

# COMPUTING BOUNDS FOR LINEAR FUNCTIONALS OF EXACT WEAK SOLUTIONS TO THE ADVECTION-DIFFUSION-REACTION EQUATION

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**Abstract.** We present a cost effective method for computing quantitative upper and lower bounds on linear functional outputs of exact weak solutions to the advection-diffusion-reaction equation and we demonstrate a simple adaptive strategy by which such outputs can be computed to a prescribed precision. The bounds are computed from independent local subproblems resulting from a standard finite element approximation to the problem. At the heart of the method lies a local dual problem by which we transform an infinite dimensional minimization problem into a finite dimensional feasibility problem. The bounds hold for all levels of refinement on polygonal domains with piecewise polynomial forcing, and the bound gap converges at twice the rate of the  $\mathcal{H}^1$ -norm of the error in the finite element solution.

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**1. Introduction.** Using simulation results to support important decisions requires a high degree of confidence in their accuracy. Three essential questions must be answered before a simulation result can be trusted. Do the mathematical equations model the relevant phenomena? Does the software actually solve the discretized mathematical model? Does the simulation result contain sufficient precision to be considered a solution of the mathematical model?

Recently, we introduced a rigorous method for computing guaranteed upper and lower bounds on linear functional outputs from Poisson's equation [16] which descended from earlier work done by Patera, Paraschivoiu, and Peraire [13, 14, 15] on two-level residual based techniques for computing output bounds. The method can answer the third question by certifying the precision of integrated outputs from finite element simulations for any level of mesh refinement. The method can help answer the second question because it has easily checkable preconditions to help verify correctness of the simulation software. Furthermore, the quantification of numerical error removes uncertainty about the fidelity of the discretization and aids the practitioner in distinguishing modelling error from numerical error when validating the simulation and thus can aid in answering the first question. Error estimates that do not have the guarantee of one-sidedness, or that approach exactness but only in the asymptotic limit, cannot certify the precision of simulations posed on arbitrary meshes and require additional work to compute a bound on the error in the error.

As the method appeals to the dual of a minimization reformulation of the original problem, it can be viewed as an extension of complementary energy techniques for error estimation, first proposed by Fraeijs de Veubeke [9] and later pursued by Ladevèze and Leguillon [12, 11], and others [10, 8], to more relevant error measures and to problems without intrinsic minimization principles such as the advection-diffusion-reaction equation. Similarly, as the method solves equilibrated elemental residual subproblems, it can be viewed as an extension of the work of Bank and Weiser [3], Ainsworth and Oden [2, 1], and others [7], which does not require exact minimums of infinite dimensional subproblems to guarantee bounds. Like Becker and Rannacher [5, 4], we are interested in the precision of integrated output quantities and focus the adap-

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tive refinement process on improving the precision of the desired output quantity in particular and not the solution in isolation.

In this paper we generalize our method in a variety of ways while extending it to the advection-diffusion-reaction equation. Beginning with the description of the model problem in §2 and continued throughout the paper, we give a more general presentation of the method which explicitly considers non-homogeneous boundary data. Section 3 launches the construction of the method with a constrained minimization reformulation of the model problem which we localize to obtain independent local subproblems. Section 4 gives a derivation of the local dual subproblem that includes the reaction term and gives a more detailed description of the local subproblems. Section 5 summarizes the products of the previous sections by laying out the complete procedure. Finally, §6 closes the paper with numerical examples which demonstrate the potential for the method to deliver simulation results of guaranteed prescribed precision through adaptive mesh refinement in addition to certifying the precision of non-adaptive results. The paper presents the method in a manner which allows the convergence results developed in the context of Poisson's equation [16] to be easily extended to the advection-diffusion-equation so we do not reproduce them here, but focus instead on the new ingredients for the advection-diffusion-reaction equation.

**2. Model Problem.** We will consider the steady scalar diffusion dominated advection-diffusion-reaction equation posed on a polygonal domain  $\Omega$  in  $d$  spatial dimensions with boundary  $\Gamma$  composed of complementary regions  $\Gamma^D$  and  $\Gamma^N$ . The problem is written in weak form as: find  $u \in \mathcal{U}$  such that

$$a(u, v) = \ell(v), \quad \forall v \in \mathcal{V}, \quad (2.1)$$

with the assumed to be continuous and coercive, but nonsymmetric, bilinear form

$$a(w, v) = \int_{\Omega} \nu \nabla w \cdot \nabla v + \mu w v + (\boldsymbol{\alpha} \cdot \nabla w) v \, d\Omega, \quad (2.2)$$

for a strictly positive real coefficient  $\nu \in \mathcal{L}^{\infty}(\Omega)$ , a nonnegative real coefficient  $\mu \in \mathcal{L}^{\infty}(\Omega)$ , and a prescribed vector field  $\boldsymbol{\alpha} \in \mathcal{H}(\text{div}; \Omega)$  which is assumed for simplicity to be incompressible,  $\nabla \cdot \boldsymbol{\alpha} = 0$ . The set of admissible functions is defined as  $\mathcal{U}(\Omega) \equiv \{v \in \mathcal{H}^1(\Omega) \mid v|_{\Gamma^D} = u_D\}$ , with Dirichlet boundary data  $u_D \in \mathcal{H}^{\frac{1}{2}}(\Gamma^D)$ , and the space of test functions is defined as  $\mathcal{V}(\Omega) \equiv \{v \in \mathcal{H}^1(\Omega) \mid v|_{\Gamma^D} = 0\}$ . Additionally, we require the prescription of the solution field on inflow boundaries, that is  $\Gamma^- \subset \Gamma^D \subset \Gamma$  for  $\Gamma^- = \{\mathbf{x} \in \Gamma \mid \boldsymbol{\alpha} \cdot \mathbf{n}(\mathbf{x}) \leq 0\}$ . The linear forcing functional

$$\ell(v) = \int_{\Omega} f v \, d\Omega + \int_{\Gamma^N} g v \, d\Gamma, \quad (2.3)$$

includes both interior  $f \in \mathcal{H}^{-1}(\Omega)$  and Neumann boundary  $g \in \mathcal{H}^{-\frac{1}{2}}(\Gamma^N)$  contributions.

We are not directly interested in the field solution  $u$ , however, but in bounded linear functional outputs from it,  $s = \ell^{\mathcal{O}}(u)$ . In particular, we will develop upper and lower bounds on the outputs produced by linear functionals such as

$$\ell^{\mathcal{O}}(w) = \int_{\Omega^{\mathcal{O}}} f^{\mathcal{O}} w \, d\Omega + \int_{\Gamma^{\mathcal{O}}} g^{\mathcal{O}} w \, d\Gamma, \quad (2.4)$$

for  $f^{\mathcal{O}} \in \mathcal{H}^{-1}(\Omega^{\mathcal{O}})$  and  $g^{\mathcal{O}} \in \mathcal{H}^{-\frac{1}{2}}(\Gamma^{\mathcal{O}})$ .

In order to guarantee bounds for any level of refinement, the method presented in this paper requires that the coefficients  $\nu$ ,  $\mu$ , and  $\alpha$ , and forcing data  $f$ ,  $f^\mathcal{O}$ ,  $g$  and  $g^\mathcal{O}$  are all piecewise polynomial. In addition, we will consider only constant coefficients  $\nu$  and  $\mu$  for simplicity.

**3. Constrained Minimization Reformulation.** In the context of our previous exposition of the method for the Poisson problem [16], we reformulated the model problem as a constrained minimization with weakly enforced continuity in order to localize the bounds computations and to obtain bounds on more informative output quantities than the abstract energy. In the present context of a nonsymmetric operator, the reformulation also provides the means by which we can treat problems without an intrinsic minimization principle.

