A LOCAL COMPUTATIONAL SCHEME FOR HIGHER ORDER FINITE ELEMENT EIGENVALUE APPROXIMATIONS*

XIAOYING DAI†, LIHUA SHEN ‡, AND AIHUI ZHOU§

Abstract. Based on some coupled discretizations, a local computational scheme is proposed and analyzed in this paper for a class of higher order finite element eigenvalue approximations. Its efficiency is proven by theoretical and numerical evidences. It is shown that the solution of an eigenvalue problem in a higher order finite element space may be reduced to the solution of an eigenvalue problem in a lower order finite element space, and the solutions of some linear algebraic systems in the higher order finite element space by some local and parallel procedure.

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1. Introduction. Motivated by efficient eigenvalue computations in quantum chemistry, in this paper, a local computation scheme is proposed and analyzed for a class of higher order finite element eigenvalue approximations. With this new proposed scheme, solving an elliptic eigenvalue problem will not be much more difficult than the local solutions of some standard elliptic boundary value problem. Our scheme is an iterative approach, which is related to that in [18, 19]. The scheme in this paper, however, is based on global and local coupled discretizations.

It is well known that efficient electronic structure computations are usually desired in quantum chemistry and nano-materials computations. In modern electronic structure computations, the so-called density functional theory is fundamental, with which Kohn-Sham equations need to be solved [7, 15, 16, 17, 21]. Note that Kohn-Sham equations are nonlinear eigenvalue systems in three dimensions, the matrices resulting from both real space and reciprocal space techniques are large, and the number of eigenvalues and eigenvectors required is proportional to the number of atoms in the molecular system. Hence, an iteration procedure of solving a large number of eigenvalues of large scale linear systems must be involved. Moreover, in order to obtain the numerical solution with satisfactory accuracy, the number of iterations are usually very large, too. In a word, efficient electronic structure computations require large scale eigenvalue computing [7, 11, 16, 17, 22, 26, 29, 30]. Therefore, it is significant to improve the approximation accuracy or reduce the computational cost in solving such linear eigenvalue problems (in three dimensions) at each iteration step.

As the finite element method is one of most effective numerical methods, we shall consider to use the finite element scheme to discretize eigenvalue problems. Although the finite element method is capable of providing accurate solutions to both all-electron [27] and pseudopotential [6, 23] formulations of Kohn-Sham equations, its application to all-electron problems in molecules and solids has so far been limited by the large number of basis functions required to adequately describe all-electron solutions near nuclei, where the solutions can have cusps and oscillate rapidly [7, 22, 31, 34].

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† LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, P.O. Box 2719, Beijing 100080, China and, Graduate University of Chinese Academy of Sciences, Beijing 100080, China,

‡Department of Mathematics, Capital Normal University, Beijing 100037, China,

§ LSEC, Institute of Computational Mathematics and Scientific/Engineering Computing, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, P.O. Box 2719, Beijing 100080, China.

To make the finite element method to be competitive with conventional methods in the all-electron context, specialize basis functions, such as isolated atomic solutions or Gaussian functions, will likely need to be added to the standard finite element basis to increase the efficiency of the representation. In the context of pseudopotential setting, however, the original Kohn-Sham equations become smooth and their solutions are much smoother and simpler [6, 7, 22, 23, 27]. Thus the finite element method with piecewise polynomial bases is immediately applicable. Since higher order finite elements are usually recommended when the data is smooth, it is very natural to apply a higher order finite element method to the pseudopotential formulation of Kohn-Sham equations. Indeed, the higher order finite element approach has been proved to be accurate and efficient in modern electronic structure computations (see, e.g., [1, 7, 14, 30, 31, 32, 34]).

The computational complexity of higher order finite element discretizations, however, is larger than that of lower order finite element discretizations. To reduce the complexity, in this paper, we will propose some new technique for fast higher order finite element eigenvalue approximations. This technique is based on our understanding of local behaviors of finite elements solutions to some elliptic problems. By using this technique, the computational complexity can be resolved through some coupled discretizations that can be carried out in local. The main idea of our new algorithm is to use a lower order finite element to approximate the low frequency of the solution and then to use some linear algebraic systems to correct the residual (which contains mostly high frequencies) in the higher order finite element space by some local and parallel procedure.

The central computation in solving Kohn-Sham equations is the repeated solution of the following model eigenvalue problem, which is also called as a Schrödinger equation, posed on a convex polygonal domain $\Omega \subset \mathbb{R}^3$:

$$\left\{ \begin{array}{rcl} -\Delta u + Vu &=& \lambda u \ \text{ in } \Omega, \\ u &=& 0 \ \text{ on } \partial\Omega, \end{array} \right. \tag{1.1}$$

where V is some potential function and is smooth in the pseudopotential setting.

Let us now use such a simple example to give a little more detailed but informal description of the main idea and the main result in this paper. Let $S_0^{h,1}(\Omega)$ and $S_0^{h,2}(\Omega)$, satisfying $S_0^{h,1}(\Omega) \subset S_0^{h,2}(\Omega) \subset H_0^1(\Omega)$, be the linear finite element space and the quadratic finite element space associated with a finite element grid $T^h(\Omega)$, respectively. We may employ the following algorithm to discretize (1.1) to obtain eigenvector approximations (on $\Omega_0 \subset \Omega$ locally) (see Section 3.1):

1. Solve an eigenvalue problem in the linear finite element space: Find $\lambda_{h,1} \in \mathbb{R}^1, u_{h,1} \in S_0^{h,1}(\Omega)$ such that $\|u_{h,1}\|_{0,\Omega} = 1$ and
$$\int_\Omega (\nabla u_{h,1} \cdot \nabla v + V u_{h,1} v) = \lambda_{h,1} \int_\Omega u_{h,1} v \quad \forall v \in S_0^{h,1}(\Omega).$$
2. Solve a linear boundary value problem in the quadratic finite element space: Find $e_{h,2} \in S_0^{h,2}(\Omega_0)$ such that
$$\begin{aligned} &\int_{\Omega_0} (\nabla e_{h,2} \cdot \nabla v + V e_{h,2} v) \\ &= \lambda_{h,1} \int_{\Omega_0} u_{h,1} v - \int_{\Omega_0} (\nabla u_{h,1} \cdot \nabla v + V u_{h,1} v) \quad \forall v \in S_0^{h,2}(\Omega_0). \end{aligned}$$

3. Set $u^{h,2} = u_{h,1} + e_{h,2}$ in Ω_0.

If, for example, $\lambda_{h,1}$ is the first eigenvalue of the problem at the first step, then under some reasonable assumption we can establish the following result (see Section 3.1)

$$\|\nabla(u - u^{h,2})\|_{0,D} = O(h^2), \tag{1.2}$$

where u is an eigenvector associated with the first eigenvalue λ of (1.1) that satisfies $\|u\|_{0,\Omega} = 1$ and $D \subset\subset \Omega_0$ that means $D \subset \Omega_0$ and dist $(\partial D \setminus \partial\Omega, \partial\Omega_0 \setminus \partial\Omega) > 0$.

This is a very satisfying result. As a consequence, for example, we can then design the following local computational scheme: first, solve the eigenvalue problem in the linear finite element space over a finite element mesh $T^h(\Omega)$, then solve some linear boundary value problems on a collection of overlapped subdomains in the quadratic finite element spaces associated with the same mesh $T^h(\Omega)$ in parallel, and finally compute some Rayleigh quotient to obtain a new eigenvalue approximation $\lambda^{h,2}$ which satisfies (see Section 3.2)

$$|\lambda^{h,2} - \lambda| = O(h^4).$$

It is easy to see that, with this new scheme, the computing scale is significantly reduced. More precisely, we can largely resolve the computational complexity and keep the same approximation accuracy as that of solving the eigenvalue problem in the global quadratic finite element space. The theoretical tool for motivating this idea is the local error estimates for finite element approximations developed in [35, 38] (see also Section 2).

The rest of the paper is organized as follows. In the next section, we shall review the local behaviors of finite element solutions discovered and studied in [35, 38], which have been introduced to design local and parallel finite element algorithms based on two-grid discretizations [35, 36, 37, 38]. Based on the local behaviors of finite element solutions and some coupled discretizations, a new local computational scheme for higher order finite element eigenvalue approximations is devised and analyzed in Section 3. In Section 4, some numerical results are reported. It is shown by the numerical results that our scheme is very efficient. Finally, some concluding remarks are given.

2. Preliminaries. In this section, we shall describe some basic notation, then provide several properties of the finite element approximation to a linear second order elliptic boundary value problem and some classic error estimates of a standard finite element discretization for elliptic eigenvalue problems.

