Computation of Eigenvalues by Upscaling

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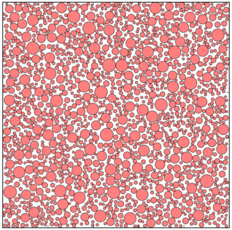
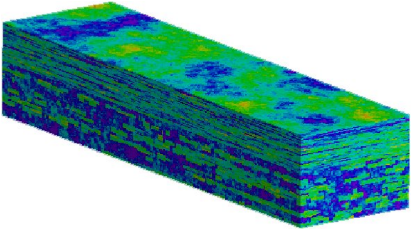
2013-06-18

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,

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

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

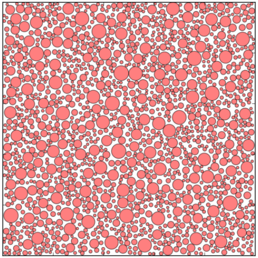
1. **Model problem**
2. Upscaling technique and error analysis
3. Numerical experiments
4. Application to a non-linear eigenvalue problem
5. Conclusions

Model multiscale eigenvalue problem

Prototypical self-adjoint eigenvalue problem

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

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

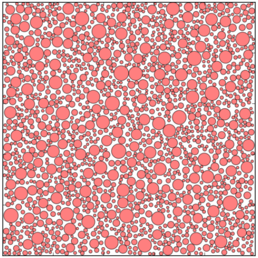


Model multiscale eigenvalue problem

Prototypical self-adjoint eigenvalue problem (variational form): find $u \in V := H_0^1(\Omega)$ 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 $0 < \alpha \le A \in L^\infty(\Omega)$

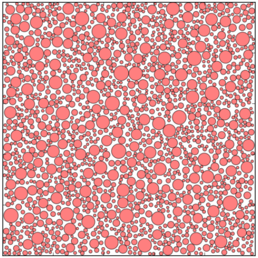


Model multiscale eigenvalue problem

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

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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.

Objectives

Investigate how well the localized orth. decomposition technique in

A. Målqvist and D. Peterseim.
Localization of Elliptic Multiscale Problems.
ArXiv e-prints, Oct. 2011.

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

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

$$\lambda_h \leq \lambda_H^{\mathrm{ms}} \leq \lambda_h + CH^4,$$
$$|||u_h - u_H^{\mathrm{ms}}||| \leq CH^2.$$

A. Målqvist and D. Peterseim.
Computation of eigenvalues by numerical upscaling.
ArXiv e-prints, Dec. 2012.

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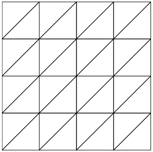
Multiscale decomposition

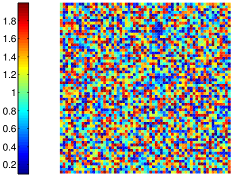
- (coarse) FE mesh $\mathcal{T}$ with parameter H
- P1-FE space $V_H := \{v \in V \mid \forall T \in \mathcal{T}, v|_T \in P_1(T)\}$
- $\mathfrak{I}_{\mathcal{T}} : V \to V_H$ a Clément interpolation operator



Decomposition

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

Example:



rough coefficient

Multiscale decomposition

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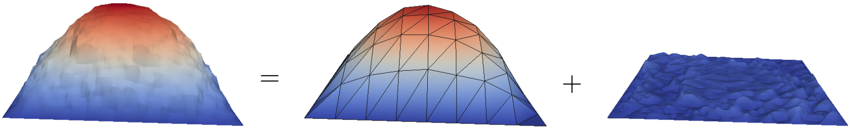


$u \in V$ = $u_H \in V_H$ + $u^{\mathrm{f}} \in V^{\mathrm{f}}$

Orthogonalization

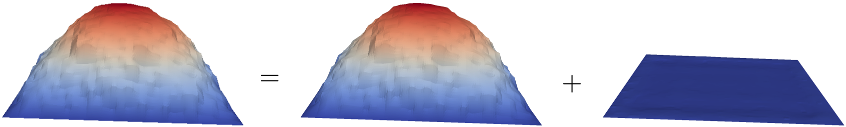
- For each $v \in V_H$ define finescale projection $\mathfrak{F}v \in V^{\mathrm{f}}$ by

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

Orthogonal Decomposition

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

Example:



