	-	4.265936007	0.232458016	0.016551520
7	82.2960238	-	3.632888104	0.355050163	0.013987920
8	92.8677605	-	6.850048057	0.377881216	0.049841235
9	99.6061234	-	10.305084010	0.469770376	0.026027378
10	109.1543283	-	-	0.476741452	0.005606426
11	129.3741945	-	-	0.505888044	0.062382302
12	138.2164330	-	-	0.554736550	0.039487317
13	141.5464639	-	-	0.540480876	0.043935515
14	145.7469718	-	-	0.765411709	0.034249528
15	152.6283573	-	-	0.712383825	0.024716759
16	155.2965039	-	-	0.761104705	0.026228034
17	158.2610708	-	-	0.749058367	0.091826207
18	164.1452194	-	-	0.840736127	0.118353184
19	171.1756923	-	-	0.946719951	0.111314058
20	179.3917590	-	-	0.928617606	0.119627862

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

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- Model problem
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- Numerical experiments
- Applications to non-linear eigenvalue problems
- Conclusions

The quadratic eigenvalue problem

Consider the quadratic eigenvalue problem (QEP): find $u \in V$, $||u||_{L^2(\Omega)} = 1$, and $\lambda \in \mathbb{C}$ such that

$$(A\nabla u, \nabla v) + \lambda c(u, v) + \lambda^2(u, v) = 0, \quad \forall v \in V.$$

This equation appears in structural mechanics and describes damped vibrations. Discretization gives an algebraic QEP,

$$Kx + \lambda Cx + \lambda^2 Mx = 0,$$

where K is stiffness, C is damping, and M is mass matrix.

If *C* is symmetric, real, and positive: the eigenvalues are complex conjugate with negative real part.

F. Tisseur and K. Meerbergen.

The quadratic eigenvalue problem SIAM Review 2001.

The quadratic eigenvalue problem

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where K is stiffness, C is damping, and M is mass matrix.

- Rayleigh damping $C = \alpha_0 M + \alpha_1 K$ leads to unchanged eigenmodes.
- Systems of Rayleigh damped components, α_0, α_1 are functions.

QEP: Linearization and approximation

Linearization: $(y = \lambda x)$

$$\begin{bmatrix} K & 0 \\ 0 & M \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} -C & -M \\ M & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

On weak form: find (u_1, u_2) and $\lambda \in \mathbb{C}$ such that,

$$a(u,v)=\lambda b(u,v),$$

$$a(u, v) = (A \nabla u_1, \nabla v_1) + (u_2, v_2),$$

 $b(u, v) = -c(u_1, v_1) - (u_2, v_1) + (u_1, v_2).$

Multiscale formulation: Find $u_{H}^{ms} \in V_{H}^{ms} \times V_{H}^{ms}$ and $\lambda_{H}^{ms} \in \mathbb{C}$ such that,

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

Numerical experiment



Numerical experiment



Numerical experiment



QEP: Analysis

We note that the operator $B: V \times V \rightarrow V \times V$ defined by,

$$\mathsf{a}(\mathsf{Bu},\mathsf{v})=\mathsf{b}(\mathsf{u},\mathsf{v}),$$

has eigenvalues $Bu = \mu u = \lambda^{-1} u$ since,

$$b(u,v) = a(Bu,v) = a(\mu u,v) = \mu a(u,v).$$

Furthermore, *a* is coercive, bounded, symmetric and *b* is bounded if $|c(u, v)| \le C||u||_{V}||v||_{V}$. If we in addition assume for some $0 \le s < 1$,

 $|c(u,v)| \leq C ||u||_{H^{s}(\Omega)} ||v||_{H^{s}(\Omega)},$

using Rellich's Lemma $H^1(\Omega) \subset H^s(\Omega)$, *B* is a compact operator. The theory for eigenvalues of non-symmetric compact operators becomes available.

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I. Babuška and J. Osborn.

Eigenvalue problems. Handbook of numerical analysis II, 1991.

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J. Descloux, N. Nassif, and J. Rappaz. On spectral approximation I & II. RAIRO 1978. (non compact)

Error in eigenvalues

Theorem (See e.g. Babuška-Osborn 1991)

Let λ be an eigenvalue of B (compact) with algebraic multiplicity m. Let $\{\tilde{\lambda}_j\}_{j=1}^m$ be Galerkin approximations using a discretized function space $\tilde{V} \subset V$. Then,

$$\left|\lambda - \left(\frac{1}{m}\sum_{j=1}^{m} (\tilde{\lambda}_{j})^{-1}\right)^{-1}\right| \leq C \sup_{u \in M(\lambda)} \inf_{\chi \in \tilde{V}} ||u - \chi||_{V} \cdot \sup_{v \in M^{*}(\lambda)} \inf_{\chi \in \tilde{V}} ||v - \chi||_{V},$$

where $M(\lambda)$ is the generalized eigenvectors and $M^*(\lambda)$ is the generalized adjoint eigenvectors associated with λ .

The choice $\tilde{V} = V_{H}^{ms}$ fulfills the requirements for this theorem.

Error in eigenvalues

Conjecture

Let λ be an eigenvalue of A (compact) with algebraic multiplicity m. Let $\{\lambda_{h,j}^{ms}\}_{j=1}^m$ be LOD approximations using a $V_H^{ms} \subset V$. Then,

$$\sup_{u\in M(\lambda)}\inf_{\chi\in V_{H}^{ms}}\|u-\chi\|_{V}\cdot \sup_{v\in M^{*}(\lambda)}\inf_{\chi\in V_{H}^{ms}}\|v-\chi\|_{V}\leq CH^{2-2s},$$

and therefore,

$$\left|\lambda - \left(\frac{1}{m}\sum_{j=1}^m (\lambda_{H,j}^{ms})^{-1}\right)^{-1}\right| \leq CH^{2-2s}.$$

This holds without assuming more regularity than $u \in H^1(\Omega)$. Localization and fine grid discretization is not considered. We lose H^2 compared to the numerical example.

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Multiscale eigenvalue problems

The Gross-Pitaevskii equation

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^{ms,h}_{H,l} 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.
- P. Henning, A. Målqvist, and D. Peterseim.
 Two-level discretization techniques for ground state computations of Bose-Einstein condensates.
 SIAM Journal on Numerical Analysis 2014.

The Gross-Pitaevskii equation

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

Theorem

$$\begin{split} \lambda &\leq \lambda_h^p \leq \lambda + CH^2 \|u - u_h\|_{H^1(\Omega)} + CH^4, \\ \|u - u_h^p\|_{H^1(\Omega)} &\leq C \|u - u_h\|_{H^1(\Omega)} + CH^3. \end{split}$$

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

Model problem

- Opscaling technique and error analysis
- Numerical experiments
- Applications to non-linear eigenvalue problems

Conclusions

Conclusion

- The Localized Orthogonal Decomposition (LOD) technique preserves the low spectrum of the operator. In particular the eigenvalue error is proportional to H⁴ after postprocessing H⁶.
- 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 without pre-asymptotic effects in the convergence.
- More work is needed in the analysis to get sharp bounds for the quadratic eigenvalue problem.
- Numerical tests with more complicated damping is needed.

Thank you for your attention!