

A posteriori error estimation of approximate boundary fluxes

T. Wildey, S. Tavener and D. Estep^{*,†}

Department of Mathematics, Colorado State University, Fort Collins, CO 80523, U.S.A.

SUMMARY

This paper describes the *a posteriori* estimation of the error in the flux of a finite element approximation on a piece of the boundary of the domain. The estimate is obtained *via* a generalized Green's function corresponding to the quantity of interest on the boundary. We investigate the effects of smoothing the data corresponding to the quantity of interest and explore the effective domain of dependence of the quantity. We relate this approach to previous work by M. F. Wheeler, G. F. Carey, I. Babuska *et al.*, and M. Larson *et al.* Copyright © 2007 John Wiley & Sons, Ltd.

Received 13 May 2006; Revised 31 December 2006; Accepted 14 April 2007

KEY WORDS: *a posteriori* error estimate; adjoint; boundary flux; effective domain of influence; extraction function; generalized Green's function; goal-oriented error estimate

1. INTRODUCTION

Goal-oriented error estimation is critically important in large-scale computational science and engineering. Indeed, the situation in which the goal of a computation is to obtain an accurate approximation of a specific quantity of interest, e.g. the normal flux of the solution on a portion of the boundary of the domain, is very common, if not the norm, in practice. Moreover, it is very often possible to compute specific quantities of interest accurately using discretizations that yield poor global accuracy in the sense of some norm. This is critically important in applications that are too complex and large to allow asymptotically resolved discretizations.

*Correspondence to: D. Estep, Department of Mathematics, Colorado State University, Fort Collins, CO 80523, U.S.A.

†E-mail: estep@math.colostate.edu

Contract/grant sponsor: Department of Energy; contract/grant numbers: DE-FG02-04ER25620, DE-FG02-05ER25699
Contract/grant sponsor: National Aeronautics and Space Administration; contract/grant number: NNG04GH63G
Contract/grant sponsor: National Science Foundation; contract/grant numbers: DMS-0107832, DGE-0221595003, MSPA-CSE-0434354
Contract/grant sponsor: Sandia Corporation; contract/grant number: PO299784

However, computing a quantity of interest with true efficiency requires an understanding of exactly how the discretization errors affect that specific quantity of interest. Several different methods have been developed to estimate the error in a linear functional of the solution along a boundary. A popular technique for calculating boundary-flux values was developed by Wheeler [1] and expanded later by Carey [2–5]. Babuska and Miller introduced another technique for estimating linear functionals in [6–8]. In [9], Larson *et al.* applied *a posteriori* error analysis techniques based on the generalized Green's function [10–18] to estimate the error in a boundary flux computed by a postprocessing technique.

In this paper, we build on the results in [9] to describe how to estimate the error in the average flux of the solution over a piece of the boundary using adjoint-based *a posteriori* techniques. Our purpose is to clarify how the adjoint problem is defined in order to obtain this quantity of interest. We also relate this approach to the prior work and draw some interesting connections between all of these approaches. Finally, we investigate the effect of smoothing the data for the adjoint problem corresponding to the quantity of interest on the effective domain of dependence of the data as determined by the generalized Green's function.

This paper is organized as follows. The first section introduces the notation and function spaces. The second section defines the appropriate adjoint problem and derives the error representation formula. In the third section we relate these results to previous work on boundary-flux computations. The last section applies these results to various test problems and one application.

2. PRELIMINARIES AND NOTATION

We consider a second-order linear elliptic problem

$$\begin{aligned} Lu &= -\nabla \cdot (A \nabla u) + \mathbf{b} \cdot \nabla u + cu = f, & x \in \Omega \\ u &= g_D, & x \in \Gamma_D \\ A \partial_n u &= g_N, & x \in \Gamma_N \\ A \partial_n u + \alpha u &= g_R, & x \in \Gamma_R \end{aligned} \tag{1}$$

posed on a bounded polygonal domain Ω with boundary $\partial\Omega$, where $\Gamma_D \cup \Gamma_N \cup \Gamma_R = \partial\Omega$, $\Gamma_D \neq \emptyset$, ∂_n denotes the unit outward normal derivative, the boundary data g_D , g_N , g_R and coefficients $A(x) \geq A_0 > 0$, \mathbf{b} , c , f , are sufficiently smooth functions.

We let $L^2(\Omega)$ denote the space of square integrable functions on Ω with inner product $(\cdot, \cdot)_\Omega$ and norm $\|\cdot\|_\Omega$. We also use $\|\cdot\|_\omega$ for a subset $\omega \subset \Omega$. We use $H^s(\Omega)$ to denote the Sobolev space with real index s [19, 20] associated with norm $\|\cdot\|_s$ and seminorm $|\cdot|_s$. We also use the subspace $H_0^1(\Omega) = \{v \in H^1(\Omega), v = 0 \text{ on } \Gamma_D\}$. The weak formulation of (1) seeks $u \in H^1(\Omega)$ such that $u = g_D$ on Γ_D and

$$a(u, v) = (f, v) + (g_N, v)_{\Gamma_N} + (g_R, v)_{\Gamma_R} \quad \text{for all } v \in H_0^1(\Omega) \tag{2}$$

with

$$a(u, v) = \int_{\Omega} (A \nabla u \cdot \nabla v + \mathbf{b} \cdot \nabla uv + cuv) \, dx + \int_{\Gamma_R} \alpha uv \, ds$$

and $(\cdot, \cdot)_{\Gamma_N}, (\cdot, \cdot)_{\Gamma_R}$ denote the integrals along Γ_N, Γ_R , respectively. We assume that a is coercive and (2) admits a unique weak solution.

