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ENHANCING LEAST-SQUARES FINITE ELEMENT METHODS THROUGH A QUANTITY-OF-INTEREST*

JEHANZEB HAMEED CHAUDHRY†, ERIC C. CYR‡, KUO LIU§, THOMAS A. MANTEUFFEL§, LUKE N. OLSON¶, AND LEI TANG§

Abstract. In this paper we introduce an approach that augments least-squares finite element formulations with user-specified quantities-of-interest. The method incorporates the quantity-of-interest into the least-squares functional and inherits the global approximation properties of the standard formulation as well as increased resolution of the quantity-of-interest. We establish theoretical properties such as optimality and enhanced convergence under a set of general assumptions. Central to the approach is that it offers an element-level estimate of the error in the quantity-of-interest. As a result, we introduce an adaptive approach that yields efficient, adaptively refined approximations. Several numerical experiments for a range of situations are presented to support the theory and highlight the effectiveness of our methodology. Notably, the results show that the new approach is effective at improving the accuracy per total computational cost.

Key words. adaptive mesh refinement, least-squares, finite element, error estimation

AMS subject classifications. 65N15, 65N30, 65N50

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1. Introduction.

In this paper, we introduce a technique for controlling the accuracy of user-specified quantities in least-squares finite element approximations. Least-squares finite element methods have been developed for a range of applications, including fluid flow [10, 21], transport [22], hyperbolic equations [14, 15], quantum chromodynamics [12], magnetohydrodynamics [3], and biomolecular simulation [11, 9]. These methods have been successful in achieving globally accurate approximations with low total computational cost [2]. However, in many simulations, accuracy in certain response quantities as well as a globally accurate solution to the PDE is desired. To this end, we develop an approach incorporating *quantities-of-interest* (QoI) into adaptive least-squares finite elements methods.

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†Department of Scientific Computing, Florida State University, Tallahassee, FL 32306 (jchaudhry@fsu.edu, http://people.sc.fsu.edu/∼jchaudhry/).
‡Computational Mathematics Department, Sandia National Laboratories, Albuquerque, NM 87185 (eccyr@sandia.gov, http://www.cs.sandia.gov/∼eccyr).
§Department of Applied Mathematics, University of Colorado at Boulder, Boulder, CO 80309 (l6tang@gmail.com, liukuo99@gmail.com, tmanteuf@colorado.edu, http://amath.colorado.edu/faculty/tmanteuf).
¶Department of Computer Science, University of Illinois at Urbana-Champaign, Urbana, IL 61801 (lukeo@illinois.edu, http://www.cs.illinois.edu/homes/lukeo).

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We consider a first-order system of PDEs,

$$\mathcal{L}u = f \quad \text{in } \Omega, \tag{1.1}$$

where $\mathcal{L}$ is a linear operator. In a least-squares finite element setting, the solution to (1.1) is determined by minimizing the least-squares functional,

$$\mathcal{F}(u; f) = \|\mathcal{L}u - f\|^2, \tag{1.2}$$

over all $u \in \mathcal{V}$, where $\|\cdot\|$ is the L^2-norm. We assume that $\mathcal{V}$ is an appropriate Hilbert space where the solution to the associated weak problem satisfies (1.1); the weak problem is as follows: find $u_* \in \mathcal{V}$ such that

$$\langle \mathcal{L}u_* - f, \mathcal{L}v \rangle = 0 \quad \forall v \in \mathcal{V}. \tag{1.3}$$

Least-squares formulations offer many attractive properties. If $\mathcal{L}$ is nonsingular, the discrete problems that follow from (1.3) result in symmetric and positive-definite systems of equations. Moreover, if $\|\mathcal{L}u\|$ is elliptic in $\mathcal{V}$, then the least-squares functional, (1.2), directly defines an effective error estimator: for a discrete function $u^h \in \mathcal{V}^h \subset \mathcal{V}$, the error $\|u_* - u^h\|_{\mathcal{V}}$ is equivalent to $\mathcal{F}(u^h, f) = \mathcal{F}(u_* - u^h; 0)$. This estimator is shown to be *locally sharp* and *globally reliable* in many settings [8, 2] and is often successful in guiding mesh refinement [2].

Many applications are primarily interested in a particular aspect of a solution, such as the lift on a wing, conservation of mass or energy, a calculated expression over a region, etc. These examples are expressed as integral quantities of the solution and are not directly considered by a standard least-squares formulation. The focus of this paper is to develop a methodology with *two* objectives:

1. maintaining convergence in global norms and
2. resolving the QoI accurately.

We denote $\mathcal{Q}$ as the QoI with $\mathcal{Q} \in \mathcal{V}'$, where $\mathcal{V}'$ is the dual space of $\mathcal{V}$. Further, we define

$$\gamma := \mathcal{Q}(u_*), \tag{1.4}$$

where u_* is the solution to the weak form (1.3).

In this paper, we introduce a new (weighted) least-squares functional that includes the QoI as an additional term:

$$\mathcal{F}_{\mathcal{Q}}(u) = \|\mathcal{L}u - f\|^2 + \beta^2 |\mathcal{Q}(u) - \gamma|^2, \tag{1.5}$$

where β is a constant. A heuristic for selecting β is introduced in section 6.4. Notice that this functional fits within the least-squares methodology: the residual is minimized in an appropriate norm. Moreover, minimizers to (1.5) still minimize (1.2); thus the new functional is a consistent modification of the original. However, because of the inclusion of the QoI, the new functional assesses *both* the quality of the approximation in satisfying the PDE as well as the accuracy of the QoI. As a result, the new functional guides the approximation process to the least-squares solution along a particular direction that yields an improved prediction of the QoI. In addition to improved convergence of the QoI, we show that the global convergence properties of the original formulation are simultaneously maintained. Similar to the original least-squares functional, we also use the new functional to develop high quality error indicators that consider both the error in the global norm and the error in the QoI.

The result is an adaptive algorithm that balances the error in both quantities, yielding rapid convergence. Balancing the two measures of error in the solution is a unique quality of the adaptive refinement algorithm developed here.

In practice, the value of the QoI, γ, is not known a priori. We show that this issue can be addressed by finding a Riesz representation of the QoI using the original least-squares functional. Using this representation, (1.5) is modified by replacing $\mathcal{Q}(u)$ and γ by the approximations $\mathcal{Q}^{\hat{h}}$ and $\gamma^{\hat{h}}$ yielding a practical method (3.9). This method bears some similarity to the goal-oriented a posteriori error estimation methods (see, for example, [6, 7, 19]) that solve an adjoint equation to determine the sensitivity of the QoI to perturbations in the PDE solution. In the text and numerical results that follow, we compare and contrast the two methods as appropriate.

In this paper, we develop the theoretical and algorithmic framework for efficiently including a QoI into the least-squares minimization process. The outline of this paper is as follows. In section 2, we outline several immediate observations for the QoI-based functional (1.5), including existence and uniqueness. In section 3, we develop bounds on the error for (1.5) and introduce a modified functional that approximates the value of the QoI. In section 4, we follow with improved error bounds for these functionals, and in section 5 we bound the error in the QoI. Finally, in section 6 we outline an adaptive refinement algorithm based on our approach, and in section 7 we support our approach with numerical results from several model problems.

2. Background and assumptions. In this section we consider the relationship between the standard least-squares functional, $\mathcal{F}$, in (1.2) and the QoI-based least-squares functional, $\mathcal{F}_{\mathcal{Q}}$, in (1.5), as well as their associated discrete forms.

2.1. Assumptions and notation. We first outline several properties of the spaces and functionals that are assumed throughout this paper. The standard least-squares functional is required to be elliptic with respect to $\mathcal{V}$, that is, to maintain coercivity and continuity over $\mathcal{V}$, which is summarized by the following assumption.

Assumption A.1 (continuity and coercivity). *Given the least-squares functional $\mathcal{F}(u; f) : \mathcal{V} \to \mathbb{R}$ defined in* (1.2) *and Sobolev space $\mathcal{V}$, assume there exist constants c_0 and c_1 such that*

$$\mathcal{F}(u; 0) = \langle \mathcal{L}u, \mathcal{L}u\rangle \geq c_0\|u\|_{\mathcal{V}}^2 \quad \textit{and} \quad \langle \mathcal{L}u, \mathcal{L}v\rangle \leq c_1\|u\|_{\mathcal{V}}\|v\|_{\mathcal{V}} \quad \forall\, u, v \in \mathcal{V}. \tag{2.1}$$

With the QoI in (1.4) and in view of functional (1.5), we restrict our attention to bounded quantities as summarized in the following assumption.

Assumption A.2 (bounded QoI). *Given the linear QoI functional $\mathcal{Q} : \mathcal{V} \to \mathbb{R}$, we assume $\mathcal{Q}$ is bounded on $\mathcal{V}$; that is, there exists a constant $c_{\mathcal{V}'} = \|\mathcal{Q}\|_{\mathcal{V}'}$ such that*

$$|\mathcal{Q}(u)| \leq c_{\mathcal{V}'}\|u\|_{\mathcal{V}} \quad \forall u \in \mathcal{V}. \tag{2.2}$$

In addition, if $\mathcal{V} \subset H^\lambda$ for some $0 \leq \lambda \leq 1$, then we say $\mathcal{Q}$ is bounded on H^λ if there exists constant $c_{-\lambda} = \|\mathcal{Q}\|_{-\lambda}$ such that

$$|\mathcal{Q}(u)| \leq c_{-\lambda}\|u\|_{\lambda} \quad \forall u \in \mathcal{V}. \tag{2.3}$$

Here, H^λ refers to the fractional Sobolev spaces H^λ for $0 < \lambda < 1$, H^1 for $\lambda = 1$, and $H^0 = L^2$ for $\lambda = 0$ [1]. In later sections we consider examples in which $\mathcal{Q}$ is specifically bounded in $H^0 = L^2$ and examples in which $\mathcal{Q}$ is not bounded in L^2 but is bounded in $H^{1/2}$. In these cases, we prove enhanced convergence to γ (see Lemma 6).