Let Ω be a bounded domain in $\mathbb{R}^d (d \geq 1)$. We shall use the standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms, see, e.g., [2, 10]. For $p = 2$, we denote $H^s(\Omega) = W^{s,2}(\Omega)$ and $H_0^1(\Omega) = \{v \in H^1(\Omega) : v\,|_{\partial\Omega} = 0\}$, where $v\,|_{\partial\Omega} = 0$ is in the sense of trace, $\|\cdot\|_{s,\Omega} = \|\cdot\|_{s,2,\Omega}$ and $\|\cdot\|_{\Omega} = \|\cdot\|_{0,2,\Omega}$. (In some places of this paper, $\|\cdot\|_{s,2,\Omega}$ should be viewed as piecewise defined if it is necessary.) The space $H^{-1}(\Omega)$, the dual of $H_0^1(\Omega)$, will also be used.

For $D \subset G \subset \Omega$, we use the notation $D \subset\subset G$ to mean that dist$(\partial D \setminus \partial\Omega, \partial G \setminus \partial\Omega) > 0$ (see Fig.2.1 for $2 - d$ cases). For simplicity, we assume that Ω and its any subdomain involved in this paper are polytopic. Note that any $w \in H_0^1(\Omega_0)$ can be naturally extended to be a function in $H_0^1(\Omega)$ with zero outside of Ω_0 when $\Omega_0 \subset \Omega$, thus we shall state this fact by the slightly abused notation $H_0^1(\Omega_0) \subset H_0^1(\Omega)$.

Throughout this paper, we shall use the letter C (with or without subscripts) to denote a generic positive constant which may stand for different values at its different

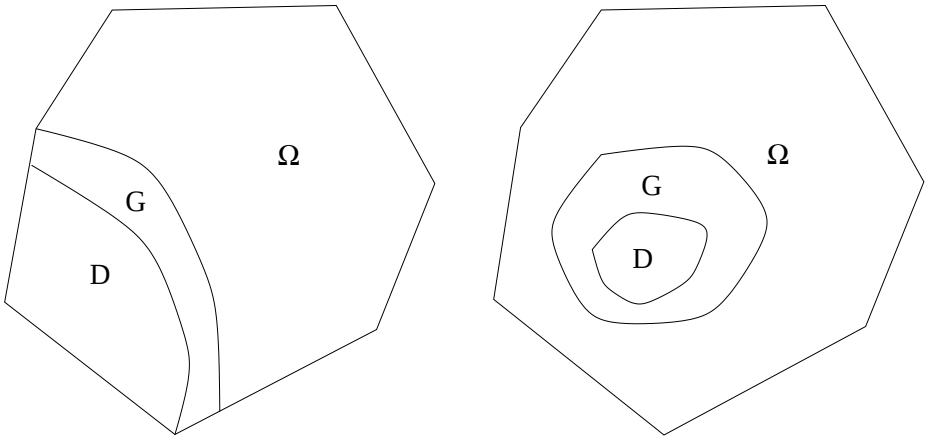

FIG. 2.1. *Subdomains*

occurrences. For convenience, the symbol $\lesssim$ will be used in this paper. That $x_1 \lesssim y_1$ means that $x_1 \leq C_1 y_1$ for some constant C_1 that is independent of mesh parameters.

Assume that $T^h(\Omega) = \{\tau\}$ is a mesh of Ω with mesh-size function $h(x)$ whose value is the diameter h_τ of the element τ containing x. One basic assumption on the mesh is that

A.0. There exists $\nu \geq 1$ such that

$$h_{_\Omega}^{\nu} \lesssim h(x), \quad x \in \Omega, \tag{2.1}$$

where $h_{_\Omega} = \max_{x\in\Omega} h(x)$ is the (largest) mesh size of $T^h(\Omega)$.

This is apparently a very mild assumption and most practical meshes should satisfy this assumption. Sometimes, we will drop the subscript in $h_{_\Omega}$ to h for the mesh size on a domain that is clear from the context.

Let $T^h(\Omega)$ consist of shape-regular simplices and define $S^{h,r}(\Omega)$ to be a space of continuous functions on Ω such that for $v \in S^{h,r}(\Omega), v$ restricted to each τ is a polynomial of total degree $\leq r$, namely

$$S^{h,r}(\Omega) = \{v \in C(\bar{\Omega}) : v\,|_\tau \in P_\tau^r \ \ \forall \tau \in T^h(\Omega)\}, \tag{2.2}$$

where P_τ^r is the space of polynomial of degree not greater than a positive integer r. Set $S_0^{h,r}(\Omega) = S^{h,r}(\Omega) \cap H_0^1(\Omega)$. These are Lagrange finite element spaces and we refer to [35] (see also [24, 25, 33]) for their basic properties that will be used in our analysis.

Given $G \subset \Omega$, we define $S^{h,r}(G)$ and $T^h(G)$ to be the restriction of $S^{h,r}(\Omega)$ and $T^h(\Omega)$ to G, respectively, and

$$S_{h,r}^0(G) = \{v \in S^{h,r}(\Omega) : \text{supp } v \subset\subset G\}.$$

For any $G \subset \Omega$ mentioned in this paper, we assume that it aligns with $T^h(\Omega)$ when it is necessary.

2.1. A linear elliptic boundary value problem. In this subsection, we shall present some basic properties of a second order elliptic boundary value problem and

its finite element approximations, which will be used in this paper. We consider the homogeneous boundary value problem

$$\left\{ \begin{array}{rl} Lu & = f \text{ in } \Omega, \\ u & = 0 \text{ on } \partial\Omega. \end{array} \right. \tag{2.3}$$

Here L is a linear second order elliptic operator:

$$Lu = -\sum_{i,j=1}^{d} \frac{\partial}{\partial x_j}(a_{ij}\frac{\partial u}{\partial x_i}) + cu$$

that satisfies $a_{ij} \in L^\infty(\Omega)$, $c \in L^\infty(\Omega)$, and (a_{ij}) is uniformly positive definite on Ω.

The weak form of (2.3) is as follows: Find $u \equiv L^{-1}f \in H_0^1(\Omega)$ such that

$$a(u,v) = (f,v) \qquad \forall v \in H_0^1(\Omega), \tag{2.4}$$

where $(\cdot,\cdot)$ is the standard inner-product of $L^2(\Omega)$ and

$$a(u,v) = \int_\Omega \sum_{i,j=1}^{d} a_{ij}\frac{\partial u}{\partial x_i}\frac{\partial v}{\partial x_j} + cuv.$$

For simplicity, we assume that

$$\|w\|_{1,\Omega}^2 \lesssim a(w,w) \quad \forall w \in H_0^1(\Omega).$$

Indeed, the results that will be obtained in this paper can be generalized to a more general case that

$$\|w\|_{1,\Omega}^2 - C^{-1}\|w\|_{0,\Omega}^2 \lesssim a(w,w) \quad \forall w \in H_0^1(\Omega)$$

hold for some constant C. We have (c.f. [13]) the following estimate for the regularity of the solution of (2.3) or (2.4): $u \in H_0^1(\Omega) \cap H^{1+\gamma}(\Omega)$ and

$$\|u\|_{1+\gamma,\Omega} \lesssim \|f\|_{-1+\gamma,\Omega} \tag{2.5}$$

for some $\gamma \in (0,1]$ depending on Ω and the coefficients of L.

For some subdomain $G \subset \Omega$, we need the following assumption.

R(G). For any $f \in L^2(G)$, there exists a $u \in H_0^1(G) \cap H^{1+\gamma}(G)$ satisfying

$$a(v,u) = (f,v) \quad \forall v \in H_0^1(G)$$

and

$$\|u\|_{1+\gamma,G} \lesssim \|f\|_{-1+\gamma,G}.$$

Define a Galerkin-projection $P_h(\equiv P_{h,r}) : H_0^1(\Omega) \mapsto S_0^{h,r}(\Omega)$ by

$$a(u - P_h u, v) = 0 \quad \forall v \in S_0^{h,r}(\Omega) \tag{2.6}$$

and apparently

$$\|P_h u\|_{1,\Omega} \lesssim \|u\|_{1,\Omega} \quad \forall u \in H_0^1(\Omega). \tag{2.7}$$

From (2.7), various global a priori error estimates for finite element approximation $P_h u$ to u can be obtained from the approximate properties of the finite element space $S^{h,r}(\Omega)$ (c.f. [10, 35]).

Now we introduce the quantity:

$$\rho_\Omega(h) = \sup_{f\in L^2(\Omega),\|f\|_{0,\Omega}=1} \inf_{v\in S_0^{h,r}(\Omega)} \|L^{-1}f - v\|_{1,\Omega}.$$

Then (see, e.g., [36]) $\rho_\Omega(h) \to 0$ as $h \to 0$ and

$$\rho_\Omega(h) \lesssim h_\Omega^\gamma. \tag{2.8}$$

Similarly, if Assumption R(G) holds, we can define $\rho_G(h)$ well, too.

The following results can be found in [35] (c.f. also [4, 36]).

PROPOSITION 2.1.

$$\|(I - P_h)L^{-1}f\|_{1,\Omega} \lesssim \rho_\Omega(h)\|f\|_{0,\Omega} \quad \forall f \in L^2(\Omega) \tag{2.9}$$

and

$$\|u - P_h u\|_{0,\Omega} \lesssim \rho_\Omega(h)\|u - P_h u\|_{1,\Omega} \quad \forall u \in H_0^1(\Omega). \tag{2.10}$$

Local error estimates for finite element approximations can be also obtained (see, e.g., [10, 24, 25, 33, 35]). For instance, we have the following a priori error estimate (see [35] for details), which will be employed in our discussions.