To discretize, we let T_h be a triangulation of Ω into elements K satisfying $\bar{\Omega} = \cup_{K \in T_h} K$. We let h_K denote the length of the longest edge of K with $h = \max_{K \in T_h} h_K$. We assume the triangulation is locally quasi-uniform. We use a Galerkin finite element method that computes a continuous, piecewise polynomial function u_h in the space

$$S_h = \{v \text{ continuous on } \Omega, v|_K \in P^q(K), K \in T_h\}$$

where $P^q(K)$ represents the space of polynomials of degree q on K . Note that $S_h \subset H^1(\Omega)$. We compute u_h satisfying $u_h = \pi_D g_D$ on Γ_D , where π_D is a projection or interpolant into V_h on Γ_D , and $a(u_h, v) = (f, v)$ for all $v \in S_h, v = 0$ on Γ_D .

3. ESTIMATING THE ERROR USING THE GENERALIZED GREEN'S FUNCTION

We briefly recall *a posteriori* error analysis using the generalized Green's function [10–18]. Green's functions have a natural importance in the numerical analysis of partial differential equations (PDEs). In particular, they can be used to compute linear functionals of the solution. The idea of a Green's function is based on the notions of duality and the adjoint. For a Banach space V , we use the bracket notation,

$$\langle \cdot, \cdot \rangle_{\Omega} = \langle \cdot, \cdot \rangle : V^* \times V \rightarrow \mathbb{R}$$

to represent the duality pairing with the dual space V^* . If we have a bounded operator $L : X \rightarrow Y$, where X and Y are Banach spaces, the adjoint operator $L^* : Y^* \rightarrow X^*$ is defined by

$$\langle y^*, Lx \rangle = \langle L^* y^*, x \rangle \quad \text{for all } x \in X, y^* \in Y^*$$

When V is a Hilbert space, e.g. $V = L^2(\Omega)$, we can assign $\langle \cdot, \cdot \rangle = (\cdot, \cdot)_{\Omega}$. In this case, we compute adjoint operators of elliptic operators by using the divergence theorem to move derivatives between trial and test functions in the weak form. However, the divergence theorem results in various types of boundary integrals. Some of the boundary terms might vanish because of the boundary conditions imposed on the solution, e.g. if $u = 0$ on Γ_D . In the classic approach to Green's functions, the adjoint is defined so the remaining boundary integral terms vanish.

For example, consider the Dirichlet problem

$$\begin{aligned} Lu &= -\nabla \cdot (A \nabla u) + \mathbf{b} \cdot \nabla u + cu = f(x), \quad x \in \Omega \\ u &= g_D, \quad x \in \partial\Omega \end{aligned}$$

with the weak formulation $a(u, v) = \langle f, v \rangle$ for any $v \in H_0^1(\Omega)$ and $f \in H^{-1}(\Omega)$. The standard adjoint boundary-value problem for the quantity of interest $\langle u, \psi \rangle$ is

$$\begin{aligned} L^* \phi &= -\nabla \cdot (A \nabla \phi) - \mathbf{b} \cdot \nabla \phi + (c - \nabla \cdot \mathbf{b}) \phi = \psi, \quad x \in \Omega \\ \phi &= 0, \quad x \in \partial\Omega \end{aligned}$$

with associated dual form $a^*(\cdot, \cdot)$.

The standard *a posteriori* error analysis follows the classic argument for Green's functions to obtain an error representation formula for the error in the quantity of interest,

$$\begin{aligned}\langle e, \psi \rangle &= a^*(\phi, e) - (A\partial_n \phi, e)_{\partial\Omega} \\ &= a(e, \phi) - (A\partial_n \phi, e)_{\partial\Omega} \\ &= a(e, \phi - P\phi) - (A\partial_n \phi, g_D - Pg_D)_{\partial\Omega}\end{aligned}\tag{3}$$

where $P\phi$ is a projection of ϕ into the finite element space S_h . If we know ϕ , we can compute $P\phi$ and determine the error in the quantity of interest. In practice, ϕ is approximated.

Carrying out the same analysis for (1) requires defining the adjoint problem to be

$$\begin{aligned}L^*\phi &= -\nabla \cdot (A\nabla \phi) - \mathbf{b} \cdot \nabla \phi + (c - \nabla \cdot \mathbf{b})\phi = \psi, \quad x \in \Omega \\ \phi &= 0, \quad x \in \Gamma_D \\ A\partial_n \phi + (\mathbf{b} \cdot \mathbf{n})\phi &= 0, \quad x \in \Gamma_N \\ A\partial_n \phi + (\alpha + \mathbf{b} \cdot \mathbf{n})\phi &= 0, \quad x \in \Gamma_R\end{aligned}\tag{4}$$

Notice that the presence of the convection term has yielded adjoint boundary conditions on the Neumann and Robin portions of the boundary.

