

# COMPUTATION OF EIGENVALUES BY NUMERICAL UPSCALING

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ABSTRACT. We discuss the possibility of computing eigenpairs of some prototypical linear second-order self-adjoint elliptic partial differential operator (or its high-resolution finite element discretization) by numerical upscaling techniques. We compute a low-dimensional generalized finite element space that preserves small eigenvalues in a superconvergent way. The approximate eigenpairs are then obtained by solving the corresponding low-dimensional algebraic eigenvalue problem. The rigorous error bounds are based on two-scale decompositions of  $H^1(\Omega)$  by means of a certain Clément-type quasi-interpolation operator.

## 1. INTRODUCTION

In this paper, we present and analyze a numerical upscaling technique for computing eigenpairs of self-adjoint linear elliptic second order differential operators with arbitrary positive bounded coefficients. The precise setting of the paper is as follows. Let  $\Omega \subset \mathbb{R}^d$  be a bounded Lipschitz domain with piecewise flat boundary and let  $A \in L^\infty(\Omega, \mathbb{R}_{\text{sym}}^{d \times d})$  be a matrix-valued coefficient with uniform spectral bounds  $0 < \alpha \leq \beta < \infty$ ,

$$(1.1) \quad \sigma(A(x)) \subset [\alpha, \beta] \quad \text{for almost all } x \in \Omega.$$

Consider the prototypical self-adjoint second order linear partial differential operator  $\mathcal{A} : H_0^1(\Omega) \rightarrow H^{-1}(\Omega)$  defined by

$$(1.2) \quad \mathcal{A}v := -\operatorname{div}(A\nabla v) \quad \text{for } v \in H_0^1(\Omega)$$

and the associated eigenproblem: find pairs consisting of an eigenvalue  $\lambda \in \mathbb{R}$  and associated non-trivial eigenfunction  $u \in V := H_0^1(\Omega)$  such

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that

$$(1.3) \quad \mathcal{A}u = \lambda u.$$

We are mainly interested in the small eigenvalues of  $\mathcal{A}$  or some accurate approximation  $\mathcal{A}_h$ . The discretized operator  $\mathcal{A}_h$  shall be related to a conforming finite element space of dimension  $N_h$  based on some, possibly very fine, mesh  $\mathcal{T}_h$  of width  $h$ .

Popular approaches for the computation of these eigenvalues include Lanczos/Arnoldi-type iterations (as implemented, e.g., in [LSY98]) or the QR-algorithm applied directly to the  $N_h$ -dimensional finite element matrices. If more structure can be exploited (e.g., a hierarchy of finite element meshes and/or spaces) some preconditioned outer iteration for the eigenvalue approximation may be performed and linear problems are solved (approximately) in every iteration step [Hac79], [KN03b], [KN03a]; see also [Ney03] and [BBS08] and references therein.

Our aim is to avoid the application of any eigenvalue solver to the large-scale matrix  $\mathcal{A}_h$  directly. Instead, inspired by [MP11], we will compute some low-dimensional approximation  $\mathcal{A}_H$  of  $\mathcal{A}$  (resp.  $\mathcal{A}_h$ ) first. This preprocessing step is done by (approximately) inverting the operator (resp. its discretization) for special right hand sides and subject to certain linear constraints. Having performed  $N_H \ll N_h$  of these computations, the solution of a low-dimensional  $N_H \times N_H$  eigenvalue problem by standard algebraic solvers yields approximations of the first  $N_H$  eigenpairs.

We emphasize that the linear problems to be solved in our method are completely independent of each other. They can be computed in parallel without any communication. Moreover, their solutions give rise to some low-dimensional discrete approximation space and the corresponding low-dimensional discrete operator  $\mathcal{A}_H$  approximates the small (leading) eigenvalues and, hence, the macroscopic response of the operator, accurately. In this sense, our method may be understood as numerical upscaling or computational homogenization.

Our method is related to some coarse finite element mesh with maximal width  $H$ . The accuracy of the approximate eigenvalues is expressed in terms of  $H$ . Without any assumptions on the smoothness of eigenfunctions, we prove that the error scales like  $H^4$ . Note that a standard first-order conforming finite element computation yields  $H^2$  under full  $H^2(\Omega)$  regularity, see e.g. [Lar00]. Under such strong assumption of high regularity, the two-grid method of [XZ01] allows certain postprocessing (solution of linear problems on the fine scale) of the coarse finite

element eigenpairs to increase the accuracy to  $H^4$ . However, the regularity assumption is essential and not justified on non-convex domains or for heterogeneous and highly variable coefficients.

Since our estimates are both, of high order (at least  $H^4$ ) and independent of the underlying regularity, the accuracy of our approximation may actually suffice to fall below the error of the fine scale discretization which scales algebraically in the fine mesh size  $h$  but depends on the regularity of the data (convexity of  $\Omega$ , differentiability and variability of  $A$ ) in a crucial way.

In cases with singular eigenfunctions (due to re-entrant corners in the domain or isolated jumps of the coefficient), it may be advantageous to use modern mesh-adaptive algorithms driven by some a posteriori error estimator as proposed and analyzed, e.g., in [Lar00], [DPR03], [CG11], [GMZ09], [GG09], [MM11], [CG12]. We are not competing with these efficient algorithms. However, adaptive mesh refinement has its limitations. For instance, if the diffusion coefficient  $A$  is highly variable, the mesh width has to be sufficiently small to resolve the oscillations [PS12]. For problems in geophysics or material sciences with characteristic geometric features on microscopic length scales, this so-called resolution condition is often so restrictive that the initial mesh must be chosen very fine and further refinement exceeds computer capacity. Our method is especially designed for such situations which require coarsening rather than refinement.

The main tools in this paper are decompositions of  $H^1(\Omega)$  into coarse and fine parts which are presented in Section 2. The method for the approximation of eigenvalues is presented and analyzed in Section 3 which further discusses practical aspects and complexity issues. Numerical experiments are presented in Section 4.