Additionally, we assume general approximation properties on the discrete subspaces of $\mathcal{V}$ as follows.

ASSUMPTION A.3 (approximation property). *Given a shape regular mesh of Ω and finite dimensional subspace, $\mathcal{V}^h \subset \mathcal{V}$, where $\mathcal{V}^h$ contains the piecewise polynomial functions of degree $t > 0$, then for any $v \in \mathcal{V}$, we have*

$$\inf_{v^h \in \mathcal{V}^h} \|v - v^h\|_{\mathcal{V}} \leq c_r h^r \|v\|_{r+1}, \tag{2.4}$$

where c_r is independent of h and $r \leq t$.

This property holds for Sobolev spaces such as H^1, $H(\text{div})$, $H(\text{curl})$, or their product spaces, and we assume this approximation property for the finite dimensional subspaces we use in our theory.

Next, consider the minimization of $\mathcal{F}$ in (1.2) over the finite element space, $\mathcal{V}^h \subset \mathcal{V}$. This is accomplished by satisfying the discrete weak form: find $u_*^h \in \mathcal{V}^h$ such that

$$\langle \mathcal{L}u_*^h - f, \mathcal{L}v^h \rangle = 0 \quad \forall v^h \in \mathcal{V}^h \subset \mathcal{V}. \tag{2.5}$$

Letting $e_*^h = u_* - u_*^h$, Assumptions A.1 and A.3 imply the following convergence bound that is used in the remainder of this paper:

$$\|\mathcal{L}e_*^h\| \leq c_r h^r \|u_*\|_{r+1}, \tag{2.6}$$

whenever $u_* \in H^{r+1}(\Omega) \cap \mathcal{V}$ for $r \leq t$.

2.2. Theoretical observations. An immediate consequence of the ellipticity of $\mathcal{F}$ is that it extends to the QoI-based functional $\mathcal{F}_{\mathcal{Q}}$. This is summarized in the following lemma, and we note that multiple (additive) QoI are also straightforward to accommodate.

LEMMA 1. *Suppose that $\mathcal{F}$ is coercive and continuous over $\mathcal{V}$, with constants c_0 and c_1, respectively. If $\mathcal{Q}$ is a bounded linear functional over $\mathcal{V} \subset H^0$ with constant $c_{\mathcal{V}'}$, then $\mathcal{F}_{\mathcal{Q}}$ is coercive and continuous over $\mathcal{V}$, with constants c_0 and $\hat{c}_1 = \sqrt{c_1^2 + \beta^2 c_{\mathcal{V}'}^2}$, respectively.*

Proof. Since

$$c_0^2 \|u\|_{\mathcal{V}}^2 \leq \|\mathcal{L}u\|^2 \leq c_1^2 \|u\|_{\mathcal{V}}^2 \quad \text{and} \quad |\mathcal{Q}(u)|^2 \leq c_{\mathcal{V}'}^2 \|u\|_{\mathcal{V}}^2 \tag{2.7}$$

hold for all $u \in \mathcal{V}$,

$$c_0^2 \|u\|_{\mathcal{V}}^2 \leq \|\mathcal{L}u\|^2 + \beta^2 |\mathcal{Q}(u)|^2 \leq (c_1^2 + \beta^2 c_{\mathcal{V}'}^2) \|u\|_{\mathcal{V}}^2 \tag{2.8}$$

immediately follows. ∎

3. Error bounds and a modified functional. In this section, we establish initial error bounds on the QoI-based functional and introduce a modified form of the QoI-based least-squares functional.

Consider the weak problem associated with the QoI-based functional, $\mathcal{F}_{\mathcal{Q}}$, in (1.5): find $u \in \mathcal{V}$ such that

$$\langle \mathcal{L}u - f, \mathcal{L}v \rangle + \beta^2 (\mathcal{Q}(u) - \gamma) \mathcal{Q}(v) = 0 \quad \forall v \in \mathcal{V}. \tag{3.1}$$

We note that $u = u_*$. Consider that the associated discrete problem to (3.1) is posed on $\mathcal{V}^h \subset \mathcal{V}$. We assume $\mathcal{V}^h$ satisfies Assumption A.3 and denote by t the polynomial degree. Then, the discrete problem is to find $u^h \in \mathcal{V}^h \subset \mathcal{V}$ such that

$$\langle \mathcal{L}u^h, \mathcal{L}v^h \rangle + \beta^2 \mathcal{Q}(u^h) \mathcal{Q}(v^h) = \langle f, \mathcal{L}v^h \rangle + \gamma \beta^2 \mathcal{Q}(v^h) \quad \forall v^h \in \mathcal{V}^h. \tag{3.2}$$

We observe that the QoI, $\gamma = \mathcal{Q}(u_*) = \mathcal{Q}(u)$, is, in general, not computable. Thus, we use the Riesz representation theorem to express $\mathcal{Q}$ in terms of the dual solution: there exists a unique $p \in \mathcal{V}$ such that

$$\mathcal{Q}(v) = \langle \mathcal{L}v, \mathcal{L}p \rangle \quad \forall v \in \mathcal{V}. \tag{3.3}$$

In particular, we have $Q(u) = \langle \mathcal{L}u, \mathcal{L}p \rangle = \langle f, \mathcal{L}p \rangle$. With this, (3.1) becomes

$$\langle \mathcal{L}u, \mathcal{L}v \rangle + \beta^2 \mathcal{Q}(u)\mathcal{Q}(v) = \langle f, \mathcal{L}v \rangle + \beta^2 \mathcal{Q}(u)\mathcal{Q}(v) \tag{3.4}$$

$$= \langle f, \mathcal{L}v \rangle + \beta^2 \langle \mathcal{L}u, \mathcal{L}p \rangle \mathcal{Q}(v) \tag{3.5}$$

$$= \langle f, \mathcal{L}v \rangle + \beta^2 \langle f, \mathcal{L}p \rangle \mathcal{Q}(v) \quad \forall v \in \mathcal{V}, \tag{3.6}$$

where we have used $u = u_*$. Here, p is unknown, so we introduce a subspace $\mathcal{W}^{\hat{h}} \subset \mathcal{V}$ and approximate p by $p^{\hat{h}} \in \mathcal{W}^{\hat{h}}$ such that

$$\langle \mathcal{L}w^{\hat{h}}, \mathcal{L}p^{\hat{h}} \rangle = \mathcal{Q}(w^{\hat{h}}) \quad \forall w^{\hat{h}} \in \mathcal{W}^{\hat{h}}. \tag{3.7}$$

We assume $\mathcal{W}^{\hat{h}}$ contains C^0 polynomial functions, satisfies Assumption A.3, and denotes by $\hat{t}$ the polynomial degree of $\mathcal{W}^{\hat{h}}$.

Using $p^{\hat{h}}$ we introduce an approximate or *modified* QoI:

$$\mathcal{Q}^{\hat{h}}(v) \,=\, \langle \mathcal{L}v, \mathcal{L}p^{\hat{h}} \rangle \quad \forall v \in \mathcal{V}. \tag{3.8}$$

Then, for exact solution u_*, we have $\mathcal{Q}^{\hat{h}}(u_*) = \langle f, \mathcal{L}p^{\hat{h}} \rangle = \gamma^{\hat{h}}$, which leads to the functional

$$\mathcal{F}_{\hat{\mathcal{Q}}}(u; f) \,=\, \|\mathcal{L}u - f\|^2 + \beta^2 \langle \mathcal{L}u - f, \mathcal{L}p^{\hat{h}} \rangle^2. \tag{3.9}$$

Then, the weak problem and discrete weak problem become the following: find $\hat{u} \in \mathcal{V}$ such that

$$\langle \mathcal{L}\hat{u}, \mathcal{L}v \rangle + \beta^2 \mathcal{Q}^{\hat{h}}(\hat{u})\mathcal{Q}^{\hat{h}}(v) = \langle f, \mathcal{L}v \rangle + \beta^2 \langle f, \mathcal{L}p^{\hat{h}} \rangle \mathcal{Q}^{\hat{h}}(v) \quad \forall v \in \mathcal{V}. \tag{3.10}$$

It is important to note that u_*, the solution to (1.3), also satisfies (3.10). Below we show that it is the unique solution. First, observe that due to Galerkin orthogonality,

$$\|\mathcal{L}p\|^2 = \|\mathcal{L}(p - p^{\hat{h}} + p^{\hat{h}})\|^2 = \|\mathcal{L}(p - p^{\hat{h}})\|^2 + \|\mathcal{L}p^{\hat{h}}\|^2, \tag{3.11}$$

and hence,

$$\|\mathcal{L}p^{\hat{h}}\| \le \|\mathcal{L}p\|. \tag{3.12}$$

By (3.8), (3.12), the Cauchy–Schwarz inequality, and Assumption A.1, we have

$$|\mathcal{Q}^{\hat{h}}(u)| \le \|\mathcal{L}u\|\|\mathcal{L}p^{\hat{h}}\| \le \|\mathcal{L}u\|\|\mathcal{L}p\| \le c_{\mathcal{V}'}\|u\|_{\mathcal{V}}, \tag{3.13}$$

where $c_{\mathcal{V}'} = c_1\|\mathcal{L}p\|$. That is, the modified QoI also defines a bounded linear functional on $\mathcal{V}$. Then Lemma 1 implies that $\mathcal{F}_{\hat{\mathcal{Q}}}$ is coercive and continuous in $\mathcal{V}$. Hence, (3.10) has a unique solution, $\hat{u} = u_* \in \mathcal{V}$. The discrete form is defined similarly with $\hat{u}^h \in \mathcal{V}^h \subset \mathcal{V}$.