3.1. Estimating the error in the flux on a portion of the boundary

Now we now consider the case when the quantity of interest is the boundary flux on a portion of the boundary for (1). Computing formally, we modify the adjoint problem (4) to get

$$\begin{aligned}L^*\phi &= 0, \quad x \in \Omega \\ \phi &= \psi, \quad x \in \Gamma \\ \phi &= 0, \quad x \in \Gamma_D \setminus \Gamma \\ A\partial_n \phi + (\mathbf{b} \cdot \mathbf{n})\phi &= 0, \quad x \in \Gamma_N \\ A\partial_n \phi + (\alpha + \mathbf{b} \cdot \mathbf{n})\phi &= 0, \quad x \in \Gamma_R\end{aligned}$$

where $\Gamma \subset \Gamma_D$ and $\psi \in H^{1/2}(\Gamma)$. The associated bilinear form is still $a^*(\phi, w)$, giving

$$0 = a^*(\phi, e) - (A\partial_n \phi, e)_\Gamma = a(e, \phi) - (A\partial_n \phi, e)_\Gamma\tag{5}$$

but the analysis for the error representation changes since the adjoint solution, ϕ , is not zero everywhere on Γ_D . Consequently, the true solution of (1) satisfies

$$a(u, \phi) = (f, \phi) + (g_N, \phi)_{\Gamma_N} + (g_R, \phi)_{\Gamma_R} - (A\partial_n u, \phi)_\Gamma$$

This also complicates the use of Galerkin orthogonality. We use a special interpolant to account for the fact that the adjoint solution is not in the finite element space. For $K \in T_h$, let $\{\eta_i\}_K$ denote

the set of nodes of K . Let $\Gamma \subset \partial\Omega$. We define $P_h^0 : H^s \rightarrow S_h$ via

$$\begin{cases} P_h^0 v(\eta_i) = \pi_h v(\eta_i), & \overline{K} \cap \Gamma = \emptyset \\ P_h^0 v(\eta_i) = \begin{cases} \pi_h v(\eta_i), & \eta_i \notin \Gamma, \\ 0, & \eta_i \in \Gamma, \end{cases} & \overline{K} \cap \Gamma \neq \emptyset, \end{cases} \quad K \in T_h, i = 1, 2, 3$$

where π_h is the Lagrange interpolant.

From 5, we get

$$\begin{aligned} 0 &= a(e, \phi) - (A\partial_n \phi, e)_{\Gamma_D} \\ &= a(e, \phi - P_h^0 \phi) - (A\partial_n \phi, e)_{\Gamma_D} \\ &= (f, \phi - P_h^0 \phi) - a(u_h, \phi - P_h^0 \phi) \\ &\quad + (g_N, \phi - \pi_h \phi)_{\Gamma_N} + (g_R, \phi - \pi_h \phi)_{\Gamma_R} \\ &\quad - (A\partial_n \phi, g_D - \pi_h g_D)_{\Gamma_D} + (A\partial_n u, \psi)_{\Gamma} \end{aligned}$$

The last line uses the fact that $\phi = \psi$ and $P_h^0 \phi = 0$ on $\partial\Omega$. We obtain

$$\begin{aligned} -(A\partial_n u, \psi)_{\Gamma} &= (f, \phi - P_h^0 \phi) - a(u_h, \phi - P_h^0 \phi) \\ &\quad + (g_N, \phi - \pi_h \phi)_{\Gamma_N} + (g_R, \phi - \pi_h \phi)_{\Gamma_R} - (A\partial_n \phi, g_D - \pi_h g_D)_{\Gamma_D} \end{aligned}$$

If we define $\pi_{\partial} \phi = P_h^0 \phi - \pi_h \phi$, we get an estimate of a linear functional of the normal derivative of the *true solution*,

$$\begin{aligned} -(A\partial_n u, \psi)_{\Gamma} &= (f, \phi - \pi_h \phi) - a(u_h, \phi - \pi_h \phi) + (f, \pi_{\partial} \phi) - a(u_h, \pi_{\partial} \phi) \\ &\quad + (g_N, \phi - \pi_h \phi)_{\Gamma_N} + (g_R, \phi - \pi_h \phi)_{\Gamma_R} - (A\partial_n \phi, g_D - \pi_h g_D)_{\Gamma_D} \end{aligned}$$

Notice that $\pi_{\partial} \phi$ is nonzero only on elements adjacent to the boundary.

To estimate a linear functional of the error in the flux on Γ , we add $(A\partial_n u_h, \phi)_{\Gamma}$ to both sides and obtain the formal error representation.

Theorem 3.1

The error $e = u - u_h$ satisfies

$$\begin{aligned} -(A\partial_n e, \psi)_{\Gamma} &= (f, \phi - \pi_h \phi) - a(u_h, \phi - \pi_h \phi) + (f, \pi_{\partial} \phi) - a(u_h, \pi_{\partial} \phi) + (A\partial_n u_h, \phi)_{\Gamma} \\ &\quad + (g_N, \phi - \pi_h \phi)_{\Gamma_N} + (g_R, \phi - \pi_h \phi)_{\Gamma_R} - (A\partial_n \phi, g_D - \pi_h g_D)_{\Gamma_D} \end{aligned} \quad (6)$$

3.2. Adaptive error control

The adjoint-based *a posteriori* error estimate provides the capability of developing a global basis for adaptivity that takes into account both the local production of error from discretization and the

global effects of stability in terms of propagation, accumulation, and cancellation of error across the domain.