In the remaining part of this paper, we will frequently make use of the notation  $a \lesssim b$  which abbreviates  $a \leq Cb$ , with some multiplicative constant  $C > 0$  which only depends on the domain  $\Omega$  and the parameter  $\rho$  (cf. (2.1) below) that measures the quality of some underlying finite element mesh. We emphasize the  $C$  does *not* depend on the mesh size, the eigenvalues, and the coefficient  $A$ . Furthermore,  $a \approx b$  abbreviates  $a \lesssim b \lesssim a$ .

## 2. TWO-SCALE DECOMPOSITIONS

Two-scale decompositions of functions  $u \in V = H_0^1(\Omega)$  into some macroscopic/coarse part  $u_{\text{cs}} \in V_{\text{cs}}$  plus some microscopic/fine part  $u_{\text{fs}} \in V_{\text{fs}}$  with a certain orthogonality relation are at the very heart of this paper. We understand macroscopic or coarse in the sense that  $V_{\text{cs}}$

is a low-dimensional generalized finite element space based on some coarse finite element mesh. We understand microscopic or fine in the sense that  $V_{\text{fs}}$  contains highly oscillating functions which cannot be represented on the coarse mesh. The decompositions will be presented in Section 2.4 after some preliminaries presented in Sections 2.1-2.3.

**2.1. Finite Element Mesh.** We denote the underlying coarse mesh by  $\mathcal{T}_H$ . The mesh is assumed to be some regular (in the sense of [Cia87]) finite element mesh of  $\Omega$  into closed simplices with mesh-size function  $0 < H \in L^\infty(\Omega)$  defined by  $H|_T = \text{diam}(T) =: H_T$  for all  $T \in \mathcal{T}$ . The mesh size may vary in space. However, we will not exploit the possible mesh adaptivity in this paper. The error bounds, typically, depend on the maximal mesh size  $\|H\|_{L^\infty(\Omega)}$ . If no confusion seems likely, we will use  $H$  also to denote the maximal mesh size (instead of writing  $\|H\|_{L^\infty(\Omega)}$ ). The use of the capital letter  $H$  for the mesh-size instead of the standard choice  $h$  shall indicate that we consider a coarse mesh and that we are not interested in asymptotics as the mesh size tends to zero. As usual, the error analysis depends on the constant  $\rho > 0$  which represents the shape regularity of the finite element mesh  $\mathcal{T}_H$ ;

$$(2.1) \quad \rho := \max_{T \in \mathcal{T}_H} \rho_T \quad \text{with} \quad \rho_T := \frac{\text{diam } T}{\text{diam } B_T} \quad \text{for } T \in \mathcal{T}_H,$$

where  $B_T$  denotes the largest ball contained in  $T$ .

**2.2. First-Order Conforming Finite Elements.** The first-order conforming finite element space corresponding to  $\mathcal{T}_H$  is given by

$$(2.2) \quad V_H := \{v \in V \mid \forall T \in \mathcal{T}_H, v|_T \text{ is a polynomial of total degree } \leq 1\}.$$

Let  $\mathcal{N}$  denote the set of interior vertices of  $\mathcal{T}_H$ . For every vertex  $z \in \mathcal{N}$ , let  $\phi_z \in V_H$  denote the corresponding nodal basis function (tent/hat function) determined by nodal values

$$\phi_z(z) = 1 \quad \text{and} \quad \phi_z(y) = 0 \quad \text{for all } y \neq z \in \mathcal{N}.$$

These nodal basis functions form a basis of  $V_H$ . The dimension of  $V_H$  equals the number of interior vertices,

$$N_H := \dim V_H = |\mathcal{N}|.$$

**2.3. Quasi-Interpolation.** The key tool in our construction will be the bounded linear surjective Clément-type (quasi-)interpolation operator  $\mathcal{I}_H : V \rightarrow V_H$  presented and analyzed in [Car99]. Given  $v \in V$ ,

$\mathcal{I}_H v := \sum_{z \in \mathcal{N}} (\mathcal{I}_H v)(z) \phi_z$  defines a (weighted) Clément interpolant with nodal values

$$(2.3) \quad (\mathcal{I}_H v)(z) := \frac{(v, \phi_z)}{(1, \phi_z)}$$

for  $z \in \mathcal{N}$ . The nodal values are weighted averages of the function over nodal patches  $\omega_z := \text{supp } \phi_z$ .

Recall the (local) approximation and stability properties of the interpolation operator  $\mathcal{I}_H$  [Car99]: There exists a generic constant  $C_{\mathcal{I}_H}$  such that for all  $v \in V$  and for all  $T \in \mathcal{T}_H$  it holds

$$(2.4.a) \quad H_T^{-1} \|v - \mathcal{I}_H v\|_{L^2(T)} + \|\nabla(v - \mathcal{I}_H v)\|_{L^2(T)} \leq C_{\mathcal{I}_H} \|\nabla v\|_{L^2(\omega_T)},$$

where  $\omega_T := \cup\{K \in \mathcal{T}_H \mid T \cap K \neq \emptyset\}$ . The constant  $C_{\mathcal{I}_H}$  depends on the shape regularity parameter  $\rho$  of the finite element mesh  $\mathcal{T}_H$  (see (2.1) above) but not on  $H_T$ . Note that there exists a constant  $C_{\text{ol}} > 0$  that only depends on  $\rho$  such that the number of elements covered by  $\omega_T$  is uniformly bounded (w.r.t.  $T$ ) by  $C_{\text{ol}}$ . Both constant,  $C_{\mathcal{I}_H}$  and  $C_{\text{ol}}$ , may be hidden in the notation “ $\lesssim$ ” introduced at the end of the Introduction on page 3.

**2.4. Decompositions.** We define the finescale space

$$V_{\text{fs}} := \text{kernel } \mathcal{I}_H,$$

which will take over the role of the microscopic/fine part in all subsequent decompositions.

Our particular choice of a quasi-interpolation operator gives rise to the following orthogonal decomposition. We write  $\|\cdot\| := \sqrt{(\cdot, \cdot)}$  to abbreviate the  $L^2$ -norm on  $\Omega$ .

