Convergence and Optimal Complexity of Adaptive Finite Element Methods

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Abstract

In this paper, we study adaptive finite element approximations in a perturbation framework, which makes use of the existing adaptive finite element analysis of a linear symmetric elliptic problem. We prove the convergence and complexity of adaptive finite element methods for a class of elliptic partial differential equations. For illustration, we apply the general approach to obtain the convergence and complexity of adaptive finite element methods for a nonsymmetric problem, a nonlinear problem as well as an unbounded coefficient eigenvalue problem.

Keywords: Adaptive finite element, convergence, complexity, eigenvalue, nonlinear, nonsymmetric, unbounded.

AMS subject classifications: 65N15, 65N25, 65N30

1 Introduction

The purpose of this paper is to study the convergence and complexity of adaptive finite element computations for a class of elliptic partial differential equations of second order and to apply our general approach to three problems: a nonsymmetric problem, a nonlinear problem, and an eigenvalue problem with an unbounded coefficient. One technical tool for motivating this work is the relationship between the general problem and a linear symmetric elliptic problem, which is derived from some perturbation arguments (see Theorem 3.1 and Lemma 3.2).

Since Babuška and Vogelius [3] gave an analysis of an adaptive finite element method (AFEM) for linear symmetric elliptic problems in 1D, there are

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a number of work on the convergence and complexity of adaptive finite element methods in the literature. For instance, Dörfler [10] presented the first multidimensional convergence result, which has been improved and generalized in [6, 9, 17, 18, 20, 23]. For a nonsymmetric problem, in particular, Mekchay and Nochetto [17] imposed a quasi-orthogonality property instead of the Pythagoras equality to prove the convergence of AFEM while Morin, Siebert, and Veeser [20] showed the convergence of error and estimator simultaneously with the strict error reduction and derived the convergence of the estimator by exploiting the (discrete) local lower but not the upper bound. To our best knowledge, however, there has been no any work on the complexity of AFEM for nonsymmetric elliptic problems in the literature. In this paper, we can get the convergence and optimal complexity of nonsymmetric problems from our general approach. For a nonlinear problem, Chen, Holst and Xu [7] proved the convergence of an adaptive finite element algorithm for Poisson-Boltzmann equation while we are able to obtain the convergence and optimal complexity of AFEM for a class of nonlinear problems now. For a smooth coefficient eigenvalue problem, Dai, Xu, and Zhou [9] gave the convergence and optimal complexity of AFEM for symmetric elliptic eigenvalue problems with piecewise smooth coefficients (see, also convergence analysis of a special case [12, 13]). In this paper we will derive similar results for unbounded coefficient eigenvalue problems from our general conclusions, too. We mention that a similar perturbation approach was used in [9].

This paper is organized as follows. In section 2 we review some existing results on the convergence and complexity analysis of AFEM for the typical problem. In section 3 we generalize results to a general model problem by using a perturbation argument. In section 4 and section 5, we provide three typical applications for illustration, including theory and numerics.

2 Adaptive FEM for a typical problem

In this section, we review some existing results on the convergence and complexity analysis of AFEM for a boundary value problem in the literature.

Let $\Omega \subset \mathbb{R}^d (d \geq 2)$ be a bounded polytopic domain. We shall use the standard notation for Sobolev spaces $W^{s,p}(\Omega)$ and their associated norms and seminorms, see, e.g., [11, 12]. 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 understood in the sense of trace, $\| \cdot \|_{s,\Omega} = \| \cdot \|_{s,2,\Omega}$. Throughout this paper, we shall use $C$ to denote a generic positive constant which may stand for different values at its different occurrences. We will also use $A \lesssim B$ to mean that $A \leq CB$ for some constant $C$ that is independent of mesh parameters. All constants involved are independent of mesh sizes.
2.1 A boundary value problem

Consider a homogeneous boundary value problem:

\[
\begin{aligned}
Lu := \nabla \cdot (A \nabla u) &= f \quad \text{in } \Omega, \\
u &= 0 \quad \text{on } \partial \Omega,
\end{aligned}
\]

(2.1)

where \( A : \Omega \to \mathbb{R}^{d \times d} \) is piecewise Lipschitz over initial triangulation \( T_0 \), for \( x \in \Omega \) matrix \( A(x) \) is symmetric and positive definite with smallest eigenvalue uniformly bounded away from 0, and \( f \in L^2(\Omega) \).

**Remark 2.1** The choice of homogeneous boundary condition is made for ease of presentation, since similar results are valid for other boundary conditions [6].

The weak form of (2.1) reads as follows: Find \( u \in H^1_0(\Omega) \) such that

\[
a(u, v) = (f, v) \quad \forall v \in H^1_0(\Omega),
\]

(2.2)

where \( a(\cdot, \cdot) = (A \nabla \cdot, \nabla \cdot) \). It is seen that \( a(\cdot, \cdot) \) is bounded and coercive on \( H^1_0(\Omega) \), i.e., for any \( w, v \in H^1(\Omega) \) there exist constants \( 0 < c_a \leq C_a < \infty \) such that

\[
|a(w, v)| \leq C_a \|w\|_{1,\Omega} \|v\|_{1,\Omega} \quad \text{and} \quad c_a \|v\|_{1,\Omega}^2 \leq a(v, v) \quad \forall v \in H^1_0(\Omega).
\]

The energy norm \( \| \cdot \|_{a,\Omega} \), which is equivalent to \( \| \cdot \|_{1,\Omega} \), is defined by \( \|w\|_{a,\Omega} = \sqrt{a(w, w)} \). It is known that (2.2) is well-posed, that is, there exists a unique solution for any \( f \in H^{-1}(\Omega) \).

Let \( \{T_h\} \) be a shape regular family of nested conforming meshes over \( \Omega \): there exists a constant \( \gamma^* \) such that

\[
\frac{h_{\tau}}{\rho_{\tau}} \leq \gamma^* \quad \forall \tau \in \bigcup_h T_h,
\]

where, for each \( \tau \in T_h \), \( h_{\tau} \) is the diameter of \( \tau \), \( \rho_{\tau} \) is the diameter of the biggest ball contained in \( \tau \), and \( h = \max_{\tau \in T_h} h_{\tau} \). Let \( E_h \) denote the set of interior sides (edges or faces) of \( T_h \). Let \( S^h_0(\Omega) \subseteq H^1_0(\Omega) \) be a family of nested finite element spaces consisting of continuous piecewise polynomials over \( T_h \) of fixed degree \( n \geq 1 \), which vanish on \( \partial \Omega \).

Define the Galerkin-projection \( P_h : H^1_0(\Omega) \to S^h_0(\Omega) \) by

\[
a(u - P_h u, v) = 0 \quad \forall v \in S^h_0(\Omega).
\]

(2.3)

For any \( u \in H^1_0(\Omega) \), there apparently hold:

\[
\|P_h u\|_{a,\Omega} \lesssim \|u\|_{a,\Omega} \quad \text{and} \quad \lim_{h \to 0} \|u - P_h u\|_{a,\Omega} = 0.
\]

Now we introduce the following quantity:

\[
\rho_\omega(h) = \sup_{f \in L^2(\Omega), \|f\|_{a,\Omega} = 1} \inf_{v \in S^h_0(\Omega)} \|L^{-1} f - v\|_{a,\Omega},
\]
then \( \rho_\Omega(h) \to 0 \) as \( h \to 0 \) (see, e.g., [28]).

A standard finite element scheme for (2.2) is: Find \( u_h \in S_h^0(\Omega) \) satisfying
\[
a(u_h, v) = (f, v) \quad \forall v \in S_h^0(\Omega). \tag{2.4}
\]

By definition (2.3), we know that \( u_h = P_h u \).

By a contradiction argument, we have (c.f., e.g., [30])

**Lemma 2.1** As operators over \( H^1_0(\Omega) \), there holds
\[
\lim_{h \to 0} \| K(I - P_h) \| = 0
\]
if \( K \) is a compact operator over \( H^1_0(\Omega) \).

### 2.2 Adaptive algorithm

Given an initial triangulation \( T_0 \), we shall generate a sequence of nested conforming triangulations \( T_k \) using the following loop:

**SOLVE \to ESTIMATE \to MARK \to REFINE.**

More precisely to get \( T_{k+1} \) from \( T_k \) we first solve the discrete equation to get \( u_k \) on \( T_k \). The error is estimated using \( u_k \) and used to mark a set of elements that are to be refined. Elements are refined in such a way that the triangulation is still shape regular and conforming. We assume that the solutions of finite-dimensional problems can be solved to any accuracy efficiently.\(^1\) Examples of such optimal solvers are multigrid method or multigrid-based preconditioned conjugate gradient method.

Now we review the residual type a posteriori error estimators for finite element solutions of (2.1). Let \( T \) denote the class of all conforming refinements by bisection of \( T_0 \). For \( T_h \in T \) and any \( v \in S_h^0(\Omega) \) we define the element residual \( \tilde{R}_\tau(v) \) and the jump residual \( \tilde{J}_e(v) \) by
\[
\tilde{R}_\tau(v) := f - L v = f + \nabla \cdot (A \nabla v) \quad \text{in } \tau \in T_h,
\]
\[
\tilde{J}_e(v) := -A \nabla v^+ \cdot \nu^+ - A \nabla v^- \cdot \nu^- := [[A \nabla v]]_e \cdot \nu_e \quad \text{on } e \in E_h,
\]
where \( e \) is the common side of elements \( \tau^+ \) and \( \tau^- \) with unit outward normals \( \nu^+ \) and \( \nu^- \), respectively, and \( \nu_e = \nu^- \).

Let \( \omega_e \) be the union of elements which share the side \( e \) and \( \omega_\tau \) be the union of elements sharing a side with \( \tau \).

For \( \tau \in T_h \), we define the local error indicator \( \tilde{\eta}_h(v, \tau) \) by
\[
\tilde{\eta}_h^2(v, \tau) := h_\tau^2 \| \tilde{R}_\tau(v) \|_{0, \tau}^2 + \sum_{e \in \partial \tau, e \subset \partial \tau} h_e \| \tilde{J}_e(v) \|_{0, e}^2
\]
and the oscillation \( \tilde{\text{osc}}_h(v, \tau) \) by
\[
\tilde{\text{osc}}_h^2(v, \tau) := h_\tau^2 \| \tilde{R}_\tau(v) - \tilde{R}_\tau(v) \|_{0, \tau}^2 + \sum_{e \in \partial \tau, e \subset \partial \tau} h_e \| \tilde{J}_e(v) - \tilde{J}_e(v) \|_{0, e}^2,
\]

\(^1\)By the similar perturbation argument, indeed, it will be seen that some approximations to the finite-dimensional problem will be sufficient.
where $\mathbf{w}$ is the $L^2$-projection of $w \in L^2(\Omega)$ to polynomials of some degree on $\tau$ or $e$.