The standard approach is to write (6) as

$$|(A\partial_n e, \psi)_\Gamma| = \left| \sum_{K \in T_h} ((f, \phi - \pi_h \phi)_K - a(u_h, \phi - \pi_h \phi)_K + (f, \pi_\partial \phi)_K - a(u_h, \pi_\partial \phi)_K \right. \\ \left. + (g_N, \phi - \pi_h \phi)_{K \cap \Gamma_N} + (g_R, \phi - \pi_h \phi)_{K \cap \Gamma_R} - (A\partial_n \phi, g_D - \pi_h g_D)_{K \cap \Gamma_D} \right. \\ \left. + (A\partial_n u_h, \phi)_{K \cap \Gamma} \right|$$

with the obvious notation for localizing the forms to elements K . The right-hand side provides a computable estimate after approximating ϕ . When the estimate is larger than the stated tolerance, an element K is marked for refinement when the local element indicator

$$\eta_K = |(f, \phi - \pi_h \phi)_K - a(u_h, \phi - \pi_h \phi)_K + (f, \pi_\partial \phi)_K - a(u_h, \pi_\partial \phi)_K \\ + (g_N, \phi - \pi_h \phi)_{K \cap \Gamma_N} + (g_R, \phi - \pi_h \phi)_{K \cap \Gamma_R} - (A\partial_n \phi, g_D - \pi_h g_D)_{K \cap \Gamma_D} \\ + (A\partial_n u_h, \phi)_{K \cap \Gamma}| \quad (7)$$

is larger than a local tolerance, typically the tolerance divided by the current number of elements.

The dual weights provided by the factors involving ϕ mean that the estimate and the local indicators reflect the stability properties of the quantity of interest. We can define a useful notion of *effective* domain of dependence [17] for a quantity of interest. In an elliptic problem, the domain of influence of the value of a solution in a localized region is formally the entire domain. However, in many cases, generalized Green's functions corresponding to local quantities of interest exhibit a decay away from the local region. We define the effective domain of influence of a quantity of interest as the region in which the local indicators η_K are significantly larger than the rest, i.e. where the mesh must be refined in order to yield the quantity of interest to a desired accuracy. A large effective domain of influence corresponds to needing to refine a large portion of the domain in order to resolve a localized quantity.

3.3. Smoothing the boundary data

Representation (6) is optimal in the case that $\Gamma = \Gamma_D$ because ϕ has the prerequisite regularity for $\phi - \pi_h \phi$ to yield $O(h^2)$ estimates. However, in general (6) does not give $O(h^2)$ convergence when $\Gamma \neq \Gamma_D$. For example, the Dirichlet portion of the boundary conditions for the quantity of interest equal to the average error $(1/|\Gamma|) \int_\Gamma A\partial_n e \, dx$, namely

$$\phi = 1/|\Gamma|, \quad x \in \Gamma \\ \phi = 0, \quad x \in \Gamma_D \setminus \Gamma$$

places discontinuities in the boundary data for the adjoint. Since the data are only in $H^{1/2-\varepsilon}(\Gamma_D)$, for $\varepsilon > 0$, ϕ is no longer in $H^2(\Omega)$. Consequently, $\phi - \pi_h \phi$ no longer yields $O(h^2)$ accuracy and it becomes harder to compute ϕ accurately.

We replace the ideal Dirichlet portion of the boundary conditions,

$$\begin{aligned}\phi &= \psi, & x &\in \Gamma \\ \phi &= 0, & x &\in \Gamma_D \setminus \Gamma\end{aligned}\tag{8}$$

by

$$\phi = \tilde{\psi}, \quad x \in \Gamma_D \tag{9}$$

where $\tilde{\psi} \in H^1(\Gamma_D)$, $\tilde{\psi} \approx \psi$ on Γ , and $\tilde{\psi} \approx 0$ on $\Gamma_D \setminus \Gamma$. Note that this means that we do not compute the quantity of interest exactly. The gain is a smooth Green's function that is easier to compute. The effect of the smoothing can be bounded analytically or estimated using an additional adjoint problem.

There is no unique way to construct $\tilde{\psi}$. Below, we consider a couple of different choices for a model problem and demonstrate that the choice of $\tilde{\psi}$ can have a strong impact on the generalized Green's function and the effective domain of dependence. In addition, the closer we choose $\tilde{\psi}$ to the nonsmooth data (8), the more difficult it is to approximate the Green's function.

4. COMPARISONS WITH PREVIOUS TECHNIQUES

First, we describe the post-processing technique developed by Wheeler [1] and Carey [2–5] to compute boundary fluxes. They consider the case $\Gamma = \Gamma_D = \partial\Omega$. Denoting the set of elements that intersect the boundary by

$$B_h = \{K \in T_h \mid \bar{K} \cap \partial\Omega \neq \emptyset\}$$

we define the space

$$W_h = \{v \in P^1(K) \text{ with } K \in B_h, \ v(\eta_i) = 0 \text{ if } \eta_i \notin \partial\Omega\}$$

where $\{\eta_i\}$ denotes the nodes of element K . To clarify, the degrees of freedom in this piecewise linear polynomial space correspond to the nodes on the boundary. The approximation is $\sigma \in W_h$ satisfying

$$-(\sigma, v)_{\partial\Omega} = (f, v) - a(u_h, v) \quad \text{for all } v \in W_h \tag{10}$$

It is clear from Green's identity that σ gives an approximation to the normal flux on the boundary while σ is relatively cheap to compute.