**Lemma 2.1** ( $L^2$ -orthogonal two-scale decomposition). Any function  $v \in V$  can be decomposed uniquely into the sum of  $v_H := \mathcal{I}_H|_{V_H}^{-1}(\mathcal{I}_H(v)) \in V_H$  and  $v_{\text{fs}} := v - v_H \in V_{\text{fs}}$  with

$$(2.5) \quad (v_H, v_{\text{fs}})_{L^2(\Omega)} = 0.$$

The orthogonality implies stability in the sense of

$$\|v_H\|^2 + \|v_{\text{fs}}\|^2 = \|v\|^2.$$

*Remark 2.1* ( $L^2$ -projection onto the finite element space). Lemma 2.1 shows that the  $L^2$ -orthogonal projection  $\Pi_{V_H}^{L^2} : V \rightarrow V_H$  onto the finite element space  $V_H$  may be characterized via the modified Clément interpolation (2.3),

$$\Pi_{V_H}^{L^2} = \mathcal{I}_H|_{V_H}^{-1} \mathcal{I}_H.$$

*Proof of Lemma 2.1.* It is easily verified that the restriction of  $\mathcal{I}_H$  on the finite element space  $V_H$  is invertible. This yields the decomposition. For the proof of orthogonality, let  $v_H = \sum_{z \in \mathcal{N}} v_H(z) \phi_z \in V_H$  and  $v_{\text{fs}} \in V_{\text{fs}}$ . Since  $\mathcal{I}_H(v_{\text{fs}}) = 0$ , we have that  $(\phi_z, v_{\text{fs}}) = \mathcal{I}_H(v_{\text{fs}})(z) \int_{\Omega} \phi_z = 0$  for all  $z \in \mathcal{N}$ . This yields

$$(v_H, v_{\text{fs}}) = \sum_{z \in \mathcal{N}} v_H(z) (\phi_z, v_{\text{fs}}) = 0$$

and shows that  $V_H$  and  $V_{\text{fs}}$  are orthogonal subspaces of  $V$ .  $\square$

We may rewrite Lemma 2.1 as

$$(2.6) \quad V = V_H \oplus V_{\text{fs}} \quad \text{and} \quad (V_H, V_{\text{fs}}) = 0.$$

The orthogonalization of this decomposition with respect to the scalar product  $a$  yields the definition of a modified coarse space  $V_{\text{cs}}$ , that is the  $a$ -orthogonal complement of  $V_{\text{fs}}$  in  $V$ . Given  $v \in V$ , define its the  $a$ -orthogonal fine scale projection operator  $\mathfrak{F}v \in V_{\text{fs}}$  by

$$a(\mathfrak{F}v, w) = a(v, w) \quad \text{for all } w \in V_{\text{fs}}.$$

We define the energy norm  $|||\cdot||| := \sqrt{a(\cdot, \cdot)}$  (the norm induced by the scalar product  $a$ ).

**Lemma 2.2** ( *$a$ -orthogonal two-scale decomposition*). Any function  $v \in V$  can be decomposed uniquely into  $v = v_{\text{cs}} + v_{\text{fs}}$ , where

$$v_{\text{cs}} := (1 - \mathfrak{F})v \in V_{\text{cs}} := (1 - \mathfrak{F})V_H$$

and

$$v_{\text{fs}} := \mathfrak{F}v \in V_{\text{fs}} = \text{kernel } \mathcal{I}_H.$$

The decomposition is orthogonal

$$(2.7) \quad a(v_{\text{cs}}, v_{\text{fs}})_{L^2(\Omega)} = 0,$$

and, hence, stable in the sense of

$$(2.8) \quad |||v_{\text{cs}}|||^2 + |||v_{\text{fs}}|||^2 = |||v|||^2.$$

In other words,

$$(2.9) \quad V = V_{\text{cs}} \oplus V_{\text{fs}} \quad \text{and} \quad a(V_{\text{cs}}, V_{\text{fs}}) = 0.$$

We aim to compute approximate eigenvectors in the space  $V_{\text{cs}}$ . The orthogonalization has preserved the dimension of the coarse part of the decomposition, i.e.,

$$\dim V_{\text{cs}} = \dim V_H = N_H$$

Moreover, the images of the nodal basis functions under the  $a$ -orthogonal projection  $(1 - \mathfrak{F})$  onto  $V_{\text{cs}}$  yield a basis of  $V_{\text{cs}}$ ,

$$(2.10) \quad V_{\text{cs}} = \text{span}\{(1 - \mathfrak{F})\phi_z \mid z \in \mathcal{N}\}.$$

In order to use this space for the approximation of eigenvalues and eigenvectors of (3.1), we need to approximate  $N_H$  solutions  $\psi_z = \mathfrak{F}\phi_z \in V_{\text{fs}}$  of

$$(2.11) \quad a(\psi_z, v) = a(\phi_z, v) \quad \text{for all } v \in V_{\text{fs}}.$$

These problems are linear and independent. The only difference with a standard Poisson problem is that there is some linear constraint hidden in the space  $V_{\text{fs}}$ , that is, the quasi-interpolation of trial and test functions vanishes.

The main reason why this preprocessing of the coarse space  $V_{\text{cs}}$  can be useful is the following  $L^2$ -quasi-orthogonality of the  $a$ -orthogonal decomposition (2.9).

**Theorem 2.3** ( $L^2$ -quasi-orthogonality of the  $a$ -orthogonal decomposition). *The decomposition  $V = V_{\text{cs}} \oplus V_{\text{fs}}$  from Lemma 2.2 is  $L^2$ -quasi-orthogonal in the sense that for all  $v_{\text{cs}} \in V_{\text{cs}}$  and all  $v_{\text{fs}} \in V_{\text{fs}}$ , it holds*

$$(2.12) \quad (v_{\text{cs}}, v_{\text{fs}})_{L^2(\Omega)} \lesssim H^2 \|\nabla v_{\text{cs}}\| \|\nabla v_{\text{fs}}\| \leq \alpha^{-1} H^2 \|v_{\text{cs}}\| \|v_{\text{fs}}\|.$$

*The decomposition is stable in the sense that*

$$(2.13) \quad \|v_{\text{cs}}\|^2 + \|H^{-1}v_{\text{fs}}\|^2 \lesssim \alpha^{-1} \|v_{\text{cs}} + v_{\text{fs}}\|^2$$