Given a subset $\omega \subset \Omega$, we define the error estimator $\tilde{\eta}_h(v, \omega)$ and the oscillation $\tilde{\text{o}sc}_h(v, \omega)$ by

\[
\tilde{\eta}_h^2(v, \omega) := \sum_{\tau \in T_h, \tau \subset \omega} \tilde{\eta}_h^2(v, \tau) \quad \text{and} \quad \tilde{\text{o}sc}_h^2(v, \omega) := \sum_{\tau \in T_h, \tau \subset \omega} \tilde{\text{o}sc}_h^2(v, \tau).
\]

For $\tau \in T_h$, we also need notation

\[
\eta_h^2(A, \tau) := h_{\tau}^2(\|\text{div}A\|_{0, \infty, \tau}^2 + h_{\tau}^{-2}\|A\|_{0, \infty, \omega}^2),
\]

and

\[
osc_h^2(A, \tau) := h_{\tau}^2(\|\text{div}A - \overline{\text{div}A}\|_{0, \infty, \tau}^2 + h_{\tau}^{-2}\|A - \overline{A}\|_{0, \infty, \omega}^2),
\]

where $\overline{A}$ is the best $L^\infty$-approximation in the space of discontinuous polynomials of some degree.

Given a subset $\omega \subset \Omega$ we finally set

\[
\eta_h(A, \omega) := \max_{\tau \in T_h, \tau \subset \omega} \eta_h(A, \tau) \quad \text{and} \quad osc_h(A, \omega) := \max_{\tau \in T_h, \tau \subset \omega} osc_h(A, \tau).
\]

We now recall the well-known upper and lower bounds for the energy error in terms of the residual-type estimator (see, e.g., [17, 19, 26]).

**Theorem 2.1** (Global a posteriori upper and lower bounds). Let $u \in H^1_0(\Omega)$ be the solution of (2.2) and $u_h \in S_h^0(\Omega)$ be the solution of (2.4). Then there exist constants $\tilde{C}_1, \tilde{C}_2$ and $\tilde{C}_3 > 0$ depending only on the shape regularity $\gamma^*$, $C_a$ and $c_a$ such that

\[
\|u - u_h\|_{a, \Omega}^2 \leq \tilde{C}_1 \tilde{\eta}_h^2(u_h, T_h)
\]

(2.5)

and

\[
\tilde{C}_2 \tilde{\eta}_h^2(u_h, T_h) \leq \|u - u_h\|_{a, \Omega}^2 + \tilde{C}_3 \tilde{\text{o}sc}_h^2(u_h, T_h).
\]

(2.6)

We replace the subscript $h$ by an iteration counter called $k$ and call the adaptive algorithm without oscillation marking as **Algorithm $D_0$**, which is defined as follows:

1. Choose a parameter $0 < \theta < 1$ :
   
   1. Pick any initial mesh $T_0$, and let $k = 0$.
   2. Solve the system on $T_0$ for the discrete solution $u_0$.
   3. Compute the local indicators $\tilde{\eta}_k$.
   4. Construct $\mathcal{M}_k \subset T_k$ by **Marking Strategy $E_0$** and parameter $\theta$.
   5. Refine $T_k$ to get a new conforming mesh $T_{k+1}$ by Procedure **REFINE**.
6. Solve the system on \( T_{k+1} \) for the discrete solution \( u_{k+1} \).

7. Let \( k = k + 1 \) and go to Step 3.

The marking strategy, which we call \textbf{Marking Strategy} \( E_0 \), is crucial for our adaptive methods. Now it can be stated by:

Given a parameter \( 0 < \theta < 1 \):

1. Construct a minimal subset \( \mathcal{M}_k \) of \( T_k \) by selecting some elements in \( T_k \) such that
   \[
   \tilde{\eta}_k(u_k, \mathcal{M}_k) \geq \theta \tilde{\eta}_k(u_k, T_k).
   \]

2. Mark all the elements in \( \mathcal{M}_k \).

Due to [6], the procedure \textsc{Refine} here is not required to satisfy the Interior Node Property of [17, 19].

Given a fixed number \( b \geq 1 \), for any \( T_k \in T \) and a subset \( \mathcal{M}_k \subset T_k \) of marked elements,

\[
T_{k+1} = \textsc{Refine}(T_k, \mathcal{M}_k)
\]

outputs a conforming triangulation \( T_{k+1} \in T \), where at least all elements of \( \mathcal{M}_k \) are bisected \( b \) times. We define \( R_{T_k \rightarrow T_{k+1}} := T_k \setminus (T_k \cap T_{k+1}) \) as the set of refined elements, thus \( \mathcal{M}_k \subset R_{T_k \rightarrow T_{k+1}} \).

\textbf{Lemma 2.2 (Complexity of Refine).} Assume that \( T_0 \) verifies condition (b) of section 4 in [27]. For \( k \geq 0 \) let \( \{T_k\}_{k \geq 0} \) be any sequence of refinements of \( T_0 \) where \( T_{k+1} \) is generated from \( T_k \) by \( T_{k+1} = \textsc{Refine}(T_k, \mathcal{M}_k) \) with a subset \( \mathcal{M}_k \subset T_k \). Then

\[
\#T_k - \#T_0 \lesssim \sum_{j=0}^{k-1} \#\mathcal{M}_j \quad \forall k \geq 1 \tag{2.7}
\]

is valid, where the hidden constant depends on \( T_0 \) and \( b \).

The convergence of \textbf{Algorithm} \( D_0 \) is shown in [6].

\textbf{Theorem 2.2} Let \( \{u_k\}_{k \in \mathbb{N}_0} \) be a sequence of finite element solutions corresponding to a sequence of nested finite element spaces \( \{S^k(\Omega)\}_{k \in \mathbb{N}_0} \) produced by \textbf{Algorithm} \( D_0 \). Then there exist constants \( \tilde{\gamma} > 0 \) and \( \xi \in (0, 1) \) depending only on the shape regularity of meshes, the data and the marking parameter \( \theta \), such that for any two consecutive iterates we have

\[
\|u - u_{k+1}\|_{a, \Omega}^2 + \tilde{\gamma} \tilde{\eta}^2_{k+1}(u_{k+1}, T_{k+1}) \\
\leq \xi^2 (\|u - u_k\|_{a, \Omega}^2 + \tilde{\gamma} \tilde{\eta}^2_k(u_k, T_k)).
\]

Indeed, constant \( \tilde{\gamma} \) has the following form

\[
\tilde{\gamma} := \frac{1}{(1 + \delta^{-1}) \Lambda_1 \eta_0^2(\mathbf{A}, T_0)}, \tag{2.8}
\]

where \( \eta_0^2(\mathbf{A}, T_0) := \eta_0^2(\mathbf{A}, T_0), \Lambda_1 := (d + 1)C_0^2/c_a \) with \( C_0 \) some positive constant and constant \( \delta \in (0, 1) \).
Following [6, 9], we have a link between nonlinear approximation theory and the AFEM through the marking strategy as follows.

**Lemma 2.3 (Optimal Marking).** Let \( u_k \in S_0^k(\Omega) \) and \( u_{k+1} \in S_0^{k+1}(\Omega) \) be finite element solutions of (2.2) over a conforming mesh \( T_k \) and its refinement \( T_{k+1} \) with marked element \( M_k \). Suppose that they satisfy the decrease property

\[
\|u - u_{k+1}\|^2_{a,\Omega} + \gamma_4 \tilde{\text{osc}}_k^2(u_{k+1}, T_{k+1}) \\
\leq \beta_k^2 (\|u - u_k\|^2_{a,\Omega} + \gamma_4 \tilde{\text{osc}}_k^2(u_k, T_k))
\]

with constants \( \gamma_4 > 0 \) and \( \beta_k \in (0, \sqrt{\frac{1}{2}}) \). Then the set \( R := R_{T_k \rightarrow T_{k+1}} \) satisfies the following inequality

\[
\hat{\eta}_k(u_k, R) \geq \hat{\theta} \tilde{\eta}_k(u_k, T_k)
\]

with \( \hat{\theta}^2 = \frac{\bar{C}_2(1-2\tilde{\beta}^2)}{\bar{C}_0(C_1(1+2C_1\gamma_4))} \), where \( C = \Lambda_1 \text{osc}_0^2(A, T_0) \) and \( \bar{C}_0 = \max(1, \frac{\bar{C}_3 \gamma_4}{\gamma_4}) \).

### 3 A general framework

Let \( u \in H^1_0(\Omega) \) satisfy

\[
a(u, v) + (V u, v) = (\ell u, v) \quad \forall v \in H^1_0(\Omega), \tag{3.9}
\]

where \( \ell : H^1_0(\Omega) \rightarrow L^2(\Omega) \) is a bounded operator and \( V : H^1_0(\Omega) \rightarrow L^2(\Omega) \) is a linear bounded operator.

Let \( K : L^2(\Omega) \rightarrow H^1_0(\Omega) \) be the operator defined by

\[
a(Kw, v) = (w, v) \quad \forall w, v \in L^2(\Omega).
\]

Then \( K \) is a compact operator and (3.9) becomes as

\[
u + KV u = K\ell u.
\]

Let \( u_h \in S^h_0(\Omega) \) be a solution of discretization

\[
a(u_h, v) + (V u_h, v) = (\ell_h u_h, v) \quad \forall v \in S^h_0(\Omega), \tag{3.10}
\]

where \( \ell_h : S^h_0(\Omega) \rightarrow L^2(\Omega) \) is some bounded operator. Note that we may view \( \ell_h \) as a perturbation to \( \ell \), for which we assume that there exists \( \kappa_1(h) \in (0, 1) \) such that

\[
\|K(\ell u - \ell_h u_h)\|_{a,\Omega} = O(\kappa_1(h))\|u - u_h\|_{a,\Omega}, \tag{3.11}
\]

where \( \kappa_1(h) \rightarrow 0 \) as \( h \rightarrow 0 \).