The boundary-flux method produces a piecewise polynomial approximation to $A\partial_n u$ rather than an estimate of a functional. However, since $\pi_{\partial} u \in W_h$ and $\phi = \pi_{\partial} \phi = \psi$ on $\partial\Omega$,

$$-(\sigma - A\partial_n u, \psi)_{\partial\Omega} = (f, \phi - \pi_h \phi) - a(u_h, \phi - \pi_h \phi)$$

In other words, σ provides an estimate of the functional of the boundary flux,

$$-(\sigma, \psi)_{\partial\Omega} \approx -(A\partial_n u, \psi)_{\partial\Omega}$$

if $(f, \phi - \pi_h \phi) - a(u_h, \phi - \pi_h \phi)$ decays away from $\partial\Omega$ rapidly. If we use $(\sigma - A\partial_n u_h, \psi)_{\partial\Omega}$ as an error indicator for refinement, only those elements next to the boundary are refined. If $(f, \phi - \pi_h \phi) - a(u_h, \phi - \pi_h \phi)$ does not decay away from $\partial\Omega$ rapidly, then those terms would eventually become dominant in the error indicator (7) under such a refinement scheme.

The recovery technique developed by Larson *et al.* [9] is essentially the same as the boundary-flux method. The difference is that the boundary-flux method results in a piecewise polynomial approximation of the normal flux with support on the elements touching the boundary, whereas the Larson *et al.* technique provides an estimate of the linear functional of the normal derivative.

Finally, we describe a post-processing technique developed by I. Babuska and A. Miller in the 1980s [6–8]. This technique uses a so-called extraction function to estimate a linear functional of the true solution. It turns out that the extraction function is actually the generalized Green's function, although it is not described in this way. A close inspection reveals their approach provides an alternative method for solving the adjoint problem. Consider the adjoint problem

$$\begin{aligned} L^* \phi &= 0, & x &\in \Omega \\ \phi &= \psi, & x &\in \partial\Omega \end{aligned} \quad (11)$$

We choose a function ϕ_B such that $\phi_B = \psi$ on $\partial\Omega$ and ϕ_B decays rapidly in Ω away from the boundary. We then write the adjoint solution as $\phi = \phi_I + \phi_B$. Since $\phi_B = \psi$ on the boundary, ϕ_I is zero on the boundary and therefore $\phi_I \in H_0^1(\Omega)$. In general, ϕ_I is unknown, but we insert $\phi = \phi_I + \phi_B$ into (11) to obtain

$$\begin{aligned} L^* \phi_I &= -L^* \phi_B, & x &\in \Omega \\ \phi_I &= 0, & x &\in \partial\Omega \end{aligned} \quad (12)$$

Finally, we use ϕ to obtain an *a posteriori* estimate analogous to (6), which is exactly the same if we choose $\phi_B = \pi_{\partial}\phi$.

Babuska and Miller consider Laplace's equation on simple domains, in which case it is possible to get precise estimates on ϕ_I using classic Green's function theory. In general, we could solve (12) instead of (11) under the hope that it might be easier to compute an accurate solution.

5. NUMERICAL RESULTS

In this section, we present some computations to illustrate the preceding discussion.

5.1. Example 1

For the first problem, we consider the solution of

$$\begin{aligned} -\Delta u &= f(x), & x &\in \Omega \\ u &= 0, & x &\in \Gamma_D = \partial\Omega \end{aligned} \quad (13)$$

where $\Omega = [0, 1] \times [0, 1]$. The exact quantity of interest is

$$\int_{\Gamma} \nabla u \cdot n \, ds$$

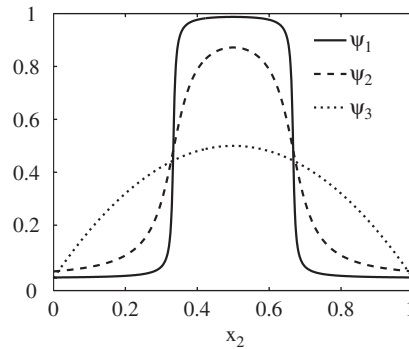


Figure 1. Profiles of the smoothed data (14) used to estimate the average value along the line segment $x_1 = 1$, $\frac{1}{3} \leq x_2 \leq \frac{2}{3}$.

which has value 0, where Γ is the line segment $x_1 = 1$, $\frac{1}{3} \leq x_2 \leq \frac{2}{3}$. We use a continuous, higher-order method to solve the three adjoint problems,

$$\begin{aligned} -\Delta \phi_i &= 0, & x &\in \Omega \\ \phi_i &= \psi_i, & x &\in \Gamma \\ \phi_i &= 0, & x &\in \Gamma_D \setminus \Gamma \end{aligned}$$

with ψ_i corresponding to three smoothed adjoint data

$$\begin{aligned} \psi_1(x_2) &= \frac{1}{3 \times 1.040266357} (\arctan(200(x_2 - 1/3)) - \arctan(200(x_2 - 2/3))) \\ \psi_2(x_2) &= \frac{1}{3 \times 0.978161737} (\arctan(20(x_2 - 1/3)) - \arctan(20(x_2 - 2/3))) \\ \psi_3(x_2) &= 2x_2(1 - x_2) \end{aligned} \quad (14)$$

each normalized to have integral norm $\frac{1}{3}$. In Figure 1, we observe that the data ψ_1 provides a very close approximation to the ideal discontinuous ψ defining the exact quantity of interest, the data ψ_2 are slightly smoother than ψ_1 , and the data ψ_3 yield an average of the normal derivative over a relatively large region resulting in an adjoint solution that is significantly smoother.

