

ROBUST ESTIMATES FOR hp -ADAPTIVE APPROXIMATIONS OF NON-SELF-ADJOINT EIGENVALUE PROBLEMS

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ABSTRACT. We present new residual estimates based on Kato’s square root theorem for spectral approximations of *diagonalizable* non-self-adjoint differential operators of convection–diffusion–reaction type. These estimates are incorporated as part of an hp -adaptive finite element algorithm for practical spectral computations, where it is shown that the resulting *a posteriori* error estimates are reliable. Provided experiments demonstrate the efficiency and reliability of our approach.

1. INTRODUCTION

This paper concerns the direct residual analysis of approximation errors involved in the variational approximation of eigenvalues and eigenvectors of linear convection–diffusion–reaction operators in bounded polygonal domains $\Omega \subset \mathbb{R}^2$, as given by the formal differential expression

$$(1.1) \quad \mathcal{A}\psi := -\nabla \cdot A\nabla\psi + b \cdot \nabla\psi + c\psi = \lambda\psi ,$$

where standard assumptions (see Section 2) on the coefficients ensure that the inverse \mathcal{A}^{-1} is a compact operator. Abstract estimates based on Kato’s square root theorem [4, 17] provide the basis for constructing a practical hp -adaptive finite element method for eigencomputations. The utilization of the Kato’s square root theorem in the context of finite element approximation is one of the main contributions of this paper, and we provide first-principle proofs wherever possible to emphasize its role in our error estimation technique.

The compactness of \mathcal{A} implies that its spectrum $\text{Spec}(\mathcal{A})$ is a countable set and that, for each eigenvalue, there is a finite dimensional eigenspace (space spanned by all eigenvectors associated with an eigenvalue). More details on the spectral theory of non-self-adjoint operators can be found in [9] and the classical reference [14]. The problem (1.1) provides an important example of a more general class of non-self-adjoint eigenvalue problems in Hilbert space for which a Riesz basis can be constructed from associated eigenvectors, see Example 2.3 and [9, 14, 24] for further discussion and references.

Definition 1.1. A sequence of vectors (functions) $(f_i)_{i \in \mathbb{N}}$ is called a *Riesz basis* of a Hilbert space H if there exists an orthonormal basis $(e_i)_{i \in \mathbb{N}}$ of H and a bounded operator \mathcal{X} with a bounded inverse \mathcal{X}^{-1} such that

$$f_i = \mathcal{X}e_i \quad \text{with} \quad i \in \mathbb{N}.$$

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Criteria for the existence of the Riesz basis of eigenvectors were given in [14, 24]. To keep the paper more self-contained, in Example 2.3 we provide a first-principle argument for the existence of a Riesz basis for some operators of type (1.1).

Remark 1.2. Since an orthonormal basis is a Riesz basis with $\mathcal{X} = I$, it is reasonable to use the quantity $\kappa(\mathcal{X}) := \|\mathcal{X}\| \|\mathcal{X}^{-1}\|$ as a measure of the “non-orthogonality” of a basis $(f_i)_{i \in \mathbb{N}}$. It is important to notice that the size of $\kappa(\mathcal{X})$ has a strong impact on the performance of the numerical linear algebra routines used to solve the discretized (algebraic) eigenvalue problems. In the context of numerical linear algebra $\kappa(\mathcal{X})$ is known as the condition number of the eigenvectors.

In practical computations one is concerned with both the efficiency and reliability of error estimates. A reliability result asserts that the true error is bounded from above by a constant times the estimated error (error is not greatly under-estimated), and an efficiency result is that it is bounded from below by a constant times the estimated error (error is not greatly over-estimated). We make explicit the dependence of the reliability of our abstract residual estimates on the condition number $\kappa(\mathcal{X})$ and the spectral gap $\lambda \in \text{Spec}(\mathcal{A})$,

$$(1.2) \quad \text{gap}(\lambda) = \max_{\xi \in \text{Spec}(\mathcal{A}) \setminus \{\lambda\}} \frac{|\xi|}{|\xi - \lambda|},$$

which, due to the compactness assumption, is a finite number. These quantities also play a clear role, as does the hp -regularity parameter γ , in the reliability of the *a posteriori* error estimates in our realization of the abstract error framework in an hp -finite element setting. A proof of efficiency is beyond the scope of the present paper, though numerical experiments provide strong evidence that the resulting error estimates are efficient. Flexibility in choosing the coefficients A, b, c in (1.1) provides for rigorous testing of our error estimates in the proposed hp -adaptive algorithm. For example, by varying the size of b one can control the increase or the decrease of the non-orthogonality measure $\kappa(\mathcal{X})$; whereas allowing discontinuities in the coefficients (particularly the diffusion matrix A) affects the regularity of the eigenvectors, making h -adaptivity necessary near the local singularities.

The paper is organized as follows. In Section 2 we introduce notation and some basic properties of the model problem (1.1). Section 3 contains the abstract reliability results based on Kato’s square root theorem, which form the basis of the hp *a posteriori* estimates in Section 4. Numerical experiments which indicate the efficiency and reliability of our hp -algorithm are presented in Section 5. In order to simplify the presentation we have put some of the more technically-involved results in the Appendix A. Here, we show that our eigenvector results are *cluster robust*, i.e., when approximating a subset of the spectrum from a subspace whose dimension is the same as the dimension of the associated spectral subspace, then the estimates depend only on the distance between the computed Ritz values and the complement of the rest of the spectrum.

2. NOTATION AND BASIC RESULTS

Let $\Omega \subset \mathbb{R}^2$ be an open, bounded polygon. For double-indices $\alpha = (\alpha_1, \alpha_2) \in \mathbb{Z}_{\geq 0}^2$, we let $|\alpha| = \alpha_1 + \alpha_2$ and $D^\alpha u = \frac{\partial^{|\alpha|} u}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2}}$. Throughout the paper we use the following standard notation: for $m \in \mathbb{N}$ and $S \subset \Omega$ we denote the standard norms and semi-norms on the

(complex) Hilbert spaces $H^m(S)$ by

$$(2.1) \quad \|\phi\|_{m,S}^2 = \sum_{|\alpha| \leq m} \|D^\alpha \phi\|_S^2 \quad \text{and} \quad |\phi|_{m,S}^2 = \sum_{|\alpha|=m} \|D^\alpha \phi\|_S^2,$$

where $\|\cdot\|_S$ denotes the L^2 -norm on S . If $S = \Omega$, we omit it from the subscript. In most cases we use the notation $\|\cdot\|$ (with no subscript) to denote the L^2 -norm on Ω , and use the previously introduced subscripts only to clarify the distinction between norms in a specific argument or claim. The Hilbert space in which we pose the variational eigenvalue problems is

$$H_0^1(\Omega) = \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega \text{ in the sense of trace}\}.$$

Definition 2.1. Given real-valued $A \in [L^\infty(\Omega)]^{2 \times 2}$, $b \in [L^\infty(\Omega)]^2$ with $\nabla \cdot b \in L^\infty(\Omega)$, and $c \in L^\infty(\Omega)$, we define the bilinear form $B : H_0^1(\Omega) \times H_0^1(\Omega) \rightarrow \mathbb{C}$ by

$$(2.2) \quad B(w, v) = \int_{\Omega} A \nabla w \cdot \nabla \bar{v} + (b \cdot \nabla w + cw) \bar{v} \, dx.$$

We make the following common assumptions on the coefficients:

- (A1) A is symmetric and uniformly positive definite a.e. in Ω , i.e., there is a $\sigma_0 > 0$ for which $(A(x)z) \cdot z \geq \sigma_0 z \cdot z$ for all $z \in \mathbb{R}^2$ and a.e. $x \in \Omega$.
- (A2) $\sigma_0 + \min(0, p c_\Omega) > 0$, where $p = \operatorname{ess\,inf}\{c(x) - \nabla \cdot b(x)/2 : x \in \Omega\}$, and c_Ω is the optimal Poincaré constant for the domain, $\|v\|_0 \leq c_\Omega \|v\|_1$ for all $v \in H_0^1(\Omega)$.

For the error estimates in Section 4, we make one further assumption on A ,

- (A3) There is a partition $\bar{\Omega} = \cup_{k=1}^p \bar{\Omega}_k$ of Ω into polygons Ω_k with disjoint interiors such that $A|_{\Omega_k} \in W^{1,\infty}(\Omega_k)$ for each k .

Since all of the coefficients are bounded, the bilinear form $B(\cdot, \cdot)$ is clearly bounded: there is a $\gamma_1 > 0$ such that $|B(w, v)| \leq \gamma_1 \|v\|_1 \|w\|_1$ for all $w, v \in H_0^1(\Omega)$. Assumptions (A1)–(A2) guarantee that $B(\cdot, \cdot)$ is also coercive (cf. [13, Theorem 3.8]): there is a $\gamma_0 > 0$ such that $|B(v, v)| \geq \operatorname{Re}(B(v, v)) \geq \gamma_0 \|v\|_1^2$ for all $v \in H_0^1(\Omega)$. For the convenience of the reader we provide the Hermitian and anti-Hermitian parts of $B(\cdot, \cdot)$,

$$B_H(u, v) = \frac{1}{2}(B(u, v) + \overline{B(v, u)}) = \int_{\Omega} A \nabla u \cdot \nabla \bar{v} + \frac{b}{2} \cdot (\bar{v} \nabla u + u \nabla \bar{v}) + cu \bar{v} \, dx,$$

$$B_A(u, v) = \frac{1}{2}(B(u, v) - \overline{B(v, u)}) = \int_{\Omega} \frac{b}{2} \cdot (\bar{v} \nabla u - u \nabla \bar{v}) \, dx,$$

and note that $B_H(\cdot, \cdot)$ is an inner-product, with

$$B_H(v, v) = \operatorname{Re}(B(v, v)) = \int_{\Omega} A \nabla v \cdot \nabla \bar{v} + (c - \nabla \cdot b/2) |v|^2 \, dx.$$

Also, recall that operators whose real parts are scalar products are called *accretive*. An operator is *maximal accretive* if it has no proper accretive extension.

By the first representation theorem from Kato [18], the operator \mathcal{A} is related to the bilinear form $B(\cdot, \cdot)$ through

$$(2.3) \quad B(\varphi, \phi) = (\mathcal{A}\varphi, \phi), \quad \varphi \in \operatorname{Dom}(\mathcal{A}), \phi \in H_0^1(\Omega).$$

We use

$$(2.4) \quad (\varphi, \phi) = \int_{\Omega} \varphi \bar{\phi} \, dx$$

to denote the standard $L^2(\Omega)$ inner-product.

We consider the following primal and dual eigenvalue problems:

Find (λ, ψ) and (λ^*, ψ^*) in $\mathbb{C} \times H_0^1(\Omega) \setminus \{0\}$ such that

$$(2.5) \quad B(\psi, \phi) = \lambda(\psi, \phi) \quad \text{and} \quad B(\varphi, \psi^*) = \lambda^*(\psi^*, \varphi) \quad \text{for all } \phi, \varphi \in H_0^1(\Omega) .$$

By analogy with the linear algebraic version of this problem, we refer to ψ and ψ^* , respectively, as right and left eigenfunctions for λ and λ^* .

We will now summarize some basic facts about the spectral theory of operators which are defined by (2.2). A recent reference is [9], see in particular [9, Example 13.4.4]. For classical references we point the reader to the monographs [14, 24] and the references therein. Since Ω is bounded, $H_0^1(\Omega)$ is compactly embedded in $L^2(\Omega)$. Since the domain of the bilinear form $B(\cdot, \cdot)$ is precisely $H_0^1(\Omega)$, we conclude that the solution operator which maps the function $f \in L^2(\Omega)$ to $u(f) \in H_0^1(\Omega) \subset L^2(\Omega)$ is also compact (as a mapping from $L^2(\Omega)$ to $L^2(\Omega)$). The solution operator is defined by

$$(2.6) \quad B(u(f), \phi) = (f, \phi), \quad \text{for all } \phi \in H_0^1(\Omega).$$

Therefore the eigenvalue problem (2.5) is attained by a sequence of eigenpairs $(\lambda_n, \psi_n) \in \mathbb{C} \times (H_0^1(\Omega) \setminus \{0\})$, $n \in \mathbb{N}$ such that $|\lambda_n| \rightarrow \infty$ as $n \rightarrow \infty$. Furthermore, the technique of [9, Example 13.4.4] assures that the vectors $(\psi_n)_{n \in \mathbb{N}}$ form a Riesz basis of the space $H_0^1(\Omega)$, which implies that the algebraic and geometric multiplicities of each distinct eigenvalue are the same, see also [14]. The eigenvalue of the smallest modulus is real and simple (of multiplicity one), and the corresponding eigenvector may be chosen to be positive almost everywhere. Since the original problem has a compact solution operator, the adjoint problem also has a compact solution operator which maps the function $f \in L^2(\Omega)$ to $u^*(f)$ and is defined by

$$(2.7) \quad B(\varphi, u^*(f)) = (f, \varphi), \quad \text{for all } \varphi \in H_0^1(\Omega).$$

The eigenvalues of the dual (adjoint) problem are the complex conjugates of the eigenvalues of the original problem. For further discussion of the abstract notions see the classical reference of Babuška and Osborn [5].

A direct generalization of the notion of an operator with a Riesz basis of eigenvectors (eigenfunctions) is the notion of a *diagonalizable operator*.

Definition 2.2. An operator \mathcal{A} in a Hilbert space $L^2(\Omega)$ is said to be diagonalizable if there exists a bounded operator \mathcal{X} which has a bounded inverse \mathcal{X}^{-1} and a normal (possibly unbounded) operator \mathcal{H} such that

$$\mathcal{A} = \mathcal{X}\mathcal{H}\mathcal{X}^{-1}$$

and $\mathcal{X}^{-1} \text{Dom}(\mathcal{A}) \subset \text{Dom}(\mathcal{H})$.