Note that (3.10) can be written as

\[
u_h + P_h KV u_h = P_h K\ell_h u_h,
\]

where \( P_h \) is defined by (2.23). We have for \( w^h = K\ell_h u_h - KV u_h \) that

\[
u_h = P_h w^h. \tag{3.12}
\]
Theorem 3.1 There exists \( \kappa(h) \in (0, 1) \) such that \( \kappa(h) \to 0 \) as \( h \to 0 \) and
\[
\|u - u_h\|_{a, \Omega} = \|w^h - P_h w^h\|_{a, \Omega} + \mathcal{O}(\kappa(h))\|u - u_h\|_{a, \Omega}.
\] (3.13)

Proof. By definition, we have
\[
u - w^h = K\ell u - KV u - (K\ell_h u_h - KV u_h) = K(\ell u - \ell_h u_h) + KV(u_h - u).
\]

Let \( \kappa_2(h) = \|KV(I - P_h)\|_a \). Since \( KV : H^1_0(\Omega) \to H^1_0(\Omega) \) is compact, we get from Lemma 2.1 that \( \kappa_2(h) \to 0 \) as \( h \to 0 \). Note that
\[
KV(u_h - u) = KV(I - P_h)(u_h - u),
\]
we obtain
\[
\|KV(u_h - u)\|_{a, \Omega} = \mathcal{O}(\kappa_2(h))\|u - u_h\|_{a, \Omega}.
\] (3.14)

Set \( \kappa(h) = \kappa_1(h) + \kappa_2(h) \), we have that \( \kappa(h) \to 0 \) as \( h \to 0 \) and
\[
\|u - w^h\|_{a, \Omega} \leq \hat{C}\kappa(h)\|u - u_h\|_{a, \Omega}.
\] (3.15)

Since (3.12) implies
\[
u - u_h = w^h - P_h w^h + u - w^h,
\]
we get (3.13) from (3.15). This completes the proof.

Theorem 3.1 sets up a relationship between the error estimates of finite element approximations of the general problem and the associated typical finite element boundary value solutions, from which various a posteriori error estimators for the general problem can be easily obtained since the a posteriori error estimators for the typical boundary value problem have been well-constructed. In fact, Theorem 3.1 implies that up to the high order term, the error of the general problem is equivalent to that of the typical problem with \( \ell_h u_h - V u_h \) as a source term. However, the high order term cannot be estimated easily in the analysis of convergence and optimal complexity of AFEM for the general problem, for instance, for a nonsymmetric problem, a nonlinear problem and an unbounded coefficient eigenvalue problem.

3.1 Adaptive algorithm

Following the element residual \( \hat{R}_\tau(u_h) \) and the jump residual \( \hat{J}_e(u_h) \) for (2.4), we define the element residual \( R_\tau(u_h) \) and the jump residual \( J_e(u_h) \) for (3.10) as follows:
\[
R_\tau(u_h) := \ell_h u_h - V u_h - L u_h = \ell_h u_h - V u_h + \nabla \cdot (A\nabla u_h) \quad \text{in} \; \tau \in \mathcal{T}_h,
\]
\[
J_e(u_h) := -A\nabla u_h^+ \cdot \nu^+ - A\nabla u_h^- \cdot \nu^- := [[A\nabla u_h]]_e \cdot \nu_e \quad \text{on} \; e \in \mathcal{E}_h.
\]

For \( \tau \in \mathcal{T}_h \), we define the local error indicator \( \eta_h(u_h, \tau) \) by
\[
\eta_h^2(u_h, \tau) := h_\tau^2 \|R_\tau(u_h)\|_{0, \tau}^2 + \sum_{e \in \mathcal{E}_h, e \subset \partial \tau} h_e \|J_e(u_h)\|_{0, e}^2
\]

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and the oscillation $\text{osc}_h(u_h, \tau)$ by

$$\text{osc}_h^2(u_h, \tau) := h^2 \| R_\tau(u_h) - R_\tau(u_h) \|_{0, \tau}^2 + \sum_{e \in \mathcal{E}_h, \tau \subset \partial e} h_e \| J_e(u_h) - J_e(u_h) \|_{0, e}^2,$$

where $e$, $\nu^+$ and $\nu^-$ are defined as those in section 2.

Given a subset $\omega \subset \Omega$, we define the error estimator $\eta_h(u_h, \omega)$ by

$$\eta^2_h(u_h, \omega) := \sum_{\tau \in \mathcal{J}_h, \tau \subset \omega} \eta^2_h(u_h, \tau) \quad (3.16)$$

and the oscillation $\text{osc}_h(u_h, \omega)$ by

$$\text{osc}_h^2(u_h, \omega) := \sum_{\tau \in \mathcal{J}_h, \tau \subset \omega} \text{osc}_h^2(u_h, \tau). \quad (3.17)$$

Let $h_0 \in (0, 1)$ be the mesh size of the initial mesh $\mathcal{T}_0$ and define

$$\tilde{\kappa}(h_0) := \sup_{h \in (0, h_0)} \kappa(h).$$

Obviously, $\tilde{\kappa}(h_0) \ll 1$ if $h_0 \ll 1$.

To analyze the convergence and complexity of finite element approximations, we need to establish some relationship between the two level approximations. We use $T_H$ to denote a coarse mesh and $T_h$ to denote a refined mesh of $T_H$. Recall that $u^h = K(\ell_h u_h - V u_h)$ and $w^H = K(\ell_H u_H - V u_H)$.

**Lemma 3.1** Let $h, H \in (0, h_0]$, then

$$\| u - u_h \|_{a, \Omega} = \| u^H - P_h w^H \|_{a, \Omega} + O(\tilde{\kappa}(h_0))(\| u - u_h \|_{a, \Omega} + \| u - u^H \|_{a, \Omega}), (3.18)$$

$$\eta_h(u_h, T_h) = \eta_h(P_h w^H, T_h) + O(\tilde{\kappa}(h_0))(\| u - u_h \|_{a, \Omega} + \| u - u^H \|_{a, \Omega}), \quad (3.19)$$

and

$$\text{osc}_h(u_h, T_h) = \tilde{\text{osc}}_h(P_h w^H, T_h) + O(\tilde{\kappa}(h_0))(\| u - u_h \|_{a, \Omega} + \| u - u^H \|_{a, \Omega}) \quad (3.20)$$

**Proof.** First, we prove (3.18). It follows that

$$\| P_h(u^h - w^H) + u - w^H \|_{a, \Omega} \lesssim \| u^h - w^H \|_{a, \Omega} + \| u - w^H \|_{a, \Omega} \lesssim \| u - w^H \|_{a, \Omega} + \| u - w^h \|_{a, \Omega},$$

which together with (3.15) implies

$$\| P_h(u^h - w^H) + w^H - u \|_{a, \Omega} \lesssim \kappa(H)\| u - u_H \|_{a, \Omega} + \kappa(h)\| u - u_h \|_{a, \Omega}.$$

Namely,

$$\| P_h(u^h - w^H) + w^H - u \|_{a, \Omega} \lesssim \tilde{\kappa}(h_0)(\| u - u_H \|_{a, \Omega} + \| u - u_h \|_{a, \Omega}). \quad (3.21)$$
Observing that identity (3.12) leads to
\[ u - u_h = w^H - P_h w^H + P_h (w^H - w^h) + u - w^H, \]
we then obtain (3.18) from (3.21).

Next, we turn to prove (3.20). Due to \( L w^h = \ell_h u_h - V u_h \) and \( L w^H = \ell_H u_H - V u_H \), we know that \( w^h - w^H \) is the solution of typical boundary value problem with \( \ell_h u_h - \ell_H u_H + V u_H - V u_h \) as a source term. Since
\[ \tilde{R}_r (P_h (w^h - w^H)) = \ell_h u_h - \ell_H u_H + V u_H - V u_h - L (P_h (w^h - w^H)), \]
we have
\[
\begin{align*}
\widetilde{osc}_h^2 (P_h (w^h - w^H), T_h) &= \sum_{\tau \in T_h} \widetilde{osc}_h^2 (E, \tau) \\
&= \sum_{\tau \in T_h} (h^2_r \| \tilde{R}_r (E) - \tilde{R}_r (E) \|_0^2 + \sum_{e \in \partial \tau} h_e \| \tilde{J}_e (E) - \tilde{J}_e (E) \|_{0,e}^2) \\
&\leq \sum_{\tau \in T_h} h^2_r \| \tilde{R}_r (E) + LE - (\tilde{R}_r (E) + LE) \|_0^2 \\
&\quad + \sum_{\tau \in T_h} (h^2_r \| LE - LE \|_0^2 + \sum_{e \in \partial \tau} h_e \| \tilde{J}_e (E) - \tilde{J}_e (E) \|_{0,e}^2), \quad (3.22)
\end{align*}
\]
where \( E = P_h (w^h - w^H) \). Following the proof of Proposition 3.3 in [6], we see that
\[
\sum_{\tau \in T_h} (h^2_r \| LE - LE \|_0^2 + \sum_{e \in \partial \tau} h_e \| \tilde{J}_e (E) - \tilde{J}_e (E) \|_{0,e}^2)
\]
can be bounded by
\[
\sum_{\tau \in T_h} C_0^2 osc_h^2 (A, \tau) \| P_h (w^h - w^H) \|_{1,\omega, \tau}^2 \lesssim osc_h^2 (A, T_h) \| P_h (w^h - w^H) \|_{a,\Omega}^2.
\]

Hence using the fact \( osc_h (A, T_h) \leq osc_0 (A, T_0) \), we obtain
\[
\sum_{\tau \in T_h} (h^2_r \| LE - LE \|_0^2 + \sum_{e \in \partial \tau} h_e \| \tilde{J}_e (E) - \tilde{J}_e (E) \|_{0,e}^2)
\]
\[
\lesssim osc_h^2 (A, T_0) \| P_h (w^h - w^H) \|_{a,\Omega}^2. \quad (3.23)
\]

Using the inverse inequality, the bounded property of \( V \) and (3.11), we get
\[
\begin{align*}
&\left( \sum_{\tau \in T_h} (h^2_r \| \tilde{R}_r (E) + LE - (\tilde{R}_r (E) + LE) \|_0^2) \right)^{1/2} \\
&\lesssim \left( \sum_{\tau \in T_h} \| h_r (\ell_h u_h - \ell_H u_H + V u_H - V u_h) \|_{0,\tau}^2 \right)^{1/2} \\
&\lesssim \| K (\ell_h u_h - \ell_H u_H) \|_{a,\Omega} + \| h u_H - u_h \|_{a,\Omega} \\
&\lesssim \| K (\ell_h u_h - \ell u) \|_{a,\Omega} + \| K (\ell_h u_H - \ell u) \|_{a,\Omega} \\
&\quad + h \| u - u_H \|_{a,\Omega} + h \| u - u_h \|_{a,\Omega} \\
&\lesssim \tilde{K} (h_0) \left( \| u - u_h \|_{a,\Omega} + \| u - u_H \|_{a,\Omega} \right).
\end{align*}
\]
Note that

\[ \| P_h(u^h - w^H)\|_{\alpha,\Omega} \lesssim \| u^h - w^H \|_{\alpha,\Omega} \]

which together with (3.15) implies

\[ \| P_h(u^h - w^H)\|_{\alpha,\Omega} \lesssim \kappa(h_0) \left( \| u - u_h \|_{\alpha,\Omega} + \| u - u_H \|_{\alpha,\Omega} \right). \] (3.25)

Combining (3.22), (3.23), (3.24) and (3.25), we conclude that

\[ \widetilde{\text{osc}}_h(P_h(w^h - w^H), T_h) \lesssim \kappa(h_0) \left( \| u - u_h \|_{\alpha,\Omega} + \| u - u_H \|_{\alpha,\Omega} \right). \] (3.26)

Due to \( u = P_h w^H + P_h (w^h - w^H) \), we obtain from the definition of oscillation that

\[ \widetilde{\text{osc}}_h(P_h w^h, T_h) \leq \widetilde{\text{osc}}_h(P_h w^H, T_h) + \widetilde{\text{osc}}_h(P_h (w^h - w^H), T_h). \] (3.27)

Hence from \( \widetilde{\text{osc}}_h(u_h, T_h) = \text{osc}_h(u_h, T_h) \), (3.26) and (3.27), we arrive at (3.20).

