

Guaranteed a posteriori bounds for eigenvalues and eigenvectors: multiplicities and clusters

Eric Cancès, Geneviève Dusson, Yvon Maday,
Benjamin Stamm, **Martin Vohralík**

Inria Paris & Ecole des Ponts

Berlin, April 15, 2019



Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Eigenvalue problem

Setting

- \mathcal{H} : real separable Hilbert space, inner product (\cdot, \cdot) , norm $\|\cdot\|$
- A : linear self-adjoint operator on \mathcal{H} with domain $D(A)$, bounded-below, with compact resolvent
- eigenvalues λ_k and eigenvectors $\varphi_k^0 \in D(A)$, $k \geq 1$, s.t.

$$A\varphi_k^0 = \lambda_k\varphi_k^0 \quad \forall k \geq 1$$

- $\lambda_k \in \mathbb{R}_+$, $\lambda_k \rightarrow +\infty$, φ_k^0 form an orthonormal basis of \mathcal{H}

Eigenvalue problem

Setting

- \mathcal{H} : real separable Hilbert space, inner product (\cdot, \cdot) , norm $\|\cdot\|$
- A : linear self-adjoint operator on \mathcal{H} with domain $D(A)$, bounded-below, with compact resolvent
- eigenvalues λ_k and eigenvectors $\varphi_k^0 \in D(A)$, $k \geq 1$, s.t.

$$A\varphi_k^0 = \lambda_k\varphi_k^0 \quad \forall k \geq 1$$

- $\lambda_k \in \mathbb{R}_+$, $\lambda_k \rightarrow +\infty$, φ_k^0 form an orthonormal basis of \mathcal{H}

Eigenvalue problem

Setting

- \mathcal{H} : real separable Hilbert space, inner product (\cdot, \cdot) , norm $\|\cdot\|$
- A : linear self-adjoint operator on \mathcal{H} with domain $D(A)$, bounded-below, with compact resolvent
- eigenvalues λ_k and eigenvectors $\varphi_k^0 \in D(A)$, $k \geq 1$, s.t.

$$A\varphi_k^0 = \lambda_k\varphi_k^0 \quad \forall k \geq 1$$

- $\lambda_k \in \mathbb{R}_+$, $\lambda_k \rightarrow +\infty$, φ_k^0 form an orthonormal basis of \mathcal{H}

Operators A^s , $s \geq 0$

•

Eigenvalue problem

Setting

- \mathcal{H} : real separable Hilbert space, inner product (\cdot, \cdot) , norm $\|\cdot\|$
- A : linear self-adjoint operator on \mathcal{H} with domain $D(A)$, bounded-below, with compact resolvent
- eigenvalues λ_k and eigenvectors $\varphi_k^0 \in D(A)$, $k \geq 1$, s.t.

$$A\varphi_k^0 = \lambda_k\varphi_k^0 \quad \forall k \geq 1$$

- $\lambda_k \in \mathbb{R}_+$, $\lambda_k \rightarrow +\infty$, φ_k^0 form an orthonormal basis of \mathcal{H}

Operators A^s , $s \geq 0$

- domain & norm

$$D(A^s) := \left\{ v \in \mathcal{H}; \quad \|A^s v\|^2 := \sum_{k \geq 1} \lambda_k^{2s} |(v, \varphi_k^0)|^2 < +\infty \right\}$$

- expression

$$v \in D(A^s) \mapsto \sum_{k \geq 1} \lambda_k^s |(v, \varphi_k^0)| \varphi_k^0 \in \mathcal{H}$$

Eigenvalue problem

Setting

- \mathcal{H} : real separable Hilbert space, inner product (\cdot, \cdot) , norm $\|\cdot\|$
- A : linear self-adjoint operator on \mathcal{H} with domain $D(A)$, bounded-below, with compact resolvent
- eigenvalues λ_k and eigenvectors $\varphi_k^0 \in D(A)$, $k \geq 1$, s.t.

$$A\varphi_k^0 = \lambda_k\varphi_k^0 \quad \forall k \geq 1$$

- $\lambda_k \in \mathbb{R}_+$, $\lambda_k \rightarrow +\infty$, φ_k^0 form an orthonormal basis of \mathcal{H}

Operators A^s , $s \geq 0$

- domain & norm

$$D(A^s) := \left\{ v \in \mathcal{H}; \quad \|A^s v\|^2 := \sum_{k \geq 1} \lambda_k^{2s} |(v, \varphi_k^0)|^2 < +\infty \right\}$$

- expression

$$A^s : v \in D(A^s) \mapsto \sum_{k \geq 1} \lambda_k^s (v, \varphi_k^0) \varphi_k^0 \in \mathcal{H}$$

Eigenvalue problem

Setting

- \mathcal{H} : real separable Hilbert space, inner product (\cdot, \cdot) , norm $\|\cdot\|$
- A : linear self-adjoint operator on \mathcal{H} with domain $D(A)$, bounded-below, with compact resolvent
- eigenvalues λ_k and eigenvectors $\varphi_k^0 \in D(A)$, $k \geq 1$, s.t.

$$A\varphi_k^0 = \lambda_k\varphi_k^0 \quad \forall k \geq 1$$

- $\lambda_k \in \mathbb{R}_+$, $\lambda_k \rightarrow +\infty$, φ_k^0 form an orthonormal basis of \mathcal{H}

Operators A^s , $s \geq 0$

- domain & norm

$$D(A^s) := \left\{ v \in \mathcal{H}; \quad \|A^s v\|^2 := \sum_{k \geq 1} \lambda_k^{2s} |(v, \varphi_k^0)|^2 < +\infty \right\}$$

- expression

$$A^s : v \in D(A^s) \mapsto \sum_{k \geq 1} \lambda_k^s (v, \varphi_k^0) \varphi_k^0 \in \mathcal{H}$$

Eigenvalue problem

Setting

- \mathcal{H} : real separable Hilbert space, inner product (\cdot, \cdot) , norm $\|\cdot\|$
- A : linear self-adjoint operator on \mathcal{H} with domain $D(A)$, bounded-below, with compact resolvent
- eigenvalues λ_k and eigenvectors $\varphi_k^0 \in D(A)$, $k \geq 1$, s.t.

$$A\varphi_k^0 = \lambda_k\varphi_k^0 \quad \forall k \geq 1$$

- $\lambda_k \in \mathbb{R}_+$, $\lambda_k \rightarrow +\infty$, φ_k^0 form an orthonormal basis of \mathcal{H}

Operators A^s , $s \geq 0$

- domain & norm

$$D(A^s) := \left\{ v \in \mathcal{H}; \quad \|A^s v\|^2 := \sum_{k \geq 1} \lambda_k^{2s} |(v, \varphi_k^0)|^2 < +\infty \right\}$$

- expression

$$A^s : v \in D(A^s) \mapsto \sum_{k \geq 1} \lambda_k^s (v, \varphi_k^0) \varphi_k^0 \in \mathcal{H}$$

Weak form, numerical approximation, examples

Weak form

- find $(\varphi_k^0, \lambda_k) \in D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_k^0, \varphi_j^0) = \delta_{kj}$, $1 \leq k, j$, s.t.

$$(A^{1/2} \varphi_k^0, A^{1/2} v) = \lambda_k (\varphi_k^0, v) \quad \forall v \in D(A^{1/2}), \forall k \geq 1$$

Conforming numerical approximation

- find $(\varphi_{kh}, \lambda_{kh}) \in V_h \subset D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_{kh}, \varphi_{jh}) = \delta_{kj}$, $1 \leq k, j \leq \dim V_h$, s.t.

$$(A^{1/2} \varphi_{kh}, A^{1/2} v_h) = \lambda_{kh} (\varphi_{kh}, v_h) \quad \forall v_h \in V_h, \forall 1 \leq k \leq \dim V_h$$

Examples

Weak form, numerical approximation, examples

Weak form

- find $(\varphi_k^0, \lambda_k) \in D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_k^0, \varphi_j^0) = \delta_{kj}$, $1 \leq k, j$, s.t.

$$(A^{1/2} \varphi_k^0, A^{1/2} v) = \lambda_k (\varphi_k^0, v) \quad \forall v \in D(A^{1/2}), \forall k \geq 1$$

Conforming numerical approximation

- find $(\varphi_{kh}, \lambda_{kh}) \in V_h \subset D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_{kh}, \varphi_{jh}) = \delta_{kj}$, $1 \leq k, j \leq \dim V_h$, s.t.