PROPOSITION 2.2. *Suppose that* $D \subset\subset \Omega_0$.

(i) If $f \in H^{-1}(\Omega)$ *and* $w \in S^{h,r}(\Omega_0)$ *satisfies*

$$a(w, v) = f(v) \quad \forall v \in S_{h,r}^0(\Omega_0), \tag{2.11}$$

then

$$\|w\|_{1,D} \lesssim \|w\|_{0,\Omega_0} + \|f\|_{-1,\Omega_0}. \tag{2.12}$$

(ii) If $u \in H_0^1(\Omega)$, *then*

$$\|u - P_h u\|_{1,D} \lesssim \inf_{v\in S_0^{h,r}(\Omega)} \|u - v\|_{1,\Omega_0} + \rho_\Omega(h)\|u - P_h u\|_{1,\Omega}.$$

2.2. A linear elliptic eigenvalue problem. A number λ is called an eigenvalue of the form $a(\cdot,\cdot)$ relative to the form $(\cdot,\cdot)$ if there is a nonzero vector $u \in H_0^1(\Omega)$, called an associated eigenvector, satisfying

$$a(u, v) = \lambda(u, v) \quad \forall v \in H_0^1(\Omega). \tag{2.13}$$

Here and hereafter, we assume that (a_{ij}) is symmetric. It is known that (2.13) has a countable sequence of real eigenvalues

$$\lambda_1 < \lambda_2 \le \lambda_3 \le \cdots$$

and corresponding eigenvectors

$$u_1, u_2, u_3, \cdots,$$

which can be assumed to satisfy

$$(u_i, u_j) = \delta_{ij},\ i, j = 1, 2, \cdots$$

In the sequence $\{\lambda_j\}$, the λ_j's are repeated according to geometric multiplicity.

A standard finite element scheme for (2.13) is: Find a pair of (λ_h, u_h), where λ_h is a number and $0 \neq u_h \in S_0^{h,r}(\Omega)$, satisfying

$$a(u_h, v) = \lambda_h(u_h, v) \quad \forall v \in S_0^{h,r}(\Omega), \tag{2.14}$$

and use λ_h and u_h as approximation to λ and u (as $h \to 0$), respectively. One sees that (2.14) has a finite sequence of eigenvalues

$$\lambda_{1,h} < \lambda_{2,h} \leq \cdots \leq \lambda_{n_h,h}, \quad n_h = \dim\ S_0^{h,r}(\Omega)$$

and corresponding eigenvectors

$$u_{1,h}, u_{2,h}, \cdots, u_{n_h,h},$$

which can be assumed to satisfy

$$(u_{i,h}, u_{j,h}) = \delta_{ij},\ i, j = 1, 2, \cdots$$

Set

$$M(\lambda_i) = \{w \in H_0^1(\Omega) : w \text{ is an eigenvector of (2.13) corresponding to } \lambda_i\}$$

and

$$\delta_h(\lambda_i)(\equiv \delta_{h,r}(\lambda_i)) = \sup_{w \in M(\lambda_i), \|w\|_{0,\Omega}=1} \inf_{v \in S_0^{h,r}(\Omega)} \|w - v\|_{1,\Omega}.$$

The following results, see [4, 5, 9] or [36], will be employed in the coming discussions.

PROPOSITION 2.3. *(i) For any $u_{i,h}$ of (2.14) ($i = 1, 2, \cdots, n_h$), there is an eigenvector u^i of (2.13) corresponding to λ_i satisfying $\|u^i\|_{0,\Omega} = 1$ and*

$$\|u^i - u_{i,h}\|_{1,\Omega} \leq C_i \delta_h(\lambda_i). \tag{2.15}$$

Moreover,

$$\|u^i - u_{i,h}\|_{0,\Omega} \leq C_i \rho_\Omega(h) \|u^i - u_{i,h}\|_{1,\Omega}. \tag{2.16}$$

(ii) For eigenvalue,

$$\lambda_i \leq \lambda_{i,h} \leq \lambda_i + C_i \delta_h^2(\lambda_i). \tag{2.17}$$

Here and hereafter C_i is some constant depending on i but not depending on the mesh parameter h.

Our analysis for eigenvalue approximations is based on the following crucial (but straightforward) property of eigenvalue and eigenvector approximation (see, e.g., [4, 5] or [36]).

PROPOSITION 2.4. *Let (λ, u) be an eigenvalue pair of (2.13). For any $w \in H_0^1(\Omega) \setminus \{0\}$,*

$$\frac{a(w, w)}{(w, w)} - \lambda = \frac{a(w - u, w - u)}{(w, w)} - \lambda \frac{(w - u, w - u)}{(w, w)}. \tag{2.18}$$

3. Local computations based on coupled discretizations. In this section we shall present some local computational schemes for higher order finite element eigenvector and eigenvalue approximations which are based on coupled discretizations. These schemes are motivated by the observation that for a solution of some elliptic problem, low frequency components can be approximated well in a lower order finite element space and high frequency is more local and can be computed in a higher order finite element space by some local procedure. The theoretical tools for analyzing these methods are the local error estimates stated in the previous section.

The local schemes we shall now present can be used to obtain approximate solution mostly by local computation. The main idea is that the more global component of a finite element solution may be obtained in a lower order finite element space and, the rest of the computation can then be localized with using a group of higher order finite element discretizations. Roughly speaking, our new schemes (for higher order finite element approximations) will be based on one lower-order finite element space on the whole domain and some higher order finite element spaces with the same mesh locally. In our analysis, we shall use an auxiliary higher order finite element space associated with the grid $T^h(\Omega)$, that is globally defined. One basic assumption for this auxiliary higher order finite element space is that it should coincide with the local higher order finite element space in the subdomain of interest.

For simplicity, we shall focus our discussion on the discretization of combination of a piecewise linear finite element space $S_0^{h,1}(\Omega)$ and a quadratic finite element space $S_0^{h,2}(\Omega)$ associated with the same grid $T^h(\Omega)$. The finite element spaces satisfy $S_0^{h,1}(\Omega) \subset S_0^{h,2}(\Omega) \subset H_0^1(\Omega)$.

We consider the approximation of any eigenvalue λ of (2.13). Here and hereafter we let $\lambda_{h,1}$ be the finite element eigenvalue of (2.14) corresponding to $S_0^{h,1}(\Omega)$ and satisfy

$$|\lambda_{h,1} - \lambda| \lesssim \delta_{h,1}^2(\lambda). \tag{3.1}$$

In our strategy, more precisely, to get an approximate solution of an eigenvalue problem in the quadratic finite element space $S_0^{h,2}(\Omega)$, we first solve the eigenvalue problem in a given linear finite element space $S_0^{h,1}(\Omega)$ and then solve a collection of linear boundary value problems in some quadratic finite element spaces $S_0^{h,2}(\Omega_j)(j = 1, 2, \cdots, m)$ locally.

3.1. Computation for eigenvectors. Let $\Omega_0 \subset\subset \Omega$ be a larger subdomain containing a subdomain $D \subset \Omega$ (namely $D \subset\subset \Omega_0$). We are interested in obtaining the approximate solution in the given subdomain D with an accuracy comparable to that from $S_0^{h,2}(\Omega)$.

A prototype of our new local computational scheme is as follows.

ALGORITHM A.

1. *Solve (2.13) in a linear finite element space: Find* $(\lambda_{h,1}, u_{h,1}) \in \mathbb{R}^1 \times S_0^{h,1}(\Omega)$ *satisfying* $\|u_{h,1}\|_{0,\Omega} = 1$ *and*

$$a(u_{h,1}, v) = \lambda_{h,1}(u_{h,1}, v) \quad \forall v \in S_0^{h,1}(\Omega).$$

2. *Solve a local linear boundary value problem in a local quadratic finite element space: Find* $e_{h,2} \in S_0^{h,2}(\Omega_0)$ *satisfying*

$$a(e_{h,2}, v) = \lambda_{h,1}(u_{h,1}, v) - a(u_{h,1}, v) \quad \forall v \in S_0^{h,2}(\Omega_0).$$

3. Set: $u^{h,2} = u_{h,1} + e_{h,2}$ *in* Ω_0.

It is seen from Proposition 2.3 that associated with the eigenvector $u_{h,1}$ obtained by Step 1 in Algorithm A, there exists an exact eigenvector u of (2.13) satisfying $\|u\|_{0,\Omega} = 1$ and

$$\|u - u_{h,1}\|_{1,\Omega} \lesssim \delta_{h,1}(\lambda), \quad \|u - u_{h,1}\|_{0,\Omega} \lesssim h^{\gamma}\delta_{h,1}(\lambda). \tag{3.2}$$

The following result, which will be used in our analysis, can be derived from Riesz-Schauder theory (c.f. [11])

PROPOSITION 3.1. *Let* $G \subset \Omega$ *and* $r \in \{1, 2\}$. *If* $M(\lambda) \subset H^s(G)(s \geq 1)$, *then*

$$\sup_{w \in M(\lambda), \|w\|_{0,\Omega}=1} \inf_{v \in S_0^{h,r}(G)} \|w - v\|_{1,G} \lesssim h^{\min(s-1,r)}. \tag{3.3}$$

In particular, if $M(\lambda) \subset H^s(\Omega)(s \geq 1))$, *then*

$$|\lambda - \lambda_{h,1}| + h^{\mu}\|u - u_{h,1}\|_{1,\Omega} \lesssim h^{2\mu}, \quad \|u - u_{h,1}\|_{0,\Omega} \lesssim h^{\gamma+\mu} \tag{3.4}$$

and

$$\|u - P_{h,r}u\|_{1,\Omega} \lesssim h^{\min(s-1,r)}, \quad \|u - P_{h,r}u\|_{0,\Omega} \lesssim h^{\gamma+\min(s-1,r)}, \tag{3.5}$$

where $\mu = \min(s - 1, 1)$.

