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Numerical Analysis

Functional a posteriori estimates for the reaction–diffusion problem

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Abstract

The Note is concerned with functional type a posteriori estimates for stationary reaction–diffusion problems. Functional a posteriori estimates are derived on purely functional grounds without using any type of the Galerkin orthogonality condition and special properties of approximation spaces. Therefore, they contain no mesh-dependent constants and provide guaranteed error bounds for any conforming approximation. Generalizations to non-conforming approximations are also possible. Estimates derived in the Note are equally efficient for the problems with constant reaction parameter and for those admitting a high variability of it in different parts of the domain. Such a robustness with respect to the reaction parameter is important because in applications the reaction parameter my often be large in one subdomain and almost zero in another one. It is shown that the a posteriori bounds obtained are directly computable and provide sharp error bounds. ***To cite this article: S. Repin, S. Sauter, C. R. Acad. Sci. Paris, Ser. I 343 (2006).***

Résumé

Estimations à posteriori de type fonctionnel pour les problèmes de réaction–diffusion. Cette Note s'intéresse aux estimations à posteriori de type fonctionnel pour les problèmes de réaction–diffusion. Ces estimations fonctionnelles à posteriori sont obtenues par des méthodes purement fonctionnelles ne faisant en particulier pas appel à des propriétés d'orthogonalité de Galerkine ou des propriétés spéciales des espaces d'approximation. De ce fait elles sont indépendantes des tailles de maillage et fournissent des erreurs fiables pour toute approximation conforme. La généralisation au cas non conforme est également possible. Les estimations établies ici sont efficaces aussi bien dans le cas de coefficients constants que de coefficients oscillant arbitrairement dans certaines parties du domaine. Une telle robustesse est importante dans les applications où certains paramètres peuvent être très grands dans certaines parties et quasi nuls dans d'autres. On montre également que les estimations à posteriori que nous obtenons sont directement calculables et fournissent des estimations optimales. ***Pour citer cet article : S. Repin, S. Sauter, C. R. Acad. Sci. Paris, Ser. I 343 (2006).***

Version française abrégée

Cette Note traite des estimations a posteriori pour le problème de réaction diffusion

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$$\begin{aligned} &\operatorname{div}(\mathbf{A}\operatorname{grad} u) - \lambda u + f = 0 && \text{in } \Omega,\\ &u = u_0 && \text{on } \Gamma_D,\\ &\langle \mathbf{A}\nabla u, \mathbf{n}\rangle = F && \text{on } \Gamma_N, \end{aligned} \tag{1}$$

Γ_D, et Γ_N sont deux parties disjointes de la frontière $\partial\Omega$, la mesure de Γ_D étant strictement positive. $\mathbf{A} = \{a_{i,j}\}$ est une matrice symétrique vérifiant pour $0 < \alpha_1 \leqslant \alpha_2$ et tout vecteur $\xi \in \mathbb{R}^d$

$$\alpha_1\|\xi\|^2 \leqslant \langle \mathbf{A}\xi, \xi\rangle \leqslant \alpha_2\|\xi\|^2,$$

et

$$u_0 \in H^1(\Omega), \quad f \in L^2(\Omega), \quad F \in L^2(\Gamma_N). \tag{2}$$

Nos estimations sont faites en fonction des normes naturellement adaptées au problème à savoir :

$$|||u||| = \left(\|\nabla u\|_{\mathbf{A}}^2 + \int_\Omega \lambda u^2\right)^{1/2}, \quad \|\nabla u\|_{\mathbf{A}}^2 = \int_\Omega \langle \mathbf{A}\nabla u, \nabla u\rangle.$$

Le but est d'obtenir une borne supérieure calculable pour $|||u - v|||$ pour tout $v \in H^1(\Omega)$ satisfaisant la condition de Dirichlet sur Γ_D. Dans le cas où $\partial\Omega = \Gamma_D$ et pour un paramètre de réaction λ constant une telle estimation est donnée dans [5–7]. Elle a la forme

$$|||u - v|||^2 \leqslant D(\nabla v, \mathbf{y}) + \frac{1}{\lambda}\|\operatorname{div}\mathbf{y} - \lambda v + f\|_{L^2(\Omega)}^2 \tag{3}$$

où

$$D(\nabla v, \mathbf{y}) = \int_\Omega \left\langle \mathbf{A}^{-1}\mathbf{y} - \nabla v, \mathbf{y} - \mathbf{A}\nabla v\right\rangle$$