$$(A^{1/2} \varphi_{kh}, A^{1/2} v_h) = \lambda_{kh} (\varphi_{kh}, v_h) \quad \forall v_h \in V_h, \forall 1 \leq k \leq \dim V_h$$

Examples

Weak form, numerical approximation, examples

Weak form

- find $(\varphi_k^0, \lambda_k) \in D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_k^0, \varphi_j^0) = \delta_{kj}$, $1 \leq k, j$, s.t.

$$(A^{1/2} \varphi_k^0, A^{1/2} v) = \lambda_k (\varphi_k^0, v) \quad \forall v \in D(A^{1/2}), \forall k \geq 1$$

Conforming numerical approximation

- find $(\varphi_{kh}, \lambda_{kh}) \in V_h \subset D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_{kh}, \varphi_{jh}) = \delta_{kj}$, $1 \leq k, j \leq \dim V_h$, s.t.

$$(A^{1/2} \varphi_{kh}, A^{1/2} v_h) = \lambda_{kh} (\varphi_{kh}, v_h) \quad \forall v_h \in V_h, \forall 1 \leq k \leq \dim V_h$$

Examples

Laplace operator on a polytope $\Omega \subset \mathbb{R}^d$ with hom. Dirichlet BCs

- $\mathcal{H} = L^2(\Omega)$, $A = -\Delta$, $D(A) = H_0^1(\Omega) \cap \{v \mid \Delta v \in L^2(\Omega)\}$,
 $D(A^{1/2}) = H_0^1(\Omega)$, $\|A^{1/2} v\| = (\int_{\Omega} |\nabla v|^2)^{1/2}$

Weak form, numerical approximation, examples

Weak form

- find $(\varphi_k^0, \lambda_k) \in D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_k^0, \varphi_j^0) = \delta_{kj}$, $1 \leq k, j$, s.t.

$$(A^{1/2} \varphi_k^0, A^{1/2} v) = \lambda_k (\varphi_k^0, v) \quad \forall v \in D(A^{1/2}), \forall k \geq 1$$

Conforming numerical approximation

- find $(\varphi_{kh}, \lambda_{kh}) \in V_h \subset D(A^{1/2}) \times \mathbb{R}_+$, $(\varphi_{kh}, \varphi_{jh}) = \delta_{kj}$, $1 \leq k, j \leq \dim V_h$, s.t.

$$(A^{1/2} \varphi_{kh}, A^{1/2} v_h) = \lambda_{kh} (\varphi_{kh}, v_h) \quad \forall v_h \in V_h, \forall 1 \leq k \leq \dim V_h$$

Examples

Schrödinger operator on a cubic box $\Omega \subset \mathbb{R}^d$ with **periodic** BCs

- $\mathcal{H} = L_{\#}^2(\Omega)$, $A = -\Delta + V$, $D(A) = H_{\#}^2(\Omega)$,
 $D(A^{1/2}) = H_{\#}^1(\Omega)$, $\|A^{1/2} v\| = (\int_{\Omega} (|\nabla v|^2 + V|v|^2))^{1/2}$

Previous results, eigenvalue bounds

- Armentano and Durán (2004), Plum (1997), Goerisch and He (1989), Still (1988), Kuttler and Sigillito (1978), Moler and Payne (1968), Fox and Rheinboldt (1966), Bazley and Fox (1961), Weinberger (1956), Forsythe (1955), Kato (1949)
- ...

Previous results, **guaranteed** eigenvalue lower bounds

- Carstensen and Gedicke (2014) & Liu (2015): \oplus **guaranteed bound, arbitrarily coarse mesh**; \ominus a priori arguments (largest mesh element diameter), only lowest-order nonconforming FEs
- Šebestová and Vejchodský (2014), Kuznetsov and Repin (2013): \oplus **general guaranteed bounds** for any conforming discretization; \ominus **suboptimal convergence speed**
- Liu and Oishi (2013): \oplus **guaranteed bound**; \ominus only lowest-order conforming FEs, **auxiliary eigenvalue problem on nonconvex domains**
- Wang, Chamoin, Ladevèze, Zhong (2016): \oplus **general bounds** for any conforming discretization; \ominus **infinite-dimensional local problem** (loss of the guaranteed bound)
- Cancès, Dusson, Maday, Stamm, Vohralík (2017, 2018): \oplus **general framework** (planewaves, conforming FEs, nonconforming FEs, mixed FEs, DGs; any order; optimal convergence); \ominus **gap condition**, simple eigenvalues

Previous results, **guaranteed eigenvalue lower bounds**

- Carstensen and Gedicke (2014) & Liu (2015): \oplus **guaranteed bound, arbitrarily coarse mesh**; \ominus a priori arguments (largest mesh element diameter), only lowest-order nonconforming FEs
- Šebestová and Vejchodský (2014), Kuznetsov and Repin (2013): \oplus **general guaranteed bounds** for any conforming discretization; \ominus **suboptimal convergence speed**
- Liu and Oishi (2013): \oplus **guaranteed bound**; \ominus only lowest-order conforming FEs, **auxiliary eigenvalue problem on nonconvex domains**
- Wang, Chamoin, Ladevèze, Zhong (2016): \oplus **general bounds** for any conforming discretization; \ominus **infinite-dimensional local problem** (loss of the guaranteed bound)
- Cancès, Dusson, Maday, Stamm, Vohralík (2017, 2018): \oplus **general framework** (planewaves, conforming FEs, nonconforming FEs, mixed FEs, DGs; any order; optimal convergence); \ominus **gap condition, simple eigenvalues**

Previous results, guaranteed eigenvalue lower bounds

- Carstensen and Gedicke (2014) & Liu (2015): \oplus guaranteed bound, arbitrarily coarse mesh; \ominus a priori arguments (largest mesh element diameter), only lowest-order nonconforming FEs
- Šebestová and Vejchodský (2014), Kuznetsov and Repin (2013): \oplus general guaranteed bounds for any conforming discretization; \ominus suboptimal convergence speed
- Liu and Oishi (2013): \oplus guaranteed bound; \ominus only lowest-order conforming FEs, auxiliary eigenvalue problem on nonconvex domains
- Wang, Chamoin, Ladevèze, Zhong (2016): \oplus general bounds for any conforming discretization; \ominus infinite-dimensional local problem (loss of the guaranteed bound)
- Cancès, Dusson, Maday, Stamm, Vohralík (2017, 2018): \oplus general framework (planewaves, conforming FEs, nonconforming FEs, mixed FEs, DGs; any order; optimal convergence); \ominus gap condition, simple eigenvalues

Previous results, eigenvector bounds

- Boffi, Gallistl, Gardini, Gastaldi (2017), Boffi, Durán, Gardini, Gastaldi (2017), Bonito and Demlow (2016), Dai, He, Zhou (2015), Gallistl (2014), Carstensen and Gedicke (2011), Bank, Grubišić, Owall (2013), Rannacher, Westenberger, Wollner (2010), Grubišić and Owall (2009), Durán, Padra, Rodríguez (2003), Heuveline and Rannacher (2002), Larson (2000), Maday and Patera (2000), Verfürth (1994) ...
- ... typically contain **uncomputable terms**, higher-order on fine enough meshes

Previous results, guaranteed eigenvector bounds

- Cancès, Dusson, Maday, Stamm, Vohralík (2017, 2018): ⊕ **general framework** (planewaves, conforming FEs, nonconforming FEs, mixed FEs, DGs; any order; optimal convergence); ⊖ **gap condition, simple eigenvalues**

Previous results, guaranteed eigenvector bounds

- Cancès, Dusson, Maday, Stamm, Vohralík (2017, 2018): \oplus **general framework** (planewaves, conforming FEs, nonconforming FEs, mixed FEs, DGs; any order; optimal convergence); \ominus **gap condition, simple eigenvalues**

Previous results, guaranteed eigenvector bounds

- Cancès, Dusson, Maday, Stamm, Vohralík (2017, 2018): ⊕ **general framework** (planewaves, conforming FEs, nonconforming FEs, mixed FEs, DGs; any order; optimal convergence); ⊖ **gap condition, simple eigenvalues**

Setting

Eigenvalue cluster

- $m, M \in \mathbb{N} \setminus \{0\}$, $m \leq M$, $J := M - m + 1$
- J eigenvalues $(\lambda_m, \dots, \lambda_M)$ (allowing for **multiplicities**)
- corresponding J eigenvectors $\Phi^0 := (\varphi_m^0, \dots, \varphi_M^0)$

Approximate eigenvalue cluster

- $(\lambda_{mh}, \dots, \lambda_{Mh})$ with $\dim V_h \geq M$, $\Phi_h := (\varphi_{mh}, \dots, \varphi_{Mh})$

Assumption A (Continuous gap condition)

There holds $\lambda_{m-1} < \lambda_m$ if $m > 1$ and $\lambda_M < \lambda_{M+1}$.