In the first set of computations, we use $f(x) = 8\pi^2 \sin(2\pi x_1) \sin(2\pi x_2)$ so $u(x) = \sin(2\pi x_1) \sin(2\pi x_2)$. In Figure 2, we plot the adjoint solutions corresponding to the three data.

In Figure 3, we plot the meshes obtained by an adaptive refinement based on (7) after five refinement levels. The localized nature of the refinement needed to resolve the desired information is clearly visible.

In Figure 4 (left), we plot the effectivity index (error estimate/true error) for the three computations. The smoother ψ approximations yield much more accurate error estimates on coarser meshes, whereas using ψ_1 requires a mesh that is fine near the layers in that function. In the context of uniform meshes, using ψ_1 to approximate the quantity of interest means having to use a much finer mesh.

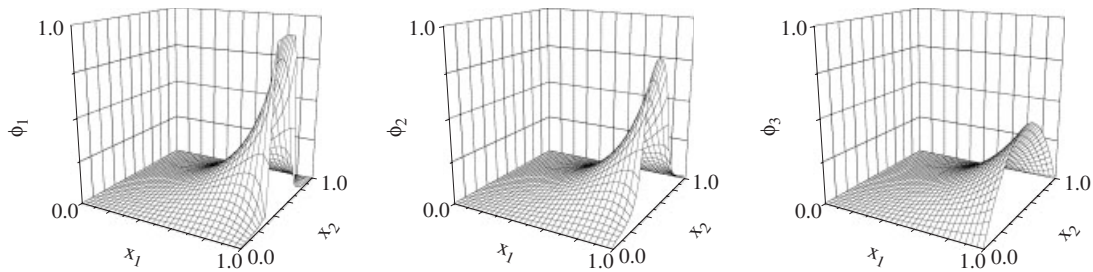


Figure 2. Adjoint solutions corresponding to ψ_1 (left), ψ_2 (middle), and ψ_3 (right).

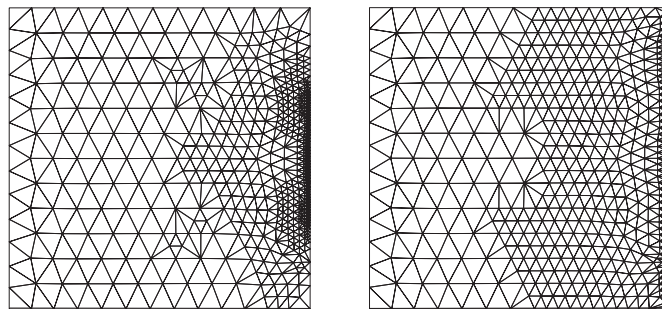


Figure 3. Final adapted meshes corresponding to ψ_1 (left) and ψ_3 (right).

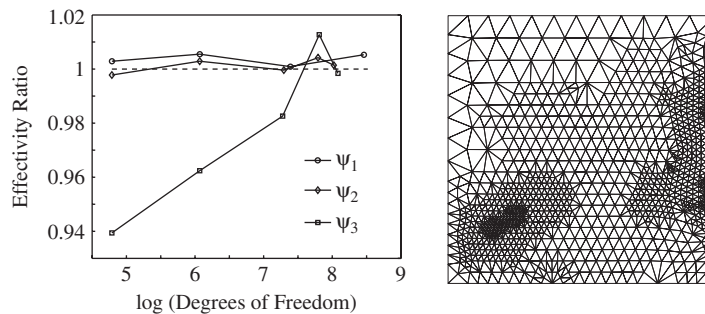


Figure 4. Left: the effectivity index for ψ_1 , ψ_2 , and ψ_3 . Right: the final adapted mesh for a problem with a highly localized forcing and data ψ_1 for the adjoint.

Finally, we plot the final adapted mesh when the function f is perturbed by an approximate delta function located away from the boundary and ψ_1 is the data for the adjoint problem. In Figure 4, we see that the adaptive mesh refinement using (7) yields a mesh that is refined near the region with the perturbation and the region where the desired information is computed. The former results from large residuals in the forward approximation and the latter results from large adjoint weights.

5.2. Example 2

We next consider Laplace's equation defined on an L-shaped domain shown in Figure 5. We impose homogeneous Dirichlet boundary conditions on the boundaries along the coordinate axes and choose Neumann boundary conditions on the remaining boundaries so that the true solution is $u(r, \theta) = r^{2/3} \sin(2\theta/3)$ in polar coordinates. The quantity of interest is the average value of the normal derivative $(1/|\Gamma_D|) \int_{\Gamma_D} \partial_n u \, ds$.