*Proof.* Given any  $v_{\text{cs}} \in V_{\text{cs}}$  and  $v_{\text{fs}} \in V_{\text{fs}}$ , Lemma 2.1, the Cauchy-Schwarz inequality, (2.4.a), and (2.1) yield

$$(v_{\text{cs}}, v_{\text{fs}}) = (v_{\text{cs}} - \mathcal{I}_H v_{\text{cs}}, v_{\text{fs}} - \mathcal{I}_H v_{\text{fs}}) \lesssim H^2 \|\nabla v_{\text{cs}}\| \|\nabla v_{\text{fs}}\|,$$

since  $(\mathcal{I}_H v_{\text{cs}}, v_{\text{fs}}) = 0$  which is the quasi-orthogonality. A similar estimate shows

$$\begin{aligned} (Hv_{\text{fs}}, Hv_{\text{fs}}) &= (H(v_{\text{fs}} - \mathcal{I}_H v_{\text{fs}}), H(v_{\text{fs}} - \mathcal{I}_H v_{\text{fs}})) \\ &\lesssim \sum_{T \in \mathcal{T}_H} \|\nabla v_{\text{fs}}\|_{L^2(\omega_T)}^2 \\ &\lesssim \alpha^{-1} \|v_{\text{fs}}\|^2. \end{aligned}$$

This, Friedrichs' inequality

$$\|v_{\text{cs}}\| \leq \pi^{-1} \text{diam } \Omega \|\nabla v_{\text{cs}}\|,$$

and (2.8) readily prove the stability estimate.  $\square$

### 3. APPROXIMATION OF EIGENVALUES AND EIGENVECTORS

This Section presents a new scheme for the approximation of eigenvalues and eigenvectors of (1.3) and its rigorous error analysis.

**3.1. Variational Formulation and Galerkin Approximation.** Recall that the eigenpairs of (1.3) are characterized equivalently as the solution to the variational problem

$$(3.1) \quad a(u^{(\ell)}, v) := \int_{\Omega} (A \nabla u^{(\ell)}) \cdot \nabla v = \lambda^{(\ell)}(u^{(\ell)}, v) \quad \text{for all } v \in V,$$

where  $(\cdot, \cdot)$  denotes the standard inner product in  $L^2(\Omega)$ . Recall that, for this problem, there exists a countable number of eigenvalues. Moreover, since  $\mathcal{A}$  is symmetric, all eigenvalues  $\lambda^{(\ell)}$  ( $\ell \in \mathbb{N}$ ) are real and positive,

$$0 < \lambda^{(1)} \leq \lambda^{(2)} \leq \lambda^{(3)} \leq \dots$$

Depending on the actual domain  $\Omega$  and the coefficient  $A$ , there may be multiple eigenvalues. A multiple eigenvalue is repeated several times according to its multiplicity in the enumeration above. Let  $u^{(\ell)}$  ( $\ell \in \mathbb{N}$ ) be normalized to one in  $L^2(\Omega)$ , i.e.,  $(u^{(\ell)}, u^{(\ell)}) = 1$ . It is well known that the eigenfunctions enjoy (or, in the case of multiple eigenvalues, may be chosen such that they fulfill) the orthogonalities

$$(3.2) \quad a(u^{(\ell)}, u^{(m)}) = (u^{(\ell)}, u^{(m)}) = 0 \quad \text{if } \ell \neq m.$$

The Galerkin discretization of (3.1) with respect to the generalized finite element space  $V_{\text{cs}}$  reads: find  $\lambda_H^{(\ell)} \in \mathbb{R}$  and non-trivial  $u_{\text{cs}}^{(\ell)} \in V_{\text{cs}}$  such that

$$(3.3) \quad a(u_{\text{cs}}^{(\ell)}, v) = \lambda_H^{(\ell)}(u_{\text{cs}}^{(\ell)}, v) \quad \text{for all } v \in V_{\text{cs}}.$$

Since  $V_{\text{cs}}$  is a finite-dimensional subspace of  $V$ , we can order the discrete eigenvalues similar as the original ones

$$0 < \lambda_H^{(1)} \leq \lambda_H^{(2)} \leq \lambda_H^{(3)} \leq \dots \leq \lambda_H^{(N_H)}.$$

Again, multiple eigenvalues are repeated according to their multiplicity. Let also  $u_{\text{cs}}^{(\ell)}$  ( $\ell = 1, 2, \dots, N_H$ ) be normalized to one in  $L^2(\Omega)$ , i.e.,  $(u_{\text{cs}}^{(\ell)}, u_{\text{cs}}^{(\ell)}) = 1$ . The discrete eigenfunctions satisfy (or, in the case of multiple eigenvalues, can be chosen such that they satisfy) the orthogonalities

$$(3.4) \quad a(u_{\text{cs}}^{(\ell)}, u_{\text{cs}}^{(m)}) = (u_{\text{cs}}^{(\ell)}, u_{\text{cs}}^{(m)}) = 0 \quad \text{if } \ell \neq m.$$



In the subsequent paragraphs we will present error bounds for the approximate eigenvalues and eigenvectors based on the variational techniques from [SF73] (which are based on [BdBSW66] on their part); see also [Bof10].

**3.2. Two-Scale Decomposition Revisited.** The eigenfunctions allow a different (with respect to Section 2) characterization of a macroscopic function, that is, any function spanned by eigenfunctions related to the  $\ell$  smallest eigenvalues. Define

$$(3.5) \quad E_\ell := \text{span}\{u^{(1)}, \dots, u^{(\ell)}\}.$$

We will have a closer look at the quasi-orthogonality results in Lemma 2.2 given some macroscopic function  $u \in E_\ell$ .