Assumption B (Discrete gap condition)

There holds $\lambda_{(m-1)h} < \lambda_{mh}$ if $m > 1$ and $\lambda_{Mh} < \lambda_{(M+1)h}$.

Assumption C (Continuous–discrete gap condition)

There holds $\lambda_{m-1} < \lambda_{mh}$ if $m > 1$ and $\lambda_{Mh} < \lambda_{M+1}$.

Setting

Eigenvalue cluster

- $m, M \in \mathbb{N} \setminus \{0\}$, $m \leq M$, $J := M - m + 1$
- J eigenvalues $(\lambda_m, \dots, \lambda_M)$ (allowing for **multiplicities**)
- corresponding J eigenvectors $\Phi^0 := (\varphi_m^0, \dots, \varphi_M^0)$

Approximate eigenvalue cluster

- $(\lambda_{mh}, \dots, \lambda_{Mh})$ with $\dim V_h \geq M$, $\Phi_h := (\varphi_{mh}, \dots, \varphi_{Mh})$

Assumption A (Continuous gap condition)

There holds $\lambda_{m-1} < \lambda_m$ if $m > 1$ and $\lambda_M < \lambda_{M+1}$.

Assumption B (Discrete gap condition)

There holds $\lambda_{(m-1)h} < \lambda_{mh}$ if $m > 1$ and $\lambda_{Mh} < \lambda_{(M+1)h}$.

Assumption C (Continuous–discrete gap condition)

There holds $\lambda_{m-1} < \lambda_{mh}$ if $m > 1$ and $\lambda_{Mh} < \lambda_{M+1}$.

Setting

Eigenvalue cluster

- $m, M \in \mathbb{N} \setminus \{0\}$, $m \leq M$, $J := M - m + 1$
- J eigenvalues $(\lambda_m, \dots, \lambda_M)$ (allowing for **multiplicities**)
- corresponding J eigenvectors $\Phi^0 := (\varphi_m^0, \dots, \varphi_M^0)$

Approximate eigenvalue cluster

- $(\lambda_{mh}, \dots, \lambda_{Mh})$ with $\dim V_h \geq M$, $\Phi_h := (\varphi_{mh}, \dots, \varphi_{Mh})$

Assumption A (Continuous gap condition)

There holds $\lambda_{m-1} < \lambda_m$ if $m > 1$ and $\lambda_M < \lambda_{M+1}$.

Assumption B (Discrete gap condition)

There holds $\lambda_{(m-1)h} < \lambda_{mh}$ if $m > 1$ and $\lambda_{Mh} < \lambda_{(M+1)h}$.

Assumption C (Continuous–discrete gap condition)

There holds $\lambda_{m-1} < \lambda_{mh}$ if $m > 1$ and $\lambda_{Mh} < \lambda_{M+1}$.

Main results

We bound

1 cluster eigenvalue error

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster eigenvector energy error

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta$$

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{opt}} (\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \eta, \eta)$$

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{eff}}(\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \text{h.o.t.})$$

✓ explicit continuous–discrete relative gap condition
 ✓ no need for an orthonormal basis

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{eff}}(\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \text{h.o.t.})$$

- ✓ explicit continuous–discrete relative gap condition
- ✓ guaranteed and optimally converging bounds
- ✗ C_{eff} depends on the continuous–discrete relative gaps and on $\tilde{\gamma}_i = \max\{(\lambda_i - \lambda_{i+1})^{-1}, 1\}$

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{eff}}(\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \text{h.o.t.})$$

- ✓ explicit continuous–discrete relative gap condition
- ✓ guaranteed and optimally converging bounds
- ✗ C_{eff} depends on the continuous–discrete relative gaps and on $\bar{c}_h := \max \left\{ \left(\frac{\lambda_{Mh}}{\lambda_1} - 1 \right)^2, 1 \right\}$
- ✗ C_{eff} depends on the mesh shape regularity (FEs Laplace)
- ✓ C_{eff} independent of polynomial degree in V_h (FEs Laplace)

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{eff}}(\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \text{h.o.t.})$$

- ✓ explicit continuous–discrete relative gap condition
- ✓ guaranteed and optimally converging bounds
- ✗ C_{eff} depends on the continuous–discrete relative gaps and on $\bar{c}_h := \max \left\{ \left(\frac{\lambda_{Mh}}{\lambda_1} - 1 \right)^2, 1 \right\}$
- ✗ C_{eff} depends on the mesh shape regularity (FEs Laplace)
- ✓ C_{eff} independent of polynomial degree in V_h (FEs Laplace)

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{eff}}(\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \text{h.o.t.})$$

- ✓ explicit continuous–discrete relative gap condition
- ✓ guaranteed and optimally converging bounds
- ✗ C_{eff} depends on the continuous–discrete relative gaps and on $\bar{c}_h := \max \left\{ \left(\frac{\lambda_{Mh}}{\lambda_1} - 1 \right)^2, 1 \right\}$
- ✗ C_{eff} depends on the mesh shape regularity (FEs Laplace)
- ✓ C_{eff} independent of polynomial degree in V_h (FEs Laplace)

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{eff}}(\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \text{h.o.t.})$$

- ✓ explicit continuous–discrete relative gap condition
- ✓ guaranteed and optimally converging bounds
- ✗ C_{eff} depends on the continuous–discrete relative gaps and on $\bar{c}_h := \max \left\{ \left(\frac{\lambda_{Mh}}{\lambda_1} - 1 \right)^2, 1 \right\}$
- ✗ C_{eff} depends on the mesh shape regularity (FEs Laplace)
- ✓ C_{eff} independent of polynomial degree in V_h (FEs Laplace)

Main results

We bound

1 cluster **eigenvalue error**

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2$$

2 cluster **eigenvector energy error**

$$\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta \leq C_{\text{eff}}(\|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} + \text{h.o.t.})$$

- ✓ explicit continuous–discrete relative gap condition
- ✓ guaranteed and optimally converging bounds
- ✗ C_{eff} depends on the continuous–discrete relative gaps and on $\bar{c}_h := \max \left\{ \left(\frac{\lambda_{Mh}}{\lambda_1} - 1 \right)^2, 1 \right\}$
- ✗ C_{eff} depends on the mesh shape regularity (FEs Laplace)
- ✓ C_{eff} independent of polynomial degree in V_h (FEs Laplace)

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Continuous and discrete orthogonal projectors

Non-uniqueness issue

- **multiple eigenvalues** $\lambda_m = \dots = \lambda_M$: for any orthogonal matrix $\mathbf{U} \in O(J) = \{\mathbf{U} \in \mathbb{R}^{J \times J}; \mathbf{U}^T \mathbf{U} = \mathbf{1}_J\}$, $\Phi^0 \mathbf{U}$ is **also** orthonormal set of **eigenvectors** for $(\lambda_m, \dots, \lambda_M)$
- measure the errors in the **spaces** spanned by **eigenvectors**, uniquely determined even for multiple eigenvalues (under Assumption A)

Continuous orthogonal projector onto $\text{Span } \Phi^0$

$$\forall v \in \mathcal{H}, \quad \gamma^0 v := \sum_{i=m}^M (v, \varphi_i^0) \varphi_i^0 \in D(A^{1/2})$$

Discrete orthogonal projector onto $\text{Span } \Phi_h$

$$\forall v \in \mathcal{H}, \quad \gamma_h v := \sum_{i=m}^M (v, \varphi_{ih}) \varphi_{ih} \in V_h$$

Continuous and discrete orthogonal projectors

Non-uniqueness issue

- **multiple eigenvalues** $\lambda_m = \dots = \lambda_M$: for any orthogonal matrix $\mathbf{U} \in O(J) = \{\mathbf{U} \in \mathbb{R}^{J \times J}; \mathbf{U}^T \mathbf{U} = \mathbf{1}_J\}$, $\Phi^0 \mathbf{U}$ is **also** orthonormal set of **eigenvectors** for $(\lambda_m, \dots, \lambda_M)$
- measure the errors in the **spaces** spanned by **eigenvectors**, uniquely determined even for multiple eigenvalues (under Assumption A)