In some cases all eigenvalues are known to be real, so $\lambda = \lambda^*$, and we naturally consider eigentriples $(\lambda, \psi, \psi^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ of (2.5). Such problems will be the focus of Sections 3–5. We provide an example of such a family of operators.

Example 2.3. Let $\mathcal{A}u := -\nabla \cdot (A\nabla u) + b \cdot \nabla u + cu$, where the coefficients A , b and c satisfy the conditions (A1)-(A2) prescribed above. Further define the multiplication operator $\mathcal{X}u := e^\beta u$ for some function $\beta \in W^{1,\infty}(\Omega)$. The following identities are obtained by direct computation:

$$\begin{aligned} e^{-\beta}[\nabla \cdot (A\nabla(e^\beta u))] &= \nabla \cdot (A\nabla u) + 2A\nabla\beta \cdot \nabla u + (\nabla \cdot (A\nabla\beta) + (A\nabla\beta) \cdot \nabla\beta)u, \\ e^{-\beta}[b \cdot \nabla(e^\beta u)] &= b \cdot \nabla u + (b \cdot \nabla\beta)u. \end{aligned}$$

If $A^{-1}b$ is a conservative vector field, then we choose β such that $\nabla\beta = \frac{1}{2}A^{-1}b$, and determine that $\mathcal{H} := \mathcal{X}^{-1}\mathcal{A}\mathcal{X}$ is self-adjoint and positive definite. In particular,

$$\mathcal{H}u = \mathcal{X}^{-1}\mathcal{A}\mathcal{X}u = -\nabla \cdot (A\nabla u) + \left(c - \frac{1}{2}\nabla \cdot b + \frac{1}{4}b \cdot (A^{-1}b) \right) u.$$

From this argument we also deduce that (λ, ϕ) is an eigenpair of \mathcal{H} if and only if $(\lambda, e^\beta\phi, e^{-\beta}\phi)$ is an eigentriple of \mathcal{A} . In the case where A and b are constant, then the choice $\beta(x) = \frac{1}{2}A^{-1}b \cdot x$, $x \in \Omega$ is obvious, and we see that the eigenvalues of \mathcal{A} only differ from those of \mathcal{B} by the additive constant $\frac{1}{4}b \cdot (A^{-1}b)$, where $\mathcal{B}u := -\nabla \cdot (A\nabla u) + cu$.

In what follows, we draw our attention to a particular class of diagonalizable operators. Particularly, we consider those diagonalizable operators which are of the convection–diffusion–reaction type with real spectrum.

Definition 2.4 (*Condition \mathfrak{S} and Square Roots*). We say that the operator \mathcal{A} satisfies the *condition \mathfrak{S}* , where \mathfrak{S} stands for the square root, if it is of the form (1.1) and is diagonalizable in the sense of Definition 2.2 with the additional assumption that the normal operator \mathcal{H} is self-adjoint and positive definite. For operators which satisfy *condition \mathfrak{S}* , we define the unique maximal accretive square root operator in the sense of the Dunford functional calculus [10] by the formula

$$\mathcal{A}^{1/2} = \mathcal{X}\mathcal{H}^{1/2}\mathcal{X}^{-1}.$$

Remark 2.5. Our main result, Theorem 3.1 below, can readily be extended to the more general case where \mathcal{H} is allowed to be a normal operator, as in the full scope of the decomposition of Definition 2.2, but we do not pursue this generality here.

Remark 2.6. Note that for any maximal accretive operator \mathcal{A} which is defined by a regularly accretive sesquilinear form associated with a differential expression (1.1) in the space $H_0^1(\Omega)$, where Ω is a polygonal domain, there exists a unique maximal accretive operator $\mathcal{A}^{1/2}$ which solves the operator equation $\mathcal{Z}^2 = \mathcal{A}$. Such an operator is called the square root of \mathcal{A} . For further references on the existence of fractional powers of maximal accretive operators as well as for precise definitions of these terms see [18, Section V.10] and [17]. In this paper we will assume that all of our operators satisfy the condition \mathfrak{S} . In the case in which claims in our theorems hold in a more general setting, we will state this explicitly.

Remark 2.7. It was a long-standing open problem, known as Kato’s conjecture or Kato’s square root problem, see [17, 23] for the origin of the problem, to determine the domain of definition of the operator $\mathcal{A}^{1/2}$. The conjecture was that the domain of the operator $\mathcal{A}^{1/2}$ should be the same as the domain of the abstract bilinear form $B(\cdot, \cdot)$ which defines the operator \mathcal{A} . This hypothesis turned out to be false for the most general abstract form of the bilinear operator, see [23, 25]. However, in the case when \mathcal{A} is a convection–diffusion–reaction operator of the form (1.1), Kato’s conjecture does hold in all dimensions, see [3,

Theorem 1.11] and [2, 4]. In particular, [4] asserts that there exist constants c_K , c_K^* , C_K and C_K^* such that

$$(2.8) \quad c_K \|\phi\|_1 \leq \|\mathcal{A}^{1/2}\phi\| \leq C_K \|\phi\|_1, \quad \phi \in H_0^1(\Omega),$$

$$(2.9) \quad c_K^* \|\phi\|_1 \leq \|\mathcal{A}^{*1/2}\phi\| \leq C_K^* \|\phi\|_1, \quad \phi \in H_0^1(\Omega).$$

Remark 2.8. Note that \mathcal{A}^* always satisfies condition \mathfrak{S} when \mathcal{A} does, and that its unique, self-adjoint and positive square root is given by the formula $\mathcal{A}^{*1/2} = \mathcal{X}^{-*}\mathcal{H}^{1/2}\mathcal{X}^*$.

3. EIGENVALUE AND EIGENVECTOR APPROXIMATION ESTIMATES

We will now present the main theoretical contribution of this paper. We obtain reliability estimates for residual eigenvalue and eigenvector approximations. We assume that the operator defined by (2.2) has a Riesz basis of eigenvectors, and that the eigenvalues are real. Example 2.3 provides a non-trivial class of operators of this type. For real eigenvalues, we naturally consider eigentriples $(\lambda, \psi, \psi^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ of (2.5), and this is reflected in the results that follow. Of course, we implicitly assume that $\psi \neq 0$ and $\psi^* \neq 0$.

3.1. Residual eigenvector error estimates. In this section we will obtain estimates of the eigenvector errors. Eigenvector approximation errors are assessed by measuring the angle between the given approximations $\widehat{\psi}$ and $\widehat{\psi}^*$ and the subspaces \mathcal{S} and \mathcal{S}^* which are spanned by all right and left eigenvectors associated with the chosen eigenvalue λ .

As a first step we introduce the right and the left residual norm. For $\varphi, \phi \in H_0^1(\Omega)$ and $\mu \in \mathbb{C}$ we define the residual form

$$\mathfrak{r}(\mu)[\varphi, \phi] = B(\varphi, \phi) - \mu(\varphi, \phi).$$

Given the vector $\varphi \in H_0^1(\Omega)$ and the scalar $\mu \in \mathbb{C}$ we define the functional

$$\phi \mapsto \mathfrak{r}(\mu)[\varphi, \phi]$$

which we call the right residual of $\varphi \in H_0^1(\Omega)$ and $\mu \in \mathbb{C}$. The number

$$(3.1) \quad \|\mathfrak{r}(\mu)[\varphi, \cdot]\|_{-1} := \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathfrak{r}(\mu)[\varphi, \phi]|}{\|\phi\|_1}$$

is the $H^{-1}(\Omega)$ -norm of the right residual. Analogously, the functional

$$\varphi \mapsto \mathfrak{r}(\mu)[\varphi, \phi]$$

is called the left residual of $\phi \in H_0^1(\Omega)$ and $\mu \in \mathbb{C}$, and the number

$$(3.2) \quad \|\mathfrak{r}(\mu)[\cdot, \phi]\|_{-1} := \sup_{\varphi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathfrak{r}(\mu)[\varphi, \phi]|}{\|\varphi\|_1}$$

denotes the $H^{-1}(\Omega)$ -norm of the left residual.

Theorem 3.1. *Let \mathcal{A} satisfy condition \mathfrak{S} and let $(\widehat{\lambda}, \widehat{\psi}, \widehat{\psi}^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ be given. Suppose $\lambda \in \mathbb{R}$ is an eigenvalue of (2.5), and let \mathbf{S}_* and \mathbf{S}_*^* be the $H_0^1(\Omega)$ -orthogonal projections onto the subspaces \mathcal{S} and \mathcal{S}^* which are spanned by all right and left eigenvectors belonging to λ , respectively. Then*

$$\begin{aligned} \|(I - \mathbf{S}_*)\widehat{\psi}\|_1 &\leq \frac{C_K^*}{c_K} \kappa(\mathcal{X}) \text{gap}(\lambda) \left(\|\mathbf{r}(\widehat{\lambda})[\widehat{\psi}, \cdot]\|_{-1} + |\widehat{\lambda} - \lambda| \right) \\ \|(I - \mathbf{S}_*^*)\widehat{\psi}^*\|_1 &\leq \frac{C_K}{c_K^*} \kappa(\mathcal{X}) \text{gap}(\lambda) \left(\|\mathbf{r}(\widehat{\lambda})[\cdot, \widehat{\psi}^*]\|_{-1} + |\widehat{\lambda} - \lambda| \right), \end{aligned}$$

where c_K , C_K and c_K^* and C_K^* are defined as in (2.8)–(2.9) and the measure of the spectral gap $\text{gap}(\lambda)$ is defined as in (1.2).

Proof. Recall that, following Definition 2.2, for a diagonalizable operator \mathcal{A} we have

$$\mathbf{r}(\lambda)[\varphi, \phi] = ((\mathcal{A} - \lambda I)\varphi, \phi)_{L^2(\Omega)} = (\mathcal{X}(\mathcal{H} - \lambda I)\mathcal{X}^{-1}\varphi, \phi)_{L^2(\Omega)},$$

where $\varphi \in \text{Dom}(\mathcal{A})$, $\phi \in H_0^1(\Omega)$.

Let $\varphi = \mathcal{A}^{-1/2}u$ and $\phi = \mathcal{A}^{*-1/2}v$ and, as in Remark 2.8, $\mathcal{A}^{*-1/2} = \mathcal{X}^{-*}\mathcal{H}^{-1/2}\mathcal{X}^*$. Then

$$\begin{aligned} \mathbf{r}(\lambda)[\varphi, \phi] &= \mathbf{r}(\lambda)[\mathcal{A}^{-1/2}u, \mathcal{A}^{*-1/2}v] = ((\mathcal{A} - \lambda I)\mathcal{A}^{-1/2}u, \mathcal{A}^{*-1/2}v)_{L^2(\Omega)} \\ &= (\mathcal{X}(I - \lambda\mathcal{H}^{-1})\mathcal{X}^{-1}u, v)_{L^2(\Omega)}, \end{aligned}$$

where $u, v \in L^2(\Omega)$.

The following proof is based on the observation that the resolvent of \mathcal{H} is compact and $\text{Spec}(\mathcal{A}) = \text{Spec}(\mathcal{H})$, and so the form $\mathbf{r}(\lambda)[\mathcal{A}^{-1/2}, \mathcal{A}^{*-1/2}]$ generates a bounded operator $\mathcal{X}(I - \lambda\mathcal{H}^{-1})\mathcal{X}^{-1}$ which has a closed range. This implies that there exists a constant C_{LBB} , see e.g., [7], such that,

$$\begin{aligned} \|(I - P_*)u\| &\leq C_{LBB} \sup_{v \in L^2(\Omega) \setminus \{0\}} \frac{|(\mathcal{X}(I - \lambda\mathcal{H}^{-1})\mathcal{X}^{-1}u, v)_{L^2(\Omega)}|}{\|v\|} \\ &= C_{LBB} \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\lambda)[\varphi, \phi]|}{\|\mathcal{A}^{*1/2}\phi\|}. \end{aligned}$$

Here P_* is the $L^2(\Omega)$ -orthogonal projection onto $\text{Ran}(\mathbf{S}_*) = \text{Ker}(\mathcal{A} - \lambda I)$ and we have used the substitution $u = \mathcal{A}^{1/2}\varphi$ and $v = \mathcal{A}^{*1/2}\phi$. Spectral calculus, e.g., [28, Theorems VIII.5 and VIII.6] for the self-adjoint operator $(I - \lambda\mathcal{H}^{-1})$ implies the estimate

$$(3.3) \quad C_{LBB} \leq \|\mathcal{X}^{-1}\| \|\mathcal{X}\| \text{gap}(\lambda) = \kappa(\mathcal{X}) \text{gap}(\lambda).$$

Moreover, we get the obvious equivalence

$$(3.4) \quad c_K^* \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\lambda)[\varphi, \phi]|}{\|\mathcal{A}^{*1/2}\phi\|} \leq \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\lambda)[\varphi, \phi]|}{\|\phi\|_1} \leq C_K^* \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\lambda)[\varphi, \phi]|}{\|\mathcal{A}^{*1/2}\phi\|},$$

for any $\varphi \in H_0^1(\Omega)$. Also, given $\varphi \in H_0^1(\Omega)$ we have

$$\|(I - \mathbf{S}_*)\varphi\|_1 \leq \|(I - P_*)\varphi\|_1 \leq \frac{1}{c_K} \|\mathcal{A}^{1/2}(I - P_*)\varphi\| = \frac{1}{c_K} \|(I - P_*)\mathcal{A}^{1/2}\varphi\|.$$

Here we have used the fact that the operator \mathcal{A} is defined in $L^2(\Omega)$ by the *Kato representation theorem* [18, Theorem VI.2.1] as given in (2.3), and therefore P_* is the $L^2(\Omega)$ -orthogonal

projection onto the eigensubspace of \mathcal{A} . Subsequently, P_* is the orthogonal projection onto the eigensubspace of $\mathcal{A}^{1/2}$ and so they commute.

