Atti Accademia Nazionale Lincei Classe Scienze Fisiche Matematiche Naturali

Rendiconti Lincei Matematica e Applicazioni

Sergey Repin

Estimates of deviations from exact solutions of initial-boundary value problem for the heat equation

Atti della Accademia Nazionale dei Lincei. Classe di Scienze Fisiche, Matematiche e Naturali. Rendiconti Lincei. Matematica e Applicazioni, Serie 9, Vol. **13** (2002), n.2, p. 121–133.

Accademia Nazionale dei Lincei

<http://www.bdim.eu/item?id=RLIN_2002_9_13_2_121_0>

Atti della Accademia Nazionale dei Lincei. Classe di Scienze Fisiche, Matematiche e Naturali. Rendiconti Lincei. Matematica e Applicazioni, Accademia Nazionale dei Lincei, 2002.

Rend. Mat. Acc. Lincei
s. 9, v. 13:121-133 (2002)

Analisi numerica. — *Estimates of deviations from exact solutions of initial-boundary value problem for the heat equation.* Nota di Sergey Repin, presentata (*) dal Socio O.A. Ladyzhenskaya.

Abstract. — The paper is concerned with deriving functionals that give upper bounds of the difference between the exact solution of the initial-boundary value problem for the heat equation and any admissible function from the functional class naturally associated with this problem. These bounds are given by nonegative functionals called *deviation majorants*, which vanish only if the function and exact solution coincide. The deviation majorants pose a new type of a posteriori estimates that can be used in numerical analysis. Also, the estimates formed by such majorants can be viewed as a certain extension of well known «energy» estimates for solutions of parabolic type problems (see [1]).

Key words: Parabolic equations; Deviations from exact solution; A posteriori estimates.

Riassunto. — *Stime delle deviazioni dalle soluzioni esatte per il problema di Cauchy-Dirichlet relativo all'equazione del calore.* Questa *Nota* è rivolta allo studio di funzionali che stabiliscono limiti superiori per la differenza tra soluzioni esatte del problema di Cauchy-Dirichlet per l'equazione del calore e qualsiasi funzione ammissibile nella classe associata in modo naturale a questo problema. Tali limiti sono espressi da funzionali non negativi, detti *maggioranti di deviazione*, che si annullano solo se la funzione coincide con la soluzione esatta. I maggioranti di deviazione pongono un nuovo tipo di stime a posteriori che possono essere utili nell'analisi numerica. Le stime date da questi maggioranti possono inoltre essere considerate come prolungamenti di *stime dell'energia* ben note per la soluzione di problemi di tipo parabolico (vedi [1]).

0. Introduction

Assume that $u \in V$ is a solution of a certain boundary-value or initial-boundary value problem, V is a proper functional space $v \in V$ is a given function, which is compared with u. Finding computable and effective estimates of the quantity $\|u - v\|$, where $\|\cdot\|$ is the respective norm, presents an important task from many viewpoints.

If v is an approximate solution, then such an estimate can be used for the explicit control of approximation errors and, therefore, presents a special interest for the numerical analysis. By evident reasons, it is called an *a posteriori* error estimate. In last decades, a posteriori estimates were intensively investigated by many authors (see, *e.g.* [2-4] and the references therein). If it is assumed that $v = v_k$, where v_k is the Galerkin approximation found for a subspace $V_k \subset V$, then one can obtain the required estimate by using the Galerkin orthogonality condition. In the literature, this method is known as the «residual method». The general form of the residual type error estimates is as follows

$$\|u - u_k\| \leq M(u_k\,, c_1\,, c_2\,, \ldots\,, c_N\,, \mathcal{D})\,, \tag{0.1}$$

(*) Nella seduta del 10 maggio 2002.