Continuous orthogonal projector onto $\text{Span } \Phi^0$

$$\forall v \in \mathcal{H}, \quad \gamma^0 v := \sum_{i=m}^M (v, \varphi_i^0) \varphi_i^0 \in D(A^{1/2})$$

Discrete orthogonal projector onto $\text{Span } \Phi_h$

$$\forall v \in \mathcal{H}, \quad \gamma_h v := \sum_{i=m}^M (v, \varphi_{ih}) \varphi_{ih} \in V_h$$

Continuous and discrete orthogonal projectors

Non-uniqueness issue

- **multiple eigenvalues** $\lambda_m = \dots = \lambda_M$: for any orthogonal matrix $\mathbf{U} \in O(J) = \{\mathbf{U} \in \mathbb{R}^{J \times J}; \mathbf{U}^T \mathbf{U} = \mathbf{1}_J\}$, $\Phi^0 \mathbf{U}$ is **also** orthonormal set of **eigenvectors** for $(\lambda_m, \dots, \lambda_M)$
- measure the errors in the **spaces** spanned by **eigenvectors**, uniquely determined even for multiple eigenvalues (under Assumption A)

Continuous orthogonal projector onto $\text{Span } \Phi^0$

$$\forall v \in \mathcal{H}, \quad \gamma^0 v := \sum_{i=m}^M (v, \varphi_i^0) \varphi_i^0 \in D(A^{1/2})$$

Discrete orthogonal projector onto $\text{Span } \Phi_h$

$$\forall v \in \mathcal{H}, \quad \gamma_h v := \sum_{i=m}^M (v, \varphi_{ih}) \varphi_{ih} \in V_h$$

Continuous and discrete orthogonal projectors

Non-uniqueness issue

- **multiple eigenvalues** $\lambda_m = \dots = \lambda_M$: for any orthogonal matrix $\mathbf{U} \in O(J) = \{\mathbf{U} \in \mathbb{R}^{J \times J}; \mathbf{U}^T \mathbf{U} = \mathbf{1}_J\}$, $\Phi^0 \mathbf{U}$ is **also** orthonormal set of **eigenvectors** for $(\lambda_m, \dots, \lambda_M)$
- measure the errors in the **spaces** spanned by **eigenvectors**, uniquely determined even for multiple eigenvalues (under Assumption A)

Continuous orthogonal projector onto $\text{Span } \Phi^0$

$$\forall v \in \mathcal{H}, \quad \gamma^0 v := \sum_{i=m}^M (v, \varphi_i^0) \varphi_i^0 \in D(A^{1/2})$$

Discrete orthogonal projector onto $\text{Span } \Phi_h$

$$\forall v \in \mathcal{H}, \quad \gamma_h v := \sum_{i=m}^M (v, \varphi_{ih}) \varphi_{ih} \in V_h$$

Unitary transformed approximate eigenvectors

Assumption D (Non-orthogonality of exact and approximate eigenspaces)

There holds

$$\forall \mathbf{v} \in \text{Span}\{\varphi_m^0, \dots, \varphi_M^0\} \setminus \{\mathbf{0}\}, \quad \|\gamma_h \mathbf{v}\| \neq 0.$$

Abstract unitary transformed approximate eigenvectors

- closest set of discrete eigenvectors

$$\Phi_h^0 := (\varphi_{mh}^0, \dots, \varphi_{Mh}^0) := \operatorname{argmin}_{\mathbf{U} \in O(J)} \|\mathbf{U} \Phi_h - \Phi^0\|$$

- unique under Assumption D
- does not change the projector

$$\forall \mathbf{v} \in \mathcal{H}, \quad \sum_{i=m}^M (v, \varphi_{ih}^0) \varphi_{ih}^0 = \gamma_h \mathbf{v} = \sum_{i=m}^M (v, \varphi_{ih}) \varphi_{ih}$$

- not needed in practice

Unitary transformed approximate eigenvectors

Assumption D (Non-orthogonality of exact and approximate eigenspaces)

There holds

$$\forall \mathbf{v} \in \text{Span}\{\varphi_m^0, \dots, \varphi_M^0\} \setminus \{0\}, \quad \|\gamma_h \mathbf{v}\| \neq 0.$$

Abstract unitary transformed approximate eigenvectors

- closest set of discrete eigenvectors

$$\Phi_h^0 := (\varphi_{mh}^0, \dots, \varphi_{Mh}^0) := \operatorname{argmin}_{\mathbf{U} \in O(J)} \|\mathbf{U} \Phi_h - \Phi^0\|$$

- unique under Assumption D
- does not change the projector

$$\forall \mathbf{v} \in \mathcal{H}, \quad \sum_{i=m}^M (v, \varphi_{ih}^0) \varphi_{ih}^0 = \gamma_h \mathbf{v} = \sum_{i=m}^M (v, \varphi_{ih}) \varphi_{ih}$$

- not needed in practice

Unitary transformed approximate eigenvectors

Assumption D (Non-orthogonality of exact and approximate eigenspaces)

There holds

$$\forall \mathbf{v} \in \text{Span}\{\varphi_m^0, \dots, \varphi_M^0\} \setminus \{0\}, \quad \|\gamma_h \mathbf{v}\| \neq 0.$$

Abstract unitary transformed approximate eigenvectors

- closest set of discrete eigenvectors

$$\Phi_h^0 := (\varphi_{mh}^0, \dots, \varphi_{Mh}^0) := \operatorname{argmin}_{\mathbf{U} \in O(J)} \|\mathbf{U} \Phi_h - \Phi^0\|$$

- unique under Assumption D
- does not change the projector

$$\forall \mathbf{v} \in \mathcal{H}, \quad \sum_{i=m}^M (v, \varphi_{ih}^0) \varphi_{ih}^0 = \gamma_h \mathbf{v} = \sum_{i=m}^M (v, \varphi_{ih}) \varphi_{ih}$$

- not needed in practice

Unitary transformed approximate eigenvectors

Assumption D (Non-orthogonality of exact and approximate eigenspaces)

There holds

$$\forall \mathbf{v} \in \text{Span}\{\varphi_m^0, \dots, \varphi_M^0\} \setminus \{0\}, \quad \|\gamma_h \mathbf{v}\| \neq 0.$$

Abstract unitary transformed approximate eigenvectors

- closest set of discrete eigenvectors

$$\Phi_h^0 := (\varphi_{mh}^0, \dots, \varphi_{Mh}^0) := \operatorname{argmin}_{\mathbf{U} \in O(J)} \|\mathbf{U} \Phi_h - \Phi^0\|$$

- unique under Assumption D
- does not change the projector

$$\forall \mathbf{v} \in \mathcal{H}, \quad \sum_{i=m}^M (\mathbf{v}, \varphi_{ih}^0) \varphi_{ih}^0 = \gamma_h \mathbf{v} = \sum_{i=m}^M (\mathbf{v}, \varphi_{ih}) \varphi_{ih}$$

- not needed in practice

Unitary transformed approximate eigenvectors

Assumption D (Non-orthogonality of exact and approximate eigenspaces)

There holds

$$\forall \mathbf{v} \in \text{Span}\{\varphi_m^0, \dots, \varphi_M^0\} \setminus \{0\}, \quad \|\gamma_h \mathbf{v}\| \neq 0.$$

Abstract unitary transformed approximate eigenvectors

- closest set of discrete eigenvectors

$$\Phi_h^0 := (\varphi_{mh}^0, \dots, \varphi_{Mh}^0) := \operatorname{argmin}_{\mathbf{U} \in O(J)} \|\mathbf{U} \Phi_h - \Phi^0\|$$

- unique under Assumption D
- does not change the projector

$$\forall \mathbf{v} \in \mathcal{H}, \quad \sum_{i=m}^M (\mathbf{v}, \varphi_{ih}^0) \varphi_{ih}^0 = \gamma_h \mathbf{v} = \sum_{i=m}^M (\mathbf{v}, \varphi_{ih}) \varphi_{ih}$$

- not needed in practice

Unitary transformed approximate eigenvectors

Assumption D (Non-orthogonality of exact and approximate eigenspaces)