**Corollary 3.1** ( *$L^2$ -quasi-orthogonality of the  $a$ -orthogonal decomposition of macroscopic functions*). Let  $\ell \in \mathbb{N}$  and let  $u = u_{\text{cs}} + u_{\text{fs}} \in E_\ell$  with  $\|u\| = 1$ , where  $u_{\text{cs}} \in V_{\text{cs}}$  (resp.  $u_{\text{fs}} \in V_{\text{fs}}$ ) denotes the coarse scale part (resp. fine scale part) of  $u$  according to the  $a$ -orthogonal decomposition in Lemma 2.2. Then it holds

$$(3.6) \quad \|u_{\text{cs}}\| \leq \sqrt{\lambda^{(\ell)}},$$

$$(3.7) \quad \|u_{\text{fs}}\| \lesssim \sqrt{\ell(\lambda^{(\ell)})^3} \left(\frac{H}{\sqrt{\alpha}}\right)^2, \text{ and}$$

$$(3.8) \quad (u_{\text{cs}}, u_{\text{fs}}) \lesssim \sqrt{\ell} \left(\frac{H\sqrt{\lambda^{(\ell)}}}{\sqrt{\alpha}}\right)^4.$$

*Proof.* Let  $\delta_j \leq 1$ ,  $j = 1, 2, \dots, \ell$ , be the coefficients in the representation of  $u$  by eigenfunctions, that is,  $u = \sum_{j=1}^{\ell} \delta_j u^{(j)}$ . Then (3.6) follows from the fact that  $(1 - \mathfrak{F})$  is a projection and the obvious bound  $\|u\|^2 \leq \lambda^{(\ell)}$ .

For the proof of (3.7), we employ some algebraic manipulations and equation (3.1),

$$(3.9) \quad \|u_{\text{fs}}\|^2 = a(u, u_{\text{fs}}) = \sum_{j=1}^{\ell} \delta_j a(u^{(j)}, u_{\text{fs}}) = \sum_{j=1}^{\ell} \delta_j \lambda^{(j)} (u^{(j)}, u_{\text{fs}}).$$

Theorem 2.3 shows that

$$(3.10) \quad (u^{(j)}, u_{\text{fs}}) \lesssim \left(\frac{H}{\sqrt{\alpha}}\right)^2 \|u^{(j)}\| \|u_{\text{fs}}\|.$$

The combination of (3.9)-(3.10) together with  $\|u^{(j)}\|^2 = \lambda^{(j)} \leq \lambda^{(\ell)}$  and  $\delta_j \leq 1$  yields the upper bound of  $\|u_{\text{fs}}\|$ .

The combination of Theorem 2.3 and the bounds (3.6)–(3.7) readily yields (3.8).  $\square$

*Remark 3.1.* In certain cases, e.g., if  $\Omega$  is convex and the coefficient  $A$  is constant, we have that any macroscopic function  $u \in E_\ell$  is in  $H^2(\Omega)$  and  $\|\nabla^2 u\| \lesssim \lambda^{(\ell)}/\alpha \|u\|$ . Such an instance of regularity gives rise to an additional power of  $H/\lambda^{(\ell)}$  in the estimates (3.7) and (3.8) in Corollary 3.1. This is due to the possible modification of (3.10),

$$(u^{(j)}, u_{\text{fs}}) = (u^{(j)} - \mathcal{I}_H u^{(j)}, u_{\text{fs}} - \mathcal{I}_H u_{\text{fs}}) \lesssim \frac{H^3 \lambda^{(j)}}{\alpha^2} \|u_{\text{fs}}\|.$$

**3.3. Estimates for Approximate Eigenvalues.** We first introduce the Rayleigh quotient, which is defined for non-trivial  $v \in V$  by

$$R(v) := \frac{a(v, v)}{(v, v)}.$$

Recall that the  $\ell$ th eigenvalue may be characterized via the minmax-principle (which goes back to Poincaré [Poi90])

$$(3.11) \quad \lambda^{(\ell)} = \min_{S \in \mathcal{S}_\ell(V)} \max_{v \in S \setminus \{0\}} R(v),$$

where  $\mathcal{S}_\ell(V)$  denotes the set of  $\ell$ -dimensional subspaces of  $V$ . This principle applies equally well to the discrete problem (3.3), i.e.,

$$(3.12) \quad \lambda_H^{(\ell)} = \min_{S \in \mathcal{S}_\ell(V_{\text{cs}})} \max_{v \in S \setminus \{0\}} R(v)$$

characterizes the  $\ell$ th discrete eigenvalue ( $\ell \leq N_H$ ). The conformity  $V_{\text{cs}} \subset V$  yields monotonicity

$$(3.13) \quad \lambda^{(\ell)} \leq \lambda_H^{(\ell)} \quad \text{for all } \ell = 1, 2, \dots, N_H.$$

The following theorem gives an estimate in the opposite direction.

**Theorem 3.2** (Bound for the eigenvalue error). *Let  $H$  be sufficiently small so that  $H \lesssim \ell^{-1/4} \sqrt{\frac{\alpha}{\lambda^{(\ell)}}}$ . Then it holds*

$$(3.14) \quad \frac{\lambda_H^{(\ell)} - \lambda^{(\ell)}}{\lambda^{(\ell)}} \lesssim \sqrt{\ell} \left( H \sqrt{\frac{\lambda^{(\ell)}}{\alpha}} \right)^4 \quad \text{for all } \ell = 1, 2, \dots, N_H.$$

*Proof.* Recall the definition of  $E_\ell$  in (3.5) and define

$$\sigma_H^{(\ell)} := \max_{u \in E_\ell: (u, u) = 1} |(u_{\text{fs}}, u_{\text{fs}}) + 2(u_{\text{cs}}, u_{\text{fs}})|,$$

where  $u_{\text{cs}} \in V_{\text{cs}}$  (resp.  $u_{\text{fs}} \in V_{\text{fs}}$ ) denotes the coarse scale part (resp. fine scale part) of  $u \in E_\ell$  according to the  $a$ -orthogonal decomposition

in Lemma 2.2. Theorem 2.3 and Corollary 3.1 yield

$$\sigma_H^{(\ell)} \lesssim \sqrt{\ell} \left( \frac{H}{\sqrt{\alpha}} \right)^2 \left( \frac{H\lambda^{(\ell)}}{\sqrt{\alpha}} \right)^2,$$

where we have used that, under the condition  $H \lesssim \ell^{-1/4} \sqrt{\frac{\alpha}{\lambda^{(\ell)}}}$ , the term  $|(u_{\text{fs}}, u_{\text{fs}})|$  is of higher order when compared with  $|(u_{\text{cs}}, u_{\text{fs}})|$ ,

$$|(u_{\text{fs}}, u_{\text{fs}})| \lesssim \ell(\lambda^{(\ell)})^3 (H/\sqrt{\alpha})^6.$$