**3.1. Weak Continuity.** We begin by introducing a triangulation of the domain,  $\mathcal{T}_h$ , into non-overlapping open subdomains,  $T$ , called elements, for which  $\bigcup_{T \in \mathcal{T}_h} \bar{T} = \bar{\Omega}$ . We denote by  $\partial T$  the edges constituting the boundary of a single element  $T$ , and by  $\partial \mathcal{T}_h$  the network of all edges in the mesh. On this triangulation, we introduce the broken space

$$\hat{\mathcal{V}} \equiv \{ v \in \mathcal{L}^2 \mid v|_T \in \mathcal{H}^1(T), \forall T \in \mathcal{T}_h \}. \quad (3.1)$$

in which the continuity of  $\hat{\mathcal{V}}$  is broken across the mesh edges,  $\partial \mathcal{T}_h$ . Note that the broken space relaxes the Dirichlet boundaries in addition to the inter-element continuity so that we have  $\mathcal{V} \subset \hat{\mathcal{V}}$  and  $\mathcal{U} \subset \hat{\mathcal{V}}$ .

We enforce continuity between the elemental subdomains weakly through the bilinear form  $b : \hat{\mathcal{V}} \times \Lambda \rightarrow \mathbb{R}$

$$b(\hat{w}, \lambda) = \sum_{T \in \mathcal{T}_h} \int_{\partial T} \sigma_T \hat{w} \lambda \, d\Gamma,$$

where, for  $T_N \in \mathcal{T}_h$  and an arbitrary ordering of the elements,  $T < T_N$ ,

$$\sigma_T(x) = \begin{cases} -1 & x \in \bar{T} \cap \bar{T}_N, T < T_N \\ +1 & \text{otherwise} \end{cases} \quad (3.2)$$

is a constant on each edge, and the edge functions  $\lambda$  are members of the dual trace space  $\Lambda = \prod_{T \in \mathcal{T}_h} \mathcal{H}^{-\frac{1}{2}}(\partial T)$ .

In addition to weak enforcement of interelement continuity, the Dirichlet data will also be enforced weakly in our reformulation through the forcing provided by the linear functional  $\ell^D : \Lambda \rightarrow \mathbb{R}$

$$\ell^D(\lambda) = \sum_{T \in \mathcal{T}_h} \int_{\Gamma_T^D} \sigma_T u_D \lambda \, d\Gamma, \quad (3.3)$$

so that  $b(\hat{w}, \lambda) = \ell^D(\lambda)$  for all  $\hat{w} \in \mathcal{U}$  and  $\lambda \in \Lambda$ .

**3.2. Operator Decomposition.** A nonsymmetric operator can be split into symmetric,  $a^s(w, v) = a^s(v, w)$ , and antisymmetric,  $a^{ss}(w, v) = -a^{ss}(v, w)$ , contributions

$$a^s(w, v) = \frac{1}{2} [a(w, v) + a^*(v, w)], \quad a^{ss}(w, v) = \frac{1}{2} [a(w, v) - a^*(v, w)], \quad (3.4)$$

where  $a^*(v, w)$  is the formal adjoint of  $a(w, v)$  for  $w \in \mathcal{U}$  and  $v \in \mathcal{V}$ . Integration by parts yields  $a(u, w) = a^*(w, u) + C^*$ , from which we note that  $a^{ss}(w, w) = \frac{1}{2}C^*$  and thus  $a(w, w) = a^s(w, w) + \frac{1}{2}C^*$ . Additionally, we note from the above that  $a(v, w) = a^s(v, w) + a^{ss}(v, w) = a^s(w, v) - a^{ss}(w, v)$ . It is easily shown for the advection-diffusion-reaction equation that

$$\begin{aligned} a^*(v, w) &= \int_{\Omega} \nu \nabla v \cdot \nabla w + \mu v w - (\boldsymbol{\alpha} \cdot \nabla v) w \, d\Omega + \int_{\Gamma^N} v (\boldsymbol{\alpha} \cdot \mathbf{n}) w \, d\Gamma, \\ C^* &= \int_{\Gamma^D} (\boldsymbol{\alpha} \cdot \mathbf{n}) u_D^2 \, d\Gamma, \end{aligned} \quad (3.5)$$

and therefore

$$\begin{aligned} a^s(w, v) &= \int_{\Omega} \nu \nabla w \cdot \nabla v + \mu w v \, d\Omega + \frac{1}{2} \int_{\Gamma^N} w (\boldsymbol{\alpha} \cdot \mathbf{n}) v \, d\Gamma, \\ \hat{a}^{ss}(w, v) &= \int_{\Omega} (\boldsymbol{\alpha} \cdot \nabla w) v \, d\Omega - \frac{1}{2} \int_{\Gamma^N} w (\boldsymbol{\alpha} \cdot \mathbf{n}) v \, d\Gamma. \end{aligned} \quad (3.6)$$

**3.3. Constrained Minimization Statement.** Using the above definitions we can write the following energy-like functional  $\varepsilon : \hat{\mathcal{V}} \rightarrow \mathbb{R}$

$$\varepsilon(\hat{w}) = a^s(\hat{w}, \hat{w}) + \frac{1}{2}C^* - \ell(\hat{w}) + \ell(\bar{u}) - a(\hat{w}, \bar{u}), \quad (3.7)$$

where  $\bar{u}$  is a member of  $\mathcal{U}$ . This functional has two essential properties. First, it is coercive on the space  $\hat{\mathcal{V}}$  for  $\mu > 0$  and for  $\mu = 0$  is coercive on the quotient space  $\hat{\mathcal{V}} \setminus \hat{\mathbb{P}}^0$ , where  $\hat{\mathbb{P}}^0$  is the space of constants over each element. Second, it produces the exact output when  $\hat{w} = u$ .

The weakly continuous constrained minimization problem for the nonsymmetric model problem can now be written as

$$\begin{aligned} \mp s &= \inf_{\hat{w}^{\pm} \in \hat{\mathcal{V}}} \mp \ell^{\mathcal{O}}(\hat{w}^{\pm}) + \frac{\kappa}{2} \varepsilon(\hat{w}^{\pm}) \\ \text{s.t.} \quad &a(\hat{w}^{\pm}, \psi) = \ell(\psi), \quad \forall \psi \in \mathcal{V}, \\ &b(\hat{w}^{\pm}, \lambda) = \ell^D(\lambda), \quad \forall \lambda \in \Lambda, \end{aligned} \quad (3.8)$$

where  $\kappa$  is a strictly positive real scaling parameter which provides dimensional consistency as well as an additionally degree of freedom which we will later use to tighten the bounds. This apparently trivial constrained minimization reformulation, first introduced in [13, 14] and whose constraints also arise in the context hybrid finite element methods [6], serves as the launching point for developing our method.