where $\mathcal{D}$ denotes the set of given data (*i.e.* boundary conditions, coefficients etc.) and c_i, $i = 1, 2, \ldots, N$ are the so-called interpolation constants that depend on properties of a special type interpolation operator acting from V to V_k (see [5]). The number N depends on the dimension of V_k and may be rather large. Note that finding the collection of sharp constants c_i presents a special and often not an easy problem (see, *e.g.*, [6]). For parabolic type problems such estimates also include the so-called stability constants that characterize stability of the initial-boundary value problem (see, *e.g.*, [7]). Estimates (0.1) are widely used in computational practice for indication of errors and subsequent mesh refinement. However, there is a restriction on the applicability of these estimates that originates from the method of their deriving: the estimates are valid only for exact solutions of the respective finite dimensional problems.

However, in many cases it is very desirable to have estimates of deviation from exact solution that are valid for any function v from a wide class of admissible functions and does not require an information on how this function was obtained. In other words, the case in point is deriving *functional* type a posteriori estimates. The general form of a functional type a posteriori error estimate is

$$\|u - v\| \leq \mathcal{M}(v, C_\Omega, \mathcal{D}), \qquad \forall v \in V, \tag{0.2}$$

where C_Ω is a constant (or several constants) depending on the domain Ω considered in the problem. Usually, C_Ω is formed by constants in embedding estimates associated with basic spaces of functions defined on Ω. The functional $\mathcal{M}$ is natural to call the *majorant of deviation from exact solution* or shortly the *deviation majorant*. It must be continuous with respect to v, vanish if $v = u$ and be practically computable for any $v \in V$. Evidently, (0.2) should in a certain way generalize the estimate of $\|u\|$ known in the theory of partial differential equations (see, *e.g.*, [1, 8]).

For elliptic boundary-value problems, majorants of type (0.2) were obtained in [9, 10] (and in some other papers cited therein). These papers are focused on convex variational problems and attracts general methods of the functional analysis and calculus of variations for deriving a posteriori error majorants. Their practical performance was investigated in [11]. In [12], they were used for estimating the accuracy of 2-D models in 3-D elasticity theory. In [13], two-sided estimates of deviations from exact solutions of elliptic type problems were obtained. For this purpose, two methods – variational and nonvariational – were used. The variational method is based on the analysis of the variational formulation of problem in question and the nonvariational one – on the analysis of the integral identity. The idea that majorants of deviations can be also obtained by analyzing integral identities was proposed by O. Ladyzhenskaya in the process of discussing the results of the author earlier obtained by variational techniques. In [13], both methods were analyzed and compared. It was stated that for linear elliptic equations they lead to the identical forms of majorants and minorants. In general, areas of applicability of the two methods are different. From one hand, it is clear that the variational method cannot be used if a problem has no variational form. From another hand, there are nonlinear problems having a variational form where using dual variational formulations is very useful (see, *e.g.*, [14]).

In this paper, deviation estimates are obtained for the initial-boundary value problem associated with the heat equation, which presents a typical problem of parabolic type. This problem has no variational form, so that the method is based upon integral identity. It is interesting, that the resulting majorants (see Theorems 2 and 3) are functionals of some new variational problems whose lower bounds give upper bounds of the deviation. They can be used for a posteriori control of errors of approximate solutions obtained by various numerical methods.

Results of the paper can be viewed as a step on the way to solving the general problem on finding computable majorants of deviations for nonvariational problems that was stated as a goal by O. Ladyzhenskaya.

