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A new equilibrated residual method improving accuracy and efficiency of flux-free error estimates

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Abstract

This paper presents a new methodology to compute guaranteed upper bounds for the energy norm of the error in the context of linear finite element approximations of the reaction–diffusion equation. The new approach revisits the ideas in Parés et al. (2009) [6, 4], with the goal of substantially reducing the computational cost of the *flux-free* method while retaining the good quality of the bounds. The new methodology provides also a technique to compute equilibrated boundary tractions improving the quality of standard equilibration strategies. The *zeroth-order* equilibration conditions are imposed using an alternative less restrictive form of the *first-order equilibration* conditions, along with a new efficient minimization criterion. This new equilibration strategy provides much more accurate upper bounds for the energy and requires only doubling the dimension of the local linear systems of equations to be solved.

Keywords: Exact/guaranteed/strict bounds; Fully computable a posteriori error estimation; Adaptivity; Reaction–diffusion equation; Flux-free; Equilibrated boundary tractions

1. Introduction

The certification of numerical simulations is fundamental in any engineering design process. In particular, most simulations are aimed at obtaining a *certified* approximation of a certain quantity of interest [1,2]. This paper focuses in obtaining bounds for the error in energy norm, which is an essential ingredient for computing bounds for any quantity of interest. Specifically, for the advection–reaction–diffusion equation, upper and lower bounds for the error in a given quantity of interest are obtained from upper bounds for the energy norm of the error of symmetrized auxiliary reaction–diffusion problems [3–5].

The two implicit residual a posteriori error estimates providing computable guaranteed bounds for the energy norm (and also for quantities of interest through an error representation involving an adjoint problem) are: (1) the hybrid-flux techniques which require computing equilibrated tractions around the elements, and (2) the flux-free techniques

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where the local problems are defined in patches of elements around every vertex node of the mesh and no explicit computation of equilibrated tractions is required. A comparison of the two techniques is presented in [6,4] showing that the flux-free approach provides much more accurate results while having larger computational cost.

The objective of the present work is to provide a novel flux-free strategy that while retaining the accuracy of the standard flux-free approach, its computational cost, which is the main drawback of flux-free error estimates, is comparable to the cost of hybrid-flux techniques.

The remainder of the paper is organized as follows. The model problem and the *flux-free* a posteriori error estimate are presented in Sections 2–5. Section 6 reformulates the new *flux-free* a posteriori error estimate into a new *hybrid-flux* technique allowing to obtain accurate equilibrated tractions. The paper concludes with a brief computational cost overview in Section 7 and several numerical examples in Section 8.

2. Model problem and finite element approximation

Let Ω be an open bounded polygonal domain in $\mathbb{R}^2$, with boundary $\partial\Omega = \overline{\Gamma}_{\rm N} \cup \overline{\Gamma}_{\rm D}$, where $\Gamma_{\rm N}$ and $\Gamma_{\rm D}$ form a disjoint partition of the boundary. The boundary value problem to be solved is stated as follows: find the real-valued function u such that

$$\begin{aligned} -\Delta u + \kappa^2 u &= f \quad && \text{in } \Omega, \\ u &= u_{\rm D} \quad && \text{on } \Gamma_{\rm D}, \\ \nabla u \cdot \boldsymbol{n} &= g_{\rm N} \quad && \text{on } \Gamma_{\rm N}, \end{aligned} \tag{1}$$

where $u_{\rm D}$ is assumed to be continuous and piecewise linear on the Dirichlet boundary $\Gamma_{\rm D}$. Additionally, without loss of generality κ is assumed to be a non-negative constant and in order to guarantee a unique solution of (1), either $\kappa > 0$ or $\Gamma_{\rm D}$ is a non-empty set.

The standard variational formulation of the problem consists of seeking $u \in \mathcal{U}$ with

$$a(u, v) = \ell(v) \quad \text{for all } v \in \mathcal{V}, \tag{2}$$

where

$$a(u, v) = \int_\Omega \left(\nabla u \cdot \nabla v + \kappa^2 u v \right) d\Omega \quad \text{and} \quad \ell(v) = \int_\Omega f v \, d\Omega + \int_{\Gamma_{\rm N}} g_{\rm N} v \, d\Gamma.$$

The solution and test spaces are $\mathcal{U} = \{u \in \mathcal{H}^1(\Omega),\ u|_{\Gamma_{\rm D}} = u_{\rm D}\}$ and $\mathcal{V} = \{v \in \mathcal{H}^1(\Omega),\ v|_{\Gamma_{\rm D}} = 0\}$, $\mathcal{H}^1(\Omega)$ being the standard Sobolev space of functions defined in Ω such that both the functions and their first derivatives are square-integrable.

The finite element approximation of problem (2) consists on finding $u_h \in \mathcal{U}^h$ such that

$$a(u_h, v) = \ell(v) \quad \text{for all } v \in \mathcal{V}^h.$$

Here, $\mathcal{U}^h \subset \mathcal{U}$ and $\mathcal{V}^h \subset \mathcal{V}$ denote the finite-dimensional spaces associated with a triangular finite element mesh of characteristic mesh size h, which functions are continuous, piecewise-linear functions. The mesh is the union of non-overlapping linear triangular elements, denoted by Ω_k, $k = 1, \ldots, n_{\rm el}$, such that the intersection of adjacent elements (those having nonempty intersection) is either a single common node or a single common edge.

3. Guaranteed upper bounds for the energy norm: Complementary energy relaxation

Much effort has been devoted to obtain *strict* bounds, that is, bounds guaranteed with respect to the exact solution independently of any underlying mesh (see for instance the series of references [7,3,8–12,6,4,5]). All these strategies recover strict bounds of the error (measured either using the energy norm or using a particular quantity of interest) using the standard complementary energy approach. The key idea is to relax the continuous residual error problem of finding $e = u - u_h \in \mathcal{V}$ such that

$$a(e, v) = \ell(v) - a(u_h, v) \quad \forall v \in \mathcal{V} \tag{3}$$

by introducing dual unknowns living in larger spaces with less regularity requirements.