If  $H$  is chosen small enough so that  $\sigma_H^{(\ell)} \leq \frac{1}{2}$ , then Lemma 6.1 in [SF73] shows that

$$\lambda_H^{(\ell)} \leq (1 - \sigma_H^{(\ell)})^{-1} \lambda^{(\ell)} \leq (1 + 2\sigma_H^{(\ell)}) \lambda^{(\ell)}.$$

Inserting our estimate for  $\sigma_H^{(\ell)}$  gives the assertion.  $\square$

*Remark 3.2* (Smallness of  $H$ ). Since all our estimates are explicit with respect to the eigenvalues, the condition  $H \lesssim \ell^{-1/4} \sqrt{\frac{\alpha}{\lambda^{(\ell)}}}$  in Theorem 3.2 is a qualitative condition for the smallness of  $H$ . Note that, typically, a condition  $H \lesssim 1/\lambda^{(\ell)}$  (or even more restrictive) arises [BBS08, Sau10]. The relaxed condition is possible because no regularity of the eigenfunctions has been used to establish the error bound.

*Remark 3.3* (Improved eigenvalue error bound). With regard to Remark 3.1, the error bound in Theorem 3.2 may be improved provided that the first  $\ell$  eigenfunctions are regular in the sense of  $\|\nabla^2 u^{(j)}\| \lesssim \lambda^{(j)}/\alpha$ . The improved bound reads

$$(3.15) \quad \frac{\lambda_H^{(\ell)} - \lambda^{(\ell)}}{\lambda^{(\ell)}} \lesssim \sqrt{\ell\lambda^{(\ell)}/\alpha} \left( \frac{H\sqrt{\lambda^{(\ell)}}}{\sqrt{\alpha}} \right)^5 \quad \text{for all } \ell = 1, 2, \dots, N_H.$$

This improved bound might still be pessimistic in the sense that the error in the  $\ell$ th eigenvalue/vector depends on the regularity of all previous previous eigenfunctions. The recent theory [KO06] shows that this is not necessarily true. Moreover, there might be smoothness also in the single summands of the two-scale decomposition which is not exploited.

**3.4. Estimates for Approximate Eigenvectors.** We turn to the error in the approximate eigenfunctions. Again, we follow the receipt provided in [SF73].

**Theorem 3.3** (Estimates of Eigenvector error). *Let  $\lambda^{(\ell)}$  be an eigenvalue of multiplicity  $r$ , i.e.  $\lambda^{(\ell)} = \dots = \lambda^{(\ell+r-1)}$ , with corresponding eigenspace spanned by the orthonormal basis  $\{u^{(\ell+i)}\}_{i=0}^{r-1}$ . Let the pair  $\{\lambda_H^{(\ell)}, u_{\text{cs}}^{(\ell)}\}$  be a Galerkin approximation solving equation (3.3) such that*

$\|u_{\text{cs}}^{(\ell)}\|_{L^2(\Omega)} = 1$ . Then there exists an eigenfunction in  $\text{span}(\{u^{(\ell+i)}\}_{i=0}^{r-1})$ , let us denote it  $u^{(\ell)}$ , such that

$$(3.16) \quad \left\| \|u^{(\ell)} - u_{\text{cs}}^{(\ell)}\| \right\|^2 \lesssim (\lambda^{(\ell)})^3 \ell^{1/2} \frac{H^4}{\alpha^2} + 4(1 + \rho)^2 (\lambda^{(\ell)})^4 \ell \frac{H^6}{\alpha^3},$$

where  $\rho = \max_{j \notin \{\ell, \ell+1, \dots, \ell+r-1\}} \frac{\lambda^{(\ell)}}{|\lambda^{(\ell)} - \lambda^{(j)}|}$ .

*Proof.* For any  $v \in \text{span}(\{u^{(\ell+i)}\}_{i=0}^{r-1})$  fulfilling  $\|v\|_{L^2(\Omega)} = 1$  it holds,

$$(3.17) \quad \begin{aligned} \left\| \|v - u_{\text{cs}}^{(\ell)}\| \right\|^2 &= \lambda^{(\ell)} - 2\lambda^{(\ell)}(v, u_{\text{cs}}^{(\ell)}) + \lambda_H^{(\ell)} \\ &= \lambda^{(\ell)}(2 - 2(v, u_{\text{cs}}^{(\ell)})) + \lambda_H^{(\ell)} - \lambda^{(\ell)} \\ &= \lambda^{(\ell)}\|v - u_{\text{cs}}^{(\ell)}\|_{L^2(\Omega)}^2 + \lambda_H^{(\ell)} - \lambda^{(\ell)}. \end{aligned}$$

It remains to bound the  $L^2$  norm. By applying the analysis presented in Lemma 6.4 and Theorem 6.2 in [SF73] we have that there is a normal eigenfunction  $u^{(\ell)} \in \text{span}(\{u^{(\ell+i)}\}_{i=0}^{r-1})$  such that,

$$\|u^{(\ell)} - u_{\text{cs}}^{(\ell)}\|_{L^2(\Omega)}^2 \leq 4(1 + \rho)^2 \|u_{\text{fs}}\|_{L^2(\Omega)}^2 \lesssim 4(1 + \rho)^2 H^2 \alpha^{-1} \left\| \|u_{\text{fs}}\| \right\|^2,$$

where  $u_{\text{fs}}$  denotes the fine scale part of  $u^{(\ell)}$  according to the  $a$ -orthogonal decomposition in Lemma 2.2. The theorem follows by combining equation (3.17) with  $v = u^{(\ell)}$ , Corollary 3.1, and Theorem 3.2.  $\square$

**3.5. Approximation of the Ideal Coarse Space.** The previous results have theoretical impact, but the method is not yet feasible because the definition of the coarse space  $V_{\text{cs}}$  involves the inversion of some infinite dimensional operator. That is why we consider the case where the original eigenvalue problem has been discretized first by some suitable finite element space related to some fine triangulation  $\mathcal{T}_h$ ; cf. Section 3.5.1. Moreover, we discuss complexity issues in Sections 3.5.2–3.5.3.