et $\mathbf{y}$ est une fonction arbitraire de $H(\Omega, \operatorname{div})$. Pour $\mathbf{y} = \mathbf{A}\nabla u$ (4) est une égalité. Il en résulte que la minimisation en y du membre de droite dans (3) peut donner une estimation de l'erreur aussi bonne que possible. Néanmoins (3) a le désavantage d'être sensible aux petites valeurs de λ ce qui rend son implémentation difficile. Dans cette note nous utilisons une méthode différente pour nos estimations et obtenons des bornes supérieures calculables pour l'approximation conforme du problème (1) qui sont stables pour les petites valeurs de λ. L'estimation fondamentale est la suivante :

$$|||u - v|||^2 \leqslant \sqrt{\int_\Omega \frac{\mu^2}{\lambda} r^2(v, \mathbf{y}) + D(\nabla v, \mathbf{y})} + C_1\left\|(1-\mu) r(v, \mathbf{y})\right\|_{L^2(\Omega)} + C_2\|F - y \cdot \nu\|_{L^2(\Gamma_N)} \tag{4}$$

où $r(v, \mathbf{y}) = f + \operatorname{div}\mathbf{y} - \lambda v$, $\mathbf{y} \in H(\Omega, \operatorname{div})$ et a une trace de carré sommable sur Γ_N, C_1 et C_2 sont les deux constantes dans les inégalités (8) et (9) et $\mu(x)$ est une fonction arbitraire à valeur dans $[0, 1]$. Les estimations (11) et (12) correspondent à un choix de $\mu = 0$ et $\mu = 1$ respectivement. Les estimations (13) et (14) sont obtenues en choisissant μ de façon à minimiser le membre de droite de (10). La comparaison de (10) avec (11) et (12) montre que cette estimation est meilleure que (11) et (12) pour de petites valeurs de λ comme pour des valeurs modérées ou très grandes.

1. Basic problem

Let $\Omega \subset \mathbb{R}^d$ be a connected bounded Lipschitz domain with boundary Γ. We consider the reaction–diffusion boundary value problem

$$\begin{aligned} &\operatorname{div}(\mathbf{A}\operatorname{grad} u) - \lambda u + f = 0 && \text{in } \Omega,\\ &u = u_0 && \text{on } \Gamma_D,\\ &\langle \mathbf{A}\nabla u, \mathbf{n}\rangle = F && \text{on } \Gamma_N, \end{aligned} \tag{5}$$

where Γ_D and Γ_N are the (non-intersecting) Dirichlet and Neumann parts of Γ, $\langle , \rangle$ denotes the scalar product of vectors, and $\mathbf{n}$ is the outer unit normal vector field. We assume that the matrix $\mathbf{A} = (a_{ij})_{i,j=1}^d : \Omega \to \mathbb{R}_{\mathrm{sym}}^{d \times d}$ has coefficients in $L^\infty(\Omega)$ and

$$\alpha_1 \|\mathbf{v}\|^2 \leqslant \langle \mathbf{A}(\mathbf{x})\mathbf{v}, \mathbf{v} \rangle \leqslant \alpha_2 \|\mathbf{v}\|^2 \quad \forall \mathbf{v} \in \mathbb{R}^d \ \forall \mathbf{x} \in \Omega \text{ a.e.}$$

with some positive constants $0 < \alpha_1 \leqslant \alpha_2$. It is assumed that the scalar function $\lambda \in L^\infty(\Omega)$ is positive and $c(\mathbf{x}) \geqslant c_0 > 0$ for almost all $\mathbf{x} \in \Omega$. Also we assume that $u_0 \in H^1(\Omega)$, $f \in L^2(\Omega)$, $F \in L^2(\Gamma_D)$, and the boundary conditions in (5) are understood as traces.