The space $\mathcal{W}^{\hat{h}}$ can be viewed as a "dual" space in the sense that we are establishing a representation of the QoI, γ, through the Riesz representation theorem. Therefore, we seek the representation in a *finer* space than that of the primal approximation from $\mathcal{V}$ in order to establish the role of $p^{\hat{h}}$.

ASSUMPTION A.4 (approximation and dual spaces). *Given a C^0 approximation space, $\mathcal{V}^h$, and C^0 dual space, $\mathcal{W}^{\hat{h}}$, satisfying Assumption* A.3 *with t and $\hat{t}$, respectively, we assume that $\mathcal{V}^h \subsetneq \mathcal{W}^{\hat{h}} \subset \mathcal{V}$.*

Hence, by Assumption A.4 and application of (3.7) for any $v^h \in \mathcal{V}^h$, we have

$$\mathcal{Q}^{\hat{h}}(v^h) = \langle \mathcal{L}v^h, \mathcal{L}p^{\hat{h}} \rangle = Q(v^h). \tag{3.14}$$

Next, we establish an error bound for the discrete problem.

LEMMA 2 (primal estimate: effect of $\hat{u}^h \in \mathcal{V}^h$). *Let $\hat{u}^h \in \mathcal{V}^h$ satisfy* (3.10). *If $\hat{u} \in H^{r+1}$, then*

$$\|\hat{u}^h - u_*\|_{\mathcal{V}} \leq Ch^r \|u_*\|_{r+1}, \quad r \leq t. \tag{3.15}$$

Proof. By the approximation property of $\mathcal{V}^h$ (Assumption A.3) and ellipticity of $\mathcal{F}_{\hat{\mathcal{Q}}}$,

$$\|\hat{u}^h - \hat{u}\|_{\mathcal{V}} \leq Ch^r \|\hat{u}\|_{r+1} \tag{3.16}$$

for $r \leq t$. Since $\hat{u} = u_*$ (see (3.10)), the proof is complete. ◻

The next lemma establishes the relationship between the discrete solutions when $\mathcal{W}^{\hat{h}} \subseteq \mathcal{V}^h$.

LEMMA 3. *Suppose $\mathcal{W}^{\hat{h}} \subseteq \mathcal{V}^h$. If $\hat{u}^h$ satisfies the discrete weak form associated with $\mathcal{F}_{\hat{\mathcal{Q}}}$,* (3.10)*, then it also satisfies the discrete weak form associated with $\mathcal{F}$,* (2.5).

Proof. Let u_*^h satisfy (2.5). Then u_*^h satisfies the orthogonality condition,

$$\langle \mathcal{L}(u_* - u_*^h), \mathcal{L}v^h \rangle = 0 \quad \forall v^h \in \mathcal{V}^h. \tag{3.17}$$

Using our assumption, $\mathcal{W}^{\hat{h}} \subseteq \mathcal{V}^h$, and (3.17),

$$\langle \mathcal{L}u_*^h - f, \mathcal{L}p^{\hat{h}} \rangle = \mathcal{Q}^{\hat{h}}(u_*^h) - \mathcal{Q}^{\hat{h}}(u_*) = 0.$$

Thus, u_*^h satisfies (3.10), the weak form associated with $\mathcal{F}_{\hat{\mathcal{Q}}}$. By uniqueness of the solution of the weak form, $u_*^h = \hat{u}^h$. ◻

In Table 1, we summarize the notation.

4. Enhanced error bounds. In section 3 we established bounds on the $\mathcal{V}$-norm of the error for both $\mathcal{F}_{\mathcal{Q}}$ and $\mathcal{F}_{\hat{\mathcal{Q}}}$. In this section, we derive enhanced L^2 error bounds under the assumption that $\mathcal{L}^*\mathcal{L}$ is H^2 regular, where $\mathcal{L}^*$ is the formal adjoint of $\mathcal{L}$. We then extend that result to fractional norms, which is used in the next section to establish enhanced error bounds for the error in the QoI.

ASSUMPTION A.5 (H^2 regularity). *Suppose $\mathcal{V} \subset H^\lambda$ and $\mathcal{Q} \in (H^\lambda)'$, the dual of H^λ, for some $0 \leq \lambda \leq 1$. From Assumption* A.1*, there exists $p \in \mathcal{V}$ such that*

$$\langle \mathcal{L}v, \mathcal{L}p \rangle = \mathcal{Q}(v) \quad \forall v \in \mathcal{V}. \tag{4.1}$$

Assume the weak operator $\mathcal{L}^*\mathcal{L}$ has full H^2 regularity; then, there exists constant $c_{-\lambda}$ such that

$$\|p\|_{2-\lambda} \leq c_{-\lambda} \|\mathcal{Q}\|_{-\lambda}. \tag{4.2}$$

TABLE 1
Explanation of the notation used in this paper.

Expression	Description	Reference
$\mathcal{F}$	Traditional least-squares functional	(1.2)
$\mathcal{F}_{\mathcal{Q}}$	Least-squares functional with QoI	(1.5)
$\mathcal{F}_{\hat{\mathcal{Q}}}$	Modified $\mathcal{F}_{\mathcal{Q}}$	(3.9)
$\mathcal{V}$	Space for solutions u and p	Assump. A.1
$\mathcal{V}^h$	Space for discrete solution u^h	Assump. A.3
$\mathcal{W}^{\hat{h}}$	Space for discrete dual solution $p^{\hat{h}}$	Assump. A.3
u_*, u, $\hat{u}$	Minimizers of $\mathcal{F}$, $\mathcal{F}_{\mathcal{Q}}$, $\mathcal{F}_{\hat{\mathcal{Q}}}$	(1.3), (3.1), (3.10)
u_*^h, u^h, $\hat{u}^h$	Approximation of u_*, u, $\hat{u}$	(2.5), (3.2), (3.10)
p	Exact dual solution	(3.3)
$p^{\hat{h}}$	Discrete approximation of p	(3.7)
Q	QoI	(1.4)
$Q^{\hat{h}}$	Discrete approximation of the QoI	(3.8)
e_*^h, e^h, $\hat{e}^h$	The error in u_*^h, u^h, $\hat{u}^h$	

We note that this assumption implies that $\mathcal{V} \subset H^1$.

In the following lemma, an Aubin–Nitsche type proof is used to establish enhanced L^2 convergence bounds.

LEMMA 4. *Let u^h and $\hat{u}^h$ be the discrete solution to $\mathcal{F}_{\mathcal{Q}}$ and $\mathcal{F}_{\hat{\mathcal{Q}}}$, satisfying* (3.2) *and* (3.10)*, respectively. Let the weak operator, $\mathcal{L}^*\mathcal{L}$, be H^2 regular (Assumption* A.5*). Then, the errors, $e^h = u_* - u^h$ and $\hat{e}^h = u_* - \hat{u}^h$ satisfy*

$$\|e^h\| \le Ch^{r+1}\|u_*\|_{r+1}, \qquad \|\hat{e}^h\| \le Ch^{r+1}\|u_*\|_{r+1}, \tag{4.3}$$

where $r \le t$.

Proof. The proof is a variation of the classical Aubin–Nitsche proof. Consider e^h and the solution, $w \in \mathcal{V}$, to the dual weak problem,

$$\langle \mathcal{L}v, \mathcal{L}w\rangle + \beta^2 \mathcal{Q}(v)\mathcal{Q}(w) = \langle v, e^h\rangle \quad \forall v \in \mathcal{V}. \tag{4.4}$$

Setting $v = e^h$, we arrive at a relationship with dual variable w and the error:

$$\langle \mathcal{L}e^h, \mathcal{L}w\rangle + \beta^2 \mathcal{Q}(e^h)\mathcal{Q}(w) \;=\; \langle e^h, e^h\rangle. \tag{4.5}$$

Then, from the orthogonality induced by the weak form, (3.2), we have

$$\langle e^h, e^h\rangle \;=\; \langle \mathcal{L}e^h, \mathcal{L}(w - v^h)\rangle + \beta^2 \mathcal{Q}(e^h)\mathcal{Q}(w - v^h) \quad \forall v^h \in \mathcal{V}^h, \tag{4.6}$$

which becomes

$$\begin{aligned} \|e^h\|^2 &\le \|Le^h\|\|\mathcal{L}(w - v^h)\| + \beta^2|\mathcal{Q}(e^h)||\mathcal{Q}(w - v^h)| \\ &\le \left(\|Le^h\|^2 + \beta^2\mathcal{Q}(e^h)^2\right)^{1/2}\left(\|\mathcal{L}(w - v^h)\|^2 + \beta^2\mathcal{Q}(w - v^h)^2\right)^{1/2}. \end{aligned} \tag{4.7}$$

Finally, we use the approximation property of $\mathcal{V}^h$ and H^2 regularity of $\mathcal{L}^*\mathcal{L}$ to arrive at

$$\inf_{v^h \in \mathcal{V}^h} \left(\|\mathcal{L}(w - v^h)\|^2 + \beta^2\mathcal{Q}(w - v^h)^2\right)^{1/2} \le Ch\|w\|_2 \le Ch\|e^h\|. \tag{4.8}$$

Combining the continuity of $\mathcal{F}_{\mathcal{Q}}$, the approximation property in Assumption A.3, (4.7), and (4.8) leads to

$$\|e^h\| \le Ch\left(\|\mathcal{L}e^h\|^2 + \beta^2\mathcal{Q}(e^h)^2\right)^{1/2} = Ch\mathcal{F}_{\mathcal{Q}}^{1/2}(e^h; 0) \le Ch^{r+1}\|u_*\|_{r+1} \tag{4.9}$$

for $r \leq t$.