1. Statement of the problem and main results

Let Ω be an open, connected and bounded domain in $\mathbb{R}^n$ with Lipschitz continuous boundary $\partial\Omega$, $Q_T := \Omega \times (0, T)$, and $S_T := \partial\Omega \times [0, T]$. By $\|\cdot\|_{2,\Omega}$ and $\|\cdot\|_{2,Q_T}$ we denote L_2-norms of functions defined on Ω and Q_T, respectively. By $L_{2,1}(Q_T)$, we denote the space of functions $g \in L_1(Q_T)$ such that the quantity $\int_0^T \|g(\cdot, t)\|_{2,\Omega} dt$ is finite. Also, we use the space $W_{2,0}^{\Delta,1}(Q_T)$ that consists of functions $w \in L_2(Q_T)$ having finite norm

$$\|w\|_{2,0}^{\Delta,1} := \int_{Q_T} (w^2 + w_t^2 + |\nabla w|^2 + (\Delta w)^2)\, dx\, dt$$

and vanishing on S_T. Other subsequently used spaces are as follows: the Hilbert spaces

$$W_2^{1,0}(Q_T) := L_2((0, T); W_2^1(\Omega)),$$
$$\overset{\circ}{W}{}_2^{1,0}(Q_T) := L_2((0, T); \overset{\circ}{W}{}_2^1(\Omega)),$$

the space

$$W_{2,0}^1(Q_T) := \{v \in W_2^1(Q_T) \mid v(x, t) = 0 \text{ on } S_T\}$$

and the space $V_2(Q_T)$, which is the Banach space of functions from $W_2^{1,0}(Q_T)$ having finite norm

$$|\!|\!| w |\!|\!|^2 := \operatorname*{vrai\,max}_{t\in(0,T)} \|w(\cdot, t)\|_{2,\Omega}^2 + \|\nabla w\|_{2,Q_T}^2 .$$

Here, and later on the symbol := means «equals by definition». The space

$$V_2^{1,0}(Q_T) = C([0, T]; L_2(\Omega)) \cap W_2^{1,0}(Q_T)$$

is a subspace of $V_2(Q_T)$. For all $t \in [0, T]$, elements of this space have traces from $L_2(\Omega)$ on cross-sections of Q_T that continuously change with respect to $t \in [0, T]$. By $\overset{\circ}{V}{}_2^{1,0}(Q_T)$ we denote another subspace of $V_2(Q_T)$, which is the intersection of $V_2^{1,0}(Q_T)$ and $\overset{\circ}{W}{}_2^{1,0}(Q_T)$.

In addition, for elements of the space $V_2^{1,0}(Q_T)$ we define the quantity

$$[w]_{(\gamma,\delta)}^2 := \gamma\|w(\cdot, T)\|_{2,\Omega}^2 + \delta\|\nabla w\|_{2,Q_T}^2 .$$

The energy norm $\|\!|\cdot|\!\|$ and the above quantity will be used as a measure of the difference between the exact solution and its approximation.

Consider the classical initial-boundary value problem for the heat equation: find $u(x, t)$ such that

$$\mathcal{L}u = f \qquad \text{in } Q_T \tag{1.1}$$

$$u(x, 0) = \varphi(x), \quad x \in \Omega \tag{1.2}$$

$$u(x, t) = 0, \qquad (x, t) \in S_T, \tag{1.3}$$

where

$$\mathcal{L}u := u_t - \Delta u. \tag{1.4}$$

In the framework of the well-known existence theory for the parabolic type problems (see, *e.g.*, [1]), the function $u \in \overset{\circ}{V}{}_2^{1,0}(Q_T)$ is called a (generalized) solution of (1.1)-(1.3) if it satisfies the following integral identity:

$$\begin{aligned} \int\limits_{Q_T} \nabla u \cdot \nabla \eta \, dx\, dt - \int\limits_{Q_T} u\eta_t \, dx\, dt + \int\limits_{\Omega} (u(x, T)\eta(x, T) - u(x, 0)\eta(x, 0))\, dx = \\ = \int\limits_{Q_T} f\eta \, dx\, dt \qquad \forall\, \eta \in W^1_{2,0}(Q_T). \end{aligned} \tag{1.5}$$

We recall the classical solvability results (see, *e.g.*, [1, 8]) for this problem.