Let us now use the substitution $u = \mathcal{A}^{1/2}\varphi$ and $v = \mathcal{A}^{*1/2}\phi$ again, then

$$\begin{aligned} \|(I - \mathbf{S}_*)\varphi\|_1 &\leq \frac{1}{c_K} \|(I - P_*)u\| \leq \frac{C_{LBB}}{c_K} \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\lambda)[\varphi, \phi]|}{\|\mathcal{A}^{*1/2}\phi\|} \\ &\leq \frac{\kappa(\mathcal{X})\text{gap}(\lambda)C_K^*}{c_K} \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\lambda)[\varphi, \phi]|}{\|\phi\|_1}. \end{aligned}$$

Using the obvious identity

$$\mathbf{r}(\lambda)[\varphi, \phi] = \mathbf{r}(\widehat{\lambda})[\varphi, \phi] + (\widehat{\lambda} - \lambda)(\varphi, \phi)$$

and inserting $\varphi = \widehat{\psi}$, we complete the proof of the first inequality. The proof of the dual inequality is analogous. \square

Remark 3.2. For a matrix version of this proof see [11, Theorem 3.1]. For other considerations in the finite element context see [8].

Remark 3.3. Although we may naturally think of $(\widehat{\lambda}, \widehat{\psi}, \widehat{\psi}^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ as an approximate eigentriple of \mathcal{A} in Theorem 3.1, with $\widehat{\lambda}$ “close to” λ , this theorem does not require any relation between these objects. Similarly, we do not need $(\widehat{\psi}, \widehat{\psi}^*)$ to be approximations of the left and right eigenvectors (ψ, ψ^*) in Lemma 3.6 below, though we also naturally think of them that way.

3.2. Residual eigenvalue error estimate. We begin with the following lemma, whose proof we include for completeness.

Lemma 3.4 (Lemma 3.6 [20]). *Let $(\lambda, \psi, \psi^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ be an eigentriple of (2.5). Then for all $\varphi, \phi \in H_0^1(\Omega)$, $(\varphi, \phi) \neq 0$,*

$$\frac{B(\varphi, \phi)}{(\varphi, \phi)} - \lambda = \frac{B(\varphi - \psi, \phi - \psi^*)}{(\varphi, \phi)} - \lambda \frac{(\varphi - \psi, \phi - \psi^*)}{(\varphi, \phi)}.$$

Proof. It holds that

$$\begin{aligned} \frac{B(\varphi - \psi, \phi - \psi^*)}{(\varphi, \phi)} &= \frac{B(\varphi, \phi)}{(\varphi, \phi)} + \frac{B(\psi, \psi^*) - B(\varphi, \psi^*) - B(\psi, \phi)}{(\varphi, \phi)} \\ &= \frac{B(\varphi, \phi)}{(\varphi, \phi)} + \frac{\lambda((\psi, \psi^*) - (\varphi, \psi^*) - (\psi, \phi))}{(\varphi, \phi)} \\ &= \frac{B(\varphi, \phi)}{(\varphi, \phi)} + \frac{\lambda((\psi, \psi^*) - (\varphi, \psi^*) + (\varphi, \phi) - (\psi, \phi))}{(\varphi, \phi)} - \lambda \\ &= \frac{B(\varphi, \phi)}{(\varphi, \phi)} + \frac{\lambda(\psi - \varphi, \psi^* - \phi)}{(\varphi, \phi)} - \lambda. \end{aligned}$$

Rearranging terms completes the proof. \square

Let us now prove a first order residual estimate for eigenvalues; in Numerical Linear Algebra, such a result is known as a *Bauer–Fike* type estimate, see [12].

Lemma 3.5. *Let $\widehat{\mu} > 0$ and $\widehat{\psi} \in H_0^1(\Omega)$, $\|\widehat{\psi}\| = 1$ be given and let \mathcal{A} satisfy the condition \mathfrak{S} . Then*

$$\min_{\xi \in \text{Spec}(\mathcal{A})} \frac{|\widehat{\mu} - \xi|}{\sqrt{\widehat{\mu}\xi}} \leq \frac{\kappa(\mathcal{X}) \|\mathfrak{r}(\widehat{\mu})[\widehat{\psi}, \cdot]\|_{-1}}{c_K^* \sqrt{\widehat{\mu}}}.$$

Here $\|\cdot\|$ denotes the norm on $L^2(\Omega)$, and the negative norm of the residual is defined in (3.1).

Proof. Let $\sigma_{\min}(\mathcal{X}) := \|\mathcal{X}^{-1}\|^{-1}$. This is a good definition, since \mathcal{X} is bounded and has a bounded inverse. We now compute

$$\begin{aligned} \|\mathfrak{r}(\widehat{\mu})[\widehat{\psi}, \cdot]\|_{-1} &= \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathfrak{r}(\widehat{\mu})[\widehat{\psi}, \phi]|}{\|\phi\|_1} \geq c_K^* \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathfrak{r}(\widehat{\mu})[\widehat{\psi}, \phi]|}{\|\mathcal{A}^{*1/2}\phi\|} \\ &= c_K^* \|\mathcal{A}^{1/2}\widehat{\psi} - \widehat{\mu}\mathcal{A}^{-1/2}\widehat{\psi}\| \end{aligned}$$

Since the operator \mathcal{A} satisfies condition \mathfrak{S} it follows that

$$\|\mathfrak{r}(\widehat{\mu})[\widehat{\psi}, \cdot]\|_{-1} = c_K^* \|\mathcal{X}(\mathcal{H}^{1/2} - \widehat{\mu}\mathcal{H}^{-1/2})\mathcal{X}^{-1}\widehat{\psi}\|.$$

We note that the operator $\mathcal{H}^{1/2} - \widehat{\mu}\mathcal{H}^{-1/2}$ is self-adjoint. Using the standard spectral calculus for self-adjoint operators, e.g., [28, Theorems VIII.5 and VIII.6], it follows that

$$\text{Spec}(\mathcal{H}^{1/2} - \widehat{\mu}\mathcal{H}^{-1/2}) = \left\{ \sqrt{\widehat{\mu}} \left(\frac{\sqrt{\xi}}{\sqrt{\widehat{\mu}}} - \frac{\sqrt{\widehat{\mu}}}{\sqrt{\xi}} \right) : \xi \in \text{Spec}(\mathcal{A}) \right\},$$

and the smallest in modulus eigenvalue of $\mathcal{H}^{1/2} - \widehat{\mu}\mathcal{H}^{-1/2}$ is $\sqrt{\widehat{\mu}} \min_{\xi \in \text{Spec}(\mathcal{A})} \frac{|\xi - \widehat{\mu}|}{\sqrt{\xi\widehat{\mu}}}$. This, together with norm properties and assumption $\|\widehat{\psi}\| = 1$ yields

$$\begin{aligned} \|\mathfrak{r}(\widehat{\mu})[\widehat{\psi}, \cdot]\|_{-1} &= c_K^* \|\mathcal{X}(\mathcal{H}^{1/2} - \widehat{\mu}\mathcal{H}^{-1/2})\mathcal{X}^{-1}\widehat{\psi}\| \\ &\geq c_K^* \sigma_{\min}(\mathcal{X}) \sqrt{\widehat{\mu}} \min_{\xi \in \text{Spec}(\mathcal{A})} \frac{|\xi - \widehat{\mu}|}{\sqrt{\xi\widehat{\mu}}} \|\mathcal{X}^{-1}\widehat{\psi}\|. \end{aligned}$$

The conclusion now follows directly. \square

We will now improve this result by obtaining an estimate which is higher order in the residual norm $\|\mathfrak{r}(\widehat{\mu})[\widehat{\psi}, \cdot]\|_{-1}$. In the rest of the theorems we shall make a special choice for the scalar $\widehat{\lambda}$. Given two non-zero vectors $\widehat{\psi}, \widehat{\psi}^* \in H_0^1(\Omega)$ we define the generalized Rayleigh quotient

$$\widehat{\lambda} = \frac{B(\widehat{\psi}, \widehat{\psi}^*)}{(\widehat{\psi}, \widehat{\psi}^*)}.$$

We will now prove a general residual estimate.

Lemma 3.6. *Let $\widehat{\psi}, \widehat{\psi}^* \in H_0^1(\Omega) \setminus \{0\}$, $(\widehat{\psi}, \widehat{\psi}^*) \neq 0$ be given, and let $\widehat{\lambda} = B(\widehat{\psi}, \widehat{\psi}^*)/(\widehat{\psi}, \widehat{\psi}^*)$ be the corresponding generalized Rayleigh quotient. For an eigentriple $(\lambda, \psi, \psi^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ of (2.5) the estimate*

$$(3.5) \quad |\widehat{\lambda} - \lambda| \leq \frac{\max \{ \|\mathfrak{r}(\widehat{\lambda})[\widehat{\psi}, \cdot]\|_{-1} \|\widehat{\psi}^* - \psi^*\|_1, \|\mathfrak{r}(\widehat{\lambda})[\cdot, \widehat{\psi}^*]\|_{-1} \|\widehat{\psi} - \psi\|_1 \}}{|\langle \widehat{\psi}, \widehat{\psi}^* \rangle|} \\ + \mathcal{O} \left(|\lambda - \widehat{\lambda}| \max \{ \|\widehat{\psi}^* - \psi^*\|_1, \|\widehat{\psi} - \psi\|_1 \} \right)$$

holds.

Proof. With Lemma 3.4 we obtain the following equality

$$\widehat{\lambda} - \lambda = \frac{B(\widehat{\psi}, \widehat{\psi}^*)}{(\widehat{\psi}, \widehat{\psi}^*)} - \lambda = \frac{B(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)} - \lambda \frac{(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)}.$$

For the right hand side we then have

$$\begin{aligned} & \frac{B(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)} - \lambda \frac{(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)} = \frac{B(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*) - \lambda(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)} \\ &= \frac{B(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*) - \lambda(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*) + \widehat{\lambda}(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*) - \widehat{\lambda}(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)} \\ &= \frac{B(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*) - \widehat{\lambda}(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)} + \frac{\widehat{\lambda}(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*) - \lambda(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)}. \end{aligned}$$

The linearity of $B(\cdot, \cdot)$ in the first component, equation (2.5) and the definition of the residual $\mathfrak{r}(\widehat{\lambda})[\widehat{\psi}, \cdot]$ imply

$$\widehat{\lambda} - \lambda = \frac{\mathfrak{r}(\widehat{\lambda})[\widehat{\psi}, \widehat{\psi}^* - \psi^*]}{(\widehat{\psi}, \widehat{\psi}^*)} + \frac{(\widehat{\lambda} - \lambda)(\psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)} + \frac{(\widehat{\lambda} - \lambda)(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)}{(\widehat{\psi}, \widehat{\psi}^*)}.$$

By taking the absolute value, applying triangle inequality and using the definition of the $H^{-1}(\Omega)$ -norm of the right residual we get

$$(3.6) \quad |\widehat{\lambda} - \lambda| \leq \frac{\|\mathfrak{r}(\widehat{\lambda})[\widehat{\psi}, \cdot]\|_{-1} \|\widehat{\psi}^* - \psi^*\|_1}{|\langle \widehat{\psi}, \widehat{\psi}^* \rangle|} + \frac{|\widehat{\lambda} - \lambda| |(\psi, \widehat{\psi}^* - \psi^*)|}{|\langle \widehat{\psi}, \widehat{\psi}^* \rangle|} + \frac{|\widehat{\lambda} - \lambda| |(\widehat{\psi} - \psi, \widehat{\psi}^* - \psi^*)|}{|\langle \widehat{\psi}, \widehat{\psi}^* \rangle|} \\ \leq \frac{\|\mathfrak{r}(\widehat{\lambda})[\widehat{\psi}, \cdot]\|_{-1} \|\widehat{\psi}^* - \psi^*\|_1}{|\langle \widehat{\psi}, \widehat{\psi}^* \rangle|} + \frac{|\widehat{\lambda} - \lambda| \|\widehat{\psi}^* - \psi^*\|}{|\langle \widehat{\psi}, \widehat{\psi}^* \rangle|} \left(\|\psi\| + \|\widehat{\psi} - \psi\| \right).$$

Performing the same calculations using the left residual $\mathfrak{r}(\widehat{\lambda})[\cdot, \widehat{\psi}^*]$ completes the proof. \square

We now combine Theorem 3.1 and Lemmas 3.5 and 3.6 to obtain a result which will form the basis of our eigenvalue error estimation presented in the next section. Before we proceed, let us recall the notion of the weak convergence of a sequence of vectors $v_n \in H_0^1(\Omega)$. We say that the sequence $v_n \in H_0^1(\Omega)$ converges weakly to $v_\infty \in H_0^1(\Omega)$ if $(v_n - v_\infty, u) + (\nabla(v_n - v_\infty), \nabla u) \rightarrow 0$, for all $u \in H_0^1(\Omega)$. In this case, we write $w\text{-}\lim_n v_n = v_\infty$. Recall also that in the case in which the sequence converges strongly, e.g., when $\|v_n - v_\infty\|_1 \rightarrow 0$, then it also converges weakly and $v_\infty = w\text{-}\lim_n v_n$. In other words, when both the strong and the weak limit of a sequence exist they must be equal.