There holds

$$\forall \mathbf{v} \in \text{Span}\{\varphi_m^0, \dots, \varphi_M^0\} \setminus \{0\}, \quad \|\gamma_h \mathbf{v}\| \neq 0.$$

Abstract unitary transformed approximate eigenvectors

- closest set of discrete eigenvectors

$$\Phi_h^0 := (\varphi_{mh}^0, \dots, \varphi_{Mh}^0) := \operatorname{argmin}_{\mathbf{U} \in O(J)} \|\mathbf{U} \Phi_h - \Phi^0\|$$

- unique under Assumption D
- does not change the projector

$$\forall \mathbf{v} \in \mathcal{H}, \quad \sum_{i=m}^M (\mathbf{v}, \varphi_{ih}^0) \varphi_{ih}^0 = \gamma_h \mathbf{v} = \sum_{i=m}^M (\mathbf{v}, \varphi_{ih}) \varphi_{ih}$$

- not needed in practice

Equivalence between projection & eigenvector errors

Hilbert–Schmidt norm

$$\|B\|_{\mathfrak{S}_2(\mathcal{H})} := \left\{ \sum_{k \geq 1} \|B e_k\|^2 \right\}^{1/2}, \quad e_k \text{ arbitrary orthonormal basis of } \mathcal{H}$$

Lemma (Equivalence between projection & \mathcal{H} / energy errors)

Let Assumptions *A*, *B*, and *D* hold. Then

$$\frac{1}{\sqrt{2}} \|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})} \leq \|\Phi^0 - \Phi_h^0\| \leq \|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})}.$$

Moreover,

$$\begin{aligned} & \frac{1}{\sqrt{2}} \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \\ & \leq \|A^{1/2}(\Phi^0 - \Phi_h^0)\| \\ & \leq \left(1 + \frac{\lambda_M}{4\lambda_m} \underbrace{\|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})}^2}_{\leq 4J} \right)^{1/2} \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}. \end{aligned}$$

Equivalence between projection & eigenvector errors

Hilbert–Schmidt norm

$$\|B\|_{\mathfrak{S}_2(\mathcal{H})} := \left\{ \sum_{k \geq 1} \|Be_k\|^2 \right\}^{1/2}, \quad e_k \text{ arbitrary orthonormal basis of } \mathcal{H}$$

Lemma (Equivalence between projection & \mathcal{H} / energy errors)

Let Assumptions **A**, **B**, and **D** hold. Then

$$\frac{1}{\sqrt{2}} \|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})} \leq \|\Phi^0 - \Phi_h^0\| \leq \|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})}.$$

Moreover,

$$\begin{aligned} & \frac{1}{\sqrt{2}} \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \\ & \leq \|A^{1/2}(\Phi^0 - \Phi_h^0)\| \\ & \leq \left(1 + \frac{\lambda_M}{4\lambda_m} \underbrace{\|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})}^2}_{\leq 4J} \right)^{1/2} \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}. \end{aligned}$$

Equivalence between projection & eigenvector errors

Hilbert–Schmidt norm

$$\|B\|_{\mathfrak{S}_2(\mathcal{H})} := \left\{ \sum_{k \geq 1} \|Be_k\|^2 \right\}^{1/2}, \quad e_k \text{ arbitrary orthonormal basis of } \mathcal{H}$$

Lemma (Equivalence between projection & \mathcal{H} / energy errors)

Let Assumptions **A**, **B**, and **D** hold. Then

$$\frac{1}{\sqrt{2}} \|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})} \leq \|\Phi^0 - \Phi_h^0\| \leq \|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})}.$$

Moreover,

$$\begin{aligned} & \frac{1}{\sqrt{2}} \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})} \\ & \leq \|A^{1/2}(\Phi^0 - \Phi_h^0)\| \\ & \leq \left(1 + \frac{\lambda_M}{4\lambda_m} \underbrace{\|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})}^2}_{\leq 4J} \right)^{1/2} \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}. \end{aligned}$$

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences**
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Eigenvalue–eigenvector equivalence

Theorem (Eigenvalue–eigenvector equivalence)

Let Assumptions *A* and *B* hold. Then

$$\begin{aligned}
 & \| \mathbf{A}^{1/2}(\gamma^0 - \gamma_h) \|_{\mathfrak{G}_2(\mathcal{H})}^2 - \lambda_M \| \gamma^0 - \gamma_h \|_{\mathfrak{G}_2(\mathcal{H})}^2 \\
 & \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \\
 & \leq \| \mathbf{A}^{1/2}(\gamma^0 - \gamma_h) \|_{\mathfrak{G}_2(\mathcal{H})}^2.
 \end{aligned}$$

Single eigenpair and cluster residuals

Single eigenpair residual $\text{Res}(\varphi_{ih}, \lambda_{ih}) \in D(A^{1/2})'$

$$\langle \text{Res}(\varphi_{ih}, \lambda_{ih}), \mathbf{v} \rangle_{D(A^{1/2})', D(A^{1/2})} := \lambda_{ih}(\varphi_{ih}, \mathbf{v}) - (A^{1/2}\varphi_{ih}, A^{1/2}\mathbf{v}), \quad \mathbf{v} \in D(A^{1/2})$$

$$\|\text{Res}(\varphi_{ih}, \lambda_{ih})\|_{D(A^{1/2})'} := \sup_{\mathbf{v} \in D(A^{1/2}), \|A^{1/2}\mathbf{v}\|=1} \langle \text{Res}(\varphi_{ih}, \lambda_{ih}), \mathbf{v} \rangle_{D(A^{1/2})', D(A^{1/2})}$$

Cluster residual $\text{Res}(\gamma_h) \in \mathfrak{S}_2(\mathcal{H})$

$$\text{Res}(\gamma_h) := A^{1/2}\gamma_h - A^{-1/2}(A^{1/2}\gamma_h)^\dagger A^{1/2}\gamma_h$$

Lemma (Equivalence of cluster and single eigenpair residuals)

There holds

$$\|\text{Res}(\gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}^2 = \sum_{i=m}^M \|\text{Res}(\varphi_{ih}, \lambda_{ih})\|_{D(A^{1/2})'}^2.$$

Single eigenpair and cluster residuals

Single eigenpair residual $\text{Res}(\varphi_{ih}, \lambda_{ih}) \in D(A^{1/2})'$

$$\langle \text{Res}(\varphi_{ih}, \lambda_{ih}), \mathbf{v} \rangle_{D(A^{1/2})', D(A^{1/2})} := \lambda_{ih}(\varphi_{ih}, \mathbf{v}) - (A^{1/2}\varphi_{ih}, A^{1/2}\mathbf{v}), \quad \mathbf{v} \in D(A^{1/2})$$

$$\|\text{Res}(\varphi_{ih}, \lambda_{ih})\|_{D(A^{1/2})'} := \sup_{\mathbf{v} \in D(A^{1/2}), \|A^{1/2}\mathbf{v}\|=1} \langle \text{Res}(\varphi_{ih}, \lambda_{ih}), \mathbf{v} \rangle_{D(A^{1/2})', D(A^{1/2})}$$

Cluster residual $\text{Res}(\gamma_h) \in \mathfrak{G}_2(\mathcal{H})$

$$\text{Res}(\gamma_h) := A^{1/2}\gamma_h - A^{-1/2}(A^{1/2}\gamma_h)^\dagger A^{1/2}\gamma_h$$

Lemma (Equivalence of cluster and single eigenpair residuals)

There holds

$$\|\text{Res}(\gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 = \sum_{i=m}^M \|\text{Res}(\varphi_{ih}, \lambda_{ih})\|_{D(A^{1/2})'}^2.$$

Single eigenpair and cluster residuals

Single eigenpair residual $\text{Res}(\varphi_{ih}, \lambda_{ih}) \in D(A^{1/2})'$

$$\langle \text{Res}(\varphi_{ih}, \lambda_{ih}), v \rangle_{D(A^{1/2})', D(A^{1/2})} := \lambda_{ih}(\varphi_{ih}, v) - (A^{1/2}\varphi_{ih}, A^{1/2}v), \quad v \in D(A^{1/2})$$

$$\|\text{Res}(\varphi_{ih}, \lambda_{ih})\|_{D(A^{1/2})'} := \sup_{v \in D(A^{1/2}), \|A^{1/2}v\|=1} \langle \text{Res}(\varphi_{ih}, \lambda_{ih}), v \rangle_{D(A^{1/2})', D(A^{1/2})}$$