$u \in V$ $\quad = \quad$ $u_H^{\mathrm{ms}} \in V_H^{\mathrm{ms}}$ $\quad + \quad$ $u^{\mathrm{f}} \in V^{\mathrm{f}}$

Ideal multiscale representation

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

Ideal method

Find $u_H^{\text{ms}} \in V_H^{\text{ms}}$, $\lambda_H^{\text{ms}} \in \mathbb{R}$ such that

$$a(u_H^{\text{ms}}, v) = \lambda_H^{\text{ms}}(u_H^{\text{ms}}, v), \ \forall v \in V_H^{\text{ms}}.$$

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

A priori error bound (ideal case)

For the k:th eigenvalue it holds

Theorem

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

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

$$\lambda_H^{ms,(1)} \leq \frac{a(u_c,u_c)}{(u_c,u_c)} \leq \frac{a(u,u)}{(u_c,u_c)} = \frac{a(u,u)}{(u-u_f,u-u_f)}$$
$$= \frac{\lambda^{(1)}}{(u,u) - 2(u,u_f) + (u_f,u_f)} \leq \frac{\lambda^{(1)}}{1 - 2(u,u_f)}.$$

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:

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

$$(u, u_f) = (u - \Im_{\mathcal{T}} u, u_f - \Im_{\mathcal{T}} u_f) \leq CH^2 |||u||| \cdot |||u_f||| \leq C' H^2 |||u_f|||,$$

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

- *We conclude $\lambda_H^{ms,(1)} \leq \frac{\lambda^{(1)}}{1 - CH^4} \leq \lambda^{(1)} + 2CH^4$.*

A priori error bound (ideal case)

For the k:th eigenfunction it holds

Theorem

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

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

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

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

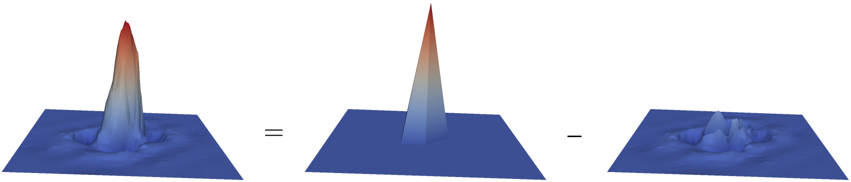
Modified nodal basis

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

Ideal multiscale FE space

$$V_H^{\mathrm{ms}} = \mathrm{span}\,\{\phi_x - \mathfrak{F}\phi_x \mid x \in \mathcal{N}\}$$

Example



$\phi_x - \mathfrak{F}\phi_x \in V_H^{\mathrm{ms}}$ $=$ $\phi_x \in V_H$ $-$ $\mathfrak{F}\phi_x \in V^{\mathrm{f}}$

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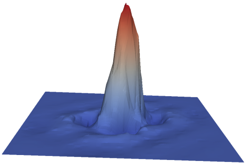
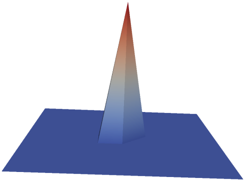


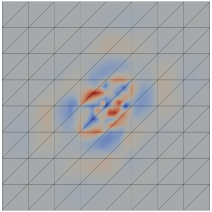
$\phi_x - \mathfrak{F}\phi_x \in V_H^{\mathrm{ms}}$

$=$



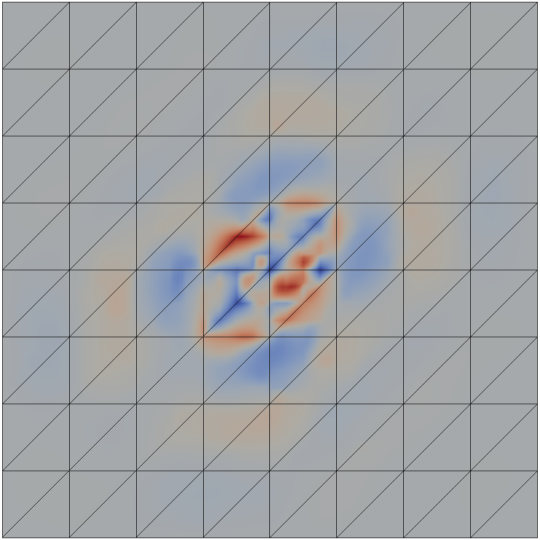
$\phi_x \in V_H$

$-$



$\mathfrak{F}\phi_x \in V^{\mathrm{f}}$

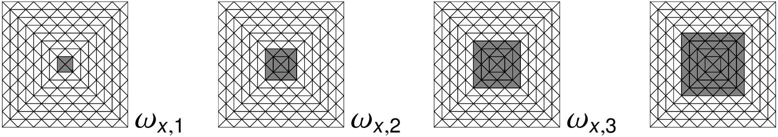
Modified nodal basis



Assuming more regularity on A we have $\phi_x - \mathfrak{I}\phi_x \in H^2(\Omega) \cap H^1_0(\Omega)$.