The key to the proof for $\hat{e}^h$ is to note that the functional, $\mathcal{F}_{\hat{\mathcal{Q}}}$, satisfies a uniform continuity constant, $\hat{c}_1$ in Lemma 1, independent of $\mathcal{W}^{\hat{h}}$. The modified weak form (3.10) is similar to that of the functional, $\mathcal{F}_{\mathcal{Q}}$, in (3.2). The proof now follows the same steps as the proof for e^h. ∎

Under Assumption A.5, we have $\mathcal{V} \subset H^1$. Thus, we have established H^1 bounds on the error in (2.6) and L^2 bounds on the error in (4.3). By application of interpolation space bounds, we next arrive at bounds in H^λ for $0 \leq \lambda \leq 1$.

LEMMA 5. *Assume that $\mathcal{V}^h \subset \mathcal{W}^{\hat{h}}$ (Assumption A.4) and that $\mathcal{L}^*\mathcal{L}$ is H^2 regular (Assumption A.5). Then, for both $\mathcal{F}_{\mathcal{Q}}$ and $\mathcal{F}_{\hat{\mathcal{Q}}}$, we have the bounds*

$$\|e^h\|_\lambda \leq Ch^{r+1-\lambda}\|u_*\|_{r+1}, \quad \|\hat{e}^h\|_\lambda \leq Ch^{r+1-\lambda}\|u_*\|_{r+1} \tag{4.10}$$

for $r \leq t$.

Proof. The proof follows from a bound on the interpolation space: given $0 \leq \lambda \leq 1$, there exists constants $c_\lambda > 0$ such that for $v \in H^1$ (cf. [1])

$$\|v\|_\lambda \leq c_\lambda \|v\|_0^{1-\lambda}\|v\|_1^\lambda. \tag{4.11}$$

From the proof of Lemma 4, coercivity bound (2.1), and Assumption A.5, we have

$$\|e^h\| \leq Ch\mathcal{F}_{\mathcal{Q}}^{1/2}(e^h; 0) \tag{4.12}$$

and

$$\|e^h\|_1 \leq c_0\mathcal{F}_{\mathcal{Q}}^{1/2}(e^h; 0). \tag{4.13}$$

From (4.12) and (4.13) with (4.11), we have

$$\|e^h\|_\lambda \leq Ch^{1-\lambda}\mathcal{F}_{\mathcal{Q}}^{1/2}(e^h; 0). \tag{4.14}$$

Finally, by Assumption A.3 and (2.6), we have

$$\|e^h\|_\lambda \leq Ch^{r+1-\lambda}\|u_*\|_{r+1}. \tag{4.15}$$

The proof for $\mathcal{F}_{\hat{\mathcal{Q}}}$ is similar. ∎

5. Bounding the QoI. In the previous section, we established enhanced convergence when $\mathcal{L}^*\mathcal{L}$ is H^2 regular. In this section, we first show that if $\mathcal{Q} \in (H^\lambda)'$ for some $0 \leq \lambda \leq 1$, the error in the QoI inherits this enhanced convergence. We then derive sharper bounds on the error in the QoI that depend on the weight factor β^2.

LEMMA 6. *Given Assumptions A.2, A.4, and A.5, let the finite element approximations $u^h, \hat{u}^h$ based on $\mathcal{F}_{\mathcal{Q}}$, $\mathcal{F}_{\hat{\mathcal{Q}}}$ satisfy (3.2), (3.10), respectively. Then, the errors, $e = u_* - u^h$ and $\hat{e} = u_* - \hat{u}^h$, satisfy*

$$\frac{|\mathcal{Q}(e^h)|}{\|\mathcal{Q}\|_{-\lambda}} \leq \|e^h\|_\lambda \leq Ch^{r+1-\lambda}\|u_*\|_{r+1}, \tag{5.1}$$

$$\frac{|\mathcal{Q}(\hat{e}^h)|}{\|\mathcal{Q}\|_{-\lambda}} \leq \|\hat{e}^h\|_\lambda \leq Ch^{r+1-\lambda}\|u_*\|_{r+1}, \tag{5.2}$$

where $0 < r \leq t$.

Proof. Suppose $\mathcal{Q}(u)$ is bounded in H^λ. Then,

$$|\mathcal{Q}(e^h)| \le \|\mathcal{Q}\|_{-\lambda}\|e^h\|_\lambda, \tag{5.3}$$

and by Lemma 5,

$$\frac{|\mathcal{Q}(e^h)|}{\|\mathcal{Q}\|_{-\lambda}} \le \|e^h\|_\lambda \le Ch^{r+1-\lambda}\|u_*\|_{r+1} \quad \text{for } r \le t. \tag{5.4}$$

The proof for $\hat{e}^h$ is similar. ∎

We have shown that if $\mathcal{Q}$ is bounded in H^λ, then enhanced convergence of $\mathcal{Q}(e^h)$ and $\mathcal{Q}(\hat{e}^h)$ is achieved. However, as we detail in the following sections, while the asymptotic rate is not changed, bounds on the error in the QoI for $\mathcal{F}_\mathcal{Q}$ and $\mathcal{F}_{\hat{\mathcal{Q}}}$ yield a smaller constant.

To bound the error in the QoI, we consider the more general scenario of an unknown value for the QoI. The next lemma establishes a sharp bound on the error in the (modified) QoI $\mathcal{Q}^{\hat{h}}(\hat{e}^h)$. A similar result holds in the case of a *known* QoI, and the approach taken is this case is similar to that of [4].

LEMMA 7 (dependence on β^2 of the error in $\mathcal{Q}^{\hat{h}}$ from $\mathcal{F}_{\hat{\mathcal{Q}}}$). *Let $\hat{u}^h$ be the solution to the discrete weak form* (3.10) *associated with modified least-squares functional, $\mathcal{F}_{\hat{\mathcal{Q}}}$. Further, assume that $\mathcal{V}^h \subset \mathcal{W}^{\hat{h}}$ by Assumption* A.4. *Then, for $\hat{e}^h = u_* - \hat{u}^h$, we have*

$$\frac{|\mathcal{Q}^{\hat{h}}(\hat{e}^h)|}{\|\mathcal{Q}\|_{-\lambda}} \le \frac{Ch^{r+1-\lambda}}{(1+\beta^2\langle \mathcal{L}w^h, \mathcal{L}w^h\rangle)}\|u_*\|_{r+1}, \quad r \le t \le \hat{t}, \tag{5.5}$$

where $w^h = \underset{v^h \in \mathcal{V}^h}{\operatorname{argmin}} \|\mathcal{L}(p - v^h)\|$.

Proof. From (3.8) and from the orthogonality in (3.10), $\hat{e}^h = u_* - \hat{u}^h$ satisfies, for all $y^h \in \mathcal{V}^h$,

$$\mathcal{Q}^{\hat{h}}(\hat{e}^h) = \langle \mathcal{L}\hat{e}^h, \mathcal{L}p^{\hat{h}}\rangle = \langle \mathcal{L}\hat{e}^h, \mathcal{L}(p^{\hat{h}} - y^h)\rangle - \beta^2\mathcal{Q}^{\hat{h}}(\hat{e}^h)\mathcal{Q}^{\hat{h}}(y^h). \tag{5.6}$$

Thus, we have

$$\mathcal{Q}^{\hat{h}}(\hat{e}^h) = \frac{\langle \mathcal{L}\hat{e}^h, \mathcal{L}(p^{\hat{h}} - y^h)\rangle}{(1+\beta^2\mathcal{Q}^{\hat{h}}(y^h))} \quad \forall\, y^h \in \mathcal{V}^h. \tag{5.7}$$

From here, we choose a particular $y^h = w^h \in \mathcal{V}^h$ so that, using (3.8),

$$\langle \mathcal{L}z^h, \mathcal{L}w^h\rangle = \langle \mathcal{L}z^h, \mathcal{L}p^{\hat{h}}\rangle = \mathcal{Q}^{\hat{h}}(z^h) \quad \forall z^h \in \mathcal{V}^h \subset \mathcal{W}^{\hat{h}}. \tag{5.8}$$

Thus, $\mathcal{Q}^{\hat{h}}(w^h) = \langle \mathcal{L}w^h, \mathcal{L}w^h\rangle$. Further, since $\mathcal{V}^h \subset \mathcal{W}^{\hat{h}} \subset \mathcal{V}$, we have the orthogonality relation $\langle \mathcal{L}(p - p^{\hat{h}}), \mathcal{L}(p^{\hat{h}} - w^h)\rangle = 0$. This implies

$$\|\mathcal{L}(p - w^h)\|^2 = \|\mathcal{L}(p - p^{\hat{h}} + p^{\hat{h}} - w^h)\|^2 = \|\mathcal{L}(p - p^{\hat{h}})\|^2 + \|\mathcal{L}(p^{\hat{h}} - w^h)\|^2$$

and hence $\|\mathcal{L}(p^{\hat{h}} - w^h)\| \le \|\mathcal{L}(p - w^h)\|$, which leads to

$$|\mathcal{Q}^{\hat{h}}(\hat{e}^h)| = \left|\frac{\langle \mathcal{L}\hat{e}^h, \mathcal{L}(p^{\hat{h}} - w^h)\rangle}{(1+\beta^2\mathcal{Q}^{\hat{h}}(w^h))}\right| \le \frac{\|\mathcal{L}\hat{e}^h\|\|\mathcal{L}(p^{\hat{h}} - w^h)\|}{1+\beta^2\langle \mathcal{L}w^h, \mathcal{L}w^h\rangle} \le \frac{\|\mathcal{L}\hat{e}^h\|\|\mathcal{L}(p - w^h)\|}{1+\beta^2\langle \mathcal{L}w^h, \mathcal{L}w^h\rangle}. \tag{5.9}$$