In the first computation, we choose Γ_D to be the line segments along $x_1 = 0$, $-1 \leq x_2 \leq 0$ and $0 \leq x_1 \leq 1$ and $x_2 = 0$. The adjoint problem is

$$\begin{aligned} -\nabla \cdot (\nabla \phi) &= 0, \quad x \in \Omega \\ \phi &= 1/2, \quad x \in \Gamma_D \\ a \partial_n \phi &= 0, \quad x \in \Gamma_N \end{aligned} \quad (15)$$

which has exact solution $\phi = \frac{1}{2}$. This implies that the adjoint weight $\phi - \pi \phi$ is negligible away from Γ . Table I displays the details of the error estimation. We use a higher-order method to solve the adjoint problem, obtaining accurate estimates at all refinement levels. Figure 5 shows the final adaptive mesh from these calculations.

Next, we test the boundary-flux technique by using

$$-(a \partial_n e, 1/2)_{\Gamma_D} \approx \sum_{K \cap \Gamma_D \neq \emptyset} (f, v)_K - a(u_h, v)_K + (a \partial_n u_h, 1/2)_{\Gamma_D}$$

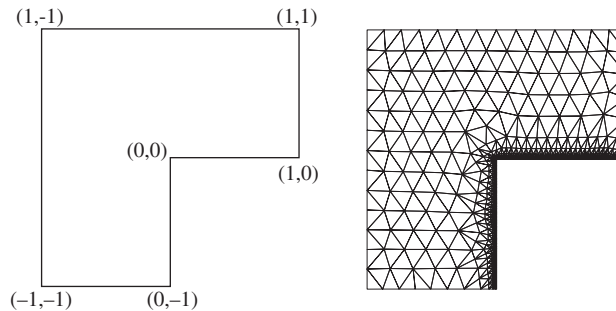


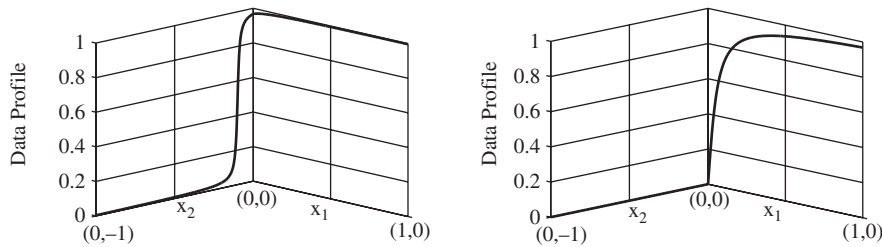
Figure 5. Left: illustration of the L-shaped domain. Right: the final adapted mesh obtained using the adjoint problem (15).

Table I. Error estimates and effectivity ratios for the first L-shaped domain computation.

Elements	DOF	Adj. est.	True error	Effect. ratio
242	156	-0.127067	-0.126349	1.0057
341	213	-0.080861	-0.080681	0.9998
531	322	-0.050952	-0.050907	1.0009
903	535	-0.032048	-0.032037	1.0003
1639	956	-0.020159	-0.020156	1.0001

Table II. Error estimates and effectivity ratios using the boundary-flux technique.

Elements	DOF	B-Flux est.	True error	Effect. ratio
242	156	−0.126342	−0.126349	0.9999
341	213	−0.080679	−0.080681	0.9999
531	322	−0.050907	−0.050907	1.0000
903	535	−0.032036	−0.032037	1.0000
1639	956	−0.020156	−0.020156	1.0000

Figure 6. Plots of the smoothed data corresponding to ψ_1 (right) and ψ_2 (left). The viewpoint is from the outside looking at the interior corner.

The error estimation results are given in Table II. We can adapt the mesh along the boundary using the resulting estimate and then refine the mesh in the interior to match. This results in exactly the same mesh as obtained using the adjoint estimate. In this special case, the boundary-flux technique compares favourably with the estimates using the adjoint problem.

Next, we consider two different smooth approximations for the data ψ in the L-shaped domain problem. The quantity of interest is the normal flux across the line segment

$$\{x \mid x_2 = 0, \ 0 \leq x_1 \leq 1\}$$

The first approximation to the discontinuous data

$$\psi = \begin{cases} 1, & x_2 = 0, \ 0 \leq x_1 \leq 1 \\ 0, & x_1 = 0, \ 0 \leq x_2 \leq 1 \end{cases}$$

we use

$$\psi_1 = \frac{1}{2} + \frac{1}{\pi} \arctan(100(x_2 + 0.1))$$

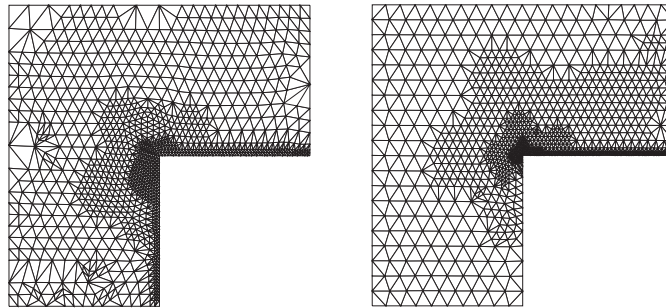
which is nearly one when $x_2 = 0$ and drops off rapidly as x_2 decreases (see Figure 6). For this problem, the exact normal flux is known, so we may use the functional

$$(\partial_n u, \psi_1)_{\Gamma_D} = -1.185761$$

to compare with the adjoint estimates in Table III. The final adaptive mesh is given in Figure 7.

Table III. Error estimates and effectivity ratios for the computations corresponding to ψ_1 .