**3.4. Localization by Lagrangian Relaxation.** The above constrained minimization (3.8) has the Lagrangian:  $L^{\pm} : \hat{\mathcal{V}} \times \mathcal{V} \times \Lambda \rightarrow \mathbb{R}$

$$\begin{aligned} L^{\pm}(\hat{w}^{\pm}; \tilde{\psi}^{\pm}, \tilde{\lambda}^{\pm}) &= \mp \ell^{\mathcal{O}}(\hat{w}^{\pm}) \\ &+ \frac{\kappa}{2} \left\{ a^s(\hat{w}^{\pm}, \hat{w}^{\pm}) + \frac{1}{2}C^* - \ell(\hat{w}^{\pm}) + \ell(\bar{u}) - a(\hat{w}^{\pm}, \bar{u}) \right\} \\ &+ \ell(\tilde{\psi}^{\pm}) - a(\hat{w}^{\pm}, \tilde{\psi}^{\pm}) + \ell^D(\tilde{\lambda}^{\pm}) - b(\hat{w}^{\pm}, \tilde{\lambda}^{\pm}), \end{aligned} \quad (3.9)$$

for given candidate Lagrange multipliers  $\tilde{\psi}^{\pm} \in \mathcal{V}$  and  $\tilde{\lambda}^{\pm} \in \Lambda$ . The Lagrangian saddle point for the constrained minimization reformulation engenders the following

relationships for all  $(\tilde{\psi}^\pm, \tilde{\lambda}^\pm) \in \mathcal{V} \times \Lambda$

$$\inf_{\hat{w}^\pm \in \hat{\mathcal{V}}} L^\pm(\hat{w}^\pm; \tilde{\psi}^\pm, \tilde{\lambda}^\pm) \leq \sup_{\substack{\psi^\pm \in \mathcal{V} \\ \lambda^\pm \in \Lambda}} \inf_{\hat{w}^\pm \in \hat{\mathcal{V}}} L^\pm(\hat{w}^\pm; \psi^\pm, \lambda^\pm) = \mp s, \quad (3.10)$$

which we will exploit for developing inexpensive local subproblems for computing bounds. Equality on the right of (3.10) results from the strong duality of convex minimizations, but the bound property would still hold with weak duality.

**3.4.1. Lagrange Multiplier Approximation.** We compute approximate Lagrange multipliers using the finite element method by first choosing  $\tilde{\psi}^\pm = \pm \psi_h$ ,  $\tilde{\lambda}^\pm = -\frac{\kappa}{2} \lambda_h^u \pm \lambda_h^\psi$ , and  $\tilde{u} = u_h$ , where  $u_h$  and  $\psi_h$  are members of the usual piecewise polynomial finite element approximation set  $\mathcal{U}_h \equiv \{w \in \mathcal{U} \mid w|_T \in \mathbb{P}^p(T), \forall T \in \mathcal{T}_h\}$  and space  $\mathcal{V}_h \equiv \{v \in \mathcal{V} \mid v|_T \in \mathbb{P}^p(T), \forall T \in \mathcal{T}_h\}$ , and both  $\lambda_h^u$  and  $\lambda_h^\psi$  are members of the piecewise polynomial space  $\Lambda_h \equiv \{\lambda \in \Lambda \mid \lambda|_\gamma \in \mathbb{P}^p(\gamma), \forall \gamma \in \partial T\}$ . We have used the notation  $\mathbb{P}^p(T)$  for the space of polynomials on element  $T$  (in  $d$  spacial dimensions) with degree less than or equal to  $p$ , and  $\mathbb{P}^p(\gamma)$  for the space of polynomials on edges  $\gamma$  (in  $d-1$  spacial dimensions) with degree less than or equal to  $p$ .

By approximating  $u$ , the optimizer of the constrained minimization (3.8), with  $u_h$  and noting from (3.4) that  $a(v, u_h) = a^s(u_h, v) - a^{ss}(u_h, v)$ , we can write an approximate gradient condition

$$\begin{aligned} \frac{\kappa}{2} \{-\ell(\hat{v}) + a(\hat{v}, u_h) + b(\hat{v}, \lambda_h^u)\} \\ \pm \{-\ell^\mathcal{O}(\hat{v}) - a(\hat{v}, \psi_h) - b(\hat{v}, \lambda_h^\psi)\} = 0, \quad \forall \hat{v} \in \hat{\mathcal{V}}_h, \end{aligned} \quad (3.11)$$

with  $\hat{\mathcal{V}}_h \equiv \{\hat{v} \in \mathcal{L}^2 \mid \hat{v}|_T \in \mathbb{P}^p(T), \forall T \in \mathcal{T}_h\}$ . We can compute approximate Lagrange multipliers from (3.11) by solving the discrete problems:

1. Find  $u_h \in \mathcal{U}_h$  such that

$$a(u_h, v) = \ell(v), \quad \forall v \in \mathcal{V}_h, \quad (3.12)$$

2. Find  $\psi_h \in \mathcal{V}_h$  such that

$$a(v, \psi_h) = -\ell^\mathcal{O}(v), \quad \forall v \in \mathcal{V}_h, \quad (3.13)$$

3. Find  $\lambda_h^u \in \Lambda_h$  such that

$$b(\hat{v}, \lambda_h^u) = \ell(\hat{v}) - a(u_h, \hat{v}), \quad \forall \hat{v} \in \hat{\mathcal{V}}_h, \quad (3.14)$$

4. Find  $\lambda_h^\psi \in \Lambda_h$  such that

$$b(\hat{v}, \lambda_h^\psi) = -\ell^\mathcal{O}(\hat{v}) - a(\hat{v}, \psi_h), \quad \forall \hat{v} \in \hat{\mathcal{V}}_h. \quad (3.15)$$

The first two problems are standard finite element approximation problems and the second two problems are equilibration problems which can be solved with an asymptotic complexity that is linear in the number of vertices in the triangulation using Ladevèze's procedure [12].

**LEMMA 3.1.** *If the Lagrange multipliers  $\lambda_h^u$  and  $\lambda_h^\psi$  satisfy the equilibration conditions (3.14) and (3.15), then the minimizations*

$$\inf_{\hat{w}^\pm \in \hat{\mathcal{V}}} L^\pm(\hat{w}^\pm; \pm \psi_h, -\frac{\kappa}{2} \lambda_h^u \pm \lambda_h^\psi) \quad (3.16)$$

are bounded from below.

*Proof.* A strictly positive reaction term in  $a^s(\hat{w}^\pm, \hat{w}^\pm)$  ensures that the lower bounding minimization (3.10) is bounded below without the aid of equilibration. For  $\mu = 0$ , the constant function is not controlled by  $a^s(\hat{w}^\pm, \hat{w}^\pm)$  and without equilibration it would become possible for the subproblems, which only have Neumann boundary conditions, to be driven to arbitrarily large negative values of the Lagrangian functional. Equilibration ensures the nullification of the constant function, as can be checked by setting  $\hat{v} = \text{const}$  in (3.14) and (3.15).  $\square$

**4. Elemental Subproblems.** The continuity relaxation of §3.4 decomposes the triangulation so that after computing the approximate Lagrange multipliers we may consider each element *independently* when computing the bounds. We perform the global lower bounding minimization (3.10) by minimizing the local contribution of the Lagrangian on each elemental subdomain and accumulating the results to produce upper and lower bounds on the exact output

$$\sum_{T \in \mathcal{T}_h} s_T^- \leq s \leq \sum_{T \in \mathcal{T}_h} s_T^+ \quad (4.1)$$

We can write the local contribution of the Lagrangian on an arbitrary element  $T$  of the triangulation  $\mathcal{T}_h$  as

$$\mp s_T^\pm = \inf_{w^\pm \in \mathcal{H}^1(T)} \frac{\kappa}{2} a_T^s(w^\pm, w^\pm) + \ell_T^\pm(w^\pm) + C_T^\pm, \quad (4.2)$$

where we have collected the constant and linear contributions to the local Lagrangian with the definitions

$$\begin{aligned} \ell_T^\pm(v) = \frac{\kappa}{2} \left\{ -\ell_T(v) - a_T(v, u_h) + b_T(v, \lambda_h^u) \right\} \\ \pm \left\{ -\ell_T^\mathcal{O}(v) - a_T(v, \psi_h) - b_T(v, \lambda_h^\psi) \right\}, \end{aligned} \quad (4.3)$$

$$\begin{aligned} C_T^\pm = \frac{\kappa}{2} \left\{ \ell_T(u_h) - \ell_T^D(\lambda_h^u) + \frac{1}{2} C_T^* \right\} \\ \pm \left\{ \ell_T(\psi_h) + \ell_T^D(\lambda_h^\psi) \right\}. \end{aligned} \quad (4.4)$$

The subscript  $T$  denotes restrictions to a single element of the triangulation. For example, we have

$$\begin{aligned} a_T(w, v) &= \int_T \nu \nabla w \cdot \nabla v + \mu w v + (\boldsymbol{\alpha} \cdot \nabla w) v \, d\Omega, \\ \ell_T(v) &= \int_T f v \, d\Omega + \int_{\Gamma_T^N} g v \, d\Gamma, \end{aligned}$$

in which  $\Gamma_T^N$  denotes the local Neumann edges,  $\partial T \cap \Gamma^N$ , as well as

$$\begin{aligned} b_T(w, \lambda_h^u) &= \int_{\partial T} \sigma_T w \lambda_h^u \, d\Gamma, \\ \ell_T^D(\lambda_h^u) &= \int_{\Gamma_T^D} \sigma_T u_D \lambda_h^u \, d\Gamma \end{aligned}$$

in which  $\Gamma_T^D$  denotes the local Dirichlet edges,  $\partial T \cap \Gamma^D$ .