The generalized solution to (5) is a function

$$u \in V_0 + u_0 := \{ w \in H^1(\Omega) \mid w = w_0 + u_0, \ w_0 \in V_0 \},$$

where $V_0 := \{ w \in H^1(\Omega) \mid w = 0 \text{ on } \Gamma_D \}$ that satisfies the relation

$$\int_\Omega \langle \mathbf{A}\nabla u, \nabla v \rangle + \lambda u v = \int_\Omega f w + \int_{\Gamma_N} F w \quad \forall w \in V_0. \tag{6}$$

Existence and uniqueness of u can be proved by standard arguments. The solution continuously depends on the data with respect to the energy norm

$$|||u||| = \left(\|\nabla u\|_{\mathbf{A}}^2 + \int_\Omega \lambda u^2 \right)^{1/2} \quad \text{with } \|\nabla u\|_{\mathbf{A}}^2 := \int_\Omega \langle \mathbf{A}\nabla u, \nabla u \rangle.$$

Let $v \in V_0 + u_0$ be a certain function viewed as an approximation of u. Our aim is to derive computable upper bounds for the quantity $|||u - v|||$. Such types of estimates are called *functional a posteriori estimates*. They have been derived for various boundary value problems in [5–7] and some other papers cited therein. The topic of a posteriori error estimation for finite element methods goes back to the pioneering papers [2,3]. We omit here a detailed review of the literature but refer to the monographs [1,4,8] and the references therein. Residual-type a posteriori error estimates for singularly perturbed reaction–diffusion problems have been developed in [9].

For the case $\partial\Omega = \Gamma_N$ and $\lambda = \text{const}$, such estimates for the reaction–diffusion problem were obtained in [5] by means of a variational technique. There, it was shown that

$$|||u - v||| \leqslant D(\nabla v, \mathbf{y}) + \frac{1}{\lambda} \| \operatorname{div} \mathbf{y} - \lambda v + f \|_{L^2(\Omega)}, \tag{7}$$

where

$$D(\nabla v, \mathbf{y}) := \int_\Omega \langle \mathbf{A}^{-1}\mathbf{y} - \nabla v, \mathbf{y} - \mathbf{A}\nabla v \rangle$$

and $\mathbf{y}$ is an arbitrary vector-valued function in the space $H(\Omega, \operatorname{div})$. Estimate (7) expresses the error in terms of two quantities: $D(\nabla v, \mathbf{y})$ (which is a measure of the error in the relation $\mathbf{y} = \mathbf{A}\nabla v$) and $R(v, \mathbf{y}) := \| \operatorname{div} \mathbf{y} - \lambda v + f \|_{L^2(\Omega)}^2$ (which is a measure of the residual of the differential equation computed for an approximate solution v and a "flux" $\mathbf{y}$). The estimate is sharp in the sense that there exists $\mathbf{y}$ such that (7) holds as an equality. Indeed, if $\mathbf{y} = \mathbf{A}\nabla u$, then $R(v, \mathbf{y}) = \lambda \|u - v\|_{L^2(\Omega)}^2$ and $D(\nabla v, \mathbf{y}) = \|\nabla(u - v)\|_{\mathbf{A}}^2$. However, (7) has a drawback: its practical efficiency deteriorates if λ is small. Therefore, for small values of the reaction parameter, sensible estimates can be obtained only if $R(v, \mathbf{y})$ is sufficiently small.

In the present Note, we derive a more general estimate that is valid for a wider class of problems with $\lambda = \lambda(\mathbf{x})$ and is stable with respect to small values of λ.

2. Upper bound of the error norm

From (6) we find that

$$\int_\Omega \langle \mathbf{A}\nabla(u - v), \nabla w \rangle + \lambda(u - v)w = \int_\Omega \left(f w - \langle \mathbf{A}\nabla v, \nabla w \rangle - \lambda v w \right) + \int_{\Gamma_N} F w \quad \forall w \in V_0.$$

For any $\mathbf{y} \in \mathbf{Q} := \{\mathbf{z} \in H(\Omega, \mathrm{div}) \mid \langle \mathbf{z}, \mathbf{n} \rangle \in L^2(\Gamma_N)\}$ and $w \in V_0$ we have

$$\int_\Omega \big(w \,\mathrm{div}\, \mathbf{y} + \langle \mathbf{y}, \nabla w \rangle\big) = \int_{\Gamma_N} \langle \mathbf{y}, \mathbf{n} \rangle w.$$

Therefore, for $w = u - v$ we obtain

$$|||u - v|||^2 = I_1 + I_2 + I_3,$$

where

$$I_1 = \int_\Omega \big\{(f + \mathrm{div}\,\mathbf{y} - \lambda v)(u - v)\big\}, \quad I_2 = \int_\Omega \big\langle \mathbf{y} - \mathbf{A}\nabla v, \nabla(u - v)\big\rangle, \quad I_3 = \int_{\Gamma_N} \big\{\big(F - \langle \mathbf{y}, \mathbf{n} \rangle\big)(u - v)\big\}.$$