THEOREM 3.2. *Assume that* $u^{h,2} \in S^{h,2}(\Omega_0)$ *is obtained by Algorithm A and Assumption* $R(\Omega_0)$ *holds. Then*

$$\|P_{h,2}u - u^{h,2}\|_{1,D} \lesssim |\lambda_{h,1} - \lambda| + \|u - u_{h,1}\|_{0,\Omega} + \|P_{h,2}u - u_{h,1}\|_{0,\Omega} + h^{\gamma}\|u - u_{h,1}\|_{1,\Omega}.$$

Consequently, if $u \in H_0^1(\Omega) \cap H^{1+\theta}(\Omega) \cap H^{2+\alpha}(\Omega_0)$ *(*$\gamma \leq \theta \leq 1 + \alpha$ *and* $0 \leq \alpha \leq 1$*), then*

$$\|u - u^{h,2}\|_{1,D} \lesssim h^{\min(\gamma+\min(\theta,1),1+\alpha)}.$$

Proof. It is seen from the definition of Algorithm A that

$$a(u^{h,2} - P_{h,2}u, v) = \lambda_{h,1}(u_{h,1}, v) - \lambda(u, v) \quad \forall v \in S_{h,2}^0(\Omega_0).$$

Hence, Proposition 2.2 and the identity

$$\lambda_{h,1}(u_{h,1}, v) - \lambda(u, v) = (\lambda_{h,1} - \lambda)(u, v) + \lambda_{h,1}(u_{h,1} - u, v) \ \ \forall v \in H_0^1(\Omega)$$

imply

$$\|P_{h,2}u - u^{h,2}\|_{1,D} \lesssim |\lambda_{h,1} - \lambda| + \|u_{h,1} - u\|_{0,\Omega_0} + \|u^{h,2} - P_{h,2}u\|_{0,\Omega_0},$$

or

$$\|P_{h,2}u - u^{h,2}\|_{1,D} \lesssim |\lambda_{h,1} - \lambda| + \|u - u_{h,1}\|_{0,\Omega_0} + \|u_{h,1} - P_{h,2}u\|_{0,\Omega} + \|e_{h,2}\|_{0,\Omega_0}.$$

Next we proceed to estimate $\|e_{h,2}\|_{0,\Omega_0}$ by using the Aubin-Nitsche duality argument. Given any $\phi \in L^2(\Omega_0)$, there exists $w \in H_0^1(\Omega_0)$ such that

$$a(v, w) = (\phi, v) \quad \forall v \in H_0^1(\Omega_0). \tag{3.6}$$

Let $w_{h,2}^0 \in S_0^{h,2}(\Omega_0)$ and $w_{h,1}^0 \in S_0^{h,1}(\Omega_0)$ satisfy

$$a(v_{h,2}, w_{h,2}^0) = a(v_{h,2}, w) \quad \forall v_{h,2} \in S_0^{h,2}(\Omega_0), \tag{3.7}$$

$$a(v_{h,1}, w_{h,1}^0) = a(v_{h,1}, w) \quad \forall v_{h,1} \in S_0^{h,1}(\Omega_0). \tag{3.8}$$

Then, Proposition 2.1 implies

$$\|w - w_{h,2}^0\|_{1,\Omega_0} \lesssim h^\gamma \|\phi\|_{0,\Omega_0}, \quad \|w - w_{h,1}^0\|_{1,\Omega} \lesssim h^\gamma \|\phi\|_{0,\Omega_0}.$$

It follows from the definitions of w, $e_{h,2}$ and $w_{h,2}^0$ that

$$\begin{aligned}
&(e_{h,2}, \phi) = a(e_{h,2}, w) = a(e_{h,2}, w_{h,2}^0) = a(u^{h,2} - u_{h,1}, w_{h,2}^0) \\
&= a(P_{h,2}u - u_{h,1}, w_{h,2}^0) + a(u^{h,2}, w_{h,2}^0) - a(P_{h,2}u, w_{h,2}^0) \\
&= a(P_{h,2}u - u_{h,1}, w_{h,2}^0) + \lambda_{h,1}(u_{h,1}, w_{h,2}^0) - \lambda(u, w_{h,2}^0) \\
&= a(P_{h,2}u - u_{h,1}, w_{h,2}^0 - w) + a(P_{h,2}u - u_{h,1}, w) \\
&\qquad + \lambda_{h,1}(u_{h,1}, w_{h,2}^0) - \lambda(u, w_{h,2}^0).
\end{aligned}$$

Thus, we obtain

$$\begin{aligned}
(e_{h,2}, \phi) &= a(P_{h,2} - u_{h,1}, w_{h,2}^0 - w) + a(P_{h,2}u - u_{h,1}, w - w_{h,1}^0) \\
&\quad + a(P_{h,2}u - u_{h,1}, w_{h,1}^0) + \lambda_{h,1}(u_{h,1}, w_{h,2}^0) - \lambda(u, w_{h,2}^0) \\
&= a(P_{h,2}u - u_{h,1}, w_{h,2}^0 - w) + a(P_{h,2}u - u_{h,1}, w - w_{h,1}^0) + \lambda(u, w_{h,1}^0) \\
&\quad - \lambda_{h,1}(u_{h,1}, w_{h,1}^0) + \lambda_{h,1}(u_{h,1}, w_{h,2}^0) - \lambda(u, w_{h,2}^0) \\
&= a(P_{h,2}u - u_{h,1}, w_{h,2}^0 - w) + a(P_{h,2}u - u_{h,1}, w - w_{h,1}^0) \\
&\quad + \lambda(u, w_{h,1}^0 - w_{h,2}^0) - \lambda_{h,1}(u_{h,1}, w_{h,1}^0 - w_{h,2}^0) \\
&= a(P_{h,2}u - u_{h,1}, w_{h,2}^0 - w) + a(P_{h,2}u - u_{h,1}, w - w_{h,1}^0) \\
&\quad + (\lambda - \lambda_{h,1})(u, w_{h,1}^0 - w_{h,2}^0) + \lambda_{h,1}(u - u_{h,1}, w_{h,1}^0 - w_{h,2}^0),
\end{aligned}$$

where (3.7) and (3.8) are used. Consequently, we get the estimation for any $\phi \in L^2(\Omega)$ that

$$|(e_{h,2}, \phi)| \lesssim (h^\gamma \|P_{h,2}u - u_{h,1}\|_{1,\Omega} + |\lambda_{h,1} - \lambda| + \|u - u_{h,1}\|_{0,\Omega}) \|\phi\|_{0,\Omega_0},$$

which implies

$$\|e_{h,2}\|_{0,\Omega_0} \lesssim |\lambda_{h,1} - \lambda| + \|P_{h,2}u - u_{h,1}\|_{0,\Omega} + h^\gamma \|u - u_{h,1}\|_{1,\Omega}.$$

The desired result then follows from Proposition 3.1. □

Remark. From Proposition 3.1 and the analysis above, we may have

$$\|u - u^{h,2}\|_{1,D} \lesssim h_{\Omega_0}^s + h_\Omega^{\theta+\gamma}, \quad s \in (1,2],\ \theta \in (0,1]$$

if $u \in H_0^1(\Omega) \cap H^{1+\theta}(\Omega) \cap H^{1+s}(\Omega_0)$, where $D \subset\subset \Omega_0 \subset \Omega$. Namely, we may get higher accuracy approximations wherever the exact solution is smooth and local quadratic finite elements are used. In the subdomain where the exact solution is not smooth, according to [38], we may use a so called two-grid discretization to obtain higher

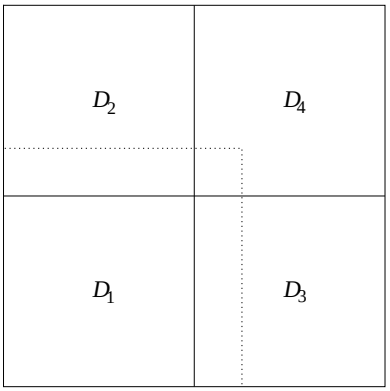

FIG. 3.1. *Domain decomposition:* $D_j \subset\subset \Omega_j$

accuracy approximation. For simplicity, in this paper, we focus our attention only to the case of smooth exact eigenvectors.