Elements	DOF	Adj. est.	True error	Effect. ratio
242	156	−0.239095	−0.210139	1.1378
881	494	−0.145261	−0.141630	1.0256
1523	829	−0.092468	−0.092524	0.9994
2171	1179	−0.057318	−0.056936	1.0067

Figure 7. Plots of the final adapted meshes corresponding to ψ_1 (right) and ψ_2 (left).Table IV. Error estimates and effectivity ratios corresponding to ψ_2 .

Elements	DOF	Adj. est.	True error	Effect. ratio
583	351	−0.024659	−0.033015	0.7469
1221	678	−0.012221	−0.015601	0.7834
1664	911	−0.005765	−0.007134	0.8081
2130	1166	−0.005765	−0.007134	0.8355
2764	1524	−0.001715	−0.001925	0.8906

Next, we consider

$$\psi_2 = \frac{2}{\pi} \arctan(20 \times x_1)$$

Using ψ_1 means regularizing the Dirichlet data on $\Gamma_D \setminus \Gamma$ so that $\phi \approx 1$ on Γ . Using ψ_2 means regularizing the data on the segment of interest. Using the analytic solution, we evaluate

$$(\partial_n u, \psi_2)_\Gamma = -0.792209$$

and summarize the results in Table IV. The final adaptive mesh is given in Figure 7.

6. CONCLUSIONS

In this paper, we carefully describe how to estimate the error in the average flux of the solution over a piece of the boundary using adjoint-based *a posteriori* analysis, concentrating on explaining how the adjoint problem is defined in order to obtain such a quantity of interest. We also explain how this approach is closely related to the earlier boundary-flux and extraction function techniques. We explore the use of various regularizations of the boundary data used to obtain an estimate of the flux over just a portion of the boundary and the trade-offs between obtaining an accurate approximation of the desired information and difficulty in solving for an accurate adjoint solution.

REFERENCES

1. Wheeler MF. A Galerkin procedure for estimating the flux for two-point boundary-value problems using continuous piecewise-polynomial spaces. *Numerische Mathematik* 1974; **2**:99–109.
2. Seager MK, Carey GF, Chow SS. Approximate boundary-flux calculations. *Computer Methods in Applied Mechanics and Engineering* 1985; **50**:107–120.
3. Carey GF. Derivative calculation from finite element solutions. *Computer Methods in Applied Mechanics and Engineering* 1982; **35**:1–14.
4. Carey GF. Some further properties of the superconvergent flux projection. *Communications in Numerical Methods in Engineering* 2002; **18**:241–250.
5. Chow S-S, Carey GF, Lazarov RD. Natural and postprocessed superconvergence in semilinear problems. *Numerical Methods for Partial Differential Equations* 2005; **7**:245–259.
6. Babuska I, Miller A. The post-processing approach in the finite element method-part 1: calculation of displacements, stresses and other higher derivatives of the displacement. *International Journal for Numerical Methods in Engineering* 1984; **20**:1085–1109.
7. Babuska I, Miller A. The post-processing approach in the finite element method-part 1: the calculation of stress intensity factors. *International Journal for Numerical Methods in Engineering* 1984; **20**:1111–1129.
8. Babuska I, Miller A. The post-processing approach in the finite element method-part 1: a-posteriori error estimates and adaptive mesh selection. *International Journal for Numerical Methods in Engineering* 1984; **20**:2311–2324.
9. Giles M, Larson MG, Levenstam JM, Suli E. Adaptive error control for finite element approximations of the lift and drag coefficients in viscous flow. *Technical Report NA-76/06*, Oxford University Computing Laboratory, 1997.
10. Estep D. *A posteriori* error bounds and global error control for approximations of ordinary differential equations. *SIAM Journal on Numerical Analysis* 1995; **32**:1–48.
11. Eriksson K, Estep D, Hansbo P, Johnson C. Introduction to adaptive methods for differential equations. *Acta Numerica* 1995; **3**:105–158.
12. Eriksson K, Estep D, Hansbo P, Johnson C. *Computational Differential Equations*. Cambridge University Press: Cambridge, 1996.
13. Estep D, Williams R, Larson M. Estimating the error of numerical solutions of systems of reaction-diffusion equations. *Memoirs of the American Mathematical Society*, vol. 146, 2000.
14. Becker R, Rannacher R. An optimal control approach to *a posteriori* error estimation in finite element methods. *Acta Numerica* 2001; **1**:1–102.
15. Giles M, Süli E. Adjoint methods for PDEs: *a posteriori* error analysis and postprocessing by duality. *Acta Numerica* 2002; **11**:145–236.
16. Bangerth W, Rannacher R. *Adaptive Finite Element Methods for Differential Equations*. Birkhauser Verlag: Basel, 2003.
17. Estep D, Holst M, Larson M. Generalized Green's functions and the effective domain of influence. *SIAM Journal on Scientific Computing* 2005; **26**:1314–1339.
18. Estep D. *A Short Course on Duality, Adjoint Operators, Green's Functions, and a Posteriori Error Analysis*. Colorado State University: Colorado, 2004.
19. Adams RA. *Sobolev Spaces*. Academic Press: New York, 1975.
20. Brenner SC, Scott LR. *The Mathematical Theory of Finite Element Methods*. Springer: Berlin, 2002.