Theorem 3.7. *Let $(\lambda, \psi, \psi^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ be an eigentriple of (2.5). Moreover, let the operator \mathcal{A} satisfy condition \mathfrak{S} . Suppose we have a sequence of triplets $(\widehat{\lambda}_\nu, \widehat{\psi}_\nu, \widehat{\psi}_\nu^*) \in \mathbb{R} \times H_0^1(\Omega) \times H_0^1(\Omega)$ such that $\|\widehat{\psi}_\nu\|_1 = \|\widehat{\psi}_\nu^*\|_1 = 1$, $(\widehat{\psi}_\nu, \widehat{\psi}_\nu^*) \neq 0$, $\widehat{\lambda}_\nu = B(\widehat{\psi}_\nu, \widehat{\psi}_\nu^*)/(\widehat{\psi}_\nu, \widehat{\psi}_\nu^*)$ and*

$$(3.7) \quad \frac{|\widehat{\lambda}_\nu - \lambda|}{\sqrt{\widehat{\lambda}_\nu \lambda}} = \min_{\xi \in \text{Spec}(\mathcal{A})} \frac{|\widehat{\lambda}_\nu - \xi|}{\sqrt{\widehat{\lambda}_\nu \xi}}$$

for each $\nu \in \mathbb{N}$. Assume that $\|\mathfrak{r}(\widehat{\lambda}_\nu)[\widehat{\psi}_\nu, \cdot]\|_{-1} \rightarrow 0$ and $\|\mathfrak{r}(\widehat{\lambda}_\nu)[\cdot, \widehat{\psi}_\nu^*]\|_{-1} \rightarrow 0$. Then for ν large enough we have the reliability estimate

$$|\widehat{\lambda}_\nu - \lambda| \leq \frac{\widehat{C}}{(\widehat{\psi}_\nu, \widehat{\psi}_\nu^*)} \|\mathfrak{r}(\widehat{\lambda}_\nu)[\widehat{\psi}_\nu, \cdot]\|_{-1} \|\mathfrak{r}(\widehat{\lambda}_\nu)[\cdot, \widehat{\psi}_\nu^*]\|_{-1} + o(\|\mathfrak{r}(\widehat{\lambda}_\nu)[\widehat{\psi}_\nu, \cdot]\|_{-1} \|\mathfrak{r}(\widehat{\lambda}_\nu)[\cdot, \widehat{\psi}_\nu^*]\|_{-1}).$$

The constant \widehat{C} depends solely on the distance of λ to the rest of the spectrum, the condition number $\kappa(\mathcal{X})$ and the equivalence constants from Kato's square root theorem.

Proof. Let \mathbf{S}_* and \mathbf{S}_*^* be the $H_0^1(\Omega)$ -orthogonal projections onto the subspaces \mathcal{S} and \mathcal{S}^* which are spanned by all right and left eigenvectors belonging to λ . Following Theorem 3.1 and Lemma 3.5 the assumptions $\|\mathfrak{r}(\widehat{\lambda}_\nu)[\widehat{\psi}_\nu, \cdot]\|_{-1} \rightarrow 0$ and $\|\mathfrak{r}(\widehat{\lambda}_\nu)[\cdot, \widehat{\psi}_\nu^*]\|_{-1} \rightarrow 0$ imply that

$$\|(I - \mathbf{S}_*)\widehat{\psi}_\nu\|_1 \rightarrow 0 \quad \text{and} \quad \|(I - \mathbf{S}_*^*)\widehat{\psi}_\nu^*\|_1 \rightarrow 0.$$

We will now present the argument for the convergence of right eigenvectors. The argument for left eigenvectors is analogous.

Since $\|\widehat{\psi}_\nu\|_1 = 1$, there exists an $H_0^1(\Omega)$ weakly convergent subsequence which we denote again by $\widehat{\psi}_\nu$. Let now $w\text{-}\lim_\nu \widehat{\psi}_\nu = \psi$, then it follows that

$$w\text{-}\lim_\nu \mathbf{S}_* \widehat{\psi}_\nu = \mathbf{S}_* \psi,$$

since \mathbf{S}_* is a bounded operator. Furthermore, we conclude that

$$w\text{-}\lim_\nu (\widehat{\psi}_\nu - \mathbf{S}_* \widehat{\psi}_\nu) = \psi - \mathbf{S}_* \psi.$$

If both the weak and strong limits exist then they are equal. Therefore $\lim_\nu (\widehat{\psi}_\nu - \mathbf{S}_* \widehat{\psi}_\nu) = 0$ implies that $\psi = \mathbf{S}_* \psi$. Subsequently, we conclude that $\psi \in \mathcal{S}$, i.e., it is an eigenvector associated with λ . Since \mathcal{S} is of finite dimension and $\|\mathbf{S}_* \widehat{\psi}_\nu\|_1 \leq 1$, it follows that there is a subsequence of $\widehat{\psi}_\nu$, which we denote again by $\widehat{\psi}_\nu$, such that $\mathbf{S}_* \widehat{\psi}_\nu$ converges strongly. Now the estimate

$$\|\widehat{\psi}_\nu - \psi\|_1 \leq \|\widehat{\psi}_\nu - \mathbf{S}_* \widehat{\psi}_\nu\|_1 + \|\mathbf{S}_* \widehat{\psi}_\nu - \psi\|_1$$

implies that $\lim_\nu \widehat{\psi}_\nu = \psi$. Recall the elementary inequalities $\arcsin x \leq x + x^3$, $0 \leq x \leq 1$ and $x \leq \arcsin x$, $0 \leq x \leq 1/2$. For each ν , we can now apply Lemma 3.6 and the estimate of Theorem 3.1. Note that $\|(I - \mathbf{S}_*)\widehat{\psi}_\nu\|_1 < 1/2$ and $\psi_\nu \in \text{Ran}(\mathbf{S}_*)$ imply

$$(3.8) \quad \|\psi_\nu - \widehat{\psi}_\nu\|_1 \leq \arcsin \|(I - \mathbf{S}_*)\widehat{\psi}_\nu\|_1 \leq \|(I - \mathbf{S}_*)\widehat{\psi}_\nu\|_1 + \|(I - \mathbf{S}_*)\widehat{\psi}_\nu\|_1^3$$

for the eigenvector $\psi_\nu = \mathbf{S}_* \widehat{\psi}_\nu / \|\mathbf{S}_* \widehat{\psi}_\nu\|_1$. Lemma 3.5 and equality (3.7) imply

$$|\widehat{\lambda}_\nu - \lambda| \leq \frac{\kappa(\mathcal{X})}{c_K^*} \sqrt{\lambda} \|\mathfrak{r}(\widehat{\lambda}_\nu)[\widehat{\psi}_\nu, \cdot]\|_{-1}$$

and the estimate of Theorem 3.1 now reads

$$(3.9) \quad \|(I - \mathbf{S}_*)\widehat{\psi}_\nu\|_1 \leq \frac{C_K^*}{c_K} \kappa(\mathcal{X}) \text{gap}(\lambda) \left(\|\mathfrak{t}(\widehat{\lambda}_\nu)[\widehat{\psi}_\nu, \cdot]\|_{-1} + \frac{\kappa(\mathcal{X})}{c_K^*} \sqrt{\lambda} \|\mathfrak{t}(\widehat{\lambda}_\nu)[\widehat{\psi}_\nu, \cdot]\|_{-1} \right)$$

An analogous estimate holds for left eigenvectors. An application of (3.8), (3.9) and Lemma 3.6 establishes the claim. \square

Remark 3.8. Note that this theorem does not say anything about eigenvector approximations, since $\psi_\nu \in \text{Ran}(\mathbf{S}_*)$ is possibly different for every ν . For the eigenvector convergence result see Appendix A. To obtain an eigenvector estimate, one would have to choose a subsequence of $\widehat{\psi}_\nu$ which converges to a fixed chosen eigenvector.

4. FINITE ELEMENT ERROR BOUNDS

Let us now discretize our model problem (2.5) using hp -finite element spaces. Let $\mathcal{T} = \mathcal{T}_h$ be a triangulation of Ω with the piecewise constant mesh function $h : \mathcal{T}_h \rightarrow (0, 1)$, $h(T) = \text{diam}(T)$ for $T \in \mathcal{T}_h$. We implicitly assume that \mathcal{T}_h is subordinate to the polygonal partition of Ω discussed in (A3) of Definition 2.1; in other words, each $T \in \mathcal{T}_h$ is contained in precisely one of the polygons Ω_k . Given a piecewise constant distribution of polynomial degrees, $p : \mathcal{T}_h \rightarrow \mathbb{N}$, we define the space

$$V = V_h^p = \{v \in H_0^1(\Omega) \cap C(\overline{\Omega}) : v|_T \in \mathbb{P}_{p(T)} \text{ for each } T \in \mathcal{T}_h\},$$

where $\mathbb{P}_{p(T)}$ is the collection of polynomials of total degree not greater than p on a given element $T \in \mathcal{T}_h$. Suppressing the mesh parameter h for convenience, we also define the set of interior edges \mathcal{E} in \mathcal{T} . Additionally, we let $\mathcal{T}(e)$ denote the two triangles having $e \in \mathcal{E}$ as an edge, and we extend p to \mathcal{E} by $p(e) = \max_{T \in \mathcal{T}(e)} p(T)$. Without loss of generality, we assume that the family of spaces satisfy the following standard *regularity properties* on \mathcal{T} and p : *There exists a constant $\gamma > 0$ for which*

(C1) $\gamma^{-1}h(T) \leq h(T') \leq \gamma h(T)$ for adjacent $T, T' \in \mathcal{T}$, $\overline{T} \cap \overline{T'} \neq \emptyset$. In other words, the diameters of adjacent elements are comparable.

(C2) $\gamma^{-1}(p(T)+1) \leq p(T')+1 \leq \gamma(p(T)+1)$ for adjacent $T, T' \in \mathcal{T}$, $\overline{T} \cap \overline{T'} \neq \emptyset$. In other words, the polynomial degrees associated with adjacent elements are comparable.

As a matter of notational convenience we use the same constant γ for (C1) and (C2).

Using a Galerkin approach we consider the following eigenvalue problem:

Find an eigentriple $(\widehat{\lambda}, \widehat{\psi}, \widehat{\psi}^*) \in \mathbb{R} \times V \times V$ such that

$$(4.1) \quad B(\widehat{\psi}, \phi) = \widehat{\lambda}(\widehat{\psi}, \phi) \quad \text{and} \quad B(\phi, \widehat{\psi}^*) = \widehat{\lambda}(\widehat{\psi}^*, \phi) \quad \text{for all } \phi \in V,$$

with $\|\widehat{\psi}\| = \|\widehat{\psi}^*\| = 1$.

With a basis $\{v_1, v_2, \dots, v_N\}$ of V , we get the algebraic eigenvalue problems

$$(4.2) \quad B\mathbf{x} = \widehat{\lambda}M\mathbf{x} \quad \text{and} \quad B^T\mathbf{y} = \widehat{\lambda}M\mathbf{y} \quad \text{with} \quad \mathbf{x}^T M\mathbf{x} = \mathbf{y}^T M\mathbf{y} = 1,$$

where $B_{ij} = B(v_j, v_i)$, $M_{ij} = (v_j, v_i) = (v_i, v_j)$. The vectors \mathbf{x} and \mathbf{y} are the coefficient vectors of $\widehat{\psi}$ and $\widehat{\psi}^*$, respectively, i.e., $\widehat{\psi} = \sum_{i=1}^N \mathbf{x}_i v_i$ and $\widehat{\psi}^* = \sum_{i=1}^N \mathbf{y}_i v_i$.

We also have the discrete analogues of (2.6) and (2.7). In particular, for $f \in L^2(\Omega)$, we define $\widehat{u}(f), \widehat{u}^*(f) \in V$ as the solutions of

$$(4.3) \quad B(\widehat{u}(f), v) = (f, v) \quad \text{and} \quad B(v, \widehat{u}^*(f)) = (f, v) \quad \text{for all } v \in V.$$

With these definitions, it is clear that $\widehat{u}(\widehat{\psi}) = \widehat{\lambda}^{-1}\widehat{\psi}$ and $\widehat{u}^*(\widehat{\psi}^*) = \widehat{\lambda}^{-1}\widehat{\psi}^*$ or, equivalently, $\widehat{u}(\widehat{\lambda}\widehat{\psi}) = \widehat{\psi}$ and $\widehat{u}^*(\widehat{\lambda}\widehat{\psi}^*) = \widehat{\psi}^*$. Using these facts, together with the Galerkin orthogonality, we obtain the following expressions for the $H^{-1}(\Omega)$ -norms of the left and right residuals:

$$(4.4) \quad \|\mathbf{r}(\widehat{\lambda})[\widehat{\psi}, \cdot]\|_{-1} = \inf_{w \in V} \sup_{v \in H_0^1(\Omega) \setminus \{0\}} \frac{\widehat{\lambda} |B(\widehat{u}(\widehat{\psi}) - u(\widehat{\psi}), v - w)|}{\|v\|_1},$$

$$(4.5) \quad \|\mathbf{r}(\widehat{\lambda})[\cdot, \widehat{\psi}^*]\|_{-1} = \inf_{w \in V} \sup_{v \in H_0^1(\Omega) \setminus \{0\}} \frac{\widehat{\lambda} |B(v - w, \widehat{u}^*(\widehat{\psi}^*) - u^*(\widehat{\psi}^*))|}{\|v\|_1}.$$

Remark 4.1. We note that the numerator in (4.4) is equivalent to $|B(\widehat{u}(\widehat{\lambda}\widehat{\psi}) - u(\widehat{\lambda}\widehat{\psi}), v - w)|$, and the numerator in (4.5) is equivalent to $|B(v - w, \widehat{u}(\widehat{\lambda}\widehat{\psi}^*) - u(\widehat{\lambda}\widehat{\psi}^*))|$.