Finally, we prove (3.19). By (2.6) and (3.26), we have

\[ \tilde{\eta}_h(P_h w^h, T_h) = \tilde{\eta}_h(P_h w^H + P_h (w^h - w^H), T_h), \]

we obtain

\[ \tilde{\eta}_h(P_h w^h, T_h) = \tilde{\eta}_h(P_h w^H, T_h) + O(\kappa(h_0)) \left( \| u - u_h \|_{\alpha,\Omega} + \| u - u_H \|_{\alpha,\Omega} \right), \]

which is nothing but (3.19) since \( \tilde{\eta}_h(P_h w^h, T_h) = \eta_h(u_h, T_h) \).

**Theorem 3.2** Let \( h_0 \ll 1 \) and \( h \in (0, h_0] \). There exist constants \( C_1, C_2 \) and \( C_3 \), which only depend on the shape regularity constant \( \gamma^* \), \( C_a \) and \( c_a \) such that

\[ \| u - u_h \|_{\alpha,\Omega}^2 \leq C_1 \eta_h^2(u_h, T_h) \] (3.29)

and

\[ C_2 \eta_h^2(u_h, T_h) \leq \| u - u_h \|_{\alpha,\Omega}^2 + C_3 \text{osc}_h^2(u_h, T_h). \] (3.30)
Proof. Recall that \( L^h w = \ell_h u_h - V u_h \). From (2.5) and (2.6) we have

\[
\| w^h - P_h w^h \|_{a,\Omega}^2 \leq \tilde{C}_1 \hat{\eta}_h^2(P_h w^h, T_h)
\]

and

\[
\tilde{C}_2 \hat{\eta}_h^2(P_h w^h, T_h) \leq \| w^h - P_h w^h \|_{a,\Omega}^2 + \tilde{C}_3 \text{osc}_h^2(P_h w^h, T_h).
\]

Thus we obtain (3.29) and (3.30) from (3.12), (3.13), (3.31) and (3.32). In particular, we may choose \( C_1, C_2 \) and \( C_3 \) satisfying

\[
C_1 = \tilde{C}_1 (1 + \tilde{C}\kappa(h_0))^2, \quad C_2 = \tilde{C}_2 (1 - \tilde{C}\kappa(h_0))^2, \quad C_3 = \tilde{C}_3 (1 - \tilde{C}\kappa(h_0))^2.
\]

**Remark 3.1** The requirement \( h_0 \ll 1 \) is somehow reasonable for finite element approximations of (3.9). We can refer to [17] for the initial mesh size requirement in adaptive finite element computations for nonsymmetric boundary value problems.

Now we address step MARK of solving (3.10) in detail, which we call **Marking Strategy E**. Similar to **Marking Strategy E\(_0\)** for (2.4), we define **Marking Strategy E** for (3.10) to enforce error reduction as follows:

Given a parameter \( 0 < \theta < 1 \):

1. Construct a minimal subset \( M_k \) of \( T_k \) by selecting some elements in \( T_k \) such that

\[
\eta_k(u_k, M_k) \geq \theta \eta_k(u_k, T_k).
\]

2. Mark all the elements in \( M_k \).

The adaptive algorithm of solving (3.10), which we call **Algorithm D**, is nothing but **Algorithm D\(_0\)** when **Marking Strategy E\(_0\)** is replaced by **Marking Strategy E**.

### 3.2 Convergence

We now prove that **Algorithm D** of (3.10) is a contraction with respect to the sum of the energy error plus the scaled error estimator.

**Theorem 3.3** Let \( \theta \in (0, 1) \) and \( \{u_k\}_{k \in \mathbb{N}_0} \) be a sequence of finite element solutions corresponding to a sequence of nested finite element spaces \( \{S_k(\Omega)\}_{k \in \mathbb{N}_0} \) produced by **Algorithm D**. Then there exist constants \( \gamma > 0 \) and \( \xi \in (0, 1) \) depending only on the shape regularity constant \( \gamma^*, C_a, c_a \) and the marking parameter \( \theta \) such that

\[
\| u - u_{k+1} \|_{a,\Omega}^2 + \gamma \eta_{k+1}^2(u_{k+1}, T_{k+1}) \leq \xi^2 (\| u - u_k \|_{a,\Omega}^2 + \gamma \eta_k^2(u_k, T_k)).
\]
Here,
\[
\gamma := \frac{\tilde{\gamma}}{1 - C_4 \delta_1^{-1} \bar{k}(h_0)}
\]  \hspace{1cm} (3.35)

with \( C_4 \) a positive constant, provided \( h_0 \ll 1 \).

**Proof.** For convenience, we use \( u_h, u_H \) to denote \( u_{k+1} \) and \( u_k \), respectively. Thus we only need to prove that for \( u_h \) and \( u_H \), there holds,
\[
\|u - u_h\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u_h, T_h) \leq \xi^2 (\|u - u_H\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u, T_h)).
\]

We conclude from Theorem 2.2, \( u \in H^1(\Omega) \), and identity \( \tilde{\gamma} > 0 \) and \( \xi \in (0,1) \) satisfying
\[
\|u - u_h\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u_h, T_h) \leq \xi^2 (\|u - u_H\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u, T_h)).
\]

Hence use the fact that \( u_H = P_H u_H \), we obtain
\[
\|u - u_H\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u, T_h) \leq \xi^2 (\|u - u_H\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u, T_h)).
\]  \hspace{1cm} (3.36)

By \( 3.18 \) and \( 3.19 \), there exists a constant \( \tilde{C} > 0 \) such that
\[
\|u - u_h\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u_h, T_h) \leq (1 + \delta_1) \|u - u_H\|_{a,\Omega} + (1 + \delta_1) \tilde{\gamma}^2 h_0^2 (P_H u_H, T_h)
\]
\[
+ \tilde{C}(1 + \delta_1^{-1}) \bar{k}^2 (h_0) (\|u - u_h\|_{a,\Omega} + \|u - u_H\|_{a,\Omega})
\]
\[
+ \tilde{C}(1 + \delta_1^{-1}) \bar{k}^2 (h_0) \tilde{\gamma} (\|u - u_h\|_{a,\Omega} + \|u - u_H\|_{a,\Omega})
\]
where the Young’s inequality is used and \( \delta_1 \in (0,1) \) satisfies
\[
(1 + \delta_1)^2 \xi^2 < 1.
\]  \hspace{1cm} (3.37)

It thus follows from \( 3.36 \), \( 3.19 \), and identity \( \tilde{\gamma} (P_H u_H, T_H) = \tilde{\gamma} (u, T_H) \) that there exists a positive constant \( C^* \) depending on \( \tilde{C} \) and \( \tilde{\gamma} \) such that
\[
\|u - u_h\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u_h, T_h) \leq (1 + \delta_1) \xi^2 \left( \|u - u_H\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u, T_h) \right)
\]
\[
+ C^* \delta_1^{-1} \bar{k}^2 (h_0) (\|u - u_h\|_{a,\Omega} + \|u - u_H\|_{a,\Omega})
\]
\[
\leq (1 + \delta_1) \xi^2 \left( (1 + \tilde{C}(h_0)) \|u - u_H\|_{a,\Omega} + \tilde{\gamma}^2 h_0^2 (u, T_H) \right)
\]
\[
+ C^* \delta_1^{-1} \bar{k}^2 (h_0) (\|u - u_h\|_{a,\Omega} + \|u - u_H\|_{a,\Omega}).
\]
Hence, if $h_0 \ll 1$, then there exists a positive constant $C_4$ depending on $C^*$ and $C$ such that

$$
\|u - u_h\|_{a, \Omega}^2 + \gamma \eta_H^2(u_h, T_h) + C_4 \mathfrak{k}(h_0)\|u - u_h\|_{a, \Omega}^2 + C_4 \delta^{-1}_1 \mathfrak{k}(h_0)\|u - u_h\|_{a, \Omega}^2.
$$

Consequently,

$$
(1 - C_4 \delta^{-1}_1 \mathfrak{k}(h_0))\|u - u_h\|_{a, \Omega}^2 + \gamma \eta_H^2(u_h, T_h)
\leq
((1 + \delta_1) \xi^2 + C_4 \mathfrak{k}(h_0))\|u - u_H\|_{a, \Omega}^2 + (1 + \delta_1) \xi^2 \gamma \eta_H^2(u_H, T_H),
$$

that is

$$
\|u - u_h\|_{a, \Omega}^2 + \gamma \eta_H^2(u_h, T_h)
\leq
\left(\frac{(1 + \delta_1) \xi^2 + C_4 \mathfrak{k}(h_0)}{1 - C_4 \delta^{-1}_1 \mathfrak{k}(h_0)}\right)^2
\|u - u_H\|_{a, \Omega}^2 + \gamma \eta_H^2(u_H, T_H).
$$

Since $h_0 \ll 1$ implies $\mathfrak{r}(h_0) \ll 1$, we have that the constant $\xi$ defined by

$$
\xi := \left(\frac{(1 + \delta_1) \xi^2 + C_4 \mathfrak{k}(h_0)}{1 - C_4 \delta^{-1}_1 \mathfrak{k}(h_0)}\right)^{1/2}
$$

satisfying $\xi \in (0, 1)$ if $h_0 \ll 1$. Therefore,

$$
\|u - u_h\|_{a, \Omega}^2 + \gamma \eta_H^2(u_h, T_h)
\leq
\xi^2 \left(\|u - u_H\|_{a, \Omega}^2 + \gamma \eta_H^2(u_H, T_H)\right).
$$

Finally, we arrive at (3.34) by using the fact that

$$
\frac{(1 + \delta_1) \xi^2 \gamma}{(1 + \delta_1) \xi^2 + C_4 \mathfrak{k}(h_0)} < \gamma.
$$

This completes the proof.