To bound $\|\mathcal{L}\hat{e}^h\|$ and $\|\mathcal{L}(p - w^h)\|$, we observe that by regularity (Assumption A.5) and by the approximation properties of $\mathcal{V}^h$ and $\mathcal{W}^{\hat{h}}$ (Assumption A.3),

$$\|\mathcal{L}\hat{e}^h\| \le ch^r \|u_*\|_{r+1} \tag{5.10}$$

and

$$\|\mathcal{L}(p - w^h)\| = \inf_{v^h \in \mathcal{V}^h} \|\mathcal{L}(p - v^h)\| \le ch^{1-\lambda}\|p\|_{2-\lambda} \le ch^{1-\lambda}\|Q\|_{-\lambda}. \tag{5.11}$$

Thus, we bound the error in the modified QoI by

$$|\mathcal{Q}^{\hat{h}}(\hat{e}^h)| \le \frac{Ch^{r+1-\lambda}}{(1 + \beta^2\langle \mathcal{L}w^h, \mathcal{L}w^h\rangle)}\|u_*\|_{r+1}\|\mathcal{Q}\|_{-\lambda} \tag{5.12}$$

for $r \le t$. ∎

From this result we see that the constant in the error bound in (5.12) becomes smaller as the weight, β^2, on the QoI constraint in (3.9) increases. That is, as we strengthen the QoI term in the least-squares functional, the approximate solution satisfies the QoI with higher accuracy, as expected.

We are now in a position to prove the major result of this section, which establishes a bound on $\mathcal{Q}(\hat{e}^h)$, the error in the exact QoI with regard to the solution obtained using the modified functional. In addition, it also shows the limitations of only increasing the weight on the QoI in the functional, (3.9).

THEOREM 5.1. *Under the same hypotheses as Lemma* 7*, we have*

$$\frac{|\mathcal{Q}(\hat{e}^h)|}{\|\mathcal{Q}\|_{-\lambda}} \le \frac{Ch^{r+1-\lambda}}{(1 + \beta^2\langle \mathcal{L}w^h, \mathcal{L}w^h\rangle)}\|u_*\|_{r+1} + C\hat{h}^{r+1-\lambda}\|u_*\|_{r+1} \tag{5.13}$$

for $r \le t \le \hat{t}$.

Proof. In order to bound $\mathcal{Q}(\hat{e}^h)$ we observe that

$$\mathcal{Q}(\hat{e}^h) = \langle \mathcal{L}\hat{e}^h, \mathcal{L}p\rangle = \langle \mathcal{L}\hat{e}^h, \mathcal{L}p^{\hat{h}}\rangle + \langle \mathcal{L}\hat{e}^h, \mathcal{L}(p - p^{\hat{h}})\rangle \tag{5.14}$$

$$= \mathcal{Q}^{\hat{h}}(\hat{e}^h) + \langle \mathcal{L}\hat{e}^h, \mathcal{L}(p - p^{\hat{h}})\rangle. \tag{5.15}$$

Since $\mathcal{V}^h \subseteq \mathcal{W}^{\hat{h}}$ by Assumption A.4,

$$\mathcal{Q}(\hat{e}^h) = \mathcal{Q}^{\hat{h}}(\hat{e}^h) + \langle \mathcal{L}(\hat{e}^h - y^{\hat{h}}), \mathcal{L}(p - p^{\hat{h}})\rangle \qquad \forall y^{\hat{h}} \in \mathcal{W}^{\hat{h}}. \tag{5.16}$$

Moreover, the second term is bounded in terms of $\hat{h}$, which yields

$$|\langle \mathcal{L}(\hat{e}^h - y^{\hat{h}}), \mathcal{L}(p - p^{\hat{h}})\rangle| \le C\hat{h}^{r+1-\lambda}\|u_*\|_{r+1}\|\mathcal{Q}\|_{-\lambda}, \quad r \le \hat{t}, \tag{5.17}$$

which yields the result. ∎

For an unknown QoI, β^2 affects only one term of the error. While the asymptotic rate is similar to the one derived in Lemma 4, here we see that if β^2 is chosen sufficiently large, then the error in the exact QoI from the modified functional (3.8) is dominated by the accuracy of the approximation, $p^{\hat{h}} \in \mathcal{W}^{\hat{h}}$. Consequently, the two terms in (5.13) highlight two important features of the error in the QoI for our least-squares approach. The first term quantifies the dependence of the primal approximation on the QoI constraint. In contrast, the second term represents the error in the dual approximation, $p^{\hat{h}}$, so that a weak representation of the dual will dominate the error if the constraint is forced too large.

Remark 1. The results in Lemma 7 and Theorem 5.1 assume that $\mathcal{Q} \in H^{-\lambda}$, and hence, $p \in H^{2-\lambda}$. If the QoI has higher regularity, then the bounds are improved. In particular, if $p \in H^{r+1}$ (and for simplicity, $h = \hat{h}$), then $|\mathcal{Q}(\hat{e}^h)| = O(h^{r^2})$. That is, the convergence rate of the error in the QoI is doubled as compared to the convergence rate in the $\mathcal{V}$ norm (see (3.15)).

In the numerical results below, $\mathcal{W}^{\hat{h}}$ is chosen on the same mesh as $\mathcal{V}^h$, but with higher-order polynomials, and β^2 is chosen adaptively on each finer mesh to ensure the enhanced rate of convergence.

6. Computation and adaptive refinement.

6.1. Discrete relationships and computation. In this section, we discuss the discrete relationships between the standard least-squares solution and the QoI-based least-squares solutions, as well as outline a method for computing the latter. Consider the weak form in (3.10). Let $\{\phi_j^h\}_{j=1}^n$ be a basis for $\mathcal{V}^h$ and write $\hat{u}^h = \sum_i u_i \phi_i^h$. From this we define matrix A with entries $A_{ij} = \langle \mathcal{L}\phi_i^h, \mathcal{L}\phi_j^h \rangle$, and vectors $\mathbf{q}$ and $\mathbf{f}$ with entries $q_i = \langle \mathcal{L}\phi_i^h, \mathcal{L}p^{\hat{h}} \rangle$ and $f_i = \langle f, \mathcal{L}\phi_i^h \rangle$, respectively. This results in the matrix problem

$$\left(A + \beta^2 \mathbf{q}\mathbf{q}^T\right) \mathbf{u} = \mathbf{f} + \beta^2 \langle f, \mathcal{L}p^{\hat{h}} \rangle \mathbf{q}. \tag{6.1}$$

Consequently, the QoI-based functional simply adds a rank-one update to our sparse matrix problem. The Sherman–Morrison formula for inverse of a rank-one update to the matrix yields

$$(A + \beta^2 \mathbf{q}\mathbf{q}^T)^{-1} = A^{-1} - \frac{\beta^2}{1 + \beta^2 \mathbf{q}^T A \mathbf{q}} (A^{-1}\mathbf{q})(A^{-1}\mathbf{q})^T. \tag{6.2}$$

Applying this to (6.1) yields

$$\mathbf{u} = A^{-1}\mathbf{f} - \beta^2 \frac{\langle f, \mathcal{L}p^{\hat{h}} \rangle - \mathbf{q}^T A^{-1} \mathbf{f}}{1 + \beta^2 \mathbf{q}^T A^{-1} \mathbf{q}} A^{-1}\mathbf{q}. \tag{6.3}$$

Note that $A^{-1}\mathbf{f}$ is the solution with $\beta = 0$, or the standard least-squares solution, u_*^h. To simplify the rest of the expression, consider the weak problem to find $p^h \in \mathcal{V}^h$ such that

$$\langle \mathcal{L}v^h, \mathcal{L}p^h \rangle = \langle \mathcal{L}v^h, \mathcal{L}p \rangle = \langle \mathcal{L}v^h, \mathcal{L}p^{\hat{h}} \rangle. \tag{6.4}$$

Note that p^h is computed as part of a multigrid algorithm to compute $p^{\hat{h}}$. The associated linear system is

$$A\mathbf{p} = \mathbf{q}. \tag{6.5}$$

Note that

$$\mathbf{q}^T A^{-1} \mathbf{q} = \mathbf{p}^T \mathbf{q} = \langle \mathcal{L}p^h, \mathcal{L}p^h \rangle \quad \text{and} \quad \mathbf{q}^T A^{-1} \mathbf{f} = \mathbf{p}^T \mathbf{f} = \langle f, \mathcal{L}p^h \rangle. \tag{6.6}$$

Combining (6.6) with (6.3) yields

$$\hat{u}^h = u_*^h + \frac{\beta^2 \langle f, \mathcal{L}(p^{\hat{h}} - p^h) \rangle}{1 + \beta^2 \langle \mathcal{L}p^h, \mathcal{L}p^h \rangle} p^h. \tag{6.7}$$

That is, the QoI-based least-squares solution can be computed in terms of u_*^h and p^h and hence can be computed efficiently. Note that, in the case of k QoI, the matrix problem results in k rank-one updates, which is solved efficiently using the method of Sherman, Morrison, and Woodbury.