We now focus on expressions such as those in the numerators in (4.4) and (4.5), and develop residual-type hp -finite element bounds. Let $f \in L^2(\Omega)$, $v \in H_0^1(\Omega)$ and $w \in V$. We set $u = u(f)$, $\widehat{u} = \widehat{u}(f)$ and get

$$(4.6) \quad \begin{aligned} B(u - \widehat{u}, v - w) &= \int_{\Omega} (f - c\widehat{u} - b \cdot \nabla \widehat{u})(v - w) - A \nabla \widehat{u} \cdot \nabla (v - w) \, dx \\ &= \sum_{T \in \mathcal{T}} \left(\int_T R_T(f)(v - w) \, dx - \int_{\partial T} A \nabla \widehat{u} \cdot \mathbf{n}(v - w) \, ds \right) \\ &= \sum_{T \in \mathcal{T}} \int_T R_T(f)(v - w) \, dx + \sum_{\varepsilon \in \mathcal{E}} \int_{\varepsilon} R_{\varepsilon}(f)(v - w) \, ds. \end{aligned}$$

Here we have defined the element residual, $R_T(f)$, and edge residual, $R_{\varepsilon}(f)$, by

$$(4.7) \quad R_T(f) := f - (-\nabla \cdot A \nabla \widehat{u} + b \cdot \nabla \widehat{u} + c\widehat{u}),$$

$$(4.8) \quad R_{\varepsilon}(f) := -(A \nabla \widehat{u})|_T \cdot \mathbf{n}_T - (A \nabla \widehat{u})|_{T'} \cdot \mathbf{n}_{T'},$$

where T and T' are the two adjacent elements of $\varepsilon \in \mathcal{E}$, having outward unit normal vectors \mathbf{n}_T and $\mathbf{n}_{T'}$, respectively. Similarly, for $u^* = u^*(f)$ and $\widehat{u}^* = \widehat{u}^*(f)$, we have

$$(4.9) \quad \begin{aligned} B(v - w, u^* - \widehat{u}^*) &= \int_{\Omega} (f - c\widehat{u}^*)(v - w) - b \cdot \nabla (v - w) \widehat{u}^* - A \nabla (v - w) \cdot \nabla \widehat{u}^* \, dx \\ &= \int_{\Omega} (f - c\widehat{u}^* + \nabla \cdot (b\widehat{u}^*))(v - w) - A \nabla (v - w) \cdot \nabla \widehat{u}^* \, dx \\ &= \sum_{T \in \mathcal{T}} \int_T R_T^*(f)(v - w) \, dx + \sum_{\varepsilon \in \mathcal{E}} \int_{\varepsilon} R_{\varepsilon}^*(f)(v - w) \, ds, \end{aligned}$$

where

$$(4.10) \quad R_T^*(f) := f - (-\nabla \cdot A \nabla \widehat{u}^* - \nabla \cdot (b\widehat{u}^*) + c\widehat{u}^*),$$

$$(4.11) \quad R_{\varepsilon}^*(f) := -(A \nabla \widehat{u}^*)|_T \cdot \mathbf{n}_T - (A \nabla \widehat{u}^*)|_{T'} \cdot \mathbf{n}_{T'}.$$

The forms of the expressions (4.6) and (4.9) motivate estimates based on a Clément-type interpolation result of [26, Theorem 2.2, Remark 2.3]. For completeness, we state this result here.

Theorem 4.2 ([26]). *There is a linear operator $\mathcal{I} : H_0^1(\Omega) \rightarrow V$ and a constant C depending only on the shape-regularity parameter γ , such that: For any vertex z and any edge ε having z as a vertex,*

$$\|v - \mathcal{I}v\|_{0,\omega_z} + \frac{h_z}{p_z} |Iv|_{1,\omega_z} + \sqrt{\frac{h_z}{p_z}} \|v - \mathcal{I}v\|_{0,\varepsilon} \leq C \frac{h_z}{p_z} |v|_{1,\Omega_z} .$$

Here, ω_z is the patch of triangles having z as a vertex, h_z is the largest of the diameters of these triangles, $p_z - 1$ is the largest of the polynomial degrees associated with these triangles, and $\Omega_z \supset \omega_z$ is a larger, but still localized, patch of triangles.

Remark 4.3. The precise definition of Ω_z is not essential here. It only matters that, if m_z is the number of triangles in Ω_z and M is the total number of triangles in \mathcal{T} , then $\sum_z m_z \leq \delta M$ for some δ which depends only on the shape-regularity parameter γ . This is a consequence of the shape-regularity assumption **(C1)** (cf. [26]).

Lemma 4.4. *Given $f \in L^2(\Omega)$, let $u, u^* \in H_0^1(\Omega)$ and $\hat{u}, \hat{u}^* \in V$ be defined as in (2.6), (2.7) and (4.3). There exists a constant C depending only on γ such that, for any $v \in H_0^1(\Omega)$,*

$$\begin{aligned} \inf_{w \in V} |B(u - \hat{u}, v - w)| &\leq C \left(\sum_{T \in \mathcal{T}} \left(\frac{h(T)}{p(T)} \right)^2 \|R_T(f)\|_{0,T}^2 + \sum_{\varepsilon \in \mathcal{E}} \frac{h(\varepsilon)}{p(\varepsilon)} \|R_\varepsilon(f)\|_{0,\varepsilon}^2 \right)^{1/2} |v|_1 , \\ \inf_{w \in V} |B(v - w, u^* - \hat{u}^*)| &\leq C \left(\sum_{T \in \mathcal{T}} \left(\frac{h(T)}{p(T)} \right)^2 \|R_T^*(f)\|_{0,T}^2 + \sum_{\varepsilon \in \mathcal{E}} \frac{h(\varepsilon)}{p(\varepsilon)} \|R_\varepsilon^*(f)\|_{0,\varepsilon}^2 \right)^{1/2} |v|_1 . \end{aligned}$$

Proof. Since the argument for the second result is the same as for the first, we only prove the former. As a notational convenience we use the common shorthand $X \lesssim Y$ when $X \leq cY$ for some constant c depending only on γ . It holds that

$$\begin{aligned} \inf_{w \in V} |B(u - \hat{u}, v - w)| &\leq \sum_{T \in \mathcal{T}} \|R_T(f)\|_{0,T} \|v - \mathcal{I}v\|_{0,T} + \sum_{\varepsilon \in \mathcal{E}} \|R_\varepsilon(f)\|_{0,\varepsilon} \|v - \mathcal{I}v\|_{0,\varepsilon} \\ &\lesssim \sum_{T \in \mathcal{T}} \|R_T(f)\|_{0,T} \frac{h_z(T)}{p_z(T)} |v|_{1,\Omega_{z(T)}} + \sum_{\varepsilon \in \mathcal{E}} \|R_\varepsilon(f)\|_{0,\varepsilon} \sqrt{\frac{h_z(\varepsilon)}{p_z(\varepsilon)}} |v|_{1,\Omega_{z(\varepsilon)}} , \end{aligned}$$

where $z(T)$ is a vertex of T and $z(\varepsilon)$ is a vertex of ε . The controlled overlap of patches (Remark 4.3) guarantees that

$$\sum_{T \in \mathcal{T}} |v|_{1,\Omega_{z(T)}}^2 \lesssim |v|_1^2 \quad , \quad \sum_{\varepsilon \in \mathcal{E}} |v|_{1,\Omega_{z(\varepsilon)}}^2 \lesssim |v|_1^2 .$$

Now using the discrete Cauchy-Schwarz inequality and the fact that triangle diameters and polynomial degrees are comparable for nearby elements and edges, we see that

$$\inf_{w \in V} |B(u - \hat{u}, v - w)| \lesssim \left(\sum_{T \in \mathcal{T}} \left(\frac{h(T)}{p(T)} \right)^2 \|R_T(f)\|_{0,T}^2 + \sum_{\varepsilon \in \mathcal{E}} \frac{h(\varepsilon)}{p(\varepsilon)} \|R_\varepsilon(f)\|_{0,\varepsilon}^2 \right)^{1/2} |v|_1 .$$

This completes the proof. \square

For a given triangle T , we define $\mathcal{E}(T)$ to be the set of interior edges of T (those not on $\partial\Omega$). We also define the (non-negative) local error indicators, $\eta_T(f)$ and $\eta_T^*(f)$, and global error estimates, $\eta(f)$ and $\eta^*(f)$, by

$$(4.12) \quad \eta_T(f)^2 := \left(\frac{h(T)}{p(T)} \right)^2 \|R_T(f)\|_{0,T}^2 + \frac{1}{2} \sum_{\varepsilon \in \mathcal{E}(T)} \frac{h(\varepsilon)}{p(\varepsilon)} \|R_\varepsilon(f)\|_{0,\varepsilon}^2 ,$$

$$(4.13) \quad \eta_T^*(f)^2 := \left(\frac{h(T)}{p(T)} \right)^2 \|R_T^*(f)\|_{0,T}^2 + \frac{1}{2} \sum_{\varepsilon \in \mathcal{E}(T)} \frac{h(\varepsilon)}{p(\varepsilon)} \|R_\varepsilon^*(\varepsilon)\|_{0,\varepsilon}^2 ,$$

$$(4.14) \quad \eta(f)^2 = \sum_{T \in \mathcal{T}} \eta_T(f)^2 = \sum_{T \in \mathcal{T}} \left(\frac{h(T)}{p(T)} \right)^2 \|R_T(f)\|_{0,T}^2 + \sum_{\varepsilon \in \mathcal{E}} \frac{h(\varepsilon)}{p(\varepsilon)} \|R_\varepsilon(f)\|_{0,\varepsilon}^2 ,$$

$$(4.15) \quad \eta^*(f)^2 := \sum_{T \in \mathcal{T}} \eta_T^*(f)^2 = \sum_{T \in \mathcal{T}} \left(\frac{h(T)}{p(T)} \right)^2 \|R_T^*(f)\|_{0,T}^2 + \sum_{\varepsilon \in \mathcal{E}} \frac{h(\varepsilon)}{p(\varepsilon)} \|R_\varepsilon^*(f)\|_{0,\varepsilon}^2 .$$

With these definitions in hand, the result below immediately follows from equalities (4.4), (4.5) and Lemma 4.4.

Theorem 4.5. *Let $(\widehat{\lambda}, \widehat{\psi}, \widehat{\psi}^*) \in \mathbb{R} \times V_h^p \times V_h^p$ be an eigentriple of (4.1). There is a constant C depending only on shape-regularity parameter γ for which*

$$\|\mathbf{r}(\widehat{\lambda})[\widehat{\psi}, \cdot]\|_{-1} \leq C \widehat{\lambda} \eta(\widehat{\psi}) \quad \text{and} \quad \|\mathbf{r}(\widehat{\lambda})[\cdot, \widehat{\psi}^*]\|_{-1} \leq C \widehat{\lambda} \eta^*(\widehat{\psi}^*) .$$

We finally obtain our key *a posteriori* error estimation results in the finite element context, which follow immediately from Theorems 3.7 and 4.5.

Theorem 4.6. *Let the operator \mathcal{A} defined by the variational form $B(\cdot, \cdot)$ satisfy condition \mathfrak{S} and let $(\widehat{\lambda}, \widehat{\psi}, \widehat{\psi}^*) \in \mathbb{R} \times V_h^p \times V_h^p$ be an eigentriple of (4.1) such that $(\widehat{\psi}, \widehat{\psi}^*) \neq 0$. Then there exists an eigenvalue λ of \mathcal{A} such that*

$$(4.16) \quad \frac{|\widehat{\lambda} - \lambda|}{\widehat{\lambda}} \leq C \widehat{\lambda} \eta(\widehat{\psi}) \eta^*(\widehat{\psi}^*) + o(\widehat{\lambda} \eta(\widehat{\psi}) \eta^*(\widehat{\psi}^*)) .$$

The constant C depends solely on the shape-regularity parameter γ , the relative distance of λ from the rest of the $\text{Spec}(\mathcal{A})$ (measured by $\text{gap}(\lambda)$), the condition number $\kappa(\mathcal{X})$ for the Ritz basis of eigenvectors of \mathcal{A} , the cosine of the angle between the left and the right computed eigenvector $(\widehat{\psi}, \widehat{\psi}^*)$ and the equivalence constants from Kato's square root theorem. Furthermore, we may choose associated right and left eigenvectors ψ and ψ^* for λ such that the following estimates hold

$$(4.17) \quad \|\psi - \widehat{\psi}\|_1 \leq C \widehat{\lambda} \eta(\widehat{\psi}), \quad \|\psi^* - \widehat{\psi}^*\|_1 \leq C \widehat{\lambda} \eta^*(\widehat{\psi}^*) .$$

Remark 4.7. Following through the arguments above, with Remark 4.1 in mind, we see that the key results in Theorem 4.6 may be re-written as:

$$|\widehat{\lambda} - \lambda| \leq C \eta(f) \eta^*(f^*) + o(\eta(f) \eta^*(f^*)) , \quad \|\psi - \widehat{\psi}\|_1 \leq C \eta(f) , \quad \|\psi^* - \widehat{\psi}^*\|_1 \leq C \eta^*(f^*) ,$$

where $f = \widehat{\lambda} \widehat{\psi}$ and $f^* = \widehat{\lambda} \widehat{\psi}^*$.