Cluster residual $\text{Res}(\gamma_h) \in \mathfrak{G}_2(\mathcal{H})$

$$\text{Res}(\gamma_h) := A^{1/2}\gamma_h - A^{-1/2}(A^{1/2}\gamma_h)^\dagger A^{1/2}\gamma_h$$

Lemma (Equivalence of cluster and single eigenpair residuals)

There holds

$$\|\text{Res}(\gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 = \sum_{i=m}^M \|\text{Res}(\varphi_{ih}, \lambda_{ih})\|_{D(A^{1/2})'}^2.$$

Eigenvector–residual equivalence I

Theorem (Upper bounds for the projection energy error)

Let Assumptions **A** and **B** hold. Then

$$\|\mathbf{A}^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 \leq \|\mathbf{Res}(\gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 + (\lambda_M + \lambda_{Mh}) \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^2.$$

Let in addition Assumptions **C** and **D** hold and set

$$c_h := \max \left[\left(\frac{\lambda_{mh}}{\lambda_{m-1}} - 1 \right)^{-1}, \left(1 - \frac{\lambda_{Mh}}{\lambda_{M+1}} \right)^{-1} \right].$$

Then

$$\|\mathbf{A}^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 \leq 2c_h^2 \|\mathbf{Res}(\gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 + \frac{\lambda_M}{2} \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^4.$$

Eigenvector–residual equivalence I

Theorem (Upper bounds for the projection energy error)

Let Assumptions **A** and **B** hold. Then

$$\|\mathbf{A}^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 \leq \|\mathbf{Res}(\gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 + (\lambda_M + \lambda_{Mh}) \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^2.$$

Let in addition Assumptions **C** and **D** hold and set

$$c_h := \max \left[\left(\frac{\lambda_{mh}}{\lambda_{m-1}} - 1 \right)^{-1}, \left(1 - \frac{\lambda_{Mh}}{\lambda_{M+1}} \right)^{-1} \right].$$

Then

$$\|\mathbf{A}^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 \leq 2c_h^2 \|\mathbf{Res}(\gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 + \frac{\lambda_M}{2} \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^4.$$

Eigenvector–residual equivalence II

Theorem (Lower bound for the projection energy error)

Let Assumptions **A**, **B**, and **D** hold. Set

$$\bar{c}_h := \max \left\{ \left(\frac{\lambda_{Mh}}{\lambda_1} - 1 \right)^2, 1 \right\}.$$

Then

$$\begin{aligned} & \|\text{Res}(\gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 \\ & \leq \bar{c}_h \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 + \frac{3(\lambda_M)^2}{4\lambda_m} \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^4 \\ & \quad + \frac{3}{\lambda_m} \left(1 + \frac{1}{4} \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^4 \right) \times \\ & \quad \left[2 \left(1 + \frac{\lambda_M}{4\lambda_m} \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^2 \right)^2 \|A^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^4 \right. \\ & \quad \left. + 2(\lambda_M)^2 \|\gamma^0 - \gamma_h\|_{\mathfrak{G}_2(\mathcal{H})}^4 \right]. \end{aligned}$$

Upper bounds for the projection \mathcal{H} error

Lemma (Upper bounds for the projection \mathcal{H} error)

Let Assumptions **A**, **B**, and **C** hold. Set

$$\tilde{c}_h := \max \left[(\lambda_{m-1})^{-1/2} \left(\frac{\lambda_{mh}}{\lambda_{m-1}} - 1 \right)^{-1}, (\lambda_{M+1})^{-1/2} \left(1 - \frac{\lambda_{Mh}}{\lambda_{M+1}} \right)^{-1} \right].$$

Then

$$\|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})} \leq \sqrt{2} c_h \|A^{-1/2} \text{Res}(\gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}$$

and

$$\|\gamma^0 - \gamma_h\|_{\mathfrak{S}_2(\mathcal{H})} \leq \sqrt{2} \tilde{c}_h \|\text{Res}(\gamma_h)\|_{\mathfrak{S}_2(\mathcal{H})}.$$

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves**
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves**
 - **Finite elements for the Laplace operator**
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Eigenvalues error I

Theorem (Guaranteed bounds for the sum of eigenvalues)

Let Assumptions **A** and **B** hold. Let $\bar{\lambda}_{m-1}$ and $\underline{\lambda}_{M+1}$ be s.t.

$$\lambda_{m-1} \leq \bar{\lambda}_{m-1} < \lambda_{mh} \text{ when } m > 1, \quad \lambda_{Mh} < \underline{\lambda}_{M+1} \leq \lambda_{M+1}.$$

Define

$$\eta_{\text{res}}^2 := \sum_{i=m}^M \|\nabla \varphi_{ih} + \sigma_{ih}\|^2 \quad \sigma_{ih} = \text{equilibrated fluxes},$$

$$c_h := \max \left[\left(\frac{\lambda_{mh}}{\bar{\lambda}_{m-1}} - 1 \right)^{-1}, \left(1 - \frac{\lambda_{Mh}}{\underline{\lambda}_{M+1}} \right)^{-1} \right],$$

$$\tilde{c}_h := \max \left[(\bar{\lambda}_{m-1})^{-1/2} \left(\frac{\lambda_{mh}}{\bar{\lambda}_{m-1}} \right)^{-1}, (\underline{\lambda}_{M+1})^{-1/2} \left(1 - \frac{\lambda_{Mh}}{\underline{\lambda}_{M+1}} \right)^{-1} \right].$$

Eigenvalues error II

Theorem (Guaranteed bounds for the sum of eigenvalues)

Then

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2.$$

Case I Let Assumption *D* hold. Then

$$\eta^2 := (2c_h^2 + 2\lambda_{Mh}\tilde{c}_h^4\eta_{\text{res}}^2)\eta_{\text{res}}^2.$$

Case II Assume that for $i = m, \dots, M$, the solutions $\zeta_{(ih)}$ of the residual *source problems* belong to $H^{1+\delta}(\Omega)$, $0 < \delta \leq 1$, so that

$$\min_{v_h \in V_h} \|\nabla(\zeta_{(ih)} - v_h)\| \leq C_I h^\delta |\zeta_{(ih)}|_{H^{1+\delta}(\Omega)},$$

$$|\zeta_{(ih)}|_{H^{1+\delta}(\Omega)} \leq C_S \|z_{(ih)}\|.$$

Then

$$\eta^2 := (1 + 4\lambda_{Mh}c_h^2 C_I^2 C_S^2 h^{2\delta})\eta_{\text{res}}^2.$$

Eigenvalues error II

Theorem (Guaranteed bounds for the sum of eigenvalues)

Then

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2.$$

Case I Let Assumption **D** hold. Then

$$\eta^2 := (2c_h^2 + 2\lambda_{Mh}\tilde{c}_h^4\eta_{\text{res}}^2)\eta_{\text{res}}^2.$$

Case II Assume that for $i = m, \dots, M$, the solutions $\zeta_{(ih)}$ of the residual *source problems* belong to $H^{1+\delta}(\Omega)$, $0 < \delta \leq 1$, so that

$$\min_{v_h \in V_h} \|\nabla(\zeta_{(ih)} - v_h)\| \leq C_I h^\delta |\zeta_{(ih)}|_{H^{1+\delta}(\Omega)},$$

$$|\zeta_{(ih)}|_{H^{1+\delta}(\Omega)} \leq C_S \|\mathfrak{z}_{(ih)}\|.$$

Then

$$\eta^2 := (1 + 4\lambda_{Mh}c_h^2 C_I^2 C_S^2 h^{2\delta})\eta_{\text{res}}^2.$$

Eigenvalues error II

Theorem (Guaranteed bounds for the sum of eigenvalues)

Then

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2.$$

Case I Let Assumption **D** hold. Then

$$\eta^2 := (2c_h^2 + 2\lambda_{Mh}\tilde{c}_h^4\eta_{res}^2)\eta_{res}^2.$$

Case II Assume that for $i = m, \dots, M$, the solutions $\zeta_{(ih)}$ of the residual **source problems** belong to $H^{1+\delta}(\Omega)$, $0 < \delta \leq 1$, so that

$$\min_{v_h \in V_h} \|\nabla(\zeta_{(ih)} - v_h)\| \leq C_I h^\delta |\zeta_{(ih)}|_{H^{1+\delta}(\Omega)},$$

$$|\zeta_{(ih)}|_{H^{1+\delta}(\Omega)} \leq C_S \|z_{(ih)}\|.$$

Then

$$\eta^2 := (1 + 4\lambda_{Mh}c_h^2 C_I^2 C_S^2 h^{2\delta})\eta_{res}^2.$$

Eigenvectors error, efficiency, and robustness

Theorem (Guaranteed bounds for the projection energy error)