THEOREM 1. *Let Ω be a bounded connected domain with Lipschitz continuous boundary $\partial\Omega$.*

(*i*) *Let $f \in L_2(Q_T)$ and $\phi(x) \in \overset{\circ}{W}{}^1_2(\Omega)$. Then problem* (1.1)-(1.3) *is uniquely solvable in the space $W^{\Delta,1}_{2,0}(Q_T)$.*

(*ii*) *If $f \in L_{2,1}(Q_T)$ and $\phi \in L_2(\Omega)$ then u belongs to the class $\overset{\circ}{V}{}_2^{1,0}(Q_T)$.*

Assume that the conditions (*i*) of Theorem 1 hold, so that the solution u exists in both spaces $W^{\Delta,1}_{2,0}(Q_T)$ and $\overset{\circ}{V}{}_2^{1,0}(Q_T)$. Let $v \in W^1_{2,0}(Q_T)$ be a given function. In particular, v can be an approximation of u obtained by a certain numerical procedure. We are interested in deriving an upper bound of the deviation $\widetilde{u} := u - v$ evaluated in the norm $\|\!|\cdot|\!\|$ (or in terms of the quantity $[\cdot]_{(\gamma,\delta)}$). Hereafter, such an upper bound is called the *deviation majorant*. The majorants derived are presented by Theorems 2 and 3 below. Theorem 3 shows that the majorant is equivalent to a cerain measure of the deviation.

2. First form of the deviation majorant

2.1. *The energy-balance equation for deviations.*

Assume that

$$f \in L_2(Q_T), \quad \phi \in \overset{\circ}{W}{}^1_2(\Omega). \tag{2.1}$$

In this case, $u \in W^{\Delta,1}_{2,0}(Q_T)$. Let the function v compared with u be such that

$$v \in W^{1}_{2,0}(Q_T). \tag{2.2}$$

From (1.5) we obtain

$$\int\limits_{Q_T} \nabla \widetilde{u} \cdot \nabla \eta \, dx\, dt - \int\limits_{Q_T} \widetilde{u}\eta_t \, dx\, dt + \int\limits_{\Omega} (\widetilde{u}(x, T)\eta(x, T) - \widetilde{u}(x, 0)\eta(x, 0))\, dx =$$
$$= \int\limits_{Q_T} (f\eta - \nabla v \cdot \nabla \eta - v_t \eta)\, dx\, dt \qquad \forall\, \eta \in W^{1}_{2,0}(Q_T).$$

Set $\eta = \widetilde{u}$ and note that

$$-\int\limits_{Q_T} \widetilde{u}\widetilde{u}_t \, dx\, dt + \int\limits_{\Omega} |\, \widetilde{u}(x, T)\,|^2 \, dx - \int\limits_{\Omega} |\, \widetilde{u}(x, 0)\,|^2 \, dx = \frac{1}{2}\|\widetilde{u}(\cdot\,, T)\|^2_{2,\Omega} - \frac{1}{2}\|\widetilde{u}(\cdot\,, 0)\|^2_{2,\Omega}.$$

This gives the integral relation

$$\|\nabla \widetilde{u}\|^2_{2,Q_T} + \frac{1}{2}\|\widetilde{u}(\cdot\,, T)\|^2_{2,\Omega} = \int\limits_{Q_T} (f\widetilde{u} - \nabla v \cdot \nabla \widetilde{u} - v_t \widetilde{u})\, dxdt + \frac{1}{2}\|\widetilde{u}(\cdot\,, 0)\|^2_{2,\Omega} \tag{2.3}$$

that presents the energy-balance in terms of deviations. The relation (2.3) can be considered as a generalization of the well-known *energy-balance equation* for the heat equation (see, *e.g.* [8]). It is easy to see that the classical energy-balance equation follows from (2.3) if set $v \equiv 0$. Subsequently, we use (2.3) as a starting point for deriving majorants of $v - u$.