6.2. Adaptive refinement algorithm. In this section, we briefly review refinement algorithms that target QoIs and present an adaptive refinement algorithm for the QoI enhanced least-squares formulation developed in the previous sections. Algorithm 1 outlines the adaptive procedure of the modified functional $\mathcal{F}_{\hat{\mathcal{Q}}}$ in (3.9). This algorithm targets the QoI, while maintaining convergence of the approximation to the global PDE.

In general, an effective refinement strategy is to distribute error equally over all mesh elements [8, 2]. To achieve this, numerous a posteriori error indicators have been developed to drive adaptive refinement algorithms toward accurate resolution of a QoI. One class of indicators integrates the weak residual by parts and then applies the Cauchy–Schwarz inequality on each element. This bounds the error in the QoI by the elementwise norm of the residual weighted by the elementwise norm of the dual solution [6, 7, 19]. An alternative solves local elementwise problems to build an error indicator [23, 24, 4, 5]. This second technique avoids Galerkin orthogonality by considering (local) high-order spaces and thereby solving the discrete dual problem in the same space as the primal problem. A final class of error indicators, which strongly motivates this work, is to evaluate the weak residual per element using the solution to a high-order dual as the test function [17, 19]. Goal-oriented refinement based on such error indicators has been applied to a large number of applications, including elasticity, fluid-flow, fluid structure interaction, and molecular biophysics [25, 20, 13, 26].

The error indicator developed for the QoI enhanced least-squares formulation shares aspects of indicators for standard least-squares formulations and for approaches developed in the references cited above. The functional $\mathcal{F}_{\hat{\mathcal{Q}}}$ involves two terms: the primal least-squares residual and the modified QoI. Letting u^h be an approximation to u, consider the error in the modified QoI,

$$
\begin{aligned}
(6.8)\qquad |\mathcal{Q}^{\hat{h}}(u_*^h) - \mathcal{Q}^{\hat{h}}(u^h)| &= |\langle \mathcal{L}(u_* - u^h), \mathcal{L}p^{\hat{h}}\rangle| = |\langle f - \mathcal{L}u^h, \mathcal{L}p^{\hat{h}}\rangle| \\
(6.9)\qquad &\le \sum_{\tau \in \text{mesh}} |\langle f - \mathcal{L}u^h, \mathcal{L}p^{\hat{h}}\rangle_\tau|.
\end{aligned}
$$

Now, consider a single term of the sum. We have

$$
(6.10)\qquad |\langle f - \mathcal{L}u^h, \mathcal{L}p^{\hat{h}}\rangle_\tau| \le \|f - \mathcal{L}u^h\|_\tau \|\mathcal{L}p^{\hat{h}}\|_\tau.
$$

From this we see that if the least-squares residual in element τ is small and if the QoI is insensitive to this element, then the associated term of the modified QoI is small. Conversely, if the residual is large, then either the least-squares residual is large or the modified QoI is particularly sensitive to this element, or both, which identifies an element that would benefit from refinement.

As a result, we consider a per element error estimator for the QoI-based least-squares finite element method of the form

$$
(6.11)\qquad \eta_\tau = \|\mathcal{L}u^h - f\|_\tau + \beta|\langle f - \mathcal{L}u^h, \mathcal{L}p^{\hat{h}}\rangle_\tau|.
$$

The presence of the QoI in both the functional (1.5) and the error estimator (6.11) is important, and we underscore this in the numerical experiments below. Specifically, the fitness of the approximation, $\hat{u}^h$, to the QoI is guided by the control of the QoI in both the weak problem and the refinement pattern. In addition, we note that the estimator, $|\langle f - \mathcal{L}u^h, \mathcal{L}p^{\hat{h}}\rangle_\tau|$ in (6.11), requires computation of the dual problem, and that the primal and dual contributions to this error estimator are combined in a multiplicative fashion (cf. [7]). The dual solution allows a local, elementwise quantification of the error in the QoI, whereas the primal problem only indicates how well the QoI is satisfied and *not* where to adapt.

Algorithm 1: QoI-based least-squares adaptive refinement algorithm.

Input: Ω^h: initial mesh
β: QoI functional weight
θ_{ref}: refinement threshold
return: Ω^h: refined mesh

$\hat{u}^h \leftarrow$ initialize
while $\mathcal{F}_{\hat{\mathcal{Q}}}(\hat{u}^h; f) > \varepsilon_{tol}$
1 construct $\mathcal{V}^h$ and $\mathcal{W}^{\hat{h}}$ on Ω^h {h `or` p `refinement`}
2 $p^{\hat{h}} \leftarrow \langle \mathcal{L}p^{\hat{h}}, \mathcal{L}w^{\hat{h}}\rangle = \mathcal{Q}(w^{\hat{h}}) \quad \forall\, w^{\hat{h}} \in \mathcal{W}^{\hat{h}}$ {`approximate QoI`}
3 $\hat{u}^h \leftarrow \min_{\mathcal{V}^h} \underbrace{\mathcal{F}_{\hat{\mathcal{Q}}}(u; f, p^{\hat{h}}, \beta)}_{\|\mathcal{L}u - f\|^2 + \beta^2\langle \mathcal{L}u - f, \mathcal{L}p^{\hat{h}}\rangle^2}$ {`QoI-based least-squares`}
for each $\tau \in \Omega^h$
4 $e_\tau^{\mathcal{F}} \leftarrow \|\mathcal{L}\hat{u}^h - f\|_\tau$ {`least-squares error`}
5 $e_\tau^{\mathcal{Q}} \leftarrow |\langle f - \mathcal{L}\hat{u}^h, \mathcal{L}p^{\hat{h}}\rangle_\tau|$ {`QoI error`}
6 $\eta_\tau = e_\tau^{\mathcal{F}} + \beta e_\tau^{\mathcal{Q}}$ {`error estimator`}
$\mathcal{E}^{\mathcal{F}} = \{e_\tau^{\mathcal{F}} \,|\, \tau \in \Omega^h\}$
$\mathcal{E}^{\mathcal{Q}} = \{e_\tau^{\mathcal{Q}} \,|\, \tau \in \Omega^h\}$
7 $\beta \leftarrow$ `compute_weight`$(\mathcal{E}^{\mathcal{F}}, \mathcal{E}^{\mathcal{Q}})$ {`determine weights`}
8 $\Omega^h \leftarrow$ `refine`$(\theta_{ref}, \Omega, \eta_\tau)$ {`refine mesh`}

Algorithm 1 requires an initial coarse representation of the mesh, Ω^h, weights for the functional and error estimator (i.e., β), and a fraction for selecting elements of the mesh to refine in line 8. In line 1, a space $\mathcal{V}^h$ is used for mesh Ω^h and a refined space, $\mathcal{W}^{\hat{h}}$, either by mesh refinement or by polynomial refinement, leading to $\mathcal{V}^h \subset \mathcal{W}^{\hat{h}}$. With these spaces, approximations to the QoI and to the modified weak problem are determined in lines 2 and 3, respectively. Based on approximations $\hat{u}^h$ and $p^{\hat{h}}$, the local error in the solution and in the QoI are approximated per element in lines 4 and 5 to form the elemental error indicator η_τ. Then, based on this elementwise view of the error, the weight β is recomputed in line 7 (see section 6.4). Finally, a certain portion of the error is selected for refinement in line 8, using θ_{ref} as a threshold. Most of the results below mark elements for refinement if they satisfy

$$e_\tau^{\mathcal{F}} + \beta e_\tau^{\mathcal{Q}} > \theta_{ref} \max_\tau \,(e_\tau^{\mathcal{F}} + \beta e_\tau^{\mathcal{Q}}). \tag{6.12}$$

However, for comparison purposes in section 7.3 a *Dörfler*-type [16] marking strategy is employed.

6.3. Relationship with traditional adjoint based methods. In addition to the modified functional, $\mathcal{F}_{\hat{\mathcal{Q}}}$, we also consider the standard least-squares functional, $\mathcal{F}$, in (1.2) and employ a QoI-based error estimator. That is, for this estimator, we minimize the functional (1.2) for our primal problem and then solve the dual problem to obtain $p^{\hat{h}}$. We utilize an additional algebraic step based on Galerkin orthogonality, common in the literature [17] for adjoint-based error estimators, namely,

$$|\langle f - \mathcal{L}u_*^h, \mathcal{L}p^{\hat{h}}\rangle| = |\langle f - \mathcal{L}u_*^h, \mathcal{L}(p^{\hat{h}} - p^h)\rangle| \quad \forall p^h \in \mathcal{V}^h. \tag{6.13}$$

As a result, a QoI-based estimator for functional (1.2) is $|\langle f - \mathcal{L}u_*^h, \mathcal{L}(p^{\hat{h}} - p^h)\rangle|_\tau$. Furthermore, p^h can be chosen in multiple ways—e.g., nodal interpolation, which is used in our experiments, or an L^2-projection of $p^{\hat{h}}$ from $\mathcal{W}^{\hat{h}}$ to $\mathcal{V}^h$.

6.4. The influence of $\boldsymbol{\beta}$. As the refinement algorithm proceeds, the least-squares and QoI terms may not remain in balance. Indeed, in section 5 we showed that if $\mathcal{Q}$ is bounded in H^λ for $0 \le \lambda < 1$, then the QoI converges at a faster rate than the functional. Since the QoI integral differs from that of the L^2-norm in the least-squares functional—i.e., it may be local and lower in dimension—we expect a dependence of β on h in order to maintain balance of the terms in the functional, $\mathcal{F}_{\hat{\mathcal{Q}}}$. A large β emphasizes the QoI in the functional and as a result, as indicated by the inequality (5.12), the approximation yields a more accurate QoI as β increases. However, the bound in (5.13) demonstrates that there is a limit to the benefit of overweighting the QoI.