Global highly accurate approximations to eigenvectors are naturally obtained from the local computation that we studied above. Given an triangulation $T^h(\Omega)$, let us assume that $D_1, \ldots, D_m$ are disjoint subdomains of Ω and then enlarge each D_j to obtain Ω_j that aligns with $T^h(\Omega)$. Note that usually $\cup_{j=1}^m D_j \subset \Omega$. The basic idea of our algorithms for global highly accurate approximations is very simple: we just apply the local computations in all Ω_j's in parallel when $\{D_1, D_2, \cdots, D_m\}$ is a partition of Ω (see Fig. 3.1 for $2-d$ cases), which is stated as follows:

ALGORITHM B.

1. *Solve (2.13) in a global linear finite element space: Find* $(\lambda_{h,1}, u_{h,1}) \in \mathbb{R}^1 \times S_0^{h,1}(\Omega)$ *satisfying* $\|u_{h,1}\|_{0,\Omega} = 1$ *and*

$$a(u_{h,1}, v) = \lambda_{h,1}(u_{h,1}, v) \quad \forall v \in S_0^{h,1}(\Omega).$$

2. *Solve local linear boundary value problems in local quadratic finite element spaces in parallel: Find* $e_{h,2}^j \in S_0^{h,2}(\Omega_j)(j = 1, 2, \cdots, m)$ *satisfying*

$$a(e_{h,2}^j, v) = \lambda_{h,1}(u_{h,1}, v) - a(u_{h,1}, v) \quad \forall v \in S_0^{h,2}(\Omega_j).$$

3. *Set* $u^{h,2} = u_{h,1} + e_{h,2}^j \quad$ *in* $D_j (j = 1, 2, \cdots, m)$.

By Theorem 3.2 and Proposition 3.1, for this algorithm, we apparently have the following result.

THEOREM 3.3. *Assume that* $u^{h,2}$ *is the solution obtained by Algorithm B and Assumptions* $R(\Omega_j)$ $(j = 1, 2, \cdots, m)$ *hold. Then*

$$\left(\sum_{j=1}^m \|P_{h,2}u - u^{h,2}\|_{1,D_j}^2 \right)^{1/2}$$
$$\lesssim |\lambda_{h,1} - \lambda| + \|u - u_{h,1}\|_{0,\Omega} + \|P_{h,2}u - u_{h,1}\|_{0,\Omega} + h^\gamma \|u_{h,2} - u_{h,1}\|_{1,\Omega}.$$

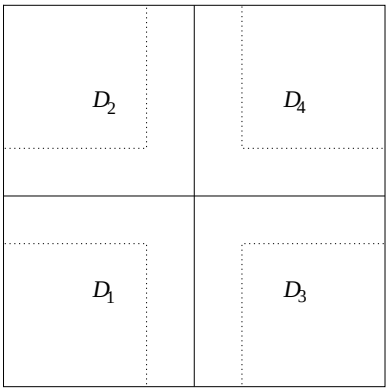

FIG. 3.2. *Domain decomposition:* $D_j \subset\subset \Omega_j$ *and* D_{m+1}

If $u \in H_0^1(\Omega) \cap H^{2+\alpha}(\Omega)(\alpha \in (0,1])$, *then*

$$\left(\sum_{j=1}^{m} \|u - u^{h,2}\|_{1,D_j}^2\right)^{1/2} \lesssim h^{1+\min(\gamma,\alpha)}.$$

3.2. Computation for eigenvalues. We note that the approximation $u^{h,2}$ obtained by Algorithm B is piecewise defined and is in general discontinuous. In this subsection, we shall propose some further modifications for this algorithm to achieve the following two goals:

- smooth $u^{h,2}$ to obtain a global $H^1(\Omega)$ approximation;
- compute $\lambda_{h,2}$ in parallel.

The first goal will be achieved by solving some local quadratic finite element problems and the second goal will be achieved by carrying out the Rayleigh quotient. We note that the second goal is realized after the first goal has been achieved.

We now proceed to present a modified algorithm that addresses both of the aforementioned two issues. To do this, we assume that $\{\Omega_1, \Omega_2, \cdots, \Omega_m\}$ is a partition of Ω (namely, $\Omega_i \cap \Omega_j = \emptyset (i \neq j)$ and $\cup_{j=1}^m \bar{\Omega}_j = \bar{\Omega}$) and set $D_{m+1} = \Omega \setminus (\cup_{j=1}^m \bar{D}_j)$, where $D_j \subset\subset \Omega_j (j = 1, 2, \cdots, m)$ (see Fig. 3.2 for $2-d$ cases).

ALGORITHM C.

1. *Solve (2.13) in a global linear finite element space: Find* $(\lambda_{h,1}, u_{h,1}) \in \mathbb{R}^1 \times S_0^{h,1}(\Omega)$ *satisfying* $\|u_{h,1}\|_{0,\Omega} = 1$ *and*

$$a(u_{h,1}, v) = \lambda_{h,1}(u_{h,1}, v) \quad \forall v \in S_0^{h,1}(\Omega).$$

2. *Solve local linear boundary value problems in local quadratic finite element spaces in parallel: Find* $e_{h,2}^j \in S_0^{h,2}(\Omega_j)(j = 1, 2, \cdots, m)$ *satisfying*

$$a(e_{h,2}^j, v) = \lambda_{h,1}(u_{h,1}, v) - a(u_{h,1}, v) \quad \forall v \in S_0^{h,2}(\Omega_j).$$

3. *Set* $u^{h,2} = u_{h,1} + e_{h,2}^j \quad$ *in* $D_j (j = 1, 2, \cdots, m)$ *and* $u^{h,2}$ *on* $\bar{D}_{m+1}$ *is defined by:* $u^{h,2}\,|_{\partial D_j \cap \partial D_{m+1}} = u_{h,1} + e_{h,2}^j (j = 1, 2, \cdots, m)$ *and satisfying*

$$a(u^{h,2}, v) = \lambda_{h,1}(u_{h,1}, v) \quad \forall v \in S_0^{h,2}(D_{m+1}).$$

4. Compute the Rayleigh quotient

$$\lambda^{h,2} = \frac{a(u^{h,2}, u^{h,2})}{(u^{h,2}, u^{h,2})}.$$

In the above algorithm, Step 3 is for obtaining a global H^1 solution and Step 4 is for the approximation of eigenvalue.

THEOREM 3.4. *Assume that $(\lambda^{h,2}, u^{h,2})$ is the pair obtained by Algorithm C and Assumptions $R(\Omega_j)(j = 1, 2, \cdots, m)$ hold. Then*

$$\|P_{h,2}u - u^{h,2}\|_{1,\Omega} \lesssim |\lambda - \lambda_{h,1}| + \|u - u_{h,1}\|_{0,\Omega} + |P_{h,2}u - u_{h,1}\|_{0,\Omega} + h^{\gamma}\|u - u_{h,1}\|_{1,\Omega}.$$

Consequently, if $u \in H_0^1(\Omega) \cap H^{2+\alpha}(\Omega)(\alpha \in (0, 1])$, then

$$|\lambda - \lambda^{h,2}| + h^{1+\min(\gamma,\alpha)}\|u - u^{h,2}\|_{1,\Omega} \lesssim h^{2+2\min(\gamma,\alpha)}.$$

Proof. From the definition of $u^{h,2}$, we have

$$a(P_{h,2}u - u^{h,2}, v) = (\lambda - \lambda_{h,1})(u, v) + \lambda_{h,1}(u - u_{h,1}, v) \quad \forall v \in S_0^{h,2}(D_{m+1}). \tag{3.9}$$

Obviously, the estimation

$$\|\nabla(P_{h,2}u - u^{h,2})\|_{0,D_{m+1}}^2 \lesssim a_{D_{m+1}}^0(P_{h,2}u - u^{h,2}, P_{h,2}u - u^{h,2})$$

is true for

$$a_{D_{m+1}}^0(w, v) = \int_{D_{m+1}} \sum_{i,j=1}^{d} a_{ij} \frac{\partial w}{\partial x_i} \frac{\partial v}{\partial x_j}, \quad w, v \in H_0^1(\Omega).$$

Hence, for any $v \in S_0^{h,2}(D_{m+1})$, we obtain

$$\begin{aligned} &\|\nabla(P_{h,2}u - u^{h,2})\|_{0,D_{m+1}}^2 \\ &\lesssim a_{D_{m+1}}^0(P_{h,2}u - u^{h,2}, P_{h,2}u - u^{h,2} - v) + (|\lambda - \lambda_{h,1}| + |\lambda_{h,1}|\|u - u_{h,1}\|_{0,\Omega})\|v\|_{1,\Omega}. \end{aligned}$$