Localization

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



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

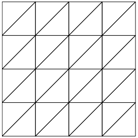
$$a(\mathfrak{F}\phi_{x,\ell}, w) = a(\phi_x, w) \quad \text{for all } w \in V^{\mathrm{f}}(\omega_{x,\ell})$$

Localized multiscale FE spaces

$$V^{\mathrm{ms}}_{H,\ell} = \mathrm{span}\{\phi_x - \mathfrak{F}\phi_{x,\ell} \mid x \in \mathcal{N}\}$$

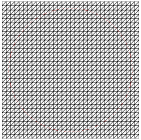
Fine scale discretization

- Finescale mesh



$\mathcal{T}$

mesh refinement $\rightsquigarrow$



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

- 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 $\mathfrak{F}\phi^h_{x,\ell} \in V^{\mathrm{f}}_h(\omega_{x,\ell}) := V^{\mathrm{f}}(\omega_{x,\ell}) \cap V_h$:

$$a(\mathfrak{F}\phi^h_{x,\ell}, w) = a(\phi_x, w) \ \text{ for all } w \in V^{\mathrm{f}}_h(\omega_{x,\ell})$$

Localized Orthogonal Decomposition (LOD)

Fully discrete multiscale FE spaces

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

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

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

Remarks:

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

A priori error analysis (discrete case)

Lemma (Truncation error)

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

$$|||\mathfrak{F}\phi_x^h - \mathfrak{F}\phi_{x,\ell}^h||| \leq C_1\gamma^\ell|||\mathfrak{F}\phi_x^h|||.$$

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.
Math. Comp., 70(233):17-25, 2001.

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

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

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

Theorem

$$\lambda_h^{(k)} \leq \lambda_h^{p,(k)} \leq \lambda_h^{(k)} + CH^8,$$
$$|||u_h^{(k)} - u_h^{p,(k)}||| \leq CH^4.$$

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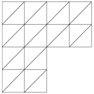
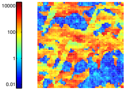
Eigenvalue Problem

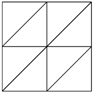


k	$\lambda_h^{(k)}$	$e^{(k)}(1/2\sqrt{2})$	$e^{(k)}(1/4\sqrt{2})$	$e^{(k)}(1/8\sqrt{2})$	$e^{(k)}(1/16\sqrt{2})$
1	9.6436869	0.003494567	0.000034466	0.000000546	0.000000010
2	15.1989274	0.009621397	0.000079887	0.000000845	0.000000010
3	19.7421815	0.023813222	0.000213097	0.000002073	0.000000023
4	29.5281571	0.096910157	0.000724615	0.000006574	0.000000076
5	31.9265496	0.094454625	0.000874659	0.000009627	0.000000138
6	41.4922250	-	0.002395227	0.000019934	0.000000254
7	44.9604884	-	0.002443271	0.000019683	0.000000223
8	49.3631826	-	0.003651870	0.000028869	0.000000308
9	49.3655623	-	0.004266472	0.000032835	0.000000355
10	56.7389993	-	0.006863742	0.000055219	0.000000618
11	65.4085991	-	0.011534878	0.000082414	0.000000856
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 $e^{(k)}(H) =: \frac{\lambda_H^{\text{ms},(k)} - \lambda_h^{(k)}}{\lambda_h^{(k)}}$ and $h = 2^{-7}\sqrt{2}$.

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

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Application to a non-linear eigenvalue problem

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 $V_{H,\ell}^{\text{ms},h}$ 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.

P. Henning, A. Målqvist, and D. Peterseim.
Two-level discretization techniques for ground state computations of Bose-Einstein condensates. *ArXiv e-prints* May 2013.

Application to a non-linear eigenvalue problem

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

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!