#### 3.5.1. Eigenvalues of High-Resolution Finite Element Discretization.

Note that the previous estimates apply verbatim to the case, where  $V$  is replaced with some fine scale finite element discretization space  $V_h \supset V_H$ . One might think of  $V_h$  being the space of conforming piecewise affines (or higher-order polynomials) with respect to some fine triangulation  $\mathcal{T}_h$  of mesh-size  $h \leq H$ .

In this regard, our approach is a method for approximating the smallest eigenvalues of the corresponding finite element discretization by first solving a few large scale linear equations and then a small scale eigenvalue problem on top of that. The accuracy of this approach is only linked with the coarse mesh-size  $H$ . Since our estimates are of high

order (at least proportional to  $H^4$ ) and independent of the underlying regularity, the accuracy may actually suffice to fall below the error of the fine scale discretization which scales algebraically in  $h$  but depends on the regularity of the data (convexity of  $\Omega$ , differentiability and variability of  $A$ ) in a crucial way.

*3.5.2. Localization of Microscopic Computations and Macroscopic Compression.* The construction of the coarse space  $V_{\text{cs}}$  is based on fine scale equations formulated on the whole domain  $\Omega$  which makes them expensive to compute. However, in [MP11] it was shown that  $\mathfrak{F}\phi_z$  decays exponentially fast outside of the support of the coarse basis function  $\phi_z$ . We specify this feature as follows. Let  $k \in \mathbb{N}$ . We define nodal patches  $\omega_{z,k}$  of  $k$  coarse grid layers centered around the node  $z \in \mathcal{N}$  by

$$(3.18) \quad \begin{aligned} \omega_{z,1} &:= \text{supp } \phi_z = \cup \{T \in \mathcal{T}_H \mid z \in T\}, \\ \omega_{z,k} &:= \cup \{T \in \mathcal{T}_H \mid T \cap \omega_{z,k-1} \neq \emptyset\} \quad \text{for } k \geq 2. \end{aligned}$$

The result in the decay of  $\mathfrak{F}\phi_z$  in [MP11] can be expressed as follows. For all vertices  $z \in \mathcal{N}$  and for all  $k \in \mathbb{N}$ , it holds

$$(3.19) \quad \|A^{1/2} \nabla \mathfrak{F}\phi_z\|_{L^2(\Omega \setminus \omega_{z,k})} \lesssim e^{-(\alpha/\beta)^{1/2}k} \|\mathfrak{F}\phi_z\|.$$

For moderate contrast  $\beta/\alpha$ , this motivates the truncation of the computations of the basis functions to local patches  $\omega_{z,k}$ . We approximate  $\psi_z = \mathfrak{F}\phi_z \in V_{\text{fs}}$  from (2.11) with  $\psi_{z,k} \in V_{\text{fs}}(\omega_{z,k}) := \{v \in V_{\text{fs}} \mid v|_{\Omega \setminus \omega_{z,k}} = 0\}$  such that

$$(3.20) \quad a(\psi_z, v) = a(\phi_z, v) \quad \text{for all } v \in V_{\text{fs}}(\omega_{z,k}).$$

This yields a modified coarse space  $V_{\text{cs}}^k$  with a local basis

$$(3.21) \quad V_{\text{cs}}^k = \text{span}\{\phi_z - \psi_{z,k} \mid z \in \mathcal{N}\}.$$

The number of non-zero entries of the corresponding stiffness matrix is proportional to  $k^d N_H$  (note that we expect  $N_H^2$  non-zero entries without the truncation). Due to the exponential decay, the very weak condition  $k \approx \log H$  implies that the perturbation of the ideal method due to this truncation is of higher order and the estimates in Theorem 3.2 and 3.3 remain valid. We refer to [MP11] for details and proofs.

*3.5.3. Complexity.* Finally, we shall comment on the overall complexity of our approach. Consider quasi-uniform meshes of size  $H$  resp.  $h$  and corresponding conforming first-order finite element space  $V_H$  and  $V_h$ . We want to approximate the eigenvalues related to  $V_h$ . Therefore, we need to solve  $N_H$  linear problems with approximately  $k^d N_h / N_H$  degrees of freedom each; the parameter  $k$  being the truncation parameter as above. Since almost linear complexity is possible (using,

e.g., multilevel preconditioning techniques), the cost for solving one of these problems up to a given accuracy is proportional to the number of degrees of freedom  $N_h/N_H$  up to possible logarithmic factors. This yields an overall complexity of  $k^d N_h \log(N_h)$  (resp.  $N_H N_h \log(N_h)$  if  $k^d \geq N_H$ ) for setting up the coarse problem. Note that this effort can be reduced drastically either by considering the independence of the linear problems in terms of parallelism or by exploiting a possible periodicity in the problem and the mesh. In the latter case, only very few of the problems have to be computed because all the other ones are equivalent up to change of coordinates.

On top of the assembling, an  $N_H$ -dimensional eigenvalue problem is to be solved. The complexity of this depends only on  $N_H$ , the number of eigenvalues of interest, and the truncation parameter  $k$  but *not* on the critically large parameter  $N_h$ .

#### 4. NUMERICAL EXPERIMENTS

Two numerical experiments shall illustrate our results. We focus on the case without localization. The localization (as discussed in Section 3.5.2) has been studied extensively for the linear problem [MP11]. In the present context of eigenvalue approximation, we are interested to observe the enormous convergence rate which is 4 or higher for the eigenvalues. In order to achieve this rate also with truncation, patches have to be large (at least 4 layers of elements) which pays off only asymptotically when  $H$  is small enough.

**4.1. Constant coefficient on L-shaped domain.** Let  $\Omega := (-1, 1)^2 \setminus [0, 1]^2$  be the L-shaped domain. Consider the constant scalar coefficient  $A_1 = 1$ . Consider uniform coarse meshes with maximal mesh widths  $\sqrt{2}H = 2^{-1}, \dots, 2^{-4}$  of  $\Omega$  as depicted in Figure 1.

The reference mesh  $\mathcal{T}_h$  has maximal mesh width  $h = 2^{-7}/\sqrt{2}$ . We consider some  $P1$  conforming finite element approximation of the eigenvalues on the reference mesh  $\mathcal{T}_h$  and compare these discrete eigenvalues  $\lambda_h^{(\ell)}$  with coarse scale approximations depending on the coarse mesh size  $H$ .