Consequently, there holds

$$\begin{aligned} &\|\nabla(P_{h,2}u - u^{h,2})\|_{0,D_{m+1}}^2 \\ &\lesssim \|\nabla(P_{h,2}u - u^{h,2})\|_{0,D_{m+1}} \inf_{\chi \in S_0^{h,2}(D_{m+1})} \|P_{h,2}u - u^{h,2} - \chi\|_{1,D_{m+1}} \\ &\quad + \xi_h \inf_{\chi \in S_0^{h,2}(D_{m+1})} (\|P_{h,2}u - u^{h,2} - \chi\|_{1,D_{m+1}} + \|P_{h,2}u - u^{h,2}\|_{1,D_{m+1}}), \end{aligned}$$

where

$$\xi_h = |\lambda - \lambda_{h,1}| + |\lambda_{h,1}|\|u - u_{h,1}\|_{0,\Omega}.$$

Note that for any $G \subset \Omega$, there holds [35]

$$\inf_{\chi \in S_0^{h,r}(G)} \|v - \chi\|_{1,G} \lesssim \|v\|_{1/2,\partial G} \quad \forall v \in S^{h,r}(G). \tag{3.10}$$

Hence we have

$$\|\nabla(P_{h,2}u-u^{h,2})\|^2_{0,D_{m+1}} \lesssim \|\nabla(P_{h,2}u-u^{h,2})\|_{0,D_{m+1}}\|P_{h,2}u-u^{h,2}\|_{1/2,\partial D_{m+1}} + \xi_h(\|P_{h,2}u-u^{h,2}\|_{1/2,\partial D_{m+1}}+\|P_{h,2}u-u^{h,2}\|_{1,D_{m+1}}).$$

Using the estimation that

$$\|P_{h,2}u-u^{h,2}\|_{1/2,\partial D_{m+1}} \lesssim \sum_{j=1}^{m}\|P_{h,2}u-u^{h,2}\|_{1/2,\partial D_j} \lesssim \sum_{j=1}^{m}\|P_{h,2}u-u^{h,2}\|_{1,D_j},$$

or

$$\|P_{h,2}u-u^{h,2}\|_{1/2,\partial D_{m+1}} \lesssim \left(\sum_{j=1}^{m}\|P_{h,2}u-u^{h,2}\|^2_{1,D_j}\right)^{1/2},$$

we get

$$\begin{aligned}&\|\nabla(P_{h,2}u-u^{h,2})\|^2_{0,D_{m+1}}\\ \lesssim\ & |\!|\!|P_{h,2}u-u^{h,2}|\!|\!|^2_{1,\Omega}+\xi_h(|\!|\!|P_{h,2}u-u^{h,2}|\!|\!|_{1,\Omega}+\|P_{h,2}u-u^{h,2}\|_{1,D_{m+1}}),\end{aligned}$$

where

$$|\!|\!|P_{h,2}u-u^{h,2}|\!|\!|_{1,\Omega} \equiv \left(\sum_{j=1}^{m}\|P_{h,2}u-u^{h,2}\|^2_{1,D_j}\right)^{1/2}.$$

Thus

$$\begin{aligned}\|P_{h,2}u-u^{h,2}\|^2_{1,\Omega} &\lesssim \|\nabla(P_{h,2}u-u^{h,2})\|^2_{0,\Omega}\\ &\lesssim |\!|\!|P_{h,2}u-u^{h,2}|\!|\!|^2_{1,\Omega}+\xi_h^2+\xi_h\|P_{h,2}u-u^{h,2}\|_{1,\Omega},\end{aligned}$$

namely,

$$\|P_{h,2}u-u^{h,2}\|_{1,\Omega} \lesssim |\!|\!|P_{h,2}u-u^{h,2}|\!|\!|_{1,\Omega}+|\lambda-\lambda_{h,1}|+\|u-u_{h,1}\|_{0,\Omega}, \tag{3.11}$$

which together with Proposition 2.3, Proposition 3.1, and Theorem 3.3 finishes the proof. □

4. Numerical experiments. In this section, we will report some numerical experiments in three dimensions, which coincide with our theory. The numerical experiments were carried out by SGI Origin 3800 in the State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences.

As we see, it is expensive to solve three dimensional problems by using uniform meshes when accurate approximate solutions are required. Thus, in our computations, we will employ adaptive meshes instead of uniform meshes. The adaptive finite element meshes are constructed from the bisection approaches [3] and the error indicators

$$\eta_\tau = \eta_{\tau,G} = \|A^{-1/2}(G_h u_h - A\nabla u_h)\|^2_{0,\tau}, \quad \tau \in T^h(\Omega)$$

when the linear finite element method is taken into account, or

$$\eta_\tau = \eta_{\tau,R} = h_\tau \|[A\nabla u_h \cdot n]\|^2_{0,\partial\tau}, \quad \tau \in T^h(\Omega)$$

when the quadratic finite elements are used. Here $A = (a_{ij})_{3\times 3}$ and the local averaging operator $G_h : S_0^{h,1}(\Omega) \to S^{h,1}(\Omega) \times S^{h,1}(\Omega)$ is defined by (see, e.g., [39, 40])

$$G_h v = \sum_{z\in\partial^2 T^h} (A\nabla v)_z \phi_z, \qquad (A\nabla v)_z = \sum_{j=1}^{J_z} \alpha_z^j (A(z)\nabla v)_{\tau_z^j} \quad \forall v \in S_0^{h,1}(\Omega),$$

where $\bigcup_{j=1}^{J_z} \tau_z^j = \omega_z$, $\sum_{j=1}^{J_z} \alpha_z^j = 1$, $\omega_z = \bigcup_{z\in\tau} \tau$, $\alpha_z^j \geq 0$ (for instance, $\alpha_z^j = \frac{1}{J_z}$ $\alpha_z^j = \frac{|\tau_z^j|}{|\omega_z|}$), J_z is the number of elements containing z, and $[g]_l$ means the jump of g across the surface l, $l \notin \partial\Omega$ (see, e.g., [20]). In the step of of correction, the fine mesh is obtained by some tetrahedral bisection strategy, too.

We will use three types of algorithms. The first one, which is denoted by Algorithm I-I, is the algorithm proposed in [38] for linear finite element eigenvalues: solve an eigenvalue problem in the linear finite element space associated with a relatively coarse mesh and then find the correction by solving some Poisson boundary value problems in linear finite element spaces associated with local refined meshes in parallel. The second one, which is named by Algorithm II-II, is a similar algorithm to Algorithm I-I (see also [38]): solve an eigenvalue problem in the quadratic finite element space associated with a relatively coarse mesh and then find the correction by solving some Poisson boundary value problems in quadratic finite element spaces associated with local refined meshes in parallel. The third one, which is called Algorithm I-II, is Algorithm C described in Section 3.2: solve an eigenvalue problem in the linear finite element space and then find the correction by solving some Poisson boundary value problems in quadratic finite element spaces associated with the same finite element mesh in parallel.

For illustration, we choose to report some simple numerical experiments only for applying two processors. Divide $\Omega \equiv (a_1, a_2) \times (b_1, b_2) \times (c_1, c_2)$ into two subdomains (see Fig. 4.1):

$$\Omega_1 = (a_1, (a_1 + a_2)/2) \times (b_1, b_2) \times (c_1, c_2), \quad \Omega_2 = ((a_1 + a_2)/2, a_2) \times (b_1, b_2) \times (c_1, c_2).$$

Set

$$D_1 = (a_1, (3a_1 + a_2)/4) \times (b_1, b_2) \times (c_1, c_2),$$

$$D_2 = ((a_1 + 3a_2)/4, a_2) \times (b_1, b_2) \times (c_1, c_2),$$

and

$$D_3 = ((3a_1 + a_2)/4, (a_1 + 3a_2)/4) \times (b_1, b_2) \times (c_1, c_2).$$

Example 1 Consider the following model problem [20]:

$$\left\{ \begin{array}{rcl} -\sum_{i=1}^{3} \frac{\partial}{\partial x_i}(x_i^2 \frac{\partial u}{\partial x_i}) & = & \lambda u \ \text{ in } \Omega, \\ u & = & 0 \ \text{ on } \partial\Omega, \end{array} \right. \tag{4.1}$$

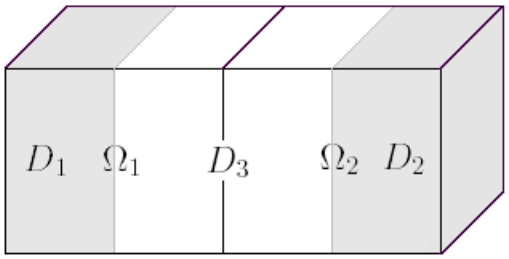

FIG. 4.1. *Domain decomposition:* $D_j \subset\subset \Omega_j (j = 1, 2)$ *and* $D_3 = \Omega \setminus (\bar{D}_1 \cup \bar{D}_2)$.

where $\Omega = (1, 3)\times(1, 2)\times(1, 2)$. The first eigenvalue of (4.1) is $\lambda = \frac{3}{4}+(\frac{2}{\ln^2 2}+\frac{1}{\ln^2 3})\pi^2 \cong 50.01212422$ and its associated eigenfunction is $u = \prod_{i=1}^{3}(x_i^{-1/2}\sin(\frac{\pi \ln x_i}{\ln \beta_i}))$, where $\beta_1 = 3, \beta_2 = \beta_3 = 2$.