Since the exact dependence on h is difficult to determine in practice, we propose a heuristic based on the observations above. A large value of β emphasizes the QoI factor, $\langle f - \mathcal{L}\hat{u}^h, \mathcal{L}p^{\hat{h}}\rangle$, in $\mathcal{F}_{\hat{\mathcal{Q}}}$. Moreover, if the approximation to $p^{\hat{h}}$ is accurate, then a large β yields a solution that resolves the QoI more accurately than standard least-squares. However, it is also necessary to balance the global least-squares error, which is represented by the term $\|\mathcal{L}\hat{u}^h - f\|$. As a result, we seek to balance these two terms in the functional by modifying β for each level of refinement in Algorithm 1. More precisely, we write the least-squares error and the approximate error in the QoI in each element τ as

$$e_\tau^{\mathcal{F}} = \|\mathcal{L}\hat{u}^h - f\|_\tau, \qquad e_\tau^{\mathcal{Q}} = |\langle f - \mathcal{L}\hat{u}^h, \mathcal{L}p^{\hat{h}}\rangle|_\tau, \tag{6.14}$$

respectively. Then, in line 7 of Algorithm 1, we compute a new weight as

$$\beta = \frac{\max_\tau e_\tau^{\mathcal{F}}}{\max_\tau e_\tau^{\mathcal{Q}}}. \tag{6.15}$$

In order to reduce the initial unrealistic influence of the QoI, a small value of β is chosen for the first iteration. Similarly, a finite bound on β is also imposed to avoid pathological cases of overweighting the QoI.

7. Numerical experiments. In this section we detail several numerical experiments comparing the traditional least-squares finite element methods with the QoI-based approach developed in this paper. Table 2 summarizes the three adaptive methods and their associated estimators and functionals.

Table 2
Adaptive strategies with the associated functional and estimator.

Method	Functional	Per element estimator
Standard least-squares	$\mathcal{F}$	$\\|\mathcal{L}u_*^h - f\\|_\tau$
QoI-based least-squares	$\mathcal{F}_{\hat{\mathcal{Q}}}$	$\\|\mathcal{L}\hat{u} - f\\|_\tau + \beta\|\langle f - \mathcal{L}\hat{u}^h, \mathcal{L}p^{\hat{h}}\rangle\|_\tau$
QoI-based only	$\mathcal{F}$	$\|\langle f - \mathcal{L}u_*^h, \mathcal{L}p^{\hat{h}} - p^h\rangle\rangle\|_\tau$

In the numerical experiments, we measure the error in the global norm given the least-squares functional, as well as the error in the QoI. For the value of QoI, we use $Q(u_*^h)$ for the standard least-squares method and the QoI-based least-squares method, while the more accurate approximation $\langle f, \mathcal{L}p^{\hat{h}}\rangle$ is employed for the QoI-based only method. The expressions used for computing the QoI for the three methods are given in Table 3. Further, we measure the efficiency of the QoI-based functional and error estimator by considering the computational work required for each approach. We define the *cost* of an adaptive refinement method to be the total work required to attain a certain accuracy. The different methods and their QoI expressions and costs are given in Table 3.

Table 3
Final QoI expression and the total at refinement level ℓ: $\dim(\mathcal{V}_\ell^h)$ and $\dim(\mathcal{W}_\ell^{\hat{h}})$ are the dimensions of $\mathcal{V}^h$ and $\mathcal{W}^{\hat{h}}$ at refinement level ℓ, respectively.

Method	QoI expression	Cost
Standard least-squares	$Q(u_*^h)$	$\sum_{i=1}^{\ell} \dim(\mathcal{V}_i^h)$
QoI-based least-squares	$\langle f, \mathcal{L}p^{\hat{h}}\rangle$	$\sum_{i=1}^{\ell} \dim(\mathcal{V}_i^h) + \dim(\mathcal{W}_i^{\hat{h}})$
QoI-based only	$\langle f, \mathcal{L}p^{\hat{h}}\rangle$	$\sum_{i=1}^{\ell} \dim(\mathcal{V}_i^h) + \dim(\mathcal{W}_i^{\hat{h}})$

This cost is representative since in the least-squares context both primal and dual problems are amenable to fast solvers such as multigrid. Moreover, the cost is consistent with the cost associated with other approaches that use a dual space. The cost of our approach, however, is potentially further reduced when implemented in a nested iteration setting, which is natural for least-squares formulations.

7.1. Diffusion. We first consider a Poisson problem described in [4]. The PDE is posed on the unit square with homogeneous Dirichlet boundary conditions. More formally, u satisfies

$$\begin{aligned} -\nabla^2 u &= f(x), \qquad x \in \Omega, \\ u(x) &= 0, \qquad x \in \partial\Omega. \end{aligned} \tag{7.1}$$

The source term, f, is defined so that the solution to (7.1) is

$$u(x, y) = 5x^2(1-x)^2(e^{10x^2} - 1)y^2(1-y)^2(e^{10y^2} - 1). \tag{7.2}$$

The QoI interest for the problem is

$$\mathcal{Q}(u) = \int_{\Omega_{\mathcal{Q}}} u, \tag{7.3}$$

where $\Omega_{\mathcal{Q}} = [0.2, 0.4]^2$. Figure 1 shows the contours of u and the region defining the QoI, $\Omega_{\mathcal{Q}}$. We see that the exact solution (7.2) yields relatively steep gradients at the

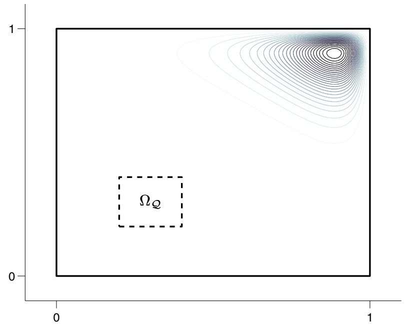


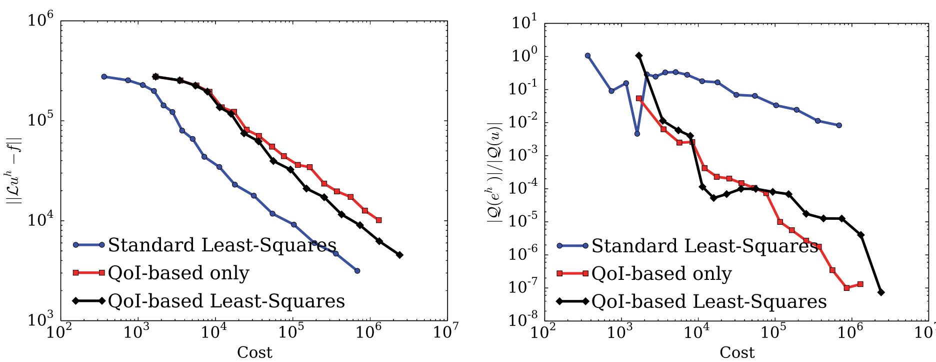
FIG. 1. *[Diffusion] Contours of the solution, u, and the region of interest, $\Omega_{\mathcal{Q}}$.*

northeast corner, while the region corresponding to the QoI-based functional is well separated from this area.

Rewriting (7.1) as a first-order system,

$$\mathcal{L}\mathbf{u} = \begin{bmatrix} -\nabla u + \mathbf{q} \\ -\nabla \cdot \mathbf{q} \\ \nabla \times \end{bmatrix} = \begin{bmatrix} 0 \\ f \\ 0 \end{bmatrix} = \mathbf{f}, \tag{7.4}$$

defines the functional, $\mathcal{F}$, and, with the addition of the QoI, $\mathcal{Q}$, defines the functional, $\mathcal{F}_{\hat{\mathcal{Q}}}$, for this problem. In our experiments, we use linear elements to discretize the primal problem, $\mathcal{V}^h = (\mathbb{P}_1^2, \mathbb{P}_1)$, and quadratic elements for the dual space, $\mathcal{W}^{\hat{h}} = (\mathbb{P}_2^2, \mathbb{P}_2)$. The parameter θ_{ref} in Algorithm 1 is chosen to be 0.3 and elements are marked according to (6.12).



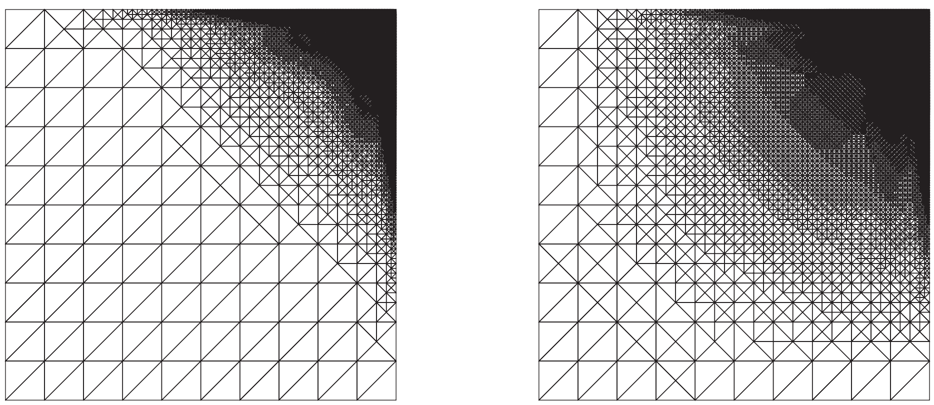
(a) Global convergence (b) QoI convergence

FIG. 2. *Results for diffusion. The methods, along with their associated functionals and estimators, are summarized in Table* 2.