Table 1 shows results for the case without truncation, i.e., all linear problems have been solved on the whole of  $\Omega$ . For fixed  $\ell$ , the rate of convergence of the eigenvalue error  $\lambda_H^{(\ell)} - \lambda_h^{(\ell)}$  in terms of  $H$  observed in Table 1 is between 6 and 7 which is even better than predicted in Theorem 3.2 and in Remark 3.1.

**4.2. Rough coefficient with multiscale features.** Let  $\Omega := (0, 1)^2$  be the unit square. The scalar coefficient  $A_2$  (see Figure 2) is piecewise

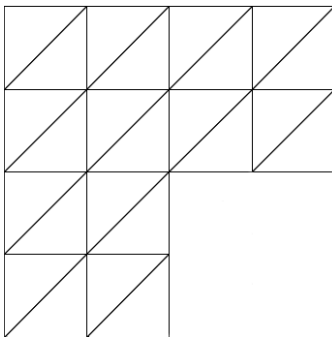


FIGURE 1. Initial uniform triangulation of the  $L$ -shape domain (5 degrees of freedom).

constant with respect to the same uniform Cartesian grid of width  $2^{-6}$ . Its values are taken from the data of the SPE10 benchmark, see <http://www.spe.org/web/csp/>. The coefficient is highly varying and strongly heterogeneous. The contrast for  $A_2$  is large,  $\beta(A_2)/\alpha(A_1) \approx 4 \cdot 10^6$ . Consider uniform coarse meshes of size  $\sqrt{2}H = 2^{-1}, 2^{-2}, \dots, 2^{-4}$  of  $\Omega$  as depicted in Figure 2. Note that none of these meshes resolves the rough coefficient  $A_2$  appropriately. Hence, (local) regularity cannot be exploited on coarse meshes.

Again, the reference mesh  $\mathcal{T}_h$  has width  $h = 2^{-7}/\sqrt{2}$  and we compare the discrete eigenvalues  $\lambda_h^{(\ell)}$  (with respect to some  $P1$  conforming finite element approximation of the eigenvalues on the reference mesh  $\mathcal{T}_h$ ) with coarse scale approximations depending on the coarse mesh size  $H$ . Table 2 shows the errors and allows us to estimate the average rate around 4 which matches our expectation from the theory. We emphasize that the large contrast does not affect the accuracy of our method in approximating the eigenvalues  $\lambda_h^{(\ell)}$ . However, the accuracy of  $\lambda_h^{(\ell)}$  is affected by the high contrast and the lack of regularity caused by the coefficient.

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$\ell$	$\lambda_h^{(\ell)}$	$e^{(\ell)}(1/2\sqrt{2})$	$e^{(\ell)}(1/4\sqrt{2})$	$e^{(\ell)}(1/8\sqrt{2})$	$e^{(\ell)}(1/16\sqrt{2})$
1	9.6436869	0.003494567	0.000034466	0.000000546	0.000000010
2	15.1989274	0.009621397	0.000079887	0.000000845	0.000000010
3	19.7421815	0.023813222	0.000213097	0.000002073	0.000000023
4	29.5281571	0.096910157	0.000724615	0.000006574	0.000000076
5	31.9265496	0.094454625	0.000874659	0.000009627	0.000000138
6	41.4922250	-	0.002395227	0.000019934	0.000000254
7	44.9604884	-	0.002443271	0.000019683	0.000000223
8	49.3631826	-	0.003651870	0.000028869	0.000000308
9	49.3655623	-	0.004266472	0.000032835	0.000000355
10	56.7389993	-	0.006863742	0.000055219	0.000000618
11	65.4085991	-	0.011534878	0.000082414	0.000000856
12	71.0947630	-	0.012596114	0.000090083	0.000001002
13	71.6064671	-	0.014249938	0.000098736	0.000001006
14	79.0043994	-	0.021801461	0.000164436	0.000001605
15	89.3706421	-	0.033550079	0.000211985	0.000002296
16	92.3648207	-	0.040060692	0.000239441	0.000002295
17	97.4459210	-	0.037438984	0.000284936	0.000002724
18	98.7545147	-	0.044544409	0.000269854	0.000002559
19	98.7545639	-	0.047835987	0.000276139	0.000002539
20	101.6755971	-	0.038203654	0.000297356	0.000002909

TABLE 1. Errors  $e^{(\ell)}(H) =: \frac{\lambda_H^{(\ell)} - \lambda_h^{(\ell)}}{\lambda_h^{(\ell)}}$  for  $\ell = 1, \dots, 20$ , constant coefficient  $A_1$ , and various choices of the coarse mesh size  $H$ .

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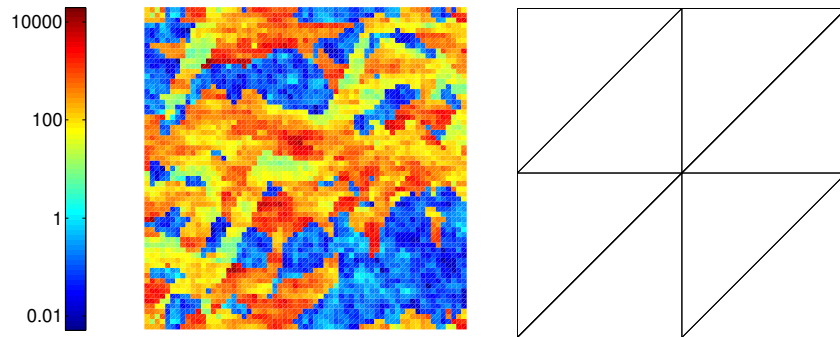


FIGURE 2. Scalar coefficient  $A_2$  used in the second numerical experiment and initial uniform triangulation of the unit square (1 degree of freedom).

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

TABLE 2. Errors  $e^{(\ell)}(H) =: \frac{\lambda_H^{(\ell)} - \lambda_h^{(\ell)}}{\lambda_h^{(\ell)}}$  for  $\ell = 1, \dots, 20$ , rough coefficient  $A_2$ , and various choices of the coarse mesh size  $H$ .

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