The numerical results obtained from the adaptive meshes are presented in Table 4.1, Table 4.2 and Table 4.3, respectively. In the tables, we have used the following notations:

N_c : the number of degrees of freedom for solving the eigenvalue problem without any correction.

N_f: the total number of degrees of freedom for solving the boundary value problems for corrections.

λ_c: the numerical eigenvalue without any correction.

λ^h: the eigenvalue approximation obtained from the Rayleigh quotient.

N_c	N_f	λ_c	$\lvert\lambda_c - \lambda\rvert/\lambda$	λ_h	$\lvert\lambda^h - \lambda\rvert/\lambda$	CPU time(s)
27	4977	6.646359e+01	3.289496e-01	5.207271e+01	4.120164e-02	5.779803e+00
78	8241	6.188943e+01	2.374885e-01	5.197303e+01	3.920860e-02	1.264343e+01
136	11013	5.633231e+01	1.263730e-01	5.105227e+01	2.079783e-02	2.008891e+01
245	20627	5.430275e+01	8.579178e-02	5.059793e+01	1.171320e-02	4.985364e+01
368	31803	5.352607e+01	7.026178e-02	5.044937e+01	8.742720e-03	9.494943e+01
769	60049	5.221756e+01	4.409808e-02	5.033467e+01	6.449292e-03	2.234454e+02
917	68901	5.180455e+01	3.583988e-02	5.028786e+01	5.513373e-03	2.715239e+02
1835	134055	5.125579e+01	2.486729e-02	5.018076e+01	3.371834e-03	7.225197e+02
2595	185979	5.098476e+01	1.944805e-02	5.013869e+01	2.530661e-03	1.256135e+03
4516	318983	5.068490e+01	1.345225e-02	5.009928e+01	1.742628e-03	3.002895e+03
6207	429559	5.053118e+01	1.037857e-02	5.008471e+01	1.451300e-03	4.532575e+03
10105	676663	5.039899e+01	7.735460e-03	5.007171e+01	1.191378e-03	8.255448e+03
17431	1135973	5.029343e+01	5.624848e-03	5.005024e+01	7.620505e-04	2.101582e+04

TABLE 4.1

Example 1, eigenvalue: linear finite elements, correction: linear finite elements

It is shown by Table 4.1, Table 4.2 and Table 4.3 that the correction approaches are very efficient and that of Algorithm I-II is the most efficient one. It is noted from the tables that the accuracy produced by Algorithm II-II is the best. However, the approximate accuracy depends on the balance between mesh sizes H and h (say, $H^2 = h$) and the optimal choice of the two-scale meshes, which requires the information of the exact eigenvectors, is not easy to take. Even though, the matching of the two-scale meshes needs to employ much more degrees of freedom. It is also noted that the band width of the stiff matrix resulting from quadratic finite elements is bigger than that of linear finite elements even the number of degrees of freedom is the same. Consequently, Algorithm I-II is the first recommendation taking into account both the computational complexity and the accuracy.

N_c	N_f	λ_c	$\lvert\lambda_c-\lambda\rvert/\lambda$	λ^h	$\lvert\lambda^h-\lambda\rvert/\lambda$	CPU time(s)
27	761	6.646359e+01	3.289496e-01	5.139070e+01	2.756488e-02	3.007081e-01
78	1169	6.188943e+01	2.374885e-01	5.078482e+01	1.545008e-02	7.330670e-01
136	1547	5.633231e+01	1.263730e-01	5.027698e+01	5.295856e-03	1.493303e+00
245	2868	5.430275e+01	8.579178e-02	5.016379e+01	3.032587e-03	3.981693e+00
368	4340	5.352607e+01	7.026178e-02	5.009714e+01	1.699970e-03	7.666605e+00
769	8061	5.221756e+01	4.409808e-02	5.004258e+01	6.090130e-04	2.169316e+01
917	9235	5.180455e+01	3.583988e-02	5.003562e+01	4.698060e-04	2.914517e+01
1835	17962	5.125579e+01	2.486729e-02	5.002505e+01	2.584108e-04	8.288357e+01
2595	24668	5.098476e+01	1.944805e-02	5.002000e+01	1.575238e-04	1.554409e+02
4516	41734	5.068490e+01	1.345225e-02	5.001496e+01	5.661246e-05	3.789464e+02
6207	56102	5.053118e+01	1.037857e-02	5.001380e+01	3.354358e-05	5.863663e+02
10105	88554	5.039899e+01	7.735459e-03	5.001316e+01	2.067981e-05	1.078481e+03
17431	148195	5.029343e+01	5.624850e-03	5.001264e+01	1.023611e-05	2.694607e+03
24832	208932	5.023192e+01	4.394847e-03	5.001229e+01	3.344226e-06	4.751123e+03

TABLE 4.2

Example 1, eigenvalue: linear finite elements, correction: quadratic finite elements

N_c	N_f	λ_c	$\lvert\lambda_c-\lambda\rvert/\lambda$	λ^h	$\lvert\lambda^h-\lambda\rvert/\lambda$	CPU time(s)
343	36065	5.063172e+01	1.238899e-02	5.002676e+01	2.927227e-04	2.448811e+02
439	42209	5.043270e+01	8.409555e-03	5.001993e+01	1.561764e-04	3.440008e+02
507	46481	5.038026e+01	7.360916e-03	5.001892e+01	1.358492e-04	4.000043e+02
693	58185	5.026263e+01	5.008938e-03	5.001575e+01	7.243368e-05	5.172422e+02
959	74449	5.017363e+01	3.229403e-03	5.001449e+01	4.725294e-05	8.242071e+02
1047	81041	5.015583e+01	2.873513e-03	5.001425e+01	4.254835e-05	8.495969e+02
1356	104957	5.011232e+01	2.003420e-03	5.001347e+01	2.686112e-05	1.414208e+03
1788	137565	5.008130e+01	1.383119e-03	5.001281e+01	1.365204e-05	1.953387e+03
1938	149525	5.007397e+01	1.236709e-03	5.001270e+01	1.155750e-05	2.287533e+03
2499	191937	5.006018e+01	9.609760e-04	5.001246e+01	6.628842e-06	3.565388e+03
3183	239793	5.004818e+01	7.210039e-04	5.001233e+01	4.021455e-06	5.066000e+03
3578	267205	5.004393e+01	6.359210e-04	5.001227e+01	2.884516e-06	6.016899e+03

TABLE 4.3

Example 1, eigenvalue: quadratic finite elements, correction: quadratic finite elements

It is seen from Fig. 4.2 that the convergence curve and the line with slope $-\frac{4}{3}$ are basically parallel, which coincide with our theory obtained in Section 3. The efficiency of the three algorithms is compared in Fig. 4.3. It is shown by the curves of relative error of eigenvalue with respect to cpu-time of the three algorithms that to reach the same accuracy, the cpu-time cost by our new algorithm is the least. Taking into account both the computational complexity and the accuracy, our new algorithm is recommended.

Example 2 Consider the following harmonic oscillator equation, which is a simple model in quantum mechanics [12]:

$$-\frac{1}{2}\Delta u+\frac{1}{2}r^2u=\lambda u \ \text{ in } \mathbb{R}^3, \tag{4.2}$$

where $r=(x_1^2+x_2^2+x_3^2)^{\frac{1}{2}}$. The first first eigenvalue of (4.2) is $\lambda=1.5$.

In our computation, we solve the following problem:

$$\begin{cases} -\frac{1}{2}\Delta u+\frac{1}{2}r^2u &= \lambda u \ \text{ in } \Omega, \\ u &= 0 \ \text{ on } \partial\Omega, \end{cases} \tag{4.3}$$

where $\Omega=(-5.5,5.5)^3$.

Some numerical results are reported in Table 4.4, Table 4.5 and Table 4.6 (see also Fig. 4.4 and Fig. 4.5). The similar conclusions to that of Example 1 are valid, too.