2.2. *General estimate.*

Introduce a new vector-valued function $y^*(x, t) \in Y^*(Q_T)$, where

$$Y^*(Q_T) := \left\{ y^*(x, t) = \{y^*_i(x, t)\} \mid y^*_i \in L_2(Q_T)\,,\ i = 1\,, 2\,, \dots\,, n \right\}$$

and rearrange (2.3) as follows:

$$\begin{aligned} &\|\nabla \widetilde{u}\|^2_{Q_T} + \frac{1}{2}\|\widetilde{u}(\cdot\,, T)\|^2_{2,\Omega} - \frac{1}{2}\|\widetilde{u}(\cdot\,, 0)\|^2_{2,\Omega} = \\ &= \int\limits_{Q_T} (f\widetilde{u} - v_t \widetilde{u} - y^* \cdot \nabla \widetilde{u})\, dx\, dt + \int\limits_{Q_T} (y^* - \nabla v) \cdot \nabla \widetilde{u} \, dx\, dt. \end{aligned} \tag{2.4}$$

For almost all $t \in [0\,, T]$, we can define the linear functional

$$\mathcal{F}_t(\,\cdot\,; v\,, y^*) : \overset{\circ}{W}{}^1_2(\Omega) \to \mathbb{R}$$

by the relation

$$\mathcal{F}_t(\eta; v\,, y^*) := \int\limits_{\Omega} \left(f\eta - v_t \eta - y^* \cdot \nabla \eta \right) dx.$$

The quantity

$$[\![\mathcal{F}_t(v, y^*)]\!]_\Omega := \sup_{\substack{\eta\in \overset{\circ}{W}{}^1_2(\Omega)\\ \eta\neq 0}} \frac{\int\limits_\Omega \left(f\eta - v_t\eta - y^*\cdot\nabla\eta\right)dx}{\|\nabla\eta\|_{2,\Omega}}$$

is evidently finite for almost all $t \in [0, T]$, and can be viewed as the norm of this functional. Moreover,

$$[\![\mathcal{F}_t(v, y^*)]\!]_\Omega \leq C_\Omega \left(\|f(\cdot, t)\|_{2,\Omega} + \|v_t(\cdot, t)\|_{2,\Omega}\right) + \|y^*(\cdot, t)\|_{2,\Omega},$$

where C_Ω is a constant in the Friedrichs-Poincaré inequality. Therefore, the quantity $[\![\mathcal{F}_t(v, y^*)]\!]_\Omega$ is square integrable on $(0, T)$.

Now, we rewrite (2.4) as follows:

$$\|\nabla\widetilde{u}\|^2_{Q_T} + \frac{1}{2}\|\widetilde{u}(\cdot, T)\|^2_{2,\Omega} - \frac{1}{2}\|\widetilde{u}(\cdot, 0)\|^2_{2,\Omega} = \int\limits_0^T \mathcal{F}_t(\widetilde{u}; v, y^*)\,dt + \int\limits_{Q_T}(y^* - \nabla v)\cdot\nabla\widetilde{u}\,dx\,dt. \tag{2.5}$$

Let δ and μ be two given constants such that

$$0 < \delta \leq 2, \qquad 0 < \mu < 1. \tag{2.6}$$

Define the set

$$\mathfrak{B}^\mu(0, T) := \{\beta(t) \in L_\infty(0, T) \mid \beta(t) \geq \mu \text{ for almost all } t \in (0, T)\}.$$

Take two scalar-valued functions $\alpha_1(t)$ and $\alpha_2(t)$, such that

$$\alpha_1(t) = \frac{1}{\delta}\left(1 + \frac{1}{\beta(t)}\right), \qquad \alpha_2(t) = \frac{1}{\delta}\left(1 + \beta(t)\right). \tag{2.7}$$