Recall from §3.2 that for the advection-diffusion-reaction equation we have

$$a_T^s(w, w) = \int_T \nu |\nabla w|^2 + \mu w^2 \, d\Omega + \frac{1}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) w^2 \, d\Gamma, \quad (4.5)$$

which is coercive on  $\mathcal{V}(T)$  for  $\mu > 0$  (and on  $\mathcal{V}(T) \setminus \mathbb{P}^0(T)$  for  $\mu = 0$ ) for all  $T$  in  $\mathcal{T}_h$  because  $\boldsymbol{\alpha} \cdot \mathbf{n}$  is perforce positive on  $\Gamma_T^N$ .

**4.1. Dualization of Local Minimization.** The localized unconstrained minimization (4.2) remains uncomputable in general, since the minimization must be performed over an infinite-dimensional space in order to guarantee the bounding property. Nevertheless, by once again applying the powerful ideas of Lagrangian saddle point theory, we can compute a lower bound to this lower bound and thus procure guaranteed computable bounds on the exact output of interest.

**PROPOSITION 4.1.** *The optimal value of the local unconstrained minimization problem (4.2) can be found by solving the local constrained maximization problem*

$$\begin{aligned} \mp s_T^\pm &= \sup_{\substack{\mathbf{q}^\pm \in (\mathcal{L}^2(T))^d \\ r^\pm \in \mathcal{L}^2(T)}} - \frac{\kappa}{2} a_T^{\text{du}}((\mathbf{q}^\pm, r^\pm), (\mathbf{q}^\pm, r^\pm)) + C_T^\pm \\ &\text{s.t. } \kappa c_T^{\text{du}}((\mathbf{q}^\pm, r^\pm), v) = -\ell_T^\pm(v), \quad \forall v \in \mathcal{H}^1(T), \end{aligned} \quad (4.6)$$

where the form  $a_T^{\text{du}} : (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T) \times (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T) \rightarrow \mathbb{R}$  is defined as

$$a_T^{\text{du}}((\mathbf{q}, r), (\mathbf{p}, v)) = \int_T \nu \mathbf{q} \cdot \mathbf{p} + \mu r v \, d\Omega + \frac{1}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) r v \, d\Gamma. \quad (4.7)$$

and the form  $c_T^{\text{du}} : (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T) \times \mathcal{H}^1(T) \rightarrow \mathbb{R}$  is defined as

$$c_T^{\text{du}}((\mathbf{q}, r), v) = \int_T \nu \mathbf{q} \cdot \nabla v + \mu r v \, d\Omega + \frac{1}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) r v \, d\Gamma. \quad (4.8)$$

*Proof.* We begin formulating the dual problem by introducing the auxiliary variable  $\boldsymbol{\pi}^\pm \in (\mathcal{L}^2(T))^d$  which satisfies the constraint

$$\kappa \int_T \nu (\nabla w^\pm - \boldsymbol{\pi}^\pm) \cdot \mathbf{p} \, d\Omega = 0, \quad \forall \mathbf{p} \in (\mathcal{L}^2(T))^d, \quad (4.9)$$

and the auxiliary variable  $\rho^\pm \in \mathcal{L}^2(T)$  which satisfies the constraint

$$\kappa \int_T \mu (w^\pm - \rho^\pm) v \, d\Omega + \frac{\kappa}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) (w^\pm - \rho^\pm) v \, d\Gamma = 0, \quad \forall v \in \mathcal{L}^2(T). \quad (4.10)$$

Defining  $\Xi$  to be the set of all triples  $(w^\pm, \boldsymbol{\pi}^\pm, \rho^\pm)$  in  $\mathcal{H}^1(T) \times (\mathcal{L}^2(T))^d \times \mathcal{L}^2(T)$  which satisfy the constraints (4.9) and (4.10), we can write the local unconstrained minimization (4.2) as an equivalent constrained minimization

$$\begin{aligned} \mp s_T^\pm &= \inf_{(w^\pm, \boldsymbol{\pi}^\pm, \rho^\pm) \in \Xi} \left\{ \frac{\kappa}{2} \left\{ \int_T \nu (\boldsymbol{\pi}^\pm)^2 + \mu (\rho^\pm)^2 \, d\Omega + \frac{1}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) (\rho^\pm)^2 \, d\Gamma \right\} \right. \\ &\quad \left. + \ell_T^\pm(w^\pm) + C_T^\pm \right\} \end{aligned} \quad (4.11)$$

This equivalent constrained minimization can be formulated as the Lagrangian saddle point problem

$$\mp s_T^\pm = \sup_{\substack{\mathbf{q}^\pm \in (\mathcal{L}^2(T))^d \\ r^\pm \in \mathcal{L}^2(T)}} \inf_{\substack{w^\pm \in \mathcal{H}^1(T) \\ \boldsymbol{\pi}^\pm \in (\mathcal{L}^2(T))^d \\ \rho^\pm \in \mathcal{L}^2(T)}} J_T^\pm(w^\pm, \boldsymbol{\pi}^\pm, \rho^\pm; \mathbf{q}^\pm, r^\pm) + C_T^\pm, \quad (4.12)$$

where the Lagrangian functional is defined as

$$\begin{aligned} J_T^\pm(w^\pm, \boldsymbol{\pi}^\pm, \rho^\pm; \mathbf{q}^\pm, r^\pm) &= \kappa \int_T \nu \left( \frac{1}{2} \boldsymbol{\pi}^\pm - \mathbf{q}^\pm \right) \boldsymbol{\pi}^\pm + \mu \left( \frac{1}{2} \rho^\pm - r^\pm \right) \rho^\pm \, d\Omega \\ &\quad + \frac{\kappa}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) \left( \frac{1}{2} \rho^\pm - r^\pm \right) \rho^\pm \, d\Gamma \\ &\quad + \kappa \left\{ \int_T \nu \nabla w^\pm \cdot \mathbf{q}^\pm + \mu w^\pm r^\pm \, d\Omega \right. \\ &\quad \quad \left. + \frac{1}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) w^\pm r^\pm \, d\Gamma \right\} \\ &\quad + \ell_T^\pm(w^\pm). \end{aligned} \quad (4.13)$$

Equality on the left of (4.12) results from the quadratic Lagrangian functional, but the bound method can also be derived when only weak duality holds.