### 3.3 Complexity

We shall study the complexity in a class of functions defined by

$$
\mathcal{A}_{\gamma} := \{v \in H^1_0(\Omega) : |v|_{s, \gamma} < \infty\},
$$

where $\gamma > 0$ is some constant,

$$
|v|_{s, \gamma} = \sup_{\varepsilon > 0} \varepsilon \inf_{T_k \subset T_0} \inf \{\|v - v_k\|_{\Omega} + (\gamma + 1) \|v_k\|_{\Omega} + \|v_k\|_{\Omega} \}^{1/2},
$$

with

$$
\# T_k - \# T_0.
$$
and $\mathcal{T}_k \subset \mathcal{T}_0$ means $\mathcal{T}_k$ is a refinement of $\mathcal{T}_0$. It is seen from the definition that, for all $\gamma > 0$, $\mathcal{A}_k^{\gamma} = \mathcal{A}_k^\gamma$. For simplicity, here and hereafter, we use $\mathcal{A}^s$ to stand for $\mathcal{A}_s^1$, and use $|v|_s$ to denote $|v|_{s,\gamma}$. So $\mathcal{A}^s$ is the class of functions that can be approximated within a given tolerance $\varepsilon$ by continuous piecewise polynomial functions over a partition $\mathcal{T}_k$ with number of degrees of freedom $\# \mathcal{T}_k - \# \mathcal{T}_0 \lesssim \varepsilon^{-1/s}|v|_{1/s}^s$.

In order to give the proof of the complexity of Algorithm D for solving (3.10), we need some preparations. Recall that associated with $u_k$, the solution of (3.10) in each mesh $\mathcal{T}_k$, $u^k = K(\ell_k u_k - V u_k)$ satisfies

$$a(w^k, v) = (\ell_k u_k - V u_k, v) \quad \forall v \in H^1_0(\Omega).$$

(3.38)

Using the similar procedure as in the proof of Theorem 3.3, we have

Lemma 3.2 Let $u_k$ and $u_{k+1}$ be discrete solutions of (3.10) over a conforming mesh $\mathcal{T}_k$ and its refinement $\mathcal{T}_{k+1}$ with marked set $\mathcal{M}_k$. Suppose that they satisfy the following property

$$\|u - u_{k+1}\|_{a,\Omega}^2 + \gamma_s \text{osc}^2_{k+1}(u_{k+1}, \mathcal{T}_{k+1}) \leq \beta^2 \left( \|u - u_k\|_{a,\Omega}^2 + \gamma_s \text{osc}^2_k(u_k, \mathcal{T}_k) \right),$$

where $\gamma_s$ and $\beta_k$ are some positive constants. Then for problem (3.38), we have

$$\|u^k - P_{k+1} w^k\|_{a,\Omega}^2 + \gamma_s \text{osc}^2_{k+1}(P_{k+1} w^k, \mathcal{T}_{k+1}) \leq \tilde{\beta}_s^2 \left( \|w^k - P_k w^k\|_{a,\Omega}^2 + \gamma_s \text{osc}^2_k(P_k w^k, \mathcal{T}_k) \right)$$

with

$$\tilde{\beta}_s := \left( \frac{1 + \delta_1}{1 - C_5 \delta_1^2 \kappa^2(h_0)} \right)^{1/2}, \quad \tilde{\gamma}_s := \frac{\gamma_s}{1 - C_5 \delta_1^2 \kappa^2(h_0)}$$

(3.39)

where $C_5$ is some positive constant and $\delta_1 \in (0, 1)$ is some constant as in the proof of Theorem 3.3.

Corollary 3.1 Let $u_k$ and $u_{k+1}$ be as those in Lemma 3.2. Suppose that they satisfy the decrease property

$$\|u - u_{k+1}\|_{a,\Omega}^2 + \gamma_s \text{osc}^2_{k+1}(u_{k+1}, \mathcal{T}_{k+1}) \leq \beta_k^2 \left( \|u - u_k\|_{a,\Omega}^2 + \gamma_s \text{osc}^2_k(u_k, \mathcal{T}_k) \right)$$

with constants $\gamma_s > 0$ and $\beta_k \in (0, \sqrt{\frac{1}{2}})$. Then the set $\mathcal{R} := R_{\mathcal{T}_k \rightarrow \mathcal{T}_{k+1}}$ satisfies the following inequality

$$\eta_k(u_k, \mathcal{R}) \geq \tilde{\theta} \eta_k(u_k, \mathcal{T}_k)$$

with $\tilde{\theta}^2 = \frac{C_2(1-2\beta_k^2)}{C_0(C_1(1+1+2C_2\gamma_s)\tilde{\gamma}_s)}$ and $C_0 = \max(1, \frac{C_1}{\gamma_s})$, where $\tilde{\beta}_s$ and $\tilde{\gamma}_s$ are defined in (3.37) with $\delta_1$ being chosen such that $\tilde{\beta}_s^2 \in (0, \frac{1}{2})$.
Proof. It is a direct consequence of combining \( u_k = P_k w^k \) with Lemma 2.3 and Lemma 3.2.

The key to relate the best mesh with AFEM triangulations is the fact that procedure **MARK** selects the marked set \( \mathcal{M}_k \) with minimal cardinality.

**Lemma 3.3** (Cardinality of \( \mathcal{M}_k \)). Let \( u \in \mathcal{A}_\tau \), \( \mathcal{T}_k \) be a conforming partition obtained from \( \mathcal{T}_0 \), and \( \theta \) satisfies \( \theta \in (0, \frac{C_2\gamma}{C_3(C_1+(1+2CC_1)\gamma)}) \). Then the following estimate is valid:

\[
\# \mathcal{M}_k \lesssim \left( \|u - u_k\|_{a,\Omega}^2 + \gamma osc_k^2(u_k, \mathcal{T}_k) \right)^{-1/2s} |u|_{s}^{1/s},
\]

where the hidden constant depends on the discrepancy between \( \theta \) and \( \frac{C_2\gamma}{C_3(C_1+(1+2CC_1)\gamma)} \), with \( C \) defined in Lemma 2.3.

**Proof.** Let \( \alpha, \alpha_1 \in (0, 1) \) satisfy 

\[
\alpha_1 \in (0, \alpha)
\]

and 

\[
\theta < \frac{C_2\gamma}{C_3(C_1+(1+2CC_1)\gamma)} (1 - \alpha^2).
\]

Choose \( \delta_1 \in (0, 1) \) to satisfy (3.37) and

\[
(1 + \delta_1)^2 \alpha_1^2 \leq \alpha^2,
\]

which implies

\[
(1 + \delta_1^2 \alpha_1^2 < 1.
\]

Set

\[
\varepsilon = \frac{1}{\sqrt{2}} \alpha_1 \left( \|u - u_k\|_{a,\Omega}^2 + \gamma osc_k^2(u_k, \mathcal{T}_k) \right)^{1/2}
\]

and let \( \mathcal{T}_\varepsilon \) be a refinement of \( \mathcal{T}_0 \) with minimal degrees of freedom satisfying

\[
\|u - u_\varepsilon\|_{a,\Omega}^2 + (\gamma + 1) osc_\varepsilon^2(u_\varepsilon, \mathcal{T}_\varepsilon) \leq \varepsilon^2.
\]

It follows from the definition of \( \mathcal{A}_\tau \) that

\[
\# \mathcal{T}_\varepsilon - \# \mathcal{T}_0 \lesssim \varepsilon^{-1/s} |u|_{s}^{1/s}.
\]

Let \( \mathcal{T}_* = \mathcal{T}_\varepsilon \oplus \mathcal{T}_k \) be the smallest common refinement of \( \mathcal{T}_k \) and \( \mathcal{T}_\varepsilon \). Note that \( w^\varepsilon = K(\ell_\varepsilon u_\varepsilon - V u_\varepsilon) \) satisfies

\[
Lw^\varepsilon = \ell_\varepsilon u_\varepsilon - V u_\varepsilon,
\]

we get from the definition of oscillation and Young’s inequality that

\[
\tilde{osc}_\varepsilon^2(P_\tau w^\varepsilon, \tau) \leq 2 \tilde{osc}_\varepsilon^2(P_\tau w^\varepsilon, \tau) + 2C_0^2 osc_\tau^2(A, \tau) \|P_\varepsilon w^\varepsilon - P_\tau w^\varepsilon\|_{a,\Omega}^2, \forall \tau \in \mathcal{T}_*,
\]

which together with the monotonicity property \( osc_\tau(A, \mathcal{T}_\tau) \leq osc_0(A, \mathcal{T}_0) \) yields