For any $\mu \in L^\infty(\Omega)$ with values in $[0, 1]$ the estimate

$$I_1 \leqslant \left\| \frac{\mu}{\sqrt{\lambda}}(f + \mathrm{div}\,\mathbf{y} - \lambda v) \right\|_{L^2(\Omega)} \big\| \sqrt{\lambda}(u - v) \big\|_{L^2(\Omega)} + \big\| (1 - \mu)(f + \mathrm{div}\,\mathbf{y} - \lambda v) \big\|_{L^2(\Omega)} C_1 \big\| \nabla(u - v) \big\|_{\mathbf{A}}$$

holds, where C_1 is the minimal constant such that the inequality

$$\|w\|_{L^2(\Omega)} \leqslant C_1 \|\nabla w\|_{\mathbf{A}} \quad \forall w \in V_0 \tag{8}$$

is satisfied. Note that C_1 depends only on α_1, Ω, and Γ_D. If $\partial\Omega = \Gamma_D$, then we have $C_1 \leqslant C_\Omega / \sqrt{\alpha_1}$, where C_Ω is the constant in the Friedrichs inequality which is not difficult to estimate from above.

The terms I_2 and I_3 can be estimated by the Hölder inequality and the trace estimate

$$\|w\|_{L^2(\Gamma_N)} \leqslant C_2 \|\nabla w\|_{\mathbf{A}} \quad \forall w \in V_0. \tag{9}$$

As a result, we arrive at the estimate

$$|||u - v||| \leqslant \left(D(\nabla v, \mathbf{y}) + \int_\Omega \frac{\mu^2}{\lambda} r^2(v, \mathbf{y}) \right)^{1/2} + C_1 \big\| (1 - \mu) r(v, \mathbf{y}) \big\|_{L^2(\Omega)} + C_2 \big\| F - \langle \mathbf{y}, \mathbf{n} \rangle \big\|_{L^2(\Gamma_N)}, \tag{10}$$

where $r(v, \mathbf{y}) := f + \mathrm{div}\,\mathbf{y} - \lambda v$ and $\mathbf{y} \in \mathbf{Q}$.

Two particular forms of (10) arise if we set $\mu = 0$ and $\mu = 1$. They are

$$|||u - v||| \leqslant D^{1/2}(\nabla v, \mathbf{y}) + C_1 \big\| r(v, \mathbf{y}) \big\|_{L^2(\Omega)} + C_2 \big\| F - \langle \mathbf{y}, \mathbf{n} \rangle \big\|_{L^2(\Gamma_N)} \tag{11}$$

and

$$|||u - v||| \leqslant \left(D(\nabla v, \mathbf{y}) + \int_\Omega \frac{r^2(v, \mathbf{y})}{\lambda} \right)^{1/2} + C_2 \big\| F - \langle \mathbf{y}, \mathbf{n} \rangle \big\|_{L^2(\Gamma_N)}. \tag{12}$$

We may also try to find $\mu(x)$ such that the right-hand side of (10) is minimal. To find the optimal function μ which minimizes (10) it is sufficient to consider the first two terms in the right-hand side of (10). We square the sum of these first two terms and use Young's inequality with a positive β. Now, the function μ is selected such that the quantity

$$(1 + \beta) D(\nabla v, \mathbf{y}) + \int_\Omega \left((1 + \beta) \frac{\mu^2}{\lambda} + \left(1 + \frac{1}{\beta} \right) C_1^2 (1 - \mu)^2 \right) r^2(v, \mathbf{y})$$

attains its minimal value. Straightforward calculus results that the minimum of the above expression with respect to μ is as follows:

$$(1 + \beta) D(\nabla v, \mathbf{y}) + \int_\Omega \frac{(\beta + 1) C_1^2 r^2(v, \mathbf{y})}{\beta + \lambda C_1^2}.$$

Thus, we obtain the estimate

$$|||u - v||| \leqslant C_2 \big\| F - \langle \mathbf{y}, \mathbf{n} \rangle \big\|_{L^2(\Gamma_N)} + \sqrt{(1 + \beta) D(\nabla v, \mathbf{y}) + \int_\Omega \frac{(\beta + 1) C_1^2 r^2(v, \mathbf{y})}{\beta + \lambda C_1^2}}$$

Table 1
The differences between the estimates (11)–(14)