A necessary condition for optimality of the inner minimization of (4.12) with respect to the principle primal variable  $w^\pm$  is

$$\kappa \left\{ \int_T \nu \nabla v \cdot \mathbf{q}^{\pm,*} + \mu v r^{\pm,*} \, d\Omega + \frac{1}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) v r^{\pm,*} \, d\Gamma \right\} = -\ell_T^\pm(v), \quad \forall v \in \mathcal{H}^1(T), \quad (4.14)$$

where the superscript  $*$  indicates optimality of the variable. Necessary conditions for optimality with respect to the two auxiliary primal variables  $\boldsymbol{\pi}^\pm$  and  $\rho^\pm$  are

$$\kappa \int_T \nu (\boldsymbol{\pi}^{\pm,*} - \mathbf{q}^{\pm,*}) \mathbf{p} \, d\Omega = 0, \quad \forall \mathbf{p} \in (\mathcal{L}^2(T))^d, \quad (4.15a)$$

$$\kappa \int_\Omega \mu (\rho^{\pm,*} - r^{\pm,*}) v \, d\Omega + \frac{\kappa}{2} \int_{\Gamma_T^N} (\boldsymbol{\alpha} \cdot \mathbf{n}) (\rho^{\pm,*} - r^{\pm,*}) v \, d\Gamma = 0, \quad \forall v \in \mathcal{L}^2(T). \quad (4.15b)$$

After substituting the auxiliary variable optimality conditions (4.15) into the Lagrangian (4.13) and retaining the principle primal variable condition (4.14) as a constraint in the outer maximization of the saddle problem (4.12), we arrive at the local dual constrained maximization (4.6) formulation of the original unconstrained local minimization (4.2).  $\square$

Significantly, we may inexpensively compute a quantitative lower bound on  $\mp s_T^\pm$ , and thereby upper and lower bounds on the exact output  $s$ , by performing the local dual constrained maximization (4.6) over a *finite* dimensional set so long as the set is rich enough to allow the dual constraint to be satisfied exactly. Indeed, while maximization will improve the sharpness of the bounds, we only require dual feasibility to obtain bounds.

**4.2. Dual Subproblems.** The local dual maximization problem (4.6) has the optimality conditions: find  $(\mathbf{q}^\pm, r^\pm, \xi^\pm) \in (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T) \times \mathcal{H}^1(T)$  such that

$$-\kappa a_T^{\text{du}}((\mathbf{q}^\pm, r^\pm), (\mathbf{p}, v)) - \kappa c_T^{\text{du}}((\mathbf{p}, v), \xi^\pm) = 0, \quad \forall (\mathbf{p}, v) \in (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T), \quad (4.16a)$$

$$-\kappa c_T^{\text{du}}((\mathbf{q}^\pm, r^\pm), v) = \ell_T^\pm(v), \quad \forall v \in \mathcal{H}^1(T), \quad (4.16b)$$

which, as a result of the linear equality constraint and convex objective functional, are both necessary and sufficient. For the purpose of computing bounds, the Lagrange multiplier  $\xi^\pm$  is an artifact of solving the constrained maximization problem and we will not make direct use of it.

As formulated, the optimality conditions depend explicitly upon the scaling parameter  $\kappa$ , but the substitutions

$$(\mathbf{q}^\pm, r^\pm, \xi^\pm) = (\nabla u_h - \frac{1}{2}\mathbf{q}^u \pm \frac{1}{\kappa}\mathbf{q}^\psi, u_h - \frac{1}{2}r^u \pm \frac{1}{\kappa}r^\psi, -\frac{1}{2}\xi^u \pm \frac{1}{\kappa}\xi^\psi)$$

will transform the above  $\kappa$ -dependent problems into the following two  $\kappa$ -independent problems: find  $(\mathbf{q}^u, r^u, \xi^u) \in (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T) \times \mathcal{H}^1(T)$  such that

$$a_T^{\text{du}}((\mathbf{q}^u, r^u), (\mathbf{p}, v)) + c_T^{\text{du}}((\mathbf{p}, v), \xi^u) = 0, \quad \forall (\mathbf{p}, v) \in (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T), \quad (4.17a)$$

$$c_T^{\text{du}}((\mathbf{q}^u, r^u), v) = \hat{R}_T^u(v), \quad \forall v \in \mathcal{H}^1(T), \quad (4.17b)$$

and find  $(\mathbf{q}^\psi, r^\psi, \xi^\psi) \in (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T) \times \mathcal{H}^1(T)$  such that

$$a_T^{\text{du}}((\mathbf{q}^\psi, r^\psi), (\mathbf{p}, v)) + c_T^{\text{du}}((\mathbf{p}, v), \xi^\psi) = 0, \quad \forall (\mathbf{p}, v) \in (\mathcal{L}^2(T))^d \times \mathcal{H}^1(T), \quad (4.18a)$$

$$c_T^{\text{du}}((\mathbf{q}^\psi, r^\psi), v) = \hat{R}_T^\psi(v), \quad \forall v \in \mathcal{H}^1(T), \quad (4.18b)$$

where we have defined the the localized residual forms

$$\hat{R}_T^u(v) = \ell_T(v) - a_T(u_h, v) - b_T(v, \lambda_h^u), \quad (4.19)$$

$$\hat{R}_T^\psi(v) = -\ell_T^\mathcal{O}(v) - a_T(v, \psi_h) - b_T(v, \lambda_h^\psi). \quad (4.20)$$

Equilibration ensures that all dual feasible functions  $(\mathbf{q}^u, r^u)$  and  $(\mathbf{q}^\psi, r^\psi)$  are orthogonal to the local finite element basis.

LEMMA 4.2. *Any pair  $(\mathbf{q}^u, r^u)$  in  $(\mathcal{L}^2(T))^d \times \mathcal{H}^1(T)$  that satisfies the constraint (4.17b) has the orthogonality property*

$$a_T^{\text{du}}((\mathbf{q}^u, r^u), (\nabla v, v)) = c_T^{\text{du}}((\mathbf{q}^u, r^u), v) = 0, \quad \forall v \in \mathcal{V}_h(T), \quad (4.21)$$

and any pair  $(\mathbf{q}^\psi, r^\psi)$  in  $(\mathcal{L}^2(T))^d \times \mathcal{H}^1(T)$  that satisfies the constraint (4.18b) has the orthogonality property

$$a_T^{\text{du}}((\mathbf{q}^\psi, r^\psi), (\nabla v, v)) = c_T^{\text{du}}((\mathbf{q}^\psi, r^\psi), v) = 0, \quad \forall v \in \mathcal{V}_h(T). \quad (4.22)$$

*Proof.* This is a direct consequence of equilibration provided by (3.14) and (3.15), and the definitions (4.19) and (4.20).  $\square$

With the above orthogonality property we can calculate the objective from dual feasible functions  $(\mathbf{q}^u, r^u)$  and  $(\mathbf{q}^\psi, r^\psi)$  using

$$\begin{aligned} \mp s_T^\pm = & -\frac{\kappa}{2} \left\{ \frac{1}{4} a_T^{\text{du}}((\mathbf{q}^u, r^u), (\mathbf{q}^u, r^u)) - C_T^u \right\} \\ & - \frac{1}{2\kappa} a_T^{\text{du}}((\mathbf{q}^\psi, r^\psi), (\mathbf{q}^\psi, r^\psi)) \\ & \pm \left\{ \frac{1}{2} a_T^{\text{du}}((\mathbf{q}^u, r^u), (\mathbf{q}^\psi, r^\psi)) + C_T^\psi \right\}, \end{aligned} \quad (4.23)$$

with the definitions

$$C_T^u = \ell_T(u_h) - a_T^s(u_h, u_h) - \ell_T^D(\lambda_h^u) + \frac{1}{2} C_T^*, \quad (4.24)$$

$$C_T^\psi = \ell_T(\psi_h) + \ell_T^D(\lambda_h^\psi). \quad (4.25)$$

**4.3. Subproblem Computation.** Recall from §4.1 that, by virtue of the dualization of the local minimization problem, we can choose a finite dimensional set within which to search for the dual functions  $(\mathbf{q}^u, r^u)$  and  $(\mathbf{q}^\psi, r^\psi)$ , so long as the set is rich enough to admit at least one pair  $(\mathbf{q}^u, r^u)$  satisfying (4.17b) and at least one pair  $(\mathbf{q}^\psi, r^\psi)$  satisfying (4.18b).