\[
\tilde{osc}_\varepsilon^2(P_\tau w^\varepsilon, \mathcal{T}_* \tau) \leq 2 \tilde{osc}_\varepsilon^2(P_\tau w^\varepsilon, \mathcal{T}_\tau) + 2C \|P_\varepsilon w^\varepsilon - P_\tau w^\varepsilon\|_{a,\Omega}^2.
\]
where $C = \Lambda_1 \text{osc}_0^2(A, T_0)$. Due to the orthogonality
\[
\|w^\varepsilon - P_* w^\varepsilon\|_{a, \Omega}^2 = \|w^\varepsilon - P_2 w^\varepsilon\|_{a, \Omega}^2 - \|P_2 w^\varepsilon - P_2 w^\varepsilon\|_{a, \Omega}^2,
\]
we arrive at
\[
\|w^\varepsilon - P_2 w^\varepsilon\|_{a, \Omega}^2 \leq \|w^\varepsilon - P_2 w^\varepsilon\|_{a, \Omega}^2 + \frac{1}{2C} \text{osc}_0^2(P_2 w^\varepsilon, T_\varepsilon).
\]
Since (2.8) implies \( \gamma \leq \frac{1}{\gamma_0} \), we obtain that
\[
\|w^\varepsilon - P_2 w^\varepsilon\|_{a, \Omega}^2 + \gamma \text{osc}_0^2(P_2 w^\varepsilon, T_\varepsilon)
\]
\[
\leq \|w^\varepsilon - P_2 w^\varepsilon\|_{a, \Omega}^2 + \frac{1}{C} \text{osc}_0^2(P_2 w^\varepsilon, T_\varepsilon).
\]
with $\sigma = \frac{1}{\gamma_0} - \tilde{\gamma} \in (0, 1)$. Applying the similar argument in the proof of Theorem 3.3 when (3.19) is replaced by (3.20), we then get
\[
\|u - u_*\|_{a, \Omega}^2 \leq \alpha_0^2 \left( \|u - u_*\|_{a, \Omega}^2 + (\gamma + \sigma) \text{osc}_0^2(P_2 w^\varepsilon, T_\varepsilon) \right)
\]
\[
\leq \alpha_0^2 \left( \|u - u_*\|_{a, \Omega}^2 + (\gamma + 1) \text{osc}_0^2(P_2 w^\varepsilon, T_\varepsilon) \right),
\]
where
\[
\alpha_0^2 := \frac{(1 + \delta_1) + C_4 \hat{h}(h_0)}{1 - C_4 \delta_1^2 \hat{h}(h_0)}
\]
and $C_4$ is the constant appearing in the proof of Theorem 3.3. Thus, by (3.43) and (3.44), it follows
\[
\|u - u_*\|_{a, \Omega}^2 + \gamma \text{osc}_0^2(u_* T_\varepsilon) \leq \hat{\alpha}^2 \left( \|u - u_k\|_{a, \Omega}^2 + \gamma \text{osc}_0^2(u_k, T_k) \right)
\]
with $\hat{\alpha} = \frac{1}{\sqrt{2}} \alpha_0 \alpha_1$. In view of (3.12), we have $\hat{\alpha}^2 \in (0, \frac{1}{4})$ when $h_0 \ll 1$. Let $\mathcal{R} := R_{T_k \rightarrow T_*}$, by Corollary 3.1 we have that $T_\varepsilon$ satisfies
\[
\eta_k(u_k, \mathcal{R}) \geq \tilde{\theta}_\eta(u_k, T_k),
\]
where
\[
\tilde{\theta}^2 = \frac{C_4(1-2\delta^2)}{C_0(c_1 + (1 + 2c_0/\gamma_1)\gamma)}, \quad \hat{\gamma} = \frac{\gamma}{1 - \delta_1 \gamma_1 \gamma(h_0)}, \quad \tilde{C}_0 = \max(1, \frac{\tilde{C}_0}{\gamma}),
\]
and
\[
\hat{\alpha}^2 = \frac{(1 + \delta_1)\hat{\alpha}^2 + C_5 \hat{h}(h_0)}{1 - C_5 \delta_1^2 \hat{h}(h_0)}.
\]
It follows from the definition of $\gamma$ (see (3.35)) and $\hat{\gamma}$ (see (2.8)) that $\hat{\gamma} < 1$ and hence $\tilde{C}_0 = \frac{\tilde{C}_0}{\gamma}$. Since $h_0 \ll 1$, we obtain that $\hat{\gamma} > \gamma$ and $\hat{\alpha} \in (0, \frac{1}{\sqrt{2}} \alpha)$ from
It is easy to see from (3.33) and \( \hat{\gamma} > \gamma \) that
\[
\tilde{\beta}^2 = \frac{\tilde{C}_2 (1 - 2\hat{\alpha}^2)}{C_\gamma (\tilde{C}_1 + (1 + 2C\tilde{C}_1)\hat{\gamma})} \geq \frac{\tilde{C}_2}{C_\gamma \gamma} (1 - \alpha^2)
\]
\[
= \frac{C_2}{C_\gamma \gamma} \frac{(1 - C\gamma (h_0))^2}{(\gamma (1 + C\gamma (h_0))^2) + 1 + 2C\gamma (h_0)^2} (1 - \alpha^2)
\]
\[
\geq \frac{C_2}{C_\gamma \gamma} \frac{(1 - \alpha^2)}{C_\gamma (1 + 2CC_1) (1 - \alpha^2) > \theta}
\]
when \( h_0 \ll 1 \). Thus
\[
\#M_k \leq \#R \leq \#T_\varepsilon - \#T_k \leq \#T_\varepsilon - \#T_0 \leq \frac{1}{\sqrt{2}} \alpha_1^{-1/s} \left( \|u - u_k\|_{\sigma, \Omega}^2 + \gamma \text{osc}_k^2(u_k, T_k) \right)^{-1/2s} |u|^{1/s},
\]
which is the desired estimate (3.40) with an explicit dependence on the discrepancy between \( \theta \) and \( \frac{C_2}{C_\gamma \gamma (1 + 2CC_1) \gamma} \) via \( \alpha_1 \). This completes the proof.

As a consequence, we obtain the optimal complexity as follows.

**Theorem 3.4** Let \( u \in A^\varepsilon \) and \( \{ u_k \}_{k \in \mathbb{N}_0} \) be a sequence of finite element solutions corresponding to a sequence of nested finite element spaces \( \{ S_k^0(\Omega) \}_{k \in \mathbb{N}_0} \) produced by **Algorithm D**. Then
\[
\|u - u_k\|_{\sigma, \Omega}^2 + \gamma \text{osc}_k^2(u_k, T_k) \lesssim (\#T_k - \#T_0)^{-2s} |u|_{s}^{2},
\]
where the hidden constant depends on the exact solution \( u \) and the discrepancy between \( \theta \) and \( \frac{C_2}{C_\gamma \gamma (1 + 2CC_1) \gamma} \).

**Proof.** It follows from (2.7) and (3.40) that
\[
\#T_k - \#T_0 \lesssim \sum_{j=0}^{k-1} \#M_j \lesssim \sum_{j=0}^{k-1} (\|u - u_j\|_{\sigma, \Omega}^2 + \gamma \text{osc}_j^2(u_j, T_j))^{-1/2s} |u|_{s}^{1/s}.
\]
Note that (3.30) implies
\[
\|u - u_j\|_{\sigma, \Omega}^2 + \gamma \eta_j^2(u_j, T_j) \leq \tilde{C} (\|u - u_j\|_{\sigma, \Omega}^2 + \gamma \text{osc}_j^2(u_j, T_j)),
\]
where \( \tilde{C} = \max(1 + \frac{\alpha}{C_2}, \frac{C_0}{C_2}) \). It then turns out
\[
\#T_k - \#T_0 \lesssim \sum_{j=0}^{k-1} (\|u - u_j\|_{\sigma, \Omega}^2 + \gamma \eta_j^2(u_j, T_j))^{-1/2s} |u|_{s}^{1/s}.
\]
Due to (3.34), we obtain for $0 \leq j < k$ that
\[
\|u - u_k\|_{a, \Omega}^2 + \gamma \eta_k^2(u_k, T_k) \leq \xi^{2(k-j)} \left(\|u - u_j\|_{a, \Omega}^2 + \gamma \eta_j^2(u_j, T_j)\right).
\]

Consequently,
\[
\#T_k - \#T_0 \leq |u|_{s}^{1/s} \left(\|u - u_k\|_{a, \Omega}^2 + \gamma \eta_k^2(u_k, T_k)\right)^{-1/2s} \sum_{j=0}^{k-1} \frac{\xi^{k-j}}{s} \leq |u|_{s}^{1/s} \left(\|u - u_k\|_{a, \Omega}^2 + \gamma \eta_k^2(u_k, T_k)\right)^{-1/2s},
\]
the last inequality holds because of the fact $\xi < 1$.

Since $\text{osc}_k(u_k, T_k) \leq \eta_k(u_k, T_k)$, we arrive at
\[
\#T_k - \#T_0 \leq \left(\|u - u_k\|_{a, \Omega}^2 + \gamma \text{osc}_k^2(u_k, T_k)\right)^{-1/2s} |u|_{s}^{1/s}.
\]
This completes the proof.

4 Applications

In this section, we provide three typical examples to show that our general theory is quite useful.

4.1 A nonsymmetric problem

The first example is a nonsymmetric elliptic partial differential equation of second order. We consider the following problem: Find $u \in H^1_0(\Omega)$ such that
\[
\begin{align*}
-\nabla \cdot (A \nabla u) + b \cdot \nabla u + cu &= f \quad \text{in } \Omega, \\
\quad u &= 0 \quad \text{on } \partial \Omega,
\end{align*}
\]
where $\Omega \subset \mathbb{R}^d (d \geq 2)$ is a bounded polytopic domain, $A : \Omega \to \mathbb{R}^{d \times d}$ is piecewise Lipschitz over initial triangulation $T_0$, for $x \in \Omega$ matrix $A(x)$ is symmetric and positive definite with smallest eigenvalue uniformly bounded away from 0, $b \in [L^\infty(\Omega)]^d$ is divergence free, $c \in L^\infty(\Omega)$, and $f \in L^2(\Omega)$.

A finite element discretization of (4.45) reads: Find $uh \in S_0^h(\Omega)$ satisfying
\[
(A \nabla uh, \nabla v) + (b \cdot \nabla uh, v) + (cuh, v) = (f, v) \quad \forall v \in S_0^h(\Omega).
\]
It is seen that (4.46) is a special case of (3.10), in which $Vu := b \cdot \nabla u + cu$ and $\ell u = \ell_h u = f$. Consequently, $\kappa_1(h) = 0$, $uh = K(f - Vu_h)$ and
\[
u - w^h = KV(u_h - u) = KV(I - P_h)(u_h - u).
\]
Obviously, $V : H^1_0(\Omega) \to L^2(\Omega)$ is a linear bounded operator and $KV$ is a compact operator over $H^1_0(\Omega)$. We have the conclusion of Theorem 3.1.
In this application, the element residual and jump residual become
\[ R_{\tau}(u_h) := f - b \cdot \nabla u_h - cu_h + \nabla \cdot (A \nabla u_h) \quad \text{in } \tau \in T_h, \]
\[ J_{e}(u_h) := [A \nabla u_h]_e \cdot \nu_e \quad \text{on } e \in E_h, \]
while the corresponding error estimator \( \eta_h(u_h, T_h) \) and the oscillation \( \text{osc}_h(u_h, T_h) \) are defined by (3.16) and (3.17), respectively. Thus Theorem 3.3 and Theorem 3.4 ensure the convergence and optimal complexity of AFEM for nonsymmetric problem (4.45).

4.2 A nonlinear problem

In this subsection, we derive the convergence and optimal complexity of AFEM for a nonlinear problem from our general theory.

Consider the following nonlinear problem: Find \( u \in H^1_0(\Omega) \) such that
\[
\begin{cases}
\mathcal{L} u := -\Delta u + f(x, u) = 0 & \text{in } \Omega, \\
u = 0 & \text{on } \partial \Omega,
\end{cases}
\] (4.47)
where \( f(x, y) \) is a smooth function on \( \mathbb{R}^3 \times \mathbb{R} \).