Figure 2a, which shows the convergence of the formulations measured in the global least-squares error, $\|\mathcal{L}u - f\|$. The standard least-squares and the QoI-based least-squares have a slightly better convergence rate as compared to a QoI-based only estimator. Figure 2b shows the error in the QoI as a function of the cost. The QoI-based only method and the QoI-based least-squares methods have a significantly better convergence rate than the standard least-squares method. As a result, the

QoI-based least-squares method targets the QoI, while retaining convergence to the solution of the PDE.

Figures 3a and 3b show the mesh after 11 levels of local adaptive refinement using the least-squares and the QoI-based least-squares methods. The figures for the meshes show that standard least-squares refines heavily in the top right corner, where the gradients in the solution are large. In contrast, the adaptively weighted QoI-based formulation refines in the top right less aggressively while refining more heavily in the region, $\Omega_{\mathcal{Q}}$, corresponding to the QoI. The more targeted refinement pattern of the QoI-based least-squares formulation attempts to balance the resolution required to satisfy the PDE with the resolution required to compute the QoI functional.



(a) Standard least-squares

(b) $\mathcal{F}_{\hat{\mathcal{Q}}}(\hat{\beta})$ with adaptive $\hat{\beta}$

Fig. 3. *[Poisson] Adaptive meshes based on standard least-squares and QoI-based least-squares after* 11 *levels of adaptive refinement. The methods, along with their associated functionals and estimators, are summarized in Table* 2.

7.2. Convection-diffusion. In this section we consider convection-diffusion in the two-dimensional domain $\Omega = [0, 10] \times [0, 2]$. This problem has been previously considered in [18]. More precisely, we seek a solution to

$$\begin{aligned} -\nabla \cdot (a(x)\nabla u(x)) + \mathbf{b} \cdot \nabla u &= 1, \qquad x \in \Omega, \\ u(x) &= 0, \qquad x \in \partial\Omega, \end{aligned} \tag{7.5}$$

where $a(x) > 0$ is a smoothly varying function, defined as

$$a(x) = 0.05 + \tanh(10(x-5)^2 + 10(y-1)^2), \tag{7.6}$$

and the vector field $\mathbf{b} = [-100, 0]^T$. Rewriting (7.5) as a first-order system results in

$$\mathbf{q} - \sqrt{a}\nabla u = 0, \tag{7.7}$$

$$-\nabla \cdot (\sqrt{a}\mathbf{q}) + \mathbf{b} \cdot \nabla u = 1, \tag{7.8}$$

$$\nabla \times (\mathbf{q}/\sqrt{a}) = 0. \tag{7.9}$$

The QoI functional of interest is to evaluate the integral of u over the small patch, $\Omega_{\mathcal{Q}} = [1, 1.25] \times [0.25, 0.5]$. Formally, in terms of the variables of the first-order system, the QoI is stated as

$$\mathcal{Q}(\mathbf{q}, u) = \int_{\Omega_{\mathcal{Q}}} u.$$

Both the domain and the QoI region are depicted in Figure 4. To solve the primal problem, piecewise linear basis functions are used, while the solution to the dual problem is approximated by quadratics; i.e., we use $\mathcal{V}^h = (\mathbb{P}_1^2, \mathbb{P}_1)$ and $\mathcal{W}^{\hat{h}} = (\mathbb{P}_2^2, \mathbb{P}_2)$. The parameter θ_{ref} in Algorithm 1 is chosen to be 0.3, and elements are marked according to (6.12).

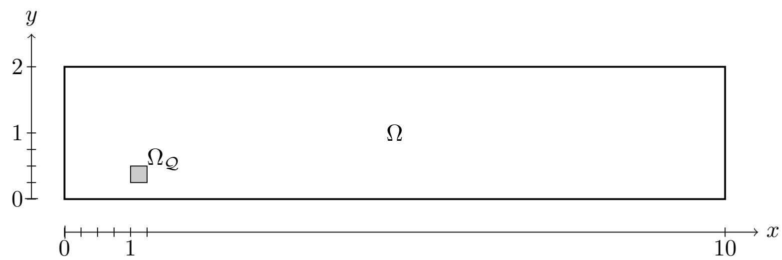
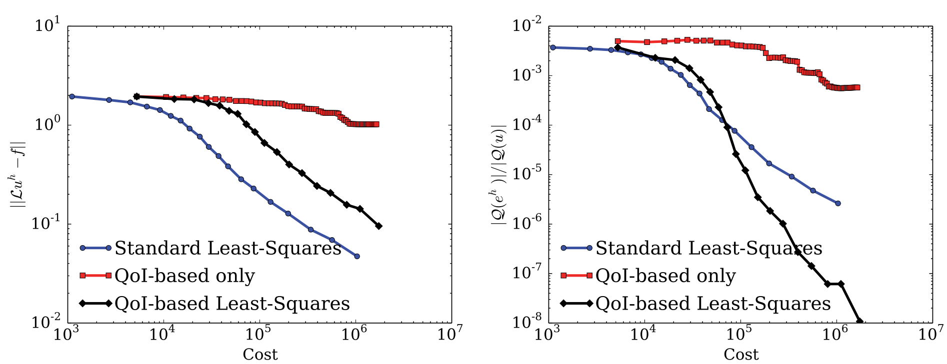


FIG. 4. *[Convection-diffusion] Computation domain with QoI region $\Omega_{\mathcal{Q}}$.*

Figure 5a shows the convergence in the global least-square error for the three methods. The standard least-squares and the QoI-based least-squares have similar convergence rates which are higher than the QoI-based only method. Figure 5b shows the convergence in the QoI. QoI-based least-squares has the best performance in this case, underscoring that global convergence of the solution may be important for this example. As will become clear in the next section, the poor performance of the QoI-based only method can be attributed to the marking strategy.

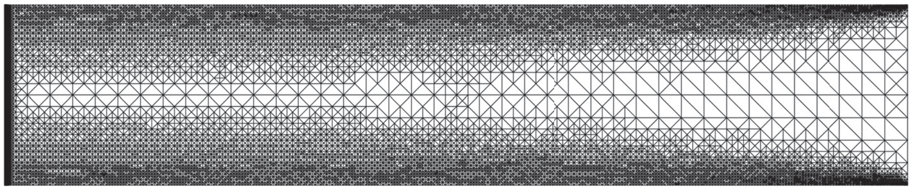


(a) Global convergence (b) QoI convergence

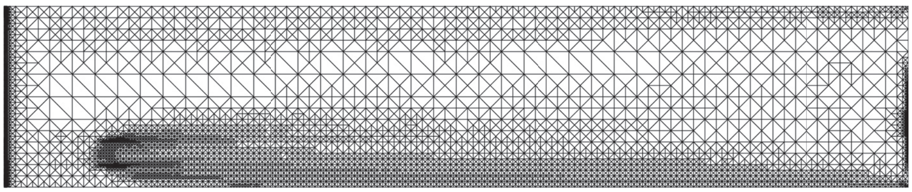
FIG. 5. *Results for convection-diffusion. The methods, along with their associated functionals and estimators, are summarized in Table* 2.

Figure 6 shows the mesh after 12 levels of adaptive, local refinement using the standard least-squares method and the QoI-based least-squares method. The figures for the meshes indicate that the QoI-based least-squares estimator refines more in the neighborhood and upwind of $\Omega_{\mathcal{Q}}$ as compared to the standard least-squares estimator.

7.3. Effect of marking strategy. The marking strategy may affect the performance of the adaptive refinement algorithm. One such effect could be that too few elements may be chosen for refinement using the marking strategy in Algorithm 1 [16]. This is the case in Figure 5, where the estimator based on QoI-based only



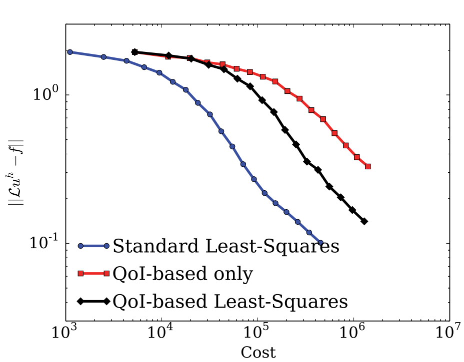
(a) Standard least-squares



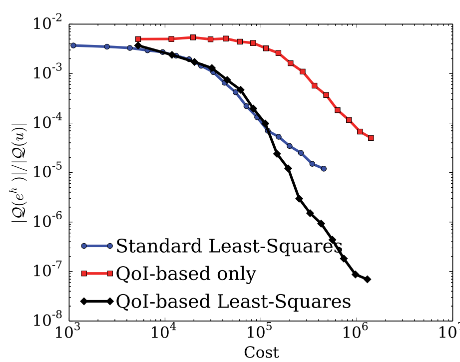
(b) QoI-based least-squares

FIG. 6. *[Convection-diffusion] Adaptive meshes based on standard least-squares and QoI-based least-squares. The methods, along with their associated functionals and estimators, are summarized in Table* 2.

estimator selects too few elements to refine. In this section, we compare the performance of estimators using a *Dörfler*-type marking strategy. This fair approach has nice theoretical properties. Yet, because a sort of the element indicators is required, this method is impractical (the computational complexity of the sort ruins the optimal linear scaling of the multigrid solves). For this marking strategy we refine the top 20% of elements with the largest error indicators. The results using this strategy for the convection-diffusion problem in section 7.2 are given in Figure 7. The results are similar in quality to Figure 5. The QoI-based least-squares method is effective at reducing both the global and QoI errors.



(a) Global convergence



(b) QoI convergence

FIG. 7. *Convection-diffusion.*

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