LEMMA 4.3. *If the interior data  $f|_T$ ,  $(\boldsymbol{\alpha} \cdot \nabla u_h)|_T$ ,  $f^\circ|_T$ , and  $(\boldsymbol{\alpha} \cdot \nabla \psi_h)|_T$  are all members of  $\mathbb{P}^m(T)$ , the boundary data  $g|_\gamma$ ,  $g^\circ|_\gamma$ , and  $((\boldsymbol{\alpha} \cdot \mathbf{n})\psi_h)|_\gamma$  are all members of  $\mathbb{P}^m(\gamma)$  for all  $\gamma \in \partial T$ , and the continuity multipliers  $\lambda_h^u$  and  $\lambda_h^\psi$  are equilibrated according to (3.14) and (3.15), then there exists at least one pair  $(\mathbf{q}_h^u, r_h^u) \in (\mathbb{P}^q(T))^d \times \mathbb{P}^q(T)$  satisfying (4.17b) and at least one pair  $(\mathbf{q}_h^\psi, r_h^\psi) \in (\mathbb{P}^q(T))^d \times \mathbb{P}^q(T)$  satisfying (4.18b) for  $q > p$  and  $q > m$ .*

*Proof.* Let  $\mathbf{q}_h^u = \mathbf{q}_D^u + \mathbf{q}_0^u$ , with  $\mathbf{q}_D^u \cdot \mathbf{n} = -\sigma_T \lambda_h^u - \nu(\nabla u_h \cdot \mathbf{n})$  on  $\partial T \setminus \Gamma_T^N$ ,  $\mathbf{q}_D^u \cdot \mathbf{n} = -\sigma_T \lambda_h^u$  on  $\Gamma_T^N$ ,  $\mathbf{q}_0^u \cdot \mathbf{n} = 0$  on  $\partial T$ , and let  $r_h^u = 0$  on  $\Gamma_T^N$ . With this lifting and a Green's formula we can write the constraint (4.17b) as

$$\int_T (-\nu \nabla \cdot \mathbf{q}_0^u + \mu r^u) v \, d\Omega = \int_T (f + \nu \Delta u_h - \mu u_h + \boldsymbol{\alpha} \cdot \nabla u_h + \nu \nabla \cdot \mathbf{q}_D^u) v \, d\Omega,$$

for all  $v$  in  $\mathbb{P}^q(T)$ . The requirements of the lemma ensure that the data on the right is in the range of the operator on the left for the case  $\mu > 0$  and  $r^u$ , and therefore at least one solution exists. Existence for the case  $\mu = 0$  is guaranteed by equilibration, as we previously addressed in [16]. Analogous reasoning applies for the pair  $(\mathbf{q}_h^\psi, r_h^\psi)$  with the exception that a Green's formula must also be applied to the advection term, which results in the additional requirement of  $(\boldsymbol{\alpha} \cdot \mathbf{n})\psi_h|_\gamma$  being in  $\mathbb{P}^m(\gamma)$ .  $\square$

Note that the requirement  $q \geq p$  suffices in the above lemma when  $\boldsymbol{\alpha} \cdot \mathbf{n} = 0$  on  $\Gamma_T^N$  or  $\Gamma_T^N = \emptyset$ , as well as when  $\mu = 0$  and both  $r_h^u$  and  $r_h^\psi$  have been set to zero.

The above proof suggests one way to solve the subproblem, but other approaches are possible. For instance, we could set  $r_h^u$  and  $r_h^\psi$  to zero from the outset in order to produce a method which treats Poisson's equation, the advection-diffusion equation and the advection-diffusion-reaction equation uniformly. Existence would be ensured by equilibration, but doing so reduces the number of available degrees of freedom in the maximization and thus would most likely reduce the sharpness of the resulting bounds.

A particularly favorable circumstance for solving the subproblem arises for both Poisson's equation and the advection-diffusion equation ( $\mu = 0$ ) when the problem

data consists only of constants ( $m = 0$ ) and linear finite elements ( $p = 1$ ) are employed with  $q = 1$ , and both  $r_h^u = 0$  and  $r_h^\psi = 0$ . Under these circumstances, the dual functions  $\mathbf{q}_h^u$  and  $\mathbf{q}_h^\psi$  can be explicitly constructed from the subproblem boundary data.

More generally, we can formulate the pair of computable subproblems as: find  $(\mathbf{q}_h^u, r_h^u, \xi_h^u) \in \mathcal{Q}_h^u(T) \times \mathbb{P}^q(T) \times \mathbb{P}^q(T)$  such that

$$a_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), (\mathbf{p}, v)) + c_T^{\text{du}}((\mathbf{p}, v), \xi^u) = 0, \quad \forall (\mathbf{p}, v) \in (\mathbb{P}^q(T))^d \times \mathbb{P}^q(T), \quad (4.26a)$$

$$c_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), v) = \hat{R}_T^u(v), \quad \forall v \in \mathbb{P}^q(T), \quad (4.26b)$$

and find  $(\mathbf{q}_h^\psi, r_h^\psi, \xi_h^\psi) \in \mathcal{Q}_h^\psi(T) \times \mathbb{P}^q(T) \times \mathbb{P}^q(T)$  such that

$$a_T^{\text{du}}((\mathbf{q}_h^\psi, r_h^\psi), (\mathbf{p}, v)) + c_T^{\text{du}}((\mathbf{p}, v), \xi^\psi) = 0, \quad \forall (\mathbf{p}, v) \in (\mathbb{P}^q(T))^d \times \mathbb{P}^q(T), \quad (4.27a)$$

$$c_T^{\text{du}}((\mathbf{q}_h^\psi, r_h^\psi), v) = \hat{R}_T^\psi(v), \quad \forall v \in \mathbb{P}^q(T), \quad (4.27b)$$

where we have defined the sets

$$\mathcal{Q}_h^u(T) = \left\{ \mathbf{q} \in (\mathbb{P}^q(T))^d \mid \mathbf{q} \cdot \mathbf{n} = \begin{cases} -\sigma_T \lambda_h^u & \text{on } \partial T \setminus \Gamma_T^N \\ -\sigma_T \lambda_h^u + g & \text{on } \Gamma_T^N \end{cases} \right\}, \quad (4.28)$$

$$\mathcal{Q}_h^\psi(T) = \left\{ \mathbf{q} \in (\mathbb{P}^q(T))^d \mid \mathbf{q} \cdot \mathbf{n} = \begin{cases} -\sigma_T \lambda_h^\psi & \text{on } \partial T \setminus \Gamma_T^N \\ -\sigma_T \lambda_h^\psi - g^\mathcal{O} & \text{on } \Gamma_T^N \end{cases} \right\}. \quad (4.29)$$

**5. Output Bound Procedure.** The elemental subproblems explicated in the previous section can be computed independently and in parallel, accumulating the local contributions (4.23) to the output bounds in the process. If we define the aggregated values

$$\begin{aligned} z_h^u &= \frac{1}{8} \sum_{T \in \mathcal{T}_h} a_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), (\mathbf{q}_h^u, r_h^u)), & z_h^\psi &= \frac{1}{2} \sum_{T \in \mathcal{T}_h} a_T^{\text{du}}((\mathbf{q}_h^\psi, r_h^\psi), (\mathbf{q}_h^\psi, r_h^\psi)), \\ \bar{z}_h &= \frac{1}{2} \sum_{T \in \mathcal{T}_h} a_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), (\mathbf{q}_h^\psi, r_h^\psi)), \end{aligned} \quad (5.1)$$

then we can write the total output bound expression as

$$s_h^\pm = -\bar{z}_h - C^{r^\psi} \pm \left\{ \kappa z_h^u + \frac{1}{\kappa} z_h^\psi \right\}, \quad (5.2)$$

in which the constant  $C^u$  defined in (4.24) is eliminated by the fact that  $\ell(u_h) - a^s(u_h, u_h) - \ell^D(\lambda_h^u) + \frac{1}{2}C^* = 0$  which results from equilibration.