$\kappa\backslash\delta$	0.02	0.1	1	10	50
0.1	0.991	0.953	0.914	0.910	0.909
	0.890	1.000	1.000	1.000	1.000
0.5	0.993	0.996	0.745	0.675	0.668
	0.406	0.774	1.000	1.000	1.000
2.0	0.997	0.983	0.745	0.394	0.346
	0.211	0.461	1.000	1.000	1.000
10.0	0.999	0.995	0.914	0.306	0.157
	0.155	0.346	1.000	1.000	1.000

for all $\beta > 0$. To simplify the minimization with respect to $\mathbf{y}$, we again square the right-hand side and apply Young's inequality to obtain finally a quadratic functional in $\mathbf{y}$ which estimates the error

$$|||u - v|||^2 \leqslant \left(1 + \frac{1}{\gamma}\right) C_2^2 \|F - \langle \mathbf{y}, \mathbf{n}\rangle\|^2_{L^2(\Gamma_N)} + (1+\gamma)\left((1+\beta) D(\nabla v, \mathbf{y}) + \int_\Omega \frac{(\beta+1) C_1^2 r^2(v,\mathbf{y})}{\beta + \lambda C_1^2}\right), \tag{13}$$

where β and γ are arbitrary positive numbers. Since $\mathbf{y}$ is at our disposal, we may take it such that $\langle \mathbf{y}, \mathbf{n}\rangle = F$ on Γ_2. Then, (13) converts into

$$|||u - v|||^2 \leqslant (1+\beta) D(\nabla v, \mathbf{y}) + \int_\Omega \frac{(1+\beta) C_1^2}{\beta + \lambda C_1^2} r^2(v, \mathbf{y}). \tag{14}$$

3. Properties of the estimates

Estimates (10)–(14) give different upper bounds for $|||u - v|||$. Their efficiency essentially depends on how accurately v and $\mathbf{y}$ satisfy the relations $r(v, \mathbf{y}) = 0$, $\mathbf{y} = \mathbf{A}\nabla v$ and the Neumann boundary condition.

It is easy to see that the substitution of the flux $p = \mathbf{A}\nabla u$ in place of $\mathbf{y}$ makes the left-hand sides of (12)–(14) equal to the right-hand ones. Indeed, in such a case $r(v, \mathbf{y}) = \lambda(u - v)$, $D(\nabla v, \mathbf{y}) = \|\nabla(u - v)\|^2_{\mathbf{A}}$, the term on Γ_N vanishes and by tending γ and β to zero we see that the right-hand sides of (12) and (13) tend to $|||u - v|||$ and $|||u - v|||^2$, respectively. Thus, the above estimates can give an upper bound as close to the exact error as it is required (for this purpose we should minimize the majorants with respect to $\mathbf{y}$ using a sufficiently rich subspace of $\mathbf{Q}$). Estimate (11) does not posses such a nice property. Moreover, for a constant λ its right-hand side exceed the left-hand one not less than $1 + \lambda\|u - v\|_{L^2(\Omega)}/\|\nabla(u - v)\|_{L^2(\Omega)}$ times, so that for large λ it may lead to a significant overestimation. Estimate (12) has the same drawback as (7): it is sensitive with respect to small λ. If $\lambda(\mathbf{x})$ takes zero values at some subdomain of Ω, then this estimate is inapplicable.

Estimates (13) and (14) are obtained with the help of an 'optimal' function μ. Therefore, they preserve the theoretical sharpness and at the same time help to handle the stability for small λ. These estimates may be especially helpful if λ is large in one part of Ω and almost zero in another. The differences between the estimates (11)–(14) are demonstrated in Table 1. We set $\delta := \sqrt{\lambda} C_1$ and $\kappa := \|r(v, \mathbf{y})\|_{L^2(\Omega)}/\sqrt{D(\nabla v, \mathbf{y})}$.

In the columns, we depict the ratios of the bounds given by the estimates with $\mu = 0$ (upper number) and $\mu = 1$ (lower number) and the bound given by (10) with the optimal μ for different values of δ and κ. It is easy to see that for small λ the estimate with $\mu = 0$ gives an upper bound close to the optimal one, however for large λ its efficiency deteriorates.

The behavior of the estimate with $\mu = 1$ is quite the opposite. For small λ it may be not efficient but for large δ it provides good results. However, the estimate with an optimization with respect to μ always gives the best possible upper bounds.

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