In virtue of the Young-Fenchel inequality, we have

$$\int\limits_0^T \mathcal{F}_t(\widetilde{u}, v, y^*)\,dt \leq \int\limits_0^T \left(\frac{\alpha_1(t)}{2}[\![\mathcal{F}_t(v, y^*)]\!]^2_\Omega + \frac{1}{2\alpha_1(t)}\|\nabla(\widetilde{u})\|^2_{2,\Omega}\right)dt$$

$$\int\limits_{Q_T}(\nabla v - y^*)\cdot\nabla\widetilde{u}\,dx\,dt \leq \int\limits_0^T \left(\frac{\alpha_2(t)}{2}\|\nabla v - y^*\|^2_{2,\Omega} + \frac{1}{2\alpha_2(t)}\|\nabla(\widetilde{u})\|^2_{2,\Omega}\right)dt.$$

Note that $\alpha_1(t)$ and $\alpha_2(t)$ satisfy the relation

$$\frac{1}{\alpha_1(t)} + \frac{1}{\alpha_2(t)} = \delta.$$

Now, (2.5) and above inequalities imply the estimate

$$(2-\delta)\|\nabla\widetilde{u}\|^2_{2,Q_T} + \|\widetilde{u}(\cdot, T)\|^2_{2,\Omega} \leq \mathcal{M}_\delta(v, y^*, \beta), \tag{2.8}$$

whose right-hand side is the functional

$$\mathcal{M}_\delta(v, y^*, \beta) := \|v(\cdot, 0) - \phi\|^2_{2,\Omega} + \tag{2.9}$$
$$+ \frac{1}{\delta} \int_0^T \left((1+\beta)\|y^* - \nabla v\|^2_{2,\Omega} + \left(1 + \frac{1}{\beta}\right) [\![\mathcal{F}_t(v, y^*)]\!]^2_\Omega \right) dt\,.$$

This estimate is valid for any $\beta(t) \in \mathfrak{B}^\mu(0, T)$ and $\delta \in (0, 2]$.

It is not difficult to see that $\mathcal{M}_\delta(v, y^*, \beta)$ vanishes if and only if

$$\mathcal{F}_t(\cdot\,; v, y^*) = 0 \quad \text{for almost all} \quad t \in (0, T)\,,$$
$$y^* = \nabla v \qquad \text{a.e. in} \qquad Q_T\,,$$
$$v(0, x) = \phi(x) \quad \text{for a.e.} \quad x \in \Omega.$$

Such a situation arises if v coincides with generalized solution of problem (1.1)-(1.3) and, therefore, $\widetilde{u} = 0$ (so that (2.8) holds as equality).

2.3. *Majorants of the deviation.*

The functional $\mathcal{M}_\delta(v, y^*, \beta)$ involve only quadratic terms. It gives upper bounds for various measures of the deviation $\widetilde{u}$. For example, if set $\delta = 1$ and $\delta = 2$, then (2.8) respectively implies the following two estimates:

$$\|\nabla \widetilde{u}\|^2_{2,Q_T} \le \mathcal{M}_1(v, y^*, \beta)\,, \tag{2.10}$$

$$\max_{t\in[0,T]} \|\widetilde{u}(\cdot, t)\|^2_{2,\Omega} \le \mathcal{M}_2(v, y^*, \beta)\,, \tag{2.11}$$

where the functions $\beta(t) \in \mathfrak{B}^\mu(0, T)$ and $y^*(x, t) \in Y^*(Q_T)$ may be taken arbitrary.

To make these estimates computationally attractive, we should replace the norm of $\mathcal{F}_t$ by an explicitly computable quantity. This can be done if take y^* in a certain subspace of $Y^*(Q_T)$. Namely, assume that

$$y^* \in Y^*_{\rm div}(Q_T) := \{y^* \in Y^*(Q_T) \mid {\rm div} y^* \in L_2(Q_T)\}. \tag{2.12}$$

Then, for almost all $t \in (0, T)$,

$$\int_\Omega \widetilde{u}(x, t){\rm div} y^*(x, t)\, dx = -\int_\Omega y^*(x, t) \cdot \nabla \widetilde{u}(x, t)\, dx$$

and we have

$$[\![\mathcal{F}_t(v, y^*)]\!]_\Omega \le C_\Omega \int_\Omega |f - v_t + {\rm div} y^*|^2\, dx. \tag{2.13}$$