Let the assumptions of the previous theorem be verified. Then the projection energy error can be bounded via

$$\|\|\nabla|(\gamma^0 - \gamma_h)\|\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta.$$

Let $\underline{\lambda}_1$ be such that $\underline{\lambda}_1 \leq \lambda_1$ and let

$$\bar{c}_h = \max \left\{ \left(\frac{\lambda_{Mh}}{\underline{\lambda}_1} - 1 \right)^2, 1 \right\}.$$

Then, under Assumption D,

$$\eta_{\text{res}}^2 \leq (d+1)^2 C_{\text{st}}^2 C_{\text{cont,PF}}^2 \bar{c}_h \|\|\nabla|(\gamma^0 - \gamma_h)\|\|_{\mathfrak{S}_2(\mathcal{H})}^2 + h.o.t.$$

Eigenvectors error, efficiency, and robustness

Theorem (Guaranteed bounds for the projection energy error)

Let the assumptions of the previous theorem be verified. Then the projection energy error can be bounded via

$$\|\|\nabla|(\gamma^0 - \gamma_h)\|\|_{\mathfrak{S}_2(\mathcal{H})} \leq \eta.$$

Let $\underline{\lambda}_1$ be such that $\underline{\lambda}_1 \leq \lambda_1$ and let

$$\bar{c}_h = \max \left\{ \left(\frac{\lambda_{Mh}}{\underline{\lambda}_1} - 1 \right)^2, 1 \right\}.$$

Then, under Assumption **D**,

$$\eta_{\text{res}}^2 \leq (d+1)^2 C_{\text{st}}^2 C_{\text{cont,PF}}^2 \bar{c}_h \|\|\nabla|(\gamma^0 - \gamma_h)\|\|_{\mathfrak{S}_2(\mathcal{H})}^2 + \text{h.o.t.}$$

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves**
 - Finite elements for the Laplace operator
 - **Planewaves for the Schrödinger operator**
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Eigenvalues error

Theorem (Guaranteed bounds for the sum of eigenvalues)

Let Assumptions **A** and **B** hold. Let $\bar{\lambda}_{m-1}$ and $\underline{\lambda}_{M+1}$ be s.t.

$$\lambda_{m-1} \leq \bar{\lambda}_{m-1} < \lambda_{mN} \text{ when } m > 1, \quad \lambda_{MN} < \underline{\lambda}_{M+1} \leq \lambda_{M+1}.$$

Define

$$\eta_{\text{res}}^2 := \sum_{i=m}^M \|\text{Res}(\varphi_{iN}, \lambda_{iN})\|_{H_{\#}^{-1}(\Omega)}^2 \quad (\text{computable}),$$

$$c_N := \max \left[\left(\frac{\lambda_{mN}}{\bar{\lambda}_{m-1}} - 1 \right)^{-1}, \left(1 - \frac{\lambda_{MN}}{\underline{\lambda}_{M+1}} \right)^{-1} \right].$$

Then

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2,$$

where

$$\eta^2 := \left(1 + \frac{1}{N^2} \frac{L^2 \lambda_{MN}}{\pi^2} c_N^2 \right) \eta_{\text{res}}^2.$$

Eigenvalues error

Theorem (Guaranteed bounds for the sum of eigenvalues)

Let Assumptions **A** and **B** hold. Let $\bar{\lambda}_{m-1}$ and $\underline{\lambda}_{M+1}$ be s.t.

$$\lambda_{m-1} \leq \bar{\lambda}_{m-1} < \lambda_{mN} \text{ when } m > 1, \quad \lambda_{MN} < \underline{\lambda}_{M+1} \leq \lambda_{M+1}.$$

Define

$$\eta_{\text{res}}^2 := \sum_{i=m}^M \|\text{Res}(\varphi_{iN}, \lambda_{iN})\|_{H_{\#}^{-1}(\Omega)}^2 \quad (\text{computable}),$$

$$c_N := \max \left[\left(\frac{\lambda_{mN}}{\bar{\lambda}_{m-1}} - 1 \right)^{-1}, \left(1 - \frac{\lambda_{MN}}{\underline{\lambda}_{M+1}} \right)^{-1} \right].$$

Then

$$0 \leq \sum_{i=m}^M (\lambda_{ih} - \lambda_i) \leq \eta^2,$$

where

$$\eta^2 := \left(1 + \frac{1}{N^2} \frac{L^2 \lambda_{MN}}{\pi^2} c_N^2 \right) \eta_{\text{res}}^2.$$

Eigenvectors error, efficiency, and robustness

Theorem (Guaranteed bounds for the projection energy error)

Let the assumptions of the previous theorem be verified. Then the projection energy error can be bounded via

$$\|(-\Delta + V)^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})} \leq \eta.$$

Let $\underline{\lambda}_1$ be such that $\underline{\lambda}_1 \leq \lambda_1$ and let

$$\bar{c}_N := \max \left\{ \left(\frac{\lambda_{MN}}{\underline{\lambda}_1} - 1 \right)^2, 1 \right\}.$$

Then, under Assumption D,

$$\eta_{\text{res}}^2 \leq \left(\sup_{\Omega} V \right) \bar{c}_N \|(-\Delta + V)^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 + h.o.t.$$

Eigenvectors error, efficiency, and robustness

Theorem (Guaranteed bounds for the projection energy error)

Let the assumptions of the previous theorem be verified. Then the projection energy error can be bounded via

$$\|(-\Delta + V)^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})} \leq \eta.$$

Let $\underline{\lambda}_1$ be such that $\underline{\lambda}_1 \leq \lambda_1$ and let

$$\bar{c}_N := \max \left\{ \left(\frac{\lambda_{MN}}{\underline{\lambda}_1} - 1 \right)^2, 1 \right\}.$$

Then, under Assumption **D**,

$$\eta_{\text{res}}^2 \leq \left(\sup_{\Omega} V \right) \bar{c}_N \|(-\Delta + V)^{1/2}(\gamma^0 - \gamma_h)\|_{\mathfrak{G}_2(\mathcal{H})}^2 + \text{h.o.t.}$$

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Setting

Errors

$$\text{Err}_\lambda := \sum_{i=m}^M (\lambda_{ih} - \lambda_i), \quad \text{Err}_{H^1} := \|\ |\nabla|(\gamma^0 - \gamma_h)\|_{\mathcal{G}_2(\mathcal{H})}, \quad \text{Err}_{L^2} := \|\gamma^0 - \gamma_h\|_{\mathcal{G}_2(\mathcal{H})}$$

Effectivity indices

$$I_\lambda^{\text{eff}} := \frac{\eta^2}{\text{Err}_\lambda}, \quad I_{H^1}^{\text{eff}} := \frac{\eta}{\text{Err}_{H^1}}, \quad I_{L^2}^{\text{eff}} := \frac{\eta_{L^2}}{\text{Err}_{L^2}}$$

Coarse meshes and $\underline{\lambda}_{M+1}$ for FEs

- nonconforming lowest-order FEs
- $\mathcal{T}_{H,1}$: 121 triangles and 320 DoFs
- $\mathcal{T}_{H,2}$: 441 triangles and 1240 DoFs

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Finite elements, unit square, Case II, clusters of size 2