We introduced the scaling parameter  $\kappa$  at the outset to allow us to optimize the sharpness of the computed bounds as well as provide dimensional consistency. Maximizing the lower bound and minimizing the upper bound with respect to  $\kappa$  yields the optimal value  $\kappa^2 = z_h^\psi / z_h^u$  with which we can write the upper and lower bounds succinctly as

$$s_h^\pm = \bar{s}_h \pm 2\sqrt{z_h^u z_h^\psi}, \quad (5.3)$$

where we have defined the bound average  $\bar{s}_h = -\bar{z}_h - C^{r^\psi}$ .

The complete method for computing output bounds can now be written as a four steps procedure.

*Step 1: Finite Element Approximation*

1. Find  $u_h \in \mathcal{U}_h$  such that

$$a(u_h, v) = \ell(v), \quad \forall v \in \mathcal{V}_h, \quad (5.4)$$

2. Find  $\psi_h \in \mathcal{V}_h$  such that

$$a(v, \psi_h) = -\ell^\mathcal{O}(v), \quad \forall v \in \mathcal{V}_h, \quad (5.5)$$

*Step 2: Finite Element Equilibration*

1. Find  $\lambda_h^u \in \Lambda_h$  such that

$$b(\hat{v}, \lambda_h^u) = \ell(\hat{v}) - a(u_h, \hat{v}), \quad \forall \hat{v} \in \hat{\mathcal{V}}_h, \quad (5.6)$$

2. Find  $\lambda_h^\psi \in \Lambda_h$  such that

$$b(\hat{v}, \lambda_h^\psi) = -\ell^\mathcal{O}(\hat{v}) - a(\hat{v}, \psi_h), \quad \forall \hat{v} \in \hat{\mathcal{V}}_h. \quad (5.7)$$

*Step 3: Elemental Subproblems*

1. Find  $(\mathbf{q}_h^u, r_h^u, \xi_h^u) \in \mathcal{Q}_h^u(T) \times \mathbb{P}^q(T) \times \mathbb{P}^q(T)$  such that

$$\begin{aligned} a_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), (\mathbf{p}, v)) + c_T^{\text{du}}((\mathbf{p}, v), \xi_h^u) &= 0, \quad \forall (\mathbf{p}, v) \in (\mathbb{P}^q(T))^d \times \mathbb{P}^q(T), \\ c_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), v) &= \hat{R}_T^u(v), \quad \forall v \in \mathbb{P}^q(T). \end{aligned} \quad (5.8)$$

2. Find  $(\mathbf{q}_h^\psi, r_h^\psi, \xi_h^\psi) \in \mathcal{Q}_h^\psi(T) \times \mathbb{P}^q(T) \times \mathbb{P}^q(T)$  such that

$$\begin{aligned} a_T^{\text{du}}((\mathbf{q}_h^\psi, r_h^\psi), (\mathbf{p}, v)) + c_T^{\text{du}}((\mathbf{p}, v), \xi_h^\psi) &= 0, \quad \forall (\mathbf{p}, v) \in (\mathbb{P}^q(T))^d \times \mathbb{P}^q(T), \\ c_T^{\text{du}}((\mathbf{q}_h^\psi, r_h^\psi), v) &= \hat{R}_T^\psi(v), \quad \forall v \in \mathbb{P}^q(T). \end{aligned} \quad (5.9)$$

3. Calculate  $\bar{z}_T$ ,  $z_T^u$ , and  $z_T^\psi$

$$\begin{aligned} z_{T,h}^u &= \frac{1}{8} a_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), (\mathbf{q}_h^u, r_h^u)), & z_{T,h}^\psi &= \frac{1}{2} a_T^{\text{du}}((\mathbf{q}_h^\psi, r_h^\psi), (\mathbf{q}_h^\psi, r_h^\psi)), \\ \bar{z}_{T,h} &= \frac{1}{2} a_T^{\text{du}}((\mathbf{q}_h^u, r_h^u), (\mathbf{q}_h^\psi, r_h^\psi)). \end{aligned} \quad (5.10)$$

*Step 4: Bounds*

$$z_h^u = \sum_{T \in \mathcal{T}_h} z_{T,h}^u, \quad z_h^\psi = \sum_{T \in \mathcal{T}_h} z_{T,h}^\psi, \quad \bar{s}_h = - \sum_{T \in \mathcal{T}_h} \bar{z}_{T,h} - C_T^\psi. \quad (5.11)$$

$$s_h^\pm = \bar{s}_h \pm 2\sqrt{z_h^u z_h^\psi} \quad (5.12)$$

The upper and lower bounding property of  $s_h^+$  and  $s_h^-$  follows directly from the Lagrangian saddle point property of the constrained minimization reformulation of the model problem. Either a strictly positive reaction coefficient,  $\mu$ , or equilibration ensure that the independent local subproblems resulting from the Lagrangian relaxation can provide non-trivial bounds. Forming the dual of the unconstrained local

minimization enables the computation of a lower bound on the infinite-dimensional minimization problem with a finite-dimensional feasibility problem. That the resulting dual subproblems are indeed computable is a consequence of the subproblem constraint data being polynomial and choosing a polynomial subset for the local dual problem. The resulting bounds converge to the exact linear functional output at twice the rate of the  $\mathcal{H}^1$ -norm measure of the error in the finite element solution, as proven in our earlier paper [16] and verified by the numerical examples.

To a large extent the subproblems are independent of the finite element approximation. We need only check that the localized data  $u_h|_T$ ,  $\psi_h|_T$ ,  $\lambda_h^u|_{\partial T}$  and  $\lambda_h^\psi|_{\partial T}$  passed to the subproblem equilibrates the element according to (5.6) and (5.7). As alluded to in the introduction, this precondition is entirely local and can easily be checked. Moreover, it has very practical implications for building correct simulation software as it acts as a verifiable contract between the relatively simple bounds subproblem and the much more complicated global approximation.

**6. Numerical Examples.** In this last section, we demonstrate the method with two numerical examples. In both examples we employ a very simple adaptive strategy that uses the local information produced during the calculation of the bounds to drive the output to a prescribed precision. At each level of refinement, only elements for which  $\Delta_T = \kappa z_{T,h}^u + \frac{1}{\kappa} z_{T,h}^\psi > \Delta_{\text{tol}}/K$  are refined, where  $\Delta_{\text{tol}}$  is a user specified tolerance for the bound gap and  $K$  is the number of elements in the triangulation at that level. The meshes are generated and adaptively refined using the freely available Triangle mesh generator [17].

**6.1. Example 1.** In our first example we consider the unit square  $(x, y) \in [0, 1]^2$  with the parameters  $\nu = 1$ ,  $\boldsymbol{\alpha} = (\alpha, 0)$ , the Dirichlet boundary conditions  $u(0, y) = 1$  on the left side and  $u(1, y) = 0$  on the right side, and homogeneous Neumann boundary conditions on the top and bottom sides. These conditions result in the well known one-dimensional solution

$$u(x, y) = \frac{e^{\beta} e^{\frac{1}{2}(\alpha-\beta)x} - e^{\frac{1}{2}(\alpha+\beta)x}}{e^{\beta} - 1}, \quad (6.1)$$

where  $\beta = \sqrt{4\mu + \alpha^2}$ .

For the output, we examine the average normal gradient on the right side of the square,  $\int_0^1 \nabla u(1, y) \cdot \mathbf{n} \, d\Gamma$ , which we write with the interior test function,  $\chi = x$ , as

$$\ell^{\mathcal{O}}(v) = \int_{\Omega} \nu \nabla v \cdot \nabla \chi + \mu v \chi + (\boldsymbol{\alpha} \cdot \nabla v) \chi \, d\Omega \quad (6.2)$$

using the technique discussed in [14].

Since we know the exact output for this example, we can calculate the effectiveness of the bounds as an indicator of the error in the finite element solution using

$$\eta = \frac{s_h^+ - s_h^-}{2|s_h - s|}. \quad (6.3)$$

Our primary goal, however, is not estimating the error in the finite element solution but providing an upper and lower bound on the exact output. The finite element solution is mostly just a means to this end.

Table 6.1 summarizes the results of uniformly refining an initial mesh of 16 elements with method parameters  $p = 1$  and  $q = 1$ . Both the output and the bound gap

$K$	$(s_h - s)/s$	$(s - s_h^-)/s$	$(s_h^+ - s)/s$	$(s_h^+ - s_h^-)/s$	$\eta$
16	0.029963	0.296452	0.160602	0.457054	7.63
256	0.001178	0.023548	0.021966	0.045514	19.32
1024	0.000295	0.006097	0.005713	0.011810	20.01
16384	0.000018	0.000385	0.000362	0.000747	20.25

TABLE 6.1

Uniform mesh refinement results for Example 1 with  $\alpha = 10$  and  $\mu = 10$ .

asymptotically converge at the optimal rate of 2. The last level of uniform refinement contains 16284 elements and produces a bound gap of 0.000747, while the simple adaptive method described above can be used to produce a bound gap of 0.000646 with a mesh containing only 4114 elements.

Table 6.2 summarizes the influence of the Peclet number,  $\alpha$ , on the effectivity of the bounds in the context of the simple adaptive method with a tolerance of  $\Delta_{\text{tol}} = 0.001s$ . Although the method is valid for nonnegative  $\alpha$ , the sharpness of the bound degrades significantly with increasing Peclet number, but the bounding property is retained.

$\alpha$	$K$	$(s_h - s)/s$	$(s - s_h^-)/s$	$(s_h^+ - s)/s$	$(s_h^+ - s_h^-)/s$	$\eta$
0	384	-0.000045	0.000342	0.000068	0.000410	4.52
1	256	-0.000051	0.000535	0.000186	0.000721	7.12
5	2883	-0.000056	0.000412	0.000404	0.000816	7.23
10	6108	-0.000005	0.000458	0.000456	0.000913	98.21

TABLE 6.2

Adaptive mesh refinement results for Example 1 with  $\mu = 1$  and various values of  $\alpha$ .

We strive to produce guaranteed, if conservative, bounds on quantities typically queried from simulations and not estimates of the error. Consequentially, we trade better estimates of the error for the confidence provided by one-sidedness. Nevertheless, various enhancements to the basic method presented here, such as the incorporation of gradient recovery heuristics, could be considered in order to improve the effectiveness of the error estimate.

**6.2. Example 2.** Our second example provides a qualitative demonstration of the method on a more complicated example problem. We consider the unit square  $(x, y) \in [0, 1]^2$  with the equation parameters  $\nu = 1$ ,  $\alpha = 500(y - \frac{1}{2}, \frac{1}{2} - x)$ ,  $\mu = 10$ , and all homogeneous Dirichlet boundary conditions. The problem is forced in the square region  $[0.7, 0.8]^2$  with  $f = 1000$  and the output is the average,  $f^{\mathcal{O}} = 1$ , over the square region  $\Omega^{\mathcal{O}} = [0.2, 0.3]^2$ . The initial mesh contains 100 elements and the method parameters are  $p = 1$  and  $q = 2$ .

We examine the result of adaptively solving the output problem with  $\Delta_{\text{tol}} = 0.0005$ . Figure 6.1 displays  $u$  and  $\psi$  for the final solution, which has a guaranteed precision of 0.000488 and contains 2917 elements. Figure 6.2 shows the distribution of elemental bound gap contributions,  $\Delta_T$ , for the initial solution and Figure 6.3 shows the final mesh obtained at the end of the adaptive process.

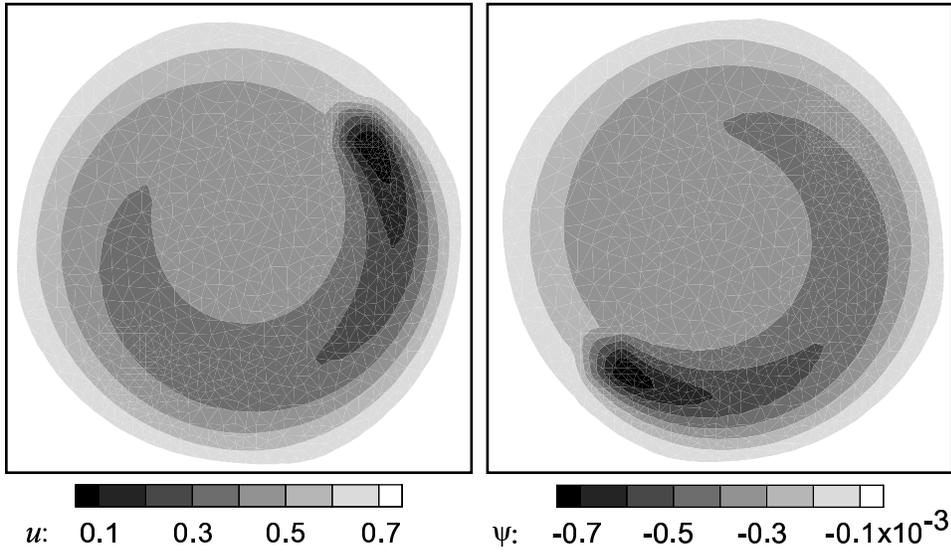


FIG. 6.1. Adaptive solution and adjoint for Example 2.

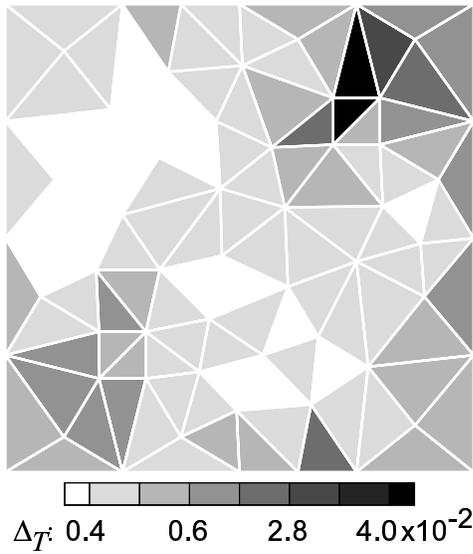


FIG. 6.2. Elemental bound gap contributions on initial mesh for Example 2.

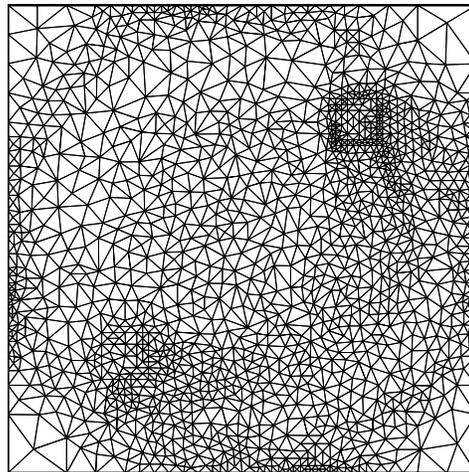


FIG. 6.3. Final mesh for Example 2.

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