Therefore, the functional

$$\widehat{\mathcal{M}}_\delta(v\,,\,y^*\,,\beta) := \int\limits_\Omega |v(x\,,0) - \phi(x)|^2\,dx + \tag{2.14}$$
$$+\frac{1}{\delta}\int\limits_{Q_T}\left((1+\beta)|y^* - \nabla v|^2 + C_\Omega^2\left(1+\frac{1}{\beta}\right)|f - v_t + \operatorname{div} y^*|^2\right) dxdt$$

gives an upper bound of $\mathcal{M}_\delta(v\,,\,y^*\,,\beta)$ if $y^* \in Y^*_{\mathrm{div}}(\Omega)$.

THEOREM 2. *Let the conditions* (2.1) *and* (2.2) *be satisfied. Then*
(*i*) *For any* $\beta \in \mathfrak{B}^\mu(0\,,T)$ *and* $y^* \in Y^*_{\mathrm{div}}(Q_T)$ *the estimates*

$$\|\nabla\widetilde{u}\|^2_{2\,,Q_T} \le \widehat{\mathcal{M}}_1(v\,,\,y^*\,,\beta)\,, \tag{2.15}$$

$$\max_{t\in[0\,,T]}\|\widetilde{u}(\cdot\,,t)\|^2_{2,\Omega} \le \widehat{\mathcal{M}}_2(v\,,\,y^*\,,\beta) \tag{2.16}$$

hold.
(*ii*) *For any* $\delta \in (0\,,2]$ *and* $\beta \in \mathfrak{B}^\mu(0\,,T)$ *the variational problem*

$$\inf_{\substack{v\in W^1_{2,0}(Q_T)\\ y^*\in Y^*_{\mathrm{div}}(Q_T)}} \widehat{\mathcal{M}}_\delta(v\,,\,y^*\,,\beta) \tag{2.17}$$

has a solution. The exact lower bound of this problem is equal to zero and is attained if and only if $v = u$ *and* $y^* = \nabla u$.

PROOF. (*i*) Estimates (2.15) and (2.16) follow from (2.10) and (2.11).
(*ii*) Existence of the pair $(v\,,y^*) \in W^1_{2,0}(Q_T) \times Y^*_{\mathrm{div}}(Q_T)$ minimizing the functional $\widehat{\mathcal{M}}_\delta(v\,,\,y^*\,,\beta)$ is proved straightforwardly. Really, set $v = u$ and $y^* = \nabla u$. Since $u \in W^{\Delta\,,1}_{2\,,1}$, we see that $\operatorname{div}\nabla u \in L_2(Q_T)$ and, therefore, $y^* \in Y^*_{\mathrm{div}}(Q_T)$. In this case, $\mathcal{M}_\delta(v\,,\,y^*\,,\beta) = 0$, so that the exact lower bound is attained.

Assume that $\mathcal{M}_\delta(v\,,\,y^*\,,\beta) = 0$. This means that the function $v(x\,,t)$ satisfies the initial and boundary conditions and, also, that for almost all $(x\,,t) \in Q_T$ the relations

$$\nabla v \;=\; y^* \in Y^*_{\mathrm{div}}(Q_T)\,, \tag{2.18}$$

$$\operatorname{div} y^* - v_t + f \;=\; 0 \tag{2.19}$$

hold. They mean that v is the exact solution of problem considered. Indeed, (2.19) implies

$$\int\limits_{Q_T}(v\eta_t - y^*\cdot\nabla\eta)\,dx\,dt - \int\limits_\Omega v(x\,,T)\eta(x\,,T)\,dx + \int\limits_\Omega v(x\,,0)\eta(x\,,0)\,dx +$$
$$+\int\limits_{Q_T} f\eta\,dx\,dt = 0 \qquad \forall\,\eta \in W^1_{2\,,0}(Q_T).$$