Remark 4.8. The second order eigenvalue estimate (4.16) holds under the assumptions of Theorem 3.7. For a fully *a posteriori* result, we would need a practical means of establishing

the requirements of that theorem, in particular, the convergence of our Galerkin eigenvalue approximations. On the other hand, the convergence of residual estimates to zero does guarantee the first order convergence of eigenvalues in the sense of Lemma 3.5. This estimate is a direct corollary of Theorem 4.5 and Lemma 3.5 and the statement reads:

For each ν , there exists an eigenvalue λ such that

$$|\widehat{\lambda}_\nu - \lambda| \leq \frac{\kappa(\mathcal{X})}{c_K^*} C \sqrt{\lambda} \widehat{\lambda}_\nu \eta(\widehat{\psi}_\nu).$$

Here the constant C depends solely on the shape regularity-parameter γ and it is the same as in Theorem 4.5. We also have the convergence of eigenvectors to the associated eigenspaces in the sense of estimate (3.9).

5. NUMERICAL EXAMPLES

In this section we provide several numerical results which illustrate the efficiency of our a posteriori error estimators and the exponential convergence of the error on a sequence of hp -adapted meshes. Following [6], we assume an eigenvalue error model of the form

$$(5.1) \quad \widehat{\lambda} = \lambda + C e^{-2\alpha\sqrt{\#\text{DOFs}}},$$

for problems with smooth eigenvectors, and

$$(5.2) \quad \widehat{\lambda} = \lambda + C e^{-2\alpha\sqrt[3]{\#\text{DOFs}}},$$

for problems defined on non-convex polygonal domains and/or possessing discontinuous coefficients, which are expected to have eigenvectors with isolated singularities. The constants C and α are determined by least-squares fitting [27], the value of α is reported for each problem and in all convergence plots a straight line of slope α is added for comparison. Although all convergence rates in the experiments are seen to be exponential, with one of the two error models above, we will abuse terminology slightly in the experiments by referring to α as the *convergence rate*; the context will make it clear if α is to be associated with the model (5.1) or (5.2). With this terminology, theory predicts that the convergence rate of the left and right eigenvectors is half of that for the eigenvalues, and we see in each of the experiments that this is essentially the case.

As in Remark 4.7, for a given approximate eigentriple $(\widehat{\lambda}, \widehat{\psi}, \widehat{\psi}^*)$, we define $f = \widehat{\lambda}\widehat{\psi}$ and $f^* = \widehat{\lambda}\widehat{\psi}^*$. Throughout this section we are interested in the following quantities: the relative eigenvalue error, its *a posteriori* estimate and the associated effectivity index, shown, respectively, below:

$$\frac{|\widehat{\lambda} - \lambda|}{\widehat{\lambda}}, \quad \frac{\eta(f)\eta^*(f^*)}{\widehat{\lambda}}, \quad \frac{|\widehat{\lambda} - \lambda|}{\eta(f)\eta^*(f^*)}.$$

Similarly for eigenvectors we analyse the eigenvector errors, their *a posteriori* estimates, and the associated effectivity indices, shown, respectively, below:

$$\begin{aligned} \|\psi - \widehat{\psi}\|_1, \quad \eta(f), \quad \|\psi - \widehat{\psi}\|_1/\eta(f), \\ \|\psi^* - \widehat{\psi}^*\|_1, \quad \eta^*(f^*), \quad \|\psi^* - \widehat{\psi}^*\|_1/\eta^*(f^*). \end{aligned}$$

For the problems with given exact eigenvalues, we use these in our error analysis. In other cases, we use highly accurate computations on very fine grids and adapted finite element

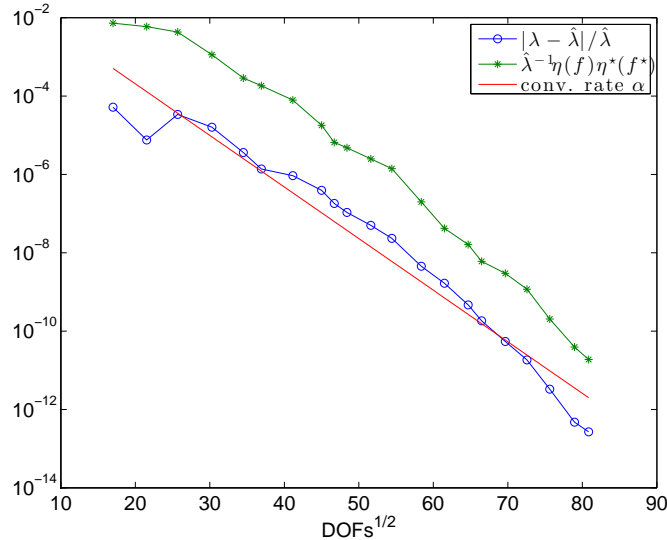


FIGURE 1. Convergence of the first eigenvalue on the unit square. Estimated convergence rate 0.1516.

spaces generated by the method described below to produce “exact eigenvalues” for our comparisons. However, in order to compute the errors for eigenvectors, we use reference eigenvectors computed on very fine grids and with adapted finite element spaces for all problems.

All the experiments have been carried out using the APTOFEM package (www.aptofem.com) on a single processor desktop machine. In particular, we have used ARPACK [21] to solve the algebraic eigenvalue problems, employing MUMPS [1] to solve the necessary linear systems.

Let us shortly summarize the adaptive algorithm used in our simulations. At first we choose the indices i of the eigenvalues of interest. On the initial coarse mesh we compute the eigenpairs $(\hat{\lambda}_{i,hp}, \hat{\psi}_{i,hp})$ and the *a posteriori* error estimators. We determine the elements $T \in \mathcal{T}$ for refinement using a simple fixed-fraction strategy based on the values of the local error estimators $\eta_T(\hat{\psi}_i)$, with different percentages for refinement and de-refinement. The choice between refining the marked elements in h or p is based on an estimation of the local analyticity of the exact eigenvectors using the computed ones, see [16] for more details. Finally, a refined space is generated and the process is restarted by taking previously calculated eigenpairs $(\hat{\lambda}_{i,hp}, \hat{\psi}_{i,hp})$ as initial values for the computations in the refined space.

5.1. Unit Square. As a simple problem for which the exact eigenvalues and eigenvectors are explicitly known, we consider the operator $\mathcal{A} = -\Delta + b \cdot \nabla$, where $b = (2, 2)$ and $\Omega = (0, 1) \times (0, 1)$. This is just a case of Example 2.3, so we see that the eigtuples are given as

$$\lambda_{j,k} = 2 + \pi^2(j^2 + k^2), \quad \psi_{j,k} = e^{x+y} \sin(j\pi x) \sin(k\pi y), \quad \psi_{j,k}^* = e^{-(x+y)} \sin(j\pi x) \sin(k\pi y),$$

for $j, k \in \mathbb{N}$.

In Figure 1 we present the relative eigenvalue errors and the error estimates for the first eigenvalue using our hp -adaptive scheme with 15% for refinement and 2% for de-refinement

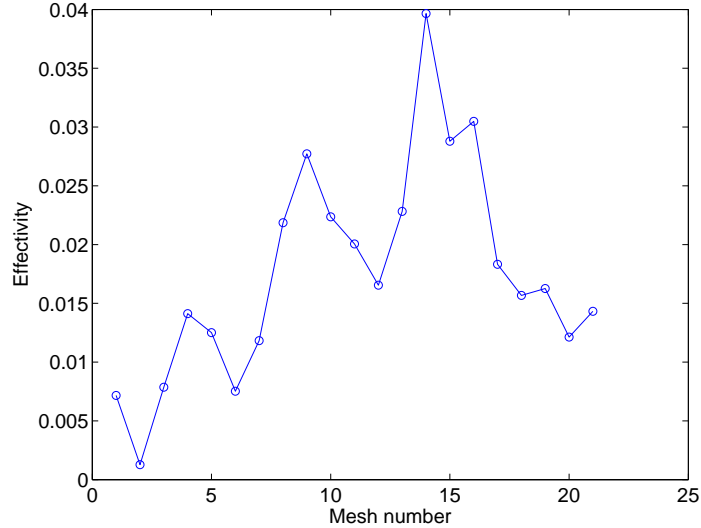


FIGURE 2. Effectivity index of the first eigenvalue on the unit square.

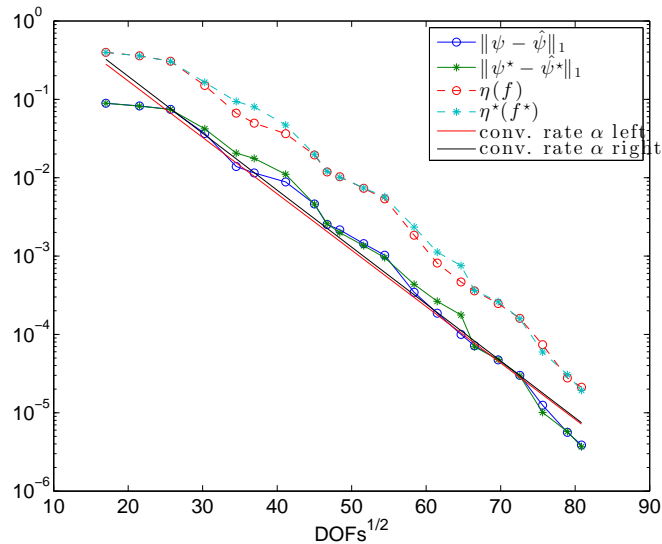


FIGURE 3. Convergence of the left and right eigenvectors (eigenfunctions) corresponding to the first eigenvalue on the unit square. Estimated convergence rates for the left and right eigenvectors (eigenfunctions) are respectively: 0.0829 and 0.0836.

in the fixed-fraction marking strategy. In this case we have that the convergence rate for the eigenvalue estimated with least-squares fitting is $\alpha = 0.1516$. The corresponding effectivity indices are shown in Figure 2.

Similarly, the right and left eigenvector errors corresponding to the first eigenvalue with the associated error estimates are depicted in Figure 3. Here the convergence rate for the right and left eigenvectors estimated with least-squares fitting are $\alpha = 0.0829, 0.0836$, respectively.

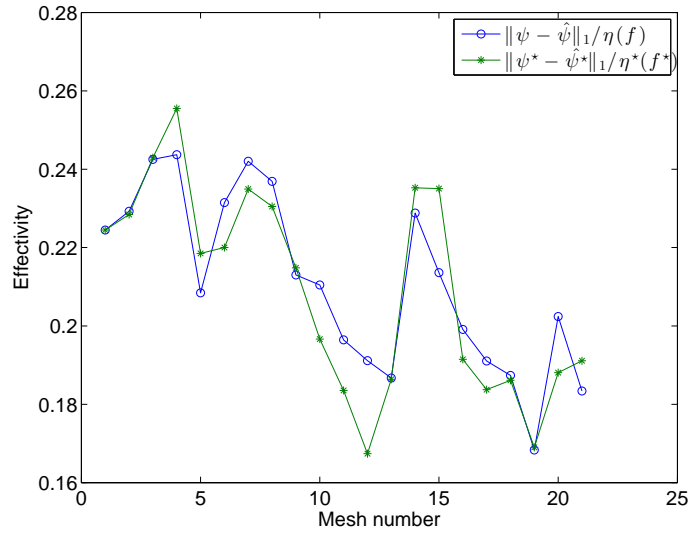


FIGURE 4. Effectivity indices of the left and right eigenvectors (eigenfunctions) corresponding to the first eigenvalue on the unit square.

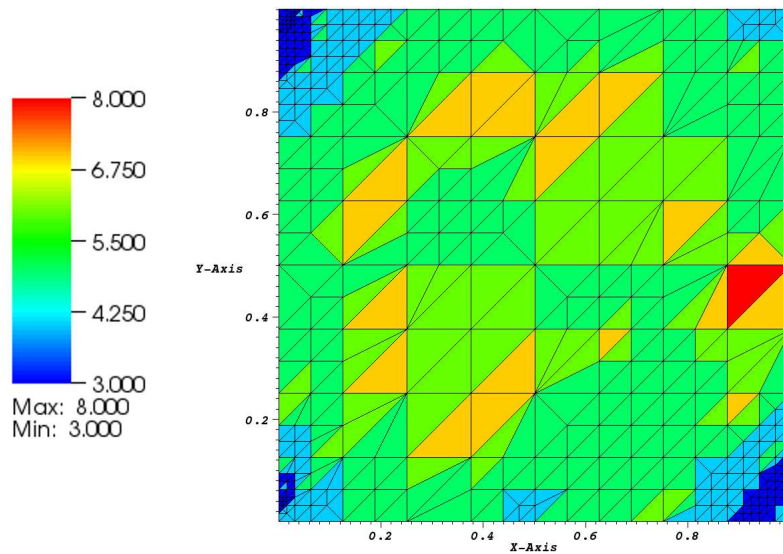


FIGURE 5. Final hp -adapted mesh for the unit square problem with the order p of polynomials expressed on the color scale.

Figure 4 presents the effectivity indices for eigenvectors. The final hp -adapted mesh is displayed in Figure 5.

5.2. L-Shape. We consider the operator $\mathcal{A} = -\Delta + b \cdot \nabla$, where $b = (2, 2)$ and Ω is the L-shaped domain pictured in Figure 10. Although there are no explicit formulas for most of

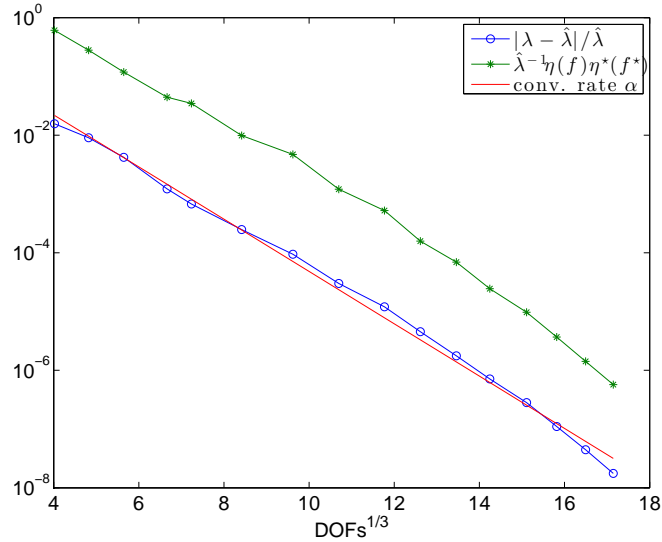


FIGURE 6. Convergence of the first eigenvalue on the L-shaped domain. Estimated convergence rate 0.5126.

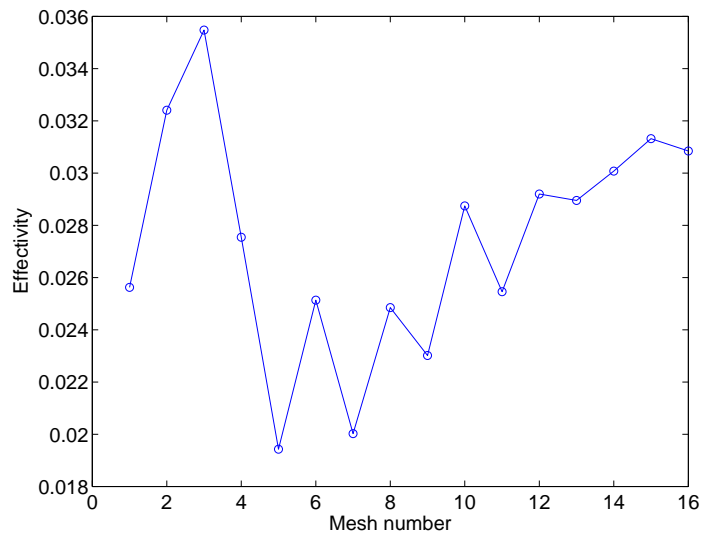


FIGURE 7. Effectivity index of the first eigenvalue on the L-shaped domain.

the eigentriples for \mathcal{A} , the first several eigenvalues of $-\Delta$ are known to very high precision (cf. [29]), and those for \mathcal{A} are readily obtained by adding 2, as discussed in Example 2.3.

Figure 6 illustrates the relative eigenvalue errors and the error estimates for the first eigenvalue using our hp -adaptive scheme with 25% for refinement and 5% for de-refinement in the fixed-fraction marking strategy [15]. In this case we have that the convergence rate for the eigenvalue estimated with least-squares fitting is $\alpha = 0.5126$. For the effectivity indices see Figure 7. Moreover, Figure 8 shows the right and left eigenvector errors corresponding to the first eigenvalue and the associated error estimates. The convergence rate for the right and left eigenvectors estimated with least-squares fitting are $\alpha = 0.2697, 0.2671$, respectively.

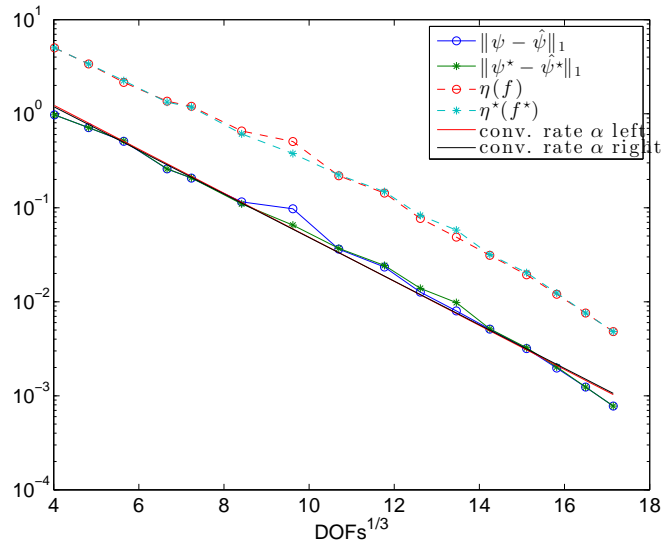


FIGURE 8. Convergence of the left and right eigenvectors (eigenfunctions) corresponding to the first eigenvalue on the L-shaped domain. Estimated convergence rates for the left and right eigenvectors (eigenfunctions) are respectively: 0.2697 and 0.2671.

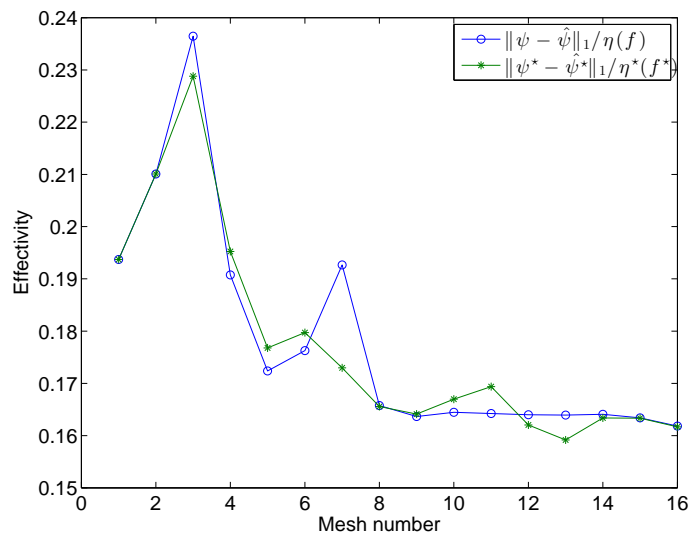


FIGURE 9. Effectivity indices of the left and right eigenvectors (eigenfunctions) corresponding to the first eigenvalue on the L-shaped domain.

Corresponding effectivity indices are displayed in Figure 9. The final hp -adapted mesh is given in Figure 10, and we see that the singularities of the left and right eigenvectors at the origin (the reentrant corner) have been recognized by our adaptive scheme, which does heavy h -refinement near the origin.

5.3. Kellogg Problem. For this example we consider the eigenvalue version of a Kellogg problem [19]: Ω is the square domain $\Omega = (-1, 1) \times (-1, 1)$, and $\mathcal{A}v = -\nabla \cdot (a\nabla v) + b \cdot \nabla v$,

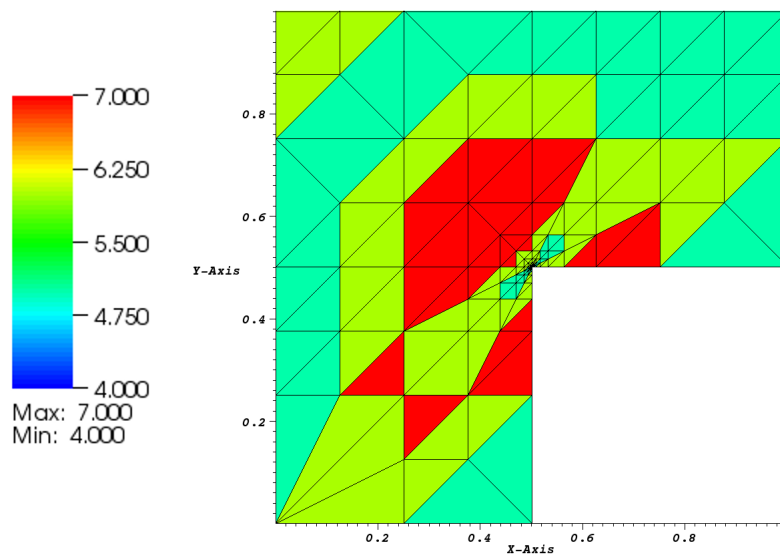


FIGURE 10. Final hp -adapted mesh for the L-shaped domain, the order of polynomials in each element is expressed in the color scheme.

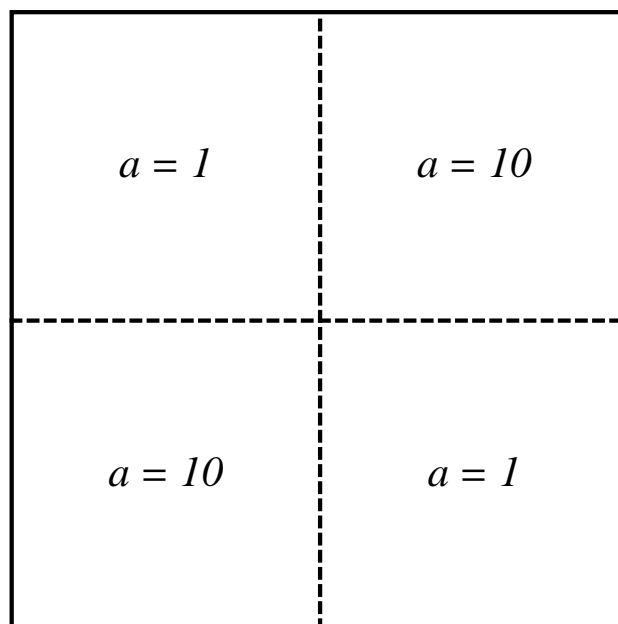


FIGURE 11. The domain and diffusion coefficients for the Kellogg problem.

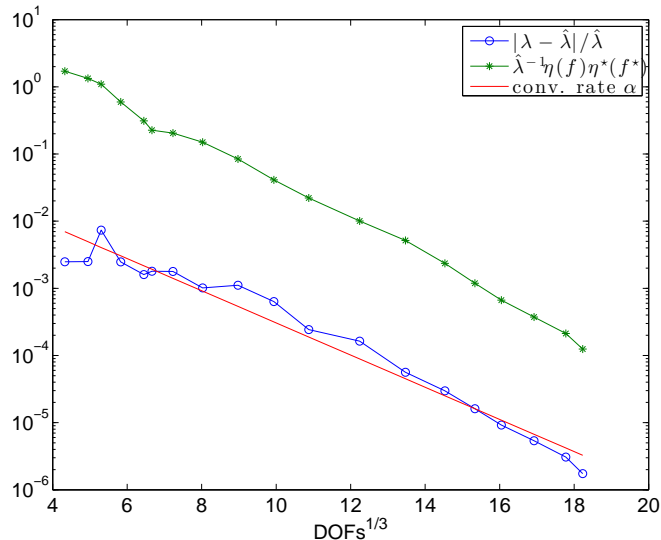


FIGURE 12. Convergence of the first eigenvalue for the Kellogg problem. Estimated convergence rate 0.2757.

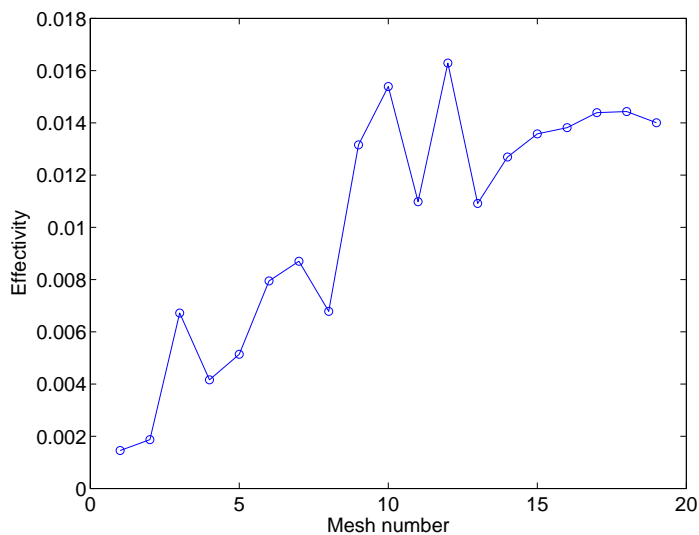


FIGURE 13. Effectivity index of the first eigenvalue for the Kellogg problem.

where $b = (2, 2)$ and $a = 10$ in quadrants I and III, and $a = 1$ in quadrants II and IV, see Figure 11. Although we have no proof that this operator fits into the framework of the error theory presented here—it is certainly not diagonalized in the manner discussed in Example 2.3—we offer numerical results which suggest that our approach works very well for the first eigenvalue, which is known to be real and simple, but whose left and right eigenvectors have strong singularities at the origin. The relative eigenvalue error and the error estimate for the first eigenvalue obtained using our hp -adaptive scheme with 15% for refinement and 4% for de-refinement are presented in Figure 12. The value of the convergence rate for the eigenvalue estimated with least-squares fitting is $\alpha = 0.2757$ and the reference

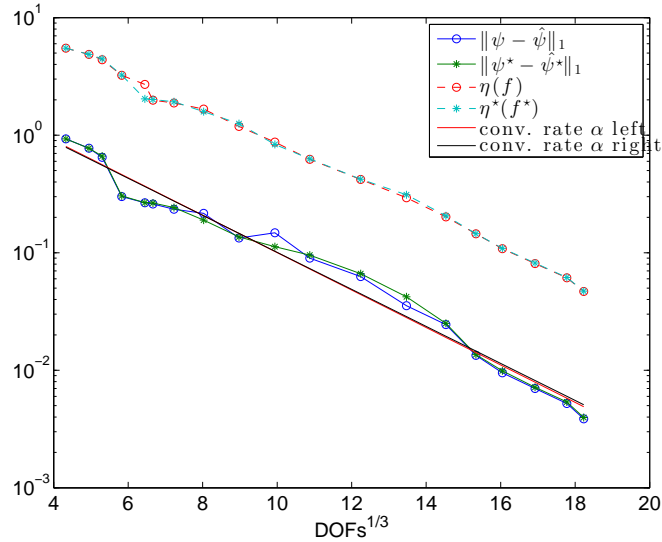


FIGURE 14. Convergence of the left and right eigenvectors (eigenfunctions) corresponding to the first eigenvalue for the Kellogg problem. Estimated convergence rates for the left and right eigenvectors (eigenfunctions) are respectively: 0.1834 and 0.1813.

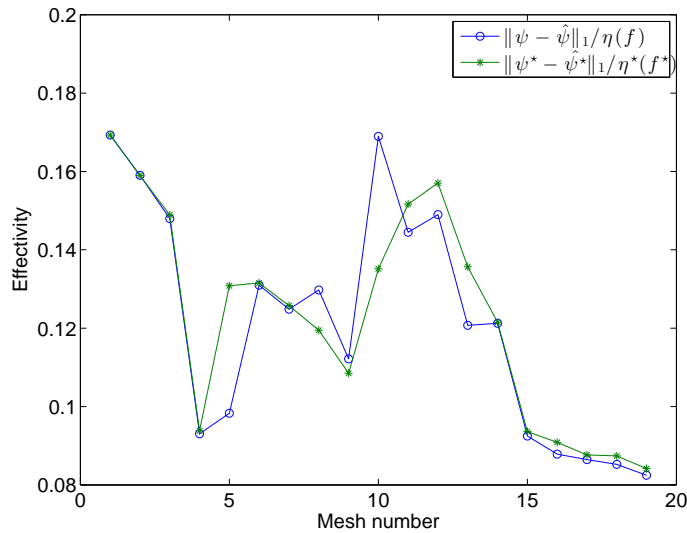


FIGURE 15. Effectivity indices of the left and right eigenvectors (eigenfunctions) corresponding to the first eigenvalue for the Kellogg problem.

value for the eigenvalue is 17.714316 with an accuracy of 10^{-6} . In Figure 13 the corresponding effectivity indices are displayed. The right and left eigenvector errors together with the associated error estimates, and the effectivity indices are given in Figure 14 and Figure 15, respectively. The convergence rate for the right and left eigenvectors estimated with least-squares fitting are $\alpha = 0.1834, 0.1813$. The final hp -adapted mesh is presented in Figure 16.

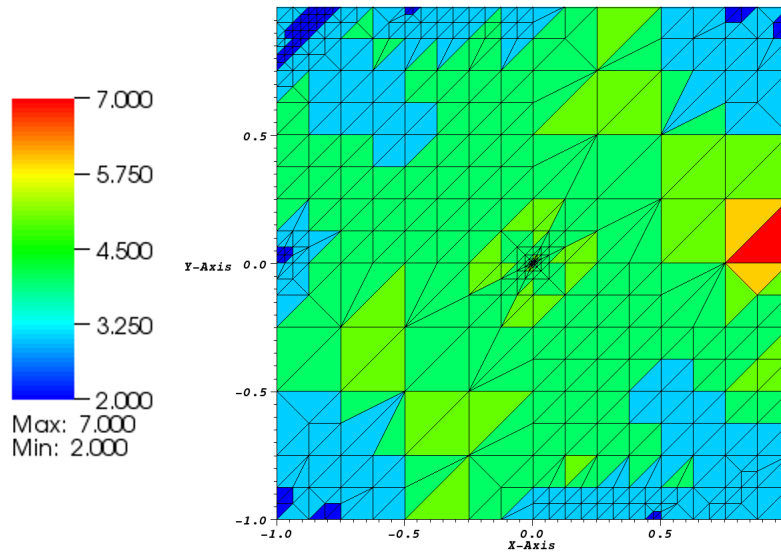


FIGURE 16. Final hp -adapted mesh for the Kellogg problem, the order of polynomials in each element is expressed in the color scheme.

As expected, the h -adaptivity is concentrated around the singularity in the center of the domain.

6. CONCLUSIONS

In this paper we have presented new relative estimates for the eigenvalue/function approximation error for a class of convection–diffusion–reaction operators. The main ingredients of our analysis have been Kato’s square root theorem, which holds for the whole class of convection–diffusion–reaction type operators with bounded coefficients, and a generalization of a Bauer-Fike type theorem (cf. discussion on [30, p. 95]), which holds only in the case when the eigenfunctions of the operator constitute a Riesz basis of the entire Hilbert space where the problem is posed. The condition number of the Riesz basis of eigenvectors measures the global sensitivity of all eigenvalues, and appears in our upper estimates of approximation errors. In the case of convection–diffusion–reaction operators which satisfy the conditions from Example 2.3, this global quantity is a good measure of the sensitivity of individual eigenvalues as well.

ACKNOWLEDGMENT

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APPENDIX A. CLUSTER ROBUST EIGENVECTOR APPROXIMATIONS

In this appendix we prove a cluster robust eigenvector approximation estimate. Namely, we establish a subspace approximation estimate which depends only on the distance between the Ritz values from the given approximation subspace to the unwanted components of the spectrum.

Before we formulate the main result, let us define a measure of the spectral separation. Let $\Lambda := \{\lambda_i : i = 1, \dots, n\}$ be an isolated subset of $\text{Spec}(\mathcal{A})$. Let $\{\widehat{\psi}_i : i = 1, \dots, n\} \subset H_0^1(\Omega)$ and $\{\widehat{\psi}_i^* : i = 1, \dots, n\} \subset H_0^1(\Omega)$ denote independent sets of vectors and let $\Xi := \{\widehat{\mu}_i, i = 1, \dots, n\} \subset \mathbb{R}$. Then we define

$$\text{gap}_2(\Xi) := \min \left\{ \frac{|\widehat{\mu}_i - \xi|}{\sqrt{\widehat{\mu}_i \xi}} : \xi \in \text{Spec}(\mathcal{A}) \setminus \Lambda \right\}.$$

Note that this gap is different from the relative gap we used in (1.2). For more information on the topological properties of various relative distance functions see [22]. Also, for a bounded operator \mathcal{X} with a bounded inverse we define $\sigma_{\min} = \|\mathcal{X}^{-1}\|^{-1}$. It plays the role of the smallest singular value from matrix analysis.

Let $f_i = \mathcal{X}e_i$, $i \in \mathbb{N}$, be a Riesz basis. Then $q_i = \mathcal{X}(\mathcal{X}^* \mathcal{X})^{-1/2}e_i$, $i \in \mathbb{N}$, is an orthonormal basis for which we have

$$(A.1) \quad |(q_i, v)| = |(\mathcal{X}(\mathcal{X}^* \mathcal{X})^{-1/2}e_i, v)| \leq \|\mathcal{X}^{-1}\| |(e_i, v)|, \quad i \in \mathbb{N}.$$

Recall that an operator A is a Hilbert-Schmidt operator providing the trace $\text{tr}(A^*A)$ is finite. For a given Hilbert-Schmidt operator A we define the Hilbert-Schmidt norm by the formula $\|A\|_{HS} = \sqrt{\text{tr}(A^*A)}$.

Theorem A.1. *Assume that the eigenvalues $\Lambda = \{\lambda_i, i = 1, \dots, n\}$ and their approximations Ξ are given such that $\text{gap}_2(\Xi) > 0$. Furthermore, let P be the L^2 -orthogonal projection onto $\mathcal{P} := \text{span}\{\widehat{\psi}_i : i = 1, \dots, n\}$ and Q be the L^2 -orthogonal projection onto $\mathcal{Q} = \text{span}\{\psi : \psi \in \text{Ker}(\mathcal{A} - \lambda I), \lambda \in \text{Spec}(\mathcal{A}) \setminus \Lambda\}$. Then*

$$\|(I - Q)P\|_{HS} \leq \frac{\kappa(\mathcal{X})}{c_K^* \lambda_{\min}(G)^{1/2}} \frac{\sqrt{\sum_{i=1}^n \|\mathfrak{r}(\widehat{\mu}_i)[\widehat{\psi}_i, \cdot]\|_{-1}^2}}{\text{gap}_2(\Xi)}.$$

Here $G_{ij} = (\widehat{\psi}_i, \widehat{\psi}_j)$, $i, j = 1, \dots, n$ is the Gram matrix of the set $\{\widehat{\psi}_i : i = 1, \dots, n\} \subset H_0^1(\Omega)$ and $\lambda_{\min}(G)$ denotes its smallest positive eigenvalue. An equivalent result, involving dual quantities, holds for left eigenvectors.

Remark A.2. In the case when $\|P - Q\| < 1$, where $\|\cdot\|$ denotes the operator norm, we have the estimate

$$\|Q - P\|_{HS} \leq \frac{\kappa(\mathcal{X})}{c_K^* \lambda_{\min}(G)^{1/2}} \frac{\sqrt{\sum_{i=1}^n \|\mathfrak{r}(\widehat{\mu}_i)[\widehat{\psi}_i, \cdot]\|_{-1}^2}}{\text{gap}_2(\Xi)},$$

and its analogue for the left eigenvectors.

Proof. Let now P and Q be the orthogonal projections as in the statement of the theorem. Obviously, $\|(I - Q)P\|_{HS} < \infty$, since $\text{Ran}(P)$ is of finite dimension.

Let $p_i, i = 1, \dots, n$ be an orthonormal basis for \mathcal{P} which is obtained from $\{\widehat{\psi}_i : i = 1, \dots, n\}$ by the Gram-Schmidt orthogonalization procedure. It follows that

$$\|(I - Q)P\|_{HS}^2 = \sum_{i=1}^n \|(I - Q)Pp_i\|^2 \leq \frac{1}{\lambda_{\min}(G)} \sum_{i=1}^n \|(I - Q)P\widehat{\psi}_i\|^2.$$

Let now $q_j, j = 1, \dots, \infty$ be an orthonormal basis for \mathcal{Q} . Analogously, we conclude that for each $\widehat{\psi}_i, i = 1, \dots, n$ we have the estimate

$$\begin{aligned} \|(I - Q)P\widehat{\psi}_i\|^2 &= \sum_{j=1}^{\infty} |(q_j, (I - Q)P\widehat{\psi}_i)|^2 \\ &\leq \|\mathcal{X}^{-1}\|^2 \sum_{j=1}^{\infty} |(f_j, (I - Q)P\widehat{\psi}_i)|^2 \\ &\leq \|\mathcal{X}^{-1}\|^2 \sum_{j=1, \lambda_j \notin \Lambda}^{\infty} |(f_j, \widehat{\psi}_i)|^2. \end{aligned}$$

In this we have used the identity (A.1) and the fact that $(I - Q)f_j = 0$ for j such that $\lambda_j \in \Lambda$. On the other hand, for a fixed i we compute

$$\begin{aligned} \|\mathbf{r}(\widehat{\mu}_i)[\widehat{\psi}_i, \cdot]\|_{-1} &= \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\widehat{\mu}_i)[\widehat{\psi}_i, \phi]|}{\|\phi\|_1} \geq c_K^* \sup_{\phi \in H_0^1(\Omega) \setminus \{0\}} \frac{|\mathbf{r}(\widehat{\mu}_i)[\widehat{\psi}_i, \phi]|}{\|\mathcal{A}^{*1/2}\phi\|} \\ &= c_K^* \|\mathcal{A}^{1/2}\widehat{\psi}_i - \widehat{\mu}_i\mathcal{A}^{-1/2}\widehat{\psi}_i\|. \end{aligned}$$

We now estimate

$$\begin{aligned} \|\mathcal{A}^{1/2}\widehat{\psi}_i - \widehat{\mu}_i\mathcal{A}^{-1/2}\widehat{\psi}_i\|_{L^2(\Omega)}^2 &= \sum_{j=1}^{\infty} |(e_j, \mathcal{A}^{1/2}\widehat{\psi}_i - \widehat{\mu}_i\mathcal{A}^{-1/2}\widehat{\psi}_i)|^2 \\ &= \sum_{j=1}^{\infty} |(\mathcal{X}^{-1}\mathcal{X}e_j, \mathcal{A}^{1/2}\widehat{\psi}_i - \widehat{\mu}_i\mathcal{A}^{-1/2}\widehat{\psi}_i)|^2 \\ &\geq \sigma_{\min}(\mathcal{X}^{-1})^2 \sum_{j=1}^{\infty} |(\mathcal{X}e_j, \mathcal{A}^{1/2}\widehat{\psi}_i - \widehat{\mu}_i\mathcal{A}^{-1/2}\widehat{\psi}_i)|^2 \\ &= \sigma_{\min}(\mathcal{X}^{-1})^2 \sum_{j=1}^{\infty} |(f_j, \mathcal{A}^{1/2}\widehat{\psi}_i - \widehat{\mu}_i\mathcal{A}^{-1/2}\widehat{\psi}_i)|^2 \\ &= \sigma_{\min}(\mathcal{X}^{-1})^2 \widehat{\mu}_i \sum_{j=1}^{\infty} \frac{|\lambda_j - \widehat{\mu}_i|^2}{\lambda_j \widehat{\mu}_i} |(f_j, \widehat{\psi}_i)|^2 \\ &\geq \sigma_{\min}(\mathcal{X}^{-1})^2 \widehat{\mu}_i \text{gap}_{\mathcal{P}_2}(\Xi) \sum_{i=1, \lambda_i \notin \Lambda}^{\infty} |(f_i, \widehat{\psi}_i)|^2. \end{aligned}$$

The conclusion of the theorem now readily follows when we note that, for a bounded \mathcal{X} with a bounded inverse, it holds $\sigma_{\min}(\mathcal{X}^{-1}) = \|\mathcal{X}\|^{-1}$. \square

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