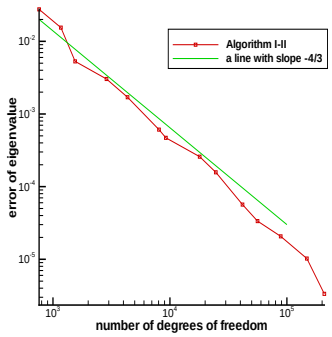

FIG. 4.2. *the convergent curve of relative error of eigenvalue with respect to the number of degrees of freedom*

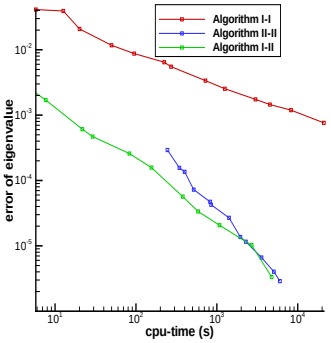

FIG. 4.3. *the relation of relative error of eigenvalue and the cpu-time*

N_c	N_f	λ_c	$\lvert\lambda_c-\lambda\rvert/\lambda$	λ^h	$\lvert\lambda^h-\lambda\rvert/\lambda$	CPU time(s)
27	4977	2.252091e+00	5.013940e-01	1.738829e+00	1.592193e-01	5.712349e+00
35	5489	2.068006e+00	3.786706e-01	1.683745e+00	1.224967e-01	6.952679e+00
47	6017	1.690342e+00	1.268949e-01	1.556450e+00	3.763324e-02	8.403858e+00
53	6521	1.669702e+00	1.131344e-01	1.531315e+00	2.087672e-02	9.971491e+00
181	14233	1.645426e+00	9.695090e-02	1.525916e+00	1.727734e-02	2.975704e+01
241	16873	1.638893e+00	9.259522e-02	1.518491e+00	1.232724e-02	4.028834e+01
469	31225	1.611284e+00	7.418938e-02	1.512807e+00	8.537748e-03	1.022111e+02
721	47593	1.571037e+00	4.735784e-02	1.511080e+00	7.386638e-03	1.831879e+02
1303	76321	1.538089e+00	2.539292e-02	1.505014e+00	3.342593e-03	3.946985e+02
2329	144745	1.526544e+00	1.769601e-02	1.502957e+00	1.971279e-03	1.059755e+03
4207	264097	1.518915e+00	1.261028e-02	1.502770e+00	1.846696e-03	2.354661e+03
7717	437117	1.510613e+00	7.075032e-03	1.501398e+00	9.318475e-04	5.157929e+03
13743	829761	1.507146e+00	4.764000e-03	1.500791e+00	5.273330e-04	1.476376e+04

TABLE 4.4
Example 2, eigenvalue: linear finite elements, correction: linear finite elements

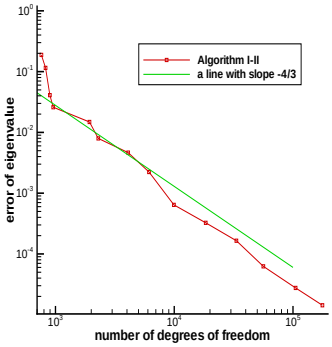

FIG. 4.4. *the convergent curve of relative error of eigenvalue with respect to the number of degrees of freedom*

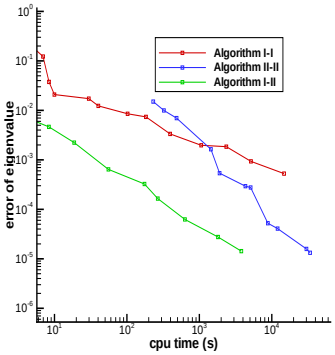

FIG. 4.5. *the relation of relative error of eigenvalue and the cpu-time*

5. Concluding remarks. Although our results and analysis are provided only for the coupling of a linear finite element space and a quadratic finite element space,

N_c	N_f	λ_c	$\lvert\lambda_c-\lambda\rvert/\lambda$	λ^h	$\lvert\lambda^h-\lambda\rvert/\lambda$	CPU time(s)
27	761	2.252091e+00	5.013940e-01	1.782641e+00	1.884274e-01	3.041508e-01
35	825	2.068006e+00	3.786706e-01	1.672741e+00	1.151608e-01	4.074850e-01
47	897	1.690342e+00	1.268949e-01	1.561519e+00	4.101254e-02	5.608289e-01
53	957	1.669702e+00	1.131344e-01	1.538927e+00	2.595134e-02	7.200279e-01
181	1933	1.645426e+00	9.695090e-02	1.522251e+00	1.483402e-02	2.278068e+00
241	2293	1.638893e+00	9.259522e-02	1.511938e+00	7.958602e-03	3.367584e+00
469	4093	1.611284e+00	7.418938e-02	1.506965e+00	4.643357e-03	8.377332e+00
721	6133	1.571037e+00	4.735785e-02	1.503343e+00	2.228966e-03	1.871426e+01
1303	9937	1.538089e+00	2.539292e-02	1.500963e+00	6.417660e-04	5.555781e+01
2329	18421	1.526544e+00	1.769601e-02	1.500488e+00	3.251057e-04	1.746728e+02
4207	33361	1.518915e+00	1.261028e-02	1.500247e+00	1.649511e-04	2.667746e+02
7717	56269	1.510613e+00	7.075031e-03	1.500094e+00	6.249937e-05	6.320155e+02
13743	105185	1.507146e+00	4.764063e-03	1.500041e+00	2.758880e-05	1.809844e+03
22715	176889	1.505164e+00	3.442762e-03	1.500021e+00	1.429715e-05	3.792496e+03

TABLE 4.5

Example 2, eigenvalue: linear finite elements, correction: quadratic finite elements

N_c	N_f	λ_c	$\lvert\lambda_c-\lambda\rvert/\lambda$	λ^h	$\lvert\lambda^h-\lambda\rvert/\lambda$	CPU time(s)
343	36065	1.659367e+00	1.062448e-01	1.522569e+00	1.504587e-02	2.308609e+02
487	45281	1.607261e+00	7.150705e-02	1.514952e+00	9.967992e-03	3.239362e+02
707	58641	1.586810e+00	5.787337e-02	1.510467e+00	6.977987e-03	4.844429e+02
1199	89409	1.542654e+00	2.843583e-02	1.502456e+00	1.637537e-03	1.443545e+03
1451	105777	1.526699e+00	1.779916e-02	1.500807e+00	5.382192e-04	1.901823e+03
2859	192049	1.512951e+00	8.634125e-03	1.500441e+00	2.937642e-04	4.319619e+03
3003	200305	1.511526e+00	7.684173e-03	1.500414e+00	2.762024e-04	5.100633e+03
3867	257521	1.504085e+00	2.723248e-03	1.500079e+00	5.237255e-05	8.825501e+03
4903	323105	1.503121e+00	2.080907e-03	1.500061e+00	4.077350e-05	1.203078e+04
8311	540257	1.501821e+00	1.213935e-03	1.500024e+00	1.584400e-05	3.006319e+04
9799	630689	1.501352e+00	9.015333e-04	1.500020e+00	1.324906e-05	3.373728e+04

TABLE 4.6

Example 2, eigenvalue: quadratic finite elements, correction: quadratic finite elements

the similar results for coupling of general polynomials subspaces may be expected. For example, let Ω be convex polytopic domain in $\mathbb{R}^d (d \geq 1)$, $D \subset\subset \Omega_0 \subset\subset \Omega$, $S_0^{h,1}(\Omega)$ denote the lower order finite element space which consists of piecewise polynomial of degree less or equal to r and $S_0^{h,2}(\Omega)$ denote the higher order finite element space which consists of piecewise polynomials of degree less or equal to p $(1 \leq r < p)$. We may obtain the following results: If $u \in H_0^1(\Omega) \cap H^{r+1+\alpha}(\Omega)$, Assumption $R(\Omega)$ holds and $u^{h,2}$ is obtained by Algorithm A, then

$$\begin{aligned}\|P_{h,2}u - u^{h,2}\|_{1,D} &\lesssim |\lambda_{h,1} - \lambda| + \|P_{h,2}u - u_{h,1}\|_{0,\Omega} + h^{\gamma}\|u - u_{h,1}\|_{1,\Omega} \\ &\lesssim h_{\Omega}^{r+\gamma}.\end{aligned}$$

Moreover, if $u \in H_0^1(\Omega) \cap H^{r+1+\alpha}(\Omega) \cap H^{p+1}(\Omega_0)$, then

$$\|u - u^{h,2}\|_{1,D} \lesssim h_{\Omega_0}^{p} + h_{\Omega}^{r+\gamma}.$$

If $(\lambda^{h,2}, u^{h,2})$ is obtained by Algorithm C, we may also have

$$\|u - u^{h,2}\|_{1,\Omega} \lesssim h^{r+\min(\gamma,\alpha)}$$

and

$$|\lambda - \lambda^{h,2}| \lesssim h^{2(r+\min(\gamma,\alpha))}.$$

It should be mentioned that it may not be so easy to obtain the above results if Ω is a domain with curved boundary. The reason is that the standard high order finite

element approximations may be polluted near the boundary. In order to maintain the high accuracy of higher order finite element discretizations, we need some other strategies on the boundary (c.f. [8, 24, 25, 33]).

In this paper, we have used a simple second order elliptic model problem to demonstrate how to use a lower order finite element space to capture the global component of the higher order finite element eigenvalue approximation and then carry out the major computation in the higher order finite element space locally. We believe that this local computational approach is a powerful technique in obtaining highly accurate approximations. Indeed, such a approach has been applied to quantum chemistry computations successfully, in which highly accurate approximations to Kohn-Sham equations can be achieved, and obtain very satisfying results. For its applications to quantum chemistry, however, there are many practical issues, including the implementation details for local density approximations, self-consistent iterations and pseudopotentials, that need to be addressed. We will report these results in our forthcoming papers.

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