For convenience, we shall drop the dependence of variable \( x \) in \( f(x, u) \) in the following exposition. We assume that \( u \in H^1_0(\Omega) \cap H^{1+s}(\Omega) \) for some \( s \in (0, 1] \). For any \( w \in H^1_0(\Omega) \cap H^{1+s}(\Omega) \), the linearized operator \( \mathcal{L}'_w \) at \( w \) (namely, the Fréchet derivative of \( \mathcal{L} \) at \( w \)) is then given by
\[ \mathcal{L}'_w = -\Delta + f'(w). \]

We assume that \( \mathcal{L}'_w : H^1_0(\Omega) \to H^{-1}(\Omega) \) is an isomorphism. As a result, \( u \in H^1_0(\Omega) \cap H^{1+s}(\Omega) \) must be an isolated solution of (4.47). The associated finite element scheme for (4.47) reads: Find \( u_h \in S^0_0(\Omega) \) satisfying
\[ (\nabla u_h, \nabla v) + (f(u_h), v) = 0 \quad \forall v \in S^0_0(\Omega). \] (4.48)

Let \( a(\cdot, \cdot) = (\nabla \cdot, \nabla \cdot), K = (-\Delta)^{-1} : L^2(\Omega) \to H^1_0(\Omega), V = 0 \) and \( \ell_h w = -f(w) \) for any \( w \in S^0_0(\Omega) \), then (4.48) becomes (3.10).

As usual, to analyze the finite element approximation of nonlinear problem (4.48), we require mesh \( T_h \) to satisfy that there exists \( \zeta \geq 1 \) such that (c.f. [29])
\[ h^s \lesssim h(x) \quad x \in \Omega, \]
where \( h(x) \) is the diameter \( h_\tau \) of the element \( \tau \) containing \( x \). We consider the case of that \( S^0_0(\Omega) \) is the conforming piecewise linear finite element space associated with \( T_h \). We assume that \( \zeta < 2s \). Thus we can choose \( p \in (3, 6\zeta/(3\zeta-2s)] \) and obtain from Theorem 3.1 and Theorem 3.2 of [29] that

**Lemma 4.1** If \( h \ll 1 \), then
\[ \|u - u_h\|_{1, \Omega} + h^s \|u_h\|_{0, \infty, \Omega} \lesssim h^s \]
and
\[ \|u - u_h\|_{0, \Omega} \lesssim r(h)\|u - u_h\|_{1, \Omega}, \]

where \( r(h) \to 0 \) as \( h \to 0 \).

Now we shall show that Theorem 3.1 is applicable for (4.47). Since \( K \) is monotone and \( f(x, y) \) is smooth, we have from Lemma 4.1 that
\[ \|K(f(u) - f(u_h))\|_{a, \Omega} \lesssim \|K(u - u_h)\|_{a, \Omega}, \]
\[ \lesssim \|u - u_h\|_{0, \Omega} \lesssim \tau(h)\|u - u_h\|_{a, \Omega}. \]

Therefore we have (3.13) when we choose \( \kappa_1(h) = \tau(h) \) and \( \kappa_2(h) = 0 \).

In this application, the element residual and jump residual become:
\[ R_\tau(u_h) := -f(u_h) + \Delta u_h \quad \text{in } \tau \in T_h, \]
\[ J_e(u_h) := -\nabla u_h^+ \cdot \nu^+ - \nabla u_h^- \cdot \nu^- := [\nabla u_h]_e \cdot \nu_e \quad \text{on } e \in E_h \]

and the corresponding error estimator \( \eta_h(u_h, T_h) \) and the oscillation \( \text{osc}_h(u_h, T_h) \) are defined by \( \text{(3.16)} \) and \( \text{(3.17)} \), respectively. Then Theorem \( \text{3.3} \) and Theorem \( \text{3.4} \) ensure the convergence and optimal complexity of AFEM for nonlinear problem (4.47).

4.3 An unbounded coefficient problem

Finally, we investigate a nonlinear eigenvalue problem, of which a coefficient is unbounded. It is known that electronic structure computations require solving the following Kohn-Sham equations [4, 14, 16]
\[ \left( \frac{1}{2} \Delta - \sum_{j=1}^{N_{\text{atom}}} \frac{Z_j}{|x - r_j|} + \int_{\mathbb{R}^3} \frac{\rho(y)}{|x - y|} dy + V_{xc}(\rho) \right) u_i = \lambda_i u_i \quad \text{in } \mathbb{R}^3, \quad (4.49) \]

where \( N_{\text{atom}} \) is the total number of atoms in the system, \( Z_j \) is the valence charge of this ion (nucleus plus core electrons), \( r_j \) is the position of the \( j \)-th atom \( (j = 1, \cdots, N_{\text{atom}}) \),
\[ \rho = \sum_{i=1}^{N_{\text{occ}}} c_i |u_i|^2 \]

with \( u_i \) the \( i \)-th smallest eigenfunction, \( c_i \) the number of electrons on the \( i \)-th orbit, and \( N_{\text{occ}} \) the total number of the occupied orbits. The central computation in solving the Kohn-Sham equation is the repeated solution of the following eigenvalue problem: Find \( (\lambda, u) \in \mathbb{R} \times H_0^1(\Omega) \) such that
\[ \begin{cases} -\frac{1}{2} \Delta u + Vu = \lambda u & \text{in } \Omega, \\ \|u\|_{0, \Omega} = 1, \end{cases} \quad (4.50) \]
where $\Omega$ is a bounded domain in $\mathbb{R}^3$, $V = V_{ne} + V_0$ is the so-called effective potential. Here, $V_0 \in L^\infty(\Omega)$ and

$$V_{ne}(x) = - \sum_{j=1}^{N_{atom}} \frac{Z_j}{|x - r_j|}.$$ 

A finite element discretization of (4.50) reads: Find $(\lambda_h, u_h) \in \mathbb{R} \times S_h^0(\Omega)$ such that

$$\frac{1}{2} (\nabla u_h, \nabla v) + (V u_h, v) = \lambda_h (u_h, v) \quad \forall v \in S_h^0(\Omega).$$

(4.51)

Let $\ell_h : S_h^0(\Omega) \to L^2(\Omega)$ be defined by

$$\ell_h v = \lambda_h v \quad \forall v \in S_h^0(\Omega),$$

then (4.51) is a special case of (3.10) when $a(\cdot, \cdot) = \frac{1}{2} (\nabla \cdot, \nabla \cdot)$ and $K = \frac{1}{2} (-\Delta)^{-1} : L^2(\Omega) \to H^1_0(\Omega)$.

Using the uncertainty principle lemma (see, e.g., [25])

$$\int_{\mathbb{R}^3} \frac{w^2(x)}{|x|^2} \leq 4 \int_{\mathbb{R}^3} |\nabla w|^2 \quad \forall w \in C_0^\infty(\mathbb{R}^3)$$

and the fact that $C_0^\infty(\Omega)$ is dense in $H^1_0(\Omega)$, we obtain

$$\int_{\Omega} \frac{w^2(x)}{|x|^2} \leq 4 \int_{\Omega} |\nabla w|^2 \quad \forall w \in H^1_0(\Omega).$$

Then for any $w \in H^1_0(\Omega)$, we have

$$\|V_{ne}w + V_0w\|_{0,\Omega} \leq C\|w\|_{1,\Omega},$$

namely, $V$ is a bounded operator over $H^1_0(\Omega)$. Thus $KV$ is a compact operator over $H^1_0(\Omega)$.

We consider the case of that $(\lambda, u) \in \mathbb{R} \times H^1_0(\Omega)$ is some simple eigenpair of (4.50) with $\|u\|_{0,\Omega} = 1$. Note that for $\ell v := \lambda v \quad \forall v \in H^1_0(\Omega)$, there holds

$$K(\ell u - \ell_h u_h) = \lambda K(u - u_h) + (\lambda - \lambda_h)K u_h,$$

So if $(\lambda_h, u_h) \in \mathbb{R} \times S_h^0(\Omega)$ is the associated finite element eigenpair of (4.51) with $\|u_h\|_{0,\Omega} = 1$ that satisfy

$$\|u - u_h\|_{0,\Omega} + |\lambda - \lambda_h| \lesssim \kappa_1(h)\|u - u_h\|_{a,\Omega},$$

we then have (c.f. [9])

$$\|K(\ell u - \ell_h u_h)\|_{a,\Omega} = O(\kappa_1(h))\|u - u_h\|_{a,\Omega},$$

where $\kappa_1(h) := \rho_1(h) + \|u - u_h\|_{a,\Omega}$ satisfying $\kappa_1(h) \to 0$ as $h \to 0$. 

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In this application, the element residual and jump residual become:

\[
R_\tau(u_h) := \lambda_h u_h - V u_h + \frac{1}{2} \Delta u_h \quad \text{in } \tau \in \mathcal{T}_h,
\]

\[
J_e(u_h) := \left[ \frac{1}{2} \nabla u_h \right]_e \cdot \nu_e \quad \text{on } e \in \mathcal{E}_h
\]

and the corresponding error estimator \( \eta_h(u_h, \mathcal{T}_h) \) and the oscillation \( \text{osc}_h(u_h, \mathcal{T}_h) \) are defined by (3.16) and (3.17), respectively. Then Theorem 3.3 and Theorem 3.4 ensure the convergence and optimal complexity of AFEM for unbounded coefficient problem (4.50) (c.f. [9]).

5 Numerical examples

In this section we will report some numerical results to illustrate our theory. Our numerical results were carried out on LSSC-II in the State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences, and our codes were based on the toolbox PHG of the State Key Laboratory of Scientific and Engineering Computing, Chinese Academy of Sciences.

Example 1. We consider (4.45) when the homogenous Dirichlet boundary condition is replaced by \( u = g \) on \( \partial \Omega \) and \( \Omega = (0,1)^3 \) with the isotropic diffusion coefficient \( A = \epsilon I, \epsilon = 10^{-2} \), convection velocity \( b = (2,3,4) \), and \( c = 0 \) (c.f. [15] for a 2D case and Remark 2.1). The exact solution is given by

\[
u = \left( x^3 - \exp \left( \frac{2(x-1)}{\epsilon} \right) \right) \left( y^2 - \exp \left( \frac{3(y-1)}{\epsilon} \right) \right) \left( z - \exp \left( \frac{4(z-1)}{\epsilon} \right) \right).
\]

For small \( \epsilon > 0 \) the solution has the typical layer behavior in the neighbourhood of \( x = 1, y = 1, z = 1 \), respectively. The Dirichlet boundary condition \( g(x, y, z) \) on \( \partial \Omega \) is given by

\[
g(x, y, z) = \begin{cases} 
0 & x = 1 \ or \ y = 1 \ or \ z = 1, 
\end{cases}
\]

\[
u(x, y, z) = \begin{cases} 
0 & x = 0 \ or \ y = 0 \ or \ z = 0.
\end{cases}
\]

Some adaptively refined meshes are displayed in Fig. 5.1 and Fig. 5.2. Our numerical results are presented in Fig. 5.3 and Fig. 5.4. It is shown from Fig. 5.4 that \( \| u - u_h \| \) is proportional to the a posteriori error estimators, which indicates the efficiency of the a posteriori error estimators given in section 4.4. Besides, it is also seen from Fig. 5.3 and Fig. 5.4 that, by using linear finite elements and quadratic finite elements, the convergence curves of errors are approximately parallel to the line with slope \(-1/3\) and the line with slope \(-2/3\), respectively. These mean that the approximation error of the exact solution has optimal convergence rate, which coincides with our theory in section 3.2.

Example 2. Consider the following nonlinear problem:

\[
\begin{cases} 
-\Delta u + u^3 = f \quad \text{in } \Omega, \\
u = 0 \quad \text{on } \partial \Omega,
\end{cases}
\]
Figure 5.1: The cross-section of an adaptive mesh of Example 1 using linear finite elements

Figure 5.2: The cross-section of an adaptive mesh of Example 1 using quadratic finite elements

Figure 5.3: The convergence curves of Example 1 using linear finite elements

Figure 5.4: The convergence curves of Example 1 using quadratic finite elements
Figure 5.5: The cross-section of an adaptive mesh of **Example 2** using linear finite elements

Figure 5.6: The cross-section of an adaptive mesh of **Example 2** using quadratic finite elements

Figure 5.7: The convergence curves of **Example 2** using linear finite elements

Figure 5.8: The convergence curves of **Example 2** using quadratic finite elements
where \( \Omega = (0, 1)^3 \). The exact solution is given by 
\[
u = \sin(\pi x_1) \sin(\pi x_2) \sin(\pi x_3)/(x_1^2 + x_2^2 + x_3^2)^{1/2}.
\]

Fig. 5.5 and Fig. 5.6 are two adaptively refined meshes, which show that the error indicator is good. It is shown from Fig. 5.7 and Fig. 5.8 that \( \|u - u_h\|_1 \) is proportional to the a posteriori error estimators, which implies the a posteriori error estimators given in section 4.2 are efficient. Besides, similar conclusions to that of Example 1 can be obtained from Fig. 5.7 and Fig. 5.8 too.

**Example 3.** Consider the Kohn-Sham equation for helium atoms:
\[
\left( -\frac{1}{2}\Delta - \frac{2}{|x|} + \int \frac{\rho(y)}{|x-y|}dy + V_{xc} \right) u = \lambda u \quad \text{in } \mathbb{R}^3,
\]
and \( \int_{\mathbb{R}^3} |u|^2 = 1 \), here \( \rho = 2|u|^2 \). In our computation of the ground state energy, we solve the following nonlinear eigenvalue problem: Find \( (\lambda, u) \in \mathbb{R} \times H_0^1(\Omega) \) such that
\[
\begin{align*}
\left( -\frac{1}{2}\Delta - \frac{2}{|x|} + \int \frac{\rho(y)}{|x-y|}dy + V_{xc} \right) u &= \lambda u \quad \text{in } \Omega, \\
u &= 0 \quad \text{on } \partial \Omega,
\end{align*}
\]
(5.52)

where \( \Omega = (-10, 10, 0)^3 \), and \( V_{xc}(\rho) = -\frac{3}{2} \alpha (\frac{3}{\pi} \rho)^{2/3} \) with \( \alpha = 0.77298 \). Since (5.52) is a nonlinear eigenvalue problem, we need to linearize and solve them iteratively, which is called the self-consistent approach \([4, 14, 16, 21]\). In our computation, a Broyden-type quasi-Newton method \([22]\) were used.

In 1989, White \([27]\) computed helium atoms over uniform cubic grids and obtained ground state energy -2.8522 a.u. by using 500,000 finite element bases. While the ground state energy of helium atoms in Software package fhi98PP \([11]\) is -2.8346 a.u., which we take as a reference.

![Figure 5.9: The ground state energy using linear finite elements](image1.png)

![Figure 5.10: The ground state energy using quadratic finite elements](image2.png)

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Figure 5.11: The cross-section of an adaptive mesh of Example 3 using linear finite elements

Figure 5.12: The cross-section of an adaptive mesh of Example 3 using quadratic finite elements

Figure 5.13: The convergence curve of Example 3 using linear finite elements

Figure 5.14: The convergence curve of Example 3 using quadratic finite elements
Our results are displayed in Fig. 5.9, Fig. 5.10, Fig. 5.11, Fig. 5.12, Fig. 5.13, and Fig. 5.14. It is seen from Fig. 5.10 that the ground state energy in our computation is close to the reference with less 100,000 degrees of freedom when the quadratic finite element discretization is used. Some cross-sections of the adaptively refined meshes are displayed in Fig. 5.11 and Fig. 5.12. Since we do not have the exact solution, we list the convergence curves of the a posteriori error estimators in Fig. 5.13 and Fig. 5.14 only. It is shown from these figures that the a posteriori error estimators given in section 4.3 are efficient.

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References

[1] R. A. Adams, *Sobolev Spaces*, Academic Press, New York, 1975.

[2] I. Babuska and J. E. Osborn, *Finite element-Galerkin approximation of the eigenvalues and eigenvectors of selfadjoint problems*, Math. Comp., 52 (1989), pp. 275-297.

[3] I. Babuska and M. Vogelius, *Feedback and adaptive finite element solution of one-dimensional boundary value problems*, Numer. Math., 44 (1984), pp. 75-102.

[4] S. L. Beck, *Real-space mesh techniques in density-function theory*, Rev. Mod. Phys., 72 (2000), pp. 1041-1080.

[5] P. Binev, W. Dahmen, and R. DeVore, *Adaptive finite element methods with convergence rates*, Numer. Math., 97 (2004), pp. 219-268.

[6] J. M. Cascon, C. Kreuzer, R. H. Nochetto, and K. G. Siebert, *Quasi-optimal convergence rate for an adaptive finite element method*, SIAM J. Numer. Anal., 46 (2008), pp. 2524-2550.

[7] L. Chen, M. J. Holst, and J. Xu, *The finite element approximation of the nonlinear Poisson-Boltzmann equation*, SIAM J. Numer. Anal., 45 (2007), pp. 2298-2320.

[8] P. G. Ciarlet and J. L. Lions, eds., *Finite Element Methods, Volume II of Handbook of Numerical Analysis*, Vol. II, North.Holland, Amsterdam, 1991.

[9] X. Dai, J. Xu, and A. Zhou, *Convergence and optimal complexity of adaptive finite element eigenvalue computations*, Numer. Math., 110 (2008), pp. 313-355.

[10] W. Dörfler, *A convergent adaptive algorithm for Poisson’s equation*, SIAM J. Numer. Anal., 33 (1996), pp. 1106-1124.
[11] M. Fuchs and M. Scheffler, *Ab initio pseudopotentials for electronic structure calculations of poly-atomic systems using density-functional theory*, Comput. Phys. Commun., 119 (1999), pp. 67-98.

[12] E. M. Garau, P. Morin, and C. Zuppa, *Convergence of adaptive finite element methods for eigenvalue problems*, Preprint, arXiv: 0803.0365v1 [math.NA] 4 Mar 2008.

[13] S. Giani and I. G. Graham, *A convergent adaptive method for elliptic eigenvalue problems*, SIAM J. Numer. Anal., 47 (2009), pp. 1067-1091.

[14] X. Gong, L. Shen, D. Zhang, and A. Zhou, *Finite element approximations for Schrödinger equations with applications to electronic structure computations*, J. Comput. Math., 26 (2008), pp. 310-323.

[15] P. Knobloch and L. Tobiska, *The $P^1_{nod}$ element: A new nonconforming finite element for convection-diffusion problems*, SIAM J. Numer. Anal., 41 (2003), pp. 436-456.

[16] W. Kohn and L. J. Sham, Self-consistent equations including exchange and correlation effects, Phys. Rev. A., 140 (1965), pp. 4743-4754.

[17] K. Mekchay and R. H. Nochetto, *Convergence of adaptive finite element methods for general second order linear elliptic PDEs*, SIAM J. Numer. Anal., 43 (2005), pp. 1803-1827.

[18] P. Morin, R. H. Nochetto, and K. Siebert, *Data oscillation and convergence of adaptive FEM*, SIAM J. Numer. Anal., 38 (2000), pp. 466-488.

[19] P. Morin, R. H. Nochetto, and K. Siebert, *Convergence of adaptive finite element methods*, SIAM Review., 44 (2002), pp. 631-658.

[20] P. Morin, K. G. Siebert, and A. Veeser, *A basic convergence result for conforming adaptive finite elements*, Math. Models Methods Appl. Sci., 18 (2008), pp. 707-737.

[21] J. P. Perdew and A. Zunger, *Self-interaction correction to density-functional approximations for many-electron*, Phys. Rev. B., 23 (1981), pp. 5048-5079.

[22] G. P. Srivastava, *Broyden’s method for self-consistent field convergence acceleration*, J. Phys. A., 17 (1984), pp. 317–321.

[23] R. Stevenson, *Optimality of a standard adaptive finite element method*, Found. Comput. Math., 7 (2007), pp. 245-269.

[24] R. Stevenson, *The completion of locally refined simplicial partitions created by bisection*, Math.Comput., 77 (2008), pp. 227-241.

[25] M. Reed and B. Simon, *Methods of Modern Mathematical Physics, II: Fourier Analysis, Self-Adjointness*, Academic Press, San Diego, 1975.
[26] R. Verfürth, *A Review of a Posteriori Error Estimates and Adaptive Mesh-Refinement Techniques*, Wiley-Teubner, New York, 1996.

[27] S. R. White, J. W. Wilkins, and M. P. Teter, *Finite-element method for electronic structure*, Phys. Rev. B., **39** (1989), pp. 5819-5833.

[28] J. Xu and A. Zhou, *Local and parallel finite element algorithms based on two-grid discretizations*, Math. Comp., **69** (2000), pp. 881-909.

[29] J. Xu and A. Zhou, *Local and parallel finite element algorithms based on two-grid discretizations for nonlinear problems*, Adv. Comput. Math., **14** (2001), pp. 293-327.

[30] A. Zhou, *Multi-level adaptive corrections in finite dimensional approximations*, J. Comput. Math., **28** (2010), to appear.