	N	h	ndof	Err_λ	η^2	l_λ^{eff}	Err_{H^1}	η	$l_{H^1}^{\text{eff}}$	Err_{L^2}	η_{L^2}	$l_{L^2}^{\text{eff}}$
$m = 2$	40	0.0354	1681	0.3351	0.4661	1.39	0.5788	0.6827	1.18	0.0041	0.0183	4.49
$M = 3$	80	0.0177	6561	0.0837	0.0972	1.16	0.2890	0.3118	1.08	0.0010	0.0046	4.47
$\mathcal{T}_{H,1}$	160	0.0088	25921	0.0209	0.0231	1.10	0.1445	0.1521	1.05	0.0003	0.0011	4.49
	320	0.0044	103041	0.0052	0.0057	1.09	0.0722	0.0755	1.05	0.0001	0.0003	4.62
$m = 9$	40	0.0354	1681	3.2698	3714.3421	1135.96	1.8235	60.9454	33.42	0.0194	0.3295	17.01
$M = 10$	80	0.0177	6561	0.8151	76.6523	94.04	0.9037	8.7551	9.69	0.0049	0.0622	12.81
$\mathcal{T}_{H,2}$	160	0.0088	25921	0.2036	4.0755	20.02	0.4508	2.0188	4.48	0.0012	0.0148	12.17
	320	0.0044	103041	0.0509	0.2842	5.58	0.2253	0.5331	2.37	0.0003	0.0036	12.03
$m = 18$	40	0.0354	1681	10.6565	10777.4005	1011.34	3.4872	103.8143	29.77	0.0729	0.5069	6.95
$M = 19$	80	0.0177	6561	2.6465	166.0018	62.73	1.6537	12.8842	7.79	0.0183	0.0887	4.86
$\mathcal{T}_{H,2}$	160	0.0088	25921	0.6605	8.7166	13.20	0.8152	2.9524	3.62	0.0046	0.0209	4.57
	320	0.0044	103041	0.1651	0.6511	3.94	0.4061	0.8069	1.99	0.0011	0.0051	4.50

Finite elements, unit square, Case II, clusters size 4/8

	N	h	ndof	Err_λ	η^2	I_λ^{eff}	Err_{H^1}	η	$I_{H^1}^{\text{eff}}$	Err_{L^2}	η_{L^2}	$I_{L^2}^{\text{eff}}$
$m = 1$	10	0.1414	121	13.5049	21673.5051	1604.86	4.1325	147.2192	35.63	0.2141	1.7415	8.13
$M = 4$	20	0.0707	441	3.4018	98.8430	29.06	1.9076	9.9420	5.21	0.0554	0.2274	4.10
$\mathcal{T}_{H,1}$	40	0.0354	1681	0.8519	5.0687	5.95	0.9297	2.2514	2.42	0.0139	0.0521	3.75
	80	0.0177	6561	0.2131	0.4708	2.21	0.4619	0.6862	1.49	0.0035	0.0128	3.67
	160	0.0088	25921	0.0533	0.0728	1.37	0.2306	0.2698	1.17	0.0009	0.0032	3.67
	320	0.0044	103041	0.0133	0.0155	1.16	0.1152	0.1243	1.08	0.0002	0.0008	3.71
$m = 1$	10	0.1414	121	72.9222	82403.2050	1130.02	9.3347	287.0596	30.75	0.3359	3.2521	9.68
$M = 8$	20	0.0707	441	18.0492	281.4040	15.59	4.3588	16.7751	3.85	0.0874	0.3923	4.49
$\mathcal{T}_{H,2}$	40	0.0354	1681	4.4994	15.9735	3.55	2.1323	3.9967	1.87	0.0221	0.0893	4.04
	80	0.0177	6561	1.1240	1.8566	1.65	1.0603	1.3626	1.29	0.0055	0.0219	3.94
	160	0.0088	25921	0.2810	0.3445	1.23	0.5294	0.5869	1.11	0.0014	0.0054	3.94
	320	0.0044	103041	0.0702	0.0788	1.12	0.2646	0.2808	1.06	0.0003	0.0014	4.00

Finite elements, L-shape, Case I, clusters of size 2

	N	h	ndof	Err_λ	η^2	l_λ^{eff}	Err_{H^1}	η	$l_{H^1}^{\text{eff}}$	Err_{L^2}	η_{L^2}	$l_{L^2}^{\text{eff}}$
$m = 3$	20	0.1703	372	2.1603	320733.4214	148468.40	1.4948	566.3333	378.87	0.0500	5.1000	101.92
$M = 5$	40	0.0817	1426	0.5710	3020.5208	5289.65	0.7607	54.9593	72.25	0.0176	2.0122	114.26
$\mathcal{T}_{H,1}$	80	0.0421	5734	0.1503	211.0547	1403.82	0.3886	14.5277	37.39	0.0066	0.9843	148.78
	160	0.0216	22001	0.0436	35.1498	806.13	0.2089	5.9287	28.38	0.0025	0.5277	208.68
	320	0.0118	86787	0.0132	8.7007	661.24	0.1149	2.9497	25.68	0.0009	0.2917	311.83
$m = 3$	10	0.3124	105	8.6772	126111.0898	14533.55	3.0801	355.1212	115.30	0.1608	6.4197	39.93
$M = 5$	20	0.1703	372	2.1603	622.3367	288.08	1.4948	24.9467	16.69	0.0500	2.2311	44.59
$\mathcal{T}_{H,2}$	40	0.0817	1426	0.5710	59.5714	104.32	0.7607	7.7182	10.15	0.0176	1.0820	61.44
	80	0.0421	5734	0.1503	11.5424	76.77	0.3886	3.3974	8.74	0.0066	0.5505	83.21
	160	0.0216	22001	0.0436	3.1223	71.61	0.2089	1.7670	8.46	0.0025	0.2980	117.86
	320	0.0118	86787	0.0132	0.9370	71.21	0.1149	0.9680	8.43	0.0009	0.1652	176.63

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Planewaves, $\Omega = (0, 2\pi) \times (0, 2\pi)$, various clusters

	N	ndof	Err_λ	η^2	I_λ^{eff}	Err_{H^1}	η	$I_{H^1}^{\text{eff}}$	Err_{L^2}	η_{L^2}	$I_{L^2}^{\text{eff}}$
$m = 1$	5	121	2.62e-05	2.02e-04	7.70	5.32e-03	1.42e-02	2.67	9.94e-04	6.18e-03	6.22
$M = 5$	15	961	4.12e-07	7.31e-07	1.77	6.45e-04	8.55e-04	1.32	4.47e-05	2.62e-04	5.85
	25	2601	5.32e-08	7.22e-08	1.36	2.31e-04	2.69e-04	1.16	9.99e-06	5.80e-05	5.81
$m = 6$	5	121	5.12e-05	2.80e-04	5.47	7.60e-03	1.67e-02	2.20	1.41e-03	5.90e-03	4.17
$M = 9$	15	961	7.51e-07	1.15e-06	1.53	8.73e-04	1.07e-03	1.23	6.05e-05	2.43e-04	4.02
	25	2601	9.63e-08	1.22e-07	1.26	3.11e-04	3.49e-04	1.12	1.35e-05	5.38e-05	4.00
$m = 10$	5	121	3.81e-05	1.79e-03	46.9	6.83e-03	4.23e-02	6.19	1.28e-03	1.30e-02	10.1
$M = 13$	15	961	4.47e-07	2.93e-06	6.55	6.77e-04	1.71e-03	2.53	4.69e-05	4.87e-04	10.4
	25	2601	5.64e-08	1.80e-07	3.18	2.39e-04	4.24e-04	1.78	1.03e-05	1.07e-04	10.4

Outline

- 1 Introduction
- 2 Orthogonal projectors
- 3 Eigenvalue–eigenvector–residual equivalences
- 4 Applications to finite elements and planewaves
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 5 Numerical experiments
 - Finite elements for the Laplace operator
 - Planewaves for the Schrödinger operator
- 6 Conclusions and outlook

Conclusions and outlook

Conclusions

- general framework based on projection operators
- allows to deal with possible degeneracies or near-degeneracies
- gap between the considered eigenvalues and the rest of the spectrum needed

Outlook

- extensions to other settings

Conclusions and outlook




Conclusions

- general framework based on projection operators
- allows to deal with possible degeneracies or near-degeneracies
- gap between the considered eigenvalues and the rest of the spectrum needed

Outlook

- extensions to other settings

References

-  CANCÈS E., DUSSON G., MADAY Y., STAMM B., VOHRALÍK M.,
Guaranteed a posteriori bounds for eigenvalues and
eigenvectors: multiplicities and clusters, in preparation, 2019.
-  CANCÈS E., DUSSON G., MADAY Y., STAMM B., VOHRALÍK M.,
Guaranteed and robust a posteriori bounds for Laplace
eigenvalues and eigenvectors: conforming approximations, *SIAM
J. Numer. Anal.* **55** (2017), 2228–2254.
-  CANCÈS E., DUSSON G., MADAY Y., STAMM B., VOHRALÍK M.,
Guaranteed and robust a posteriori bounds for Laplace
eigenvalues and eigenvectors: a unified framework, *Numer.
Math.* **140** (2018), 1033–1079.

Thank you for your attention!