In view of (2.18), this relation is equivalent to the integral identity (1.5). Hence, we conclude that $v = u$. □

COROLLARY 1. *By* (2.15) *and* (2.16) *we can estimate the deviation* $\widetilde{u}$ *in the «energy» norm as follows*

$$\|\widetilde{u}\|^2 \leq \widehat{\mathcal{M}}_1(v, y^*, \beta) + \widehat{\mathcal{M}}_2(v, y^*, \beta). \tag{2.20}$$

Also, by (2.8) *we obtain*

$$[\widetilde{u}]^2_{(1,\delta')} \leq \widehat{\mathcal{M}}_\delta(v, y^*, \beta), \quad \delta' = 2 - \delta. \tag{2.21}$$

REMARK 1. The majorant $\widehat{\mathcal{M}}_\delta(v, y^*, \beta)$ is defined if $v \in W^1_{2,0}(Q_T)$, $f \in L_2(Q_T)$, $v(x, 0) \in L_2(\Omega)$, and $\phi(x) \in L_2(\Omega)$. It is possible to extend estimates (2.15), (2.16), (2.20), and (2.21) to a wider set of functions by arguments close to those used in [8, Chapter 2, §2].

REMARK 2. The majorants $\mathcal{M}_\delta$ and $\widehat{\mathcal{M}}_\delta$ yield various estimates of type (0.2). For example, take $y^* = \nabla v$ in $\mathcal{M}_\delta$ and $y^* = \mathcal{R}\nabla v$ in $\widehat{\mathcal{M}}_\delta$, where $\mathcal{R} : Y^*(Q_T) \to Y^*_{\text{div}}(Q_T)$ is a smoothing operator (computationally inexpensive operators of such a type are known in the numerical analysis). Then the quantity $\mathcal{M}_\delta(v, \nabla v, \beta)$ or $\widehat{\mathcal{M}}_\delta(v, \mathcal{R}\nabla v, \beta)$ form the right-hand side of (0.2) provided that δ and β lies in the admissible sets.

3. SECOND FORM OF THE DEVIATION MAJORANT

3.1. *General estimate.*

Now we reform the right-hand side of (2.4) by other means. Present the right-hand side of this relation as sum of three terms, which are

$$I_1 = \int_{Q_T} \left(f\widetilde{u} - v_t\widetilde{u} - w_t\widetilde{u} - y^* \cdot \nabla\widetilde{u}\right) dxdt,$$

$$I_2 = \int_{Q_T} \left(y^* - \nabla v + \nabla w\right) \cdot \nabla\widetilde{u}\, dxdt,$$

$$I_3 = \int_{Q_T} \left(w_t\widetilde{u} - \nabla w \cdot \nabla\widetilde{u}\right) dxdt.$$

Here, $y^* \in Y^*(Q_T)$ and $w \in W^1_{2,0}(Q_T)$ are arbitrary functions (later we discuss how to chose these functions in order to obtain rigorous estimates).

For almost all $t \in (0, T)$, we define the linear functional

$$\mathcal{F}_t(\,\cdot\,; v, w, y^*) : \overset{\circ}{W}{}^1_2(\Omega) \to \mathbb{R}$$

by the relation

$$\mathcal{F}_t(\eta; v, w, y^*) := \int_\Omega \left(f\eta - v_t\eta - w_t\eta - y^* \cdot \nabla\eta\right) dx.$$

It is easy to see that the quantity

$$[\![\mathcal{F}_t(v, w, y^*)]\!]_\Omega := \sup_{\substack{\eta \in \overset{\circ}{W}{}^1_2(\Omega),\\ \eta \neq 0}} \frac{\int\limits_\Omega \left(f\eta - v_t\eta - w_t\eta - y^* \cdot \nabla\eta\right) dