Available online at www.sciencedirect.com
ScienceDirect
Mathematics and Computers in Simulation 80 (2010) 1674–1683
MATHEMATICS AND COMPUTERS IN SIMULATION
www.elsevier.com/locate/matcom

Goal-oriented a posteriori error estimates for transport problems

Dmitri Kuzmin [a,*], Sergey Korotov [b]

[a] *Institute of Applied Mathematics (LS III), Dortmund University of Technology, Vogelpothsweg 87, D-44227 Dortmund, Germany*
[b] *Institute of Mathematics, Helsinki University of Technology, P.O. Box 1100, FIN–02015 TKK, GermanyFinlandGermany*

Received 31 October 2008; received in revised form 23 January 2009; accepted 16 March 2009
Available online 28 March 2009

Abstract

Some aspects of goal-oriented a posteriori error estimation are addressed in the context of steady convection–diffusion equations. The difference between the exact and approximate values of a linear target functional is expressed in terms of integrals that depend on the solutions to the primal and dual problems. Gradient averaging techniques are employed to separate the element residual and diffusive flux errors without introducing jump terms. The dual solution is computed numerically and interpolated using higher-order basis functions. A node-based approach to localization of global errors in the quantities of interest is pursued. A possible violation of Galerkin orthogonality is taken into account. Numerical experiments are performed for centered and upwind-biased approximations of a 1D boundary value problem.

PACS: 65N15; 65N50; 76M30

Keywords: Stationary convection–diffusion equations; The finite element method; A posteriori error estimates; Goal-oriented quantities; Mesh adaptation

1. Introduction

Numerical simulation of transport phenomena (convection and/or diffusion) plays an increasingly important role in science and engineering. The accuracy and reliability of computational methods depend on the choice of discretization techniques and, to a large extent, on the quality of the underlying mesh. Nowadays, adaptive mesh refinement techniques are widely used to reduce discretization errors in a computationally efficient way. Sometimes the location of critical zones, such as boundary and interior layers, is known. However, in most cases, mesh adaptation is an iterative process which involves estimation of numerical errors by means of certain a posteriori feedback mechanisms.

The derivation of a posteriori error estimates is aimed at obtaining computable lower and/or upper bounds for certain quantities of interest. In the case of convection-dominated transport problems, the global energy norm ceases to be a good measure of the numerical error. One of the most promising current trends in Computational Fluid Dynamics is goal-oriented adaptivity, whereby the duality argument is employed to derive an estimate for the magnitude of a given target/output functional [1,6,7,16,17,19]. The most prominent representative of such error estimators is the Dual-

* Corresponding author.
E-mail addresses: kuzmin@math.uni-dortmund.de (D. Kuzmin), sergey.korotov@hut.fi (S. Korotov).

0378-4754/$36.00 © 2009 IMACS. Published by Elsevier B.V. All rights reserved.
doi:10.1016/j.matcom.2009.03.008

Weighted-Residual (DWR) method of Becker and Rannacher [3,4]. Remarkably, it is applicable not only to self-adjoint elliptic PDEs but also to hyperbolic conservation laws [9,10].

In most cases, Galerkin orthogonality is involved in the derivation of goal-oriented a posteriori estimates by the DWR method. For the numerical solution to possess this property, the discretization must be performed by the Galerkin finite element method, and the resulting algebraic equations must be solved exactly. These requirements are rarely satisfied in practice due to numerical integration, round-off errors, and slack tolerances for iterative solvers. Last but not least, various stabilization terms or flux/slope limiters may be responsible for a (local) loss of Galerkin orthogonality. As a result, an extra term needs to be included in the error estimate for the DWR method. This part is computable but its localization, i.e., distribution among individual elements/nodes is a nontrivial task. Existing localization procedures [2] exploit the nature of the underlying discretization and are not universally applicable.

In the present paper, we address goal-oriented error estimation for stationary transport equations. The methodology to be presented is completely independent of the numerical scheme used to compute the approximate solution. The underlying localization procedure differs from that for the classical DWR method in a number of respects. First, integration by parts is applied to an *averaged* gradient so as to avoid the arising of jump terms at interelement boundaries. In the context of pure diffusion problems, gradient averaging has already been used in goal-oriented estimates [11,12,15] but the approach to be presented is more general and based on different premises. Second, the error in the quantity of interest is expressed in terms of *nodal* values [18], which yields a nonoscillatory distribution of weighted residuals. Moreover, errors due to the lack of Galerkin orthogonality are localized in a simple and natural way. The conversion of nodal errors to element contributions is straightforward.

The derivation of the above error estimate is followed by a discussion of algorithmic details and application to a one-dimensional convection–diffusion problem. The availability of analytical solutions makes it possible to perform a detailed analysis of accuracy and to identify the major sources of error.

2. Goal-oriented error estimation

Consider the Dirichlet problem that models steady convection and diffusion of a conserved scalar quantity $u(\mathbf{x})$ in a domain Ω with boundary Γ

$$\begin{cases} \nabla \cdot (\mathbf{v}u - \varepsilon \nabla u) = f & \text{in}\Omega, \\ u = b & \text{on}\Gamma, \end{cases} \tag{1}$$

where $\mathbf{v}(\mathbf{x})$ is a known velocity field, $\varepsilon > 0$ is a constant diffusion coefficient, $f(\mathbf{x})$ is a volumetric source/sink, and $b(\mathbf{x})$ is the prescribed boundary data.

A variational form of problem (1) can be constructed by the weighted residual method using integration by parts. Let $H^1(\Omega)$ be the Sobolev space of square integrable functions with first derivatives in $L^2(\Omega)$. Furthermore, let $H_0^1(\Omega)$ denote a subspace of functions from $H^1(\Omega)$ vanishing on the boundary Γ. The problem statement becomes: Find $u \in H^1(\Omega)$ such that $u = b$ on Γ and

$$a(w, u) = (w, f), \quad \forall w \in H_0^1(\Omega), \tag{2}$$

where the bilinear form $a(\cdot, \cdot)$ and the L^2 scalar product $(\cdot, \cdot)$ are defined by

$$a(w, u) = \int_\Omega w \nabla \cdot (\mathbf{v}u) \mathrm{d}x + \int_\Omega \nabla w \cdot (\varepsilon \nabla u) \mathrm{d}x, \quad \forall w, u \in H^1(\Omega), \tag{3}$$

$$(w, f) = \int_\Omega w f \mathrm{d}x, \quad \forall w, f \in L^2(\Omega). \tag{4}$$

Let $u_h \in H^1(\Omega)$ be a numerical solution of problem (2) satisfying the Dirichlet boundary condition $u_h = b$ on Γ. It is convenient to define u_h as a finite element interpolant of nodal values computed by an arbitrary numerical scheme.

Numerical errors can be quantified using the residual of the weak form (2)

$$\rho(w, u_h) = (w, f) - a(w, u_h), \quad \forall w \in H_0^1(\Omega). \tag{5}$$

Note that the value of $\rho(w, u_h)$ depends on the choice of w. This weight should carry information about the propagation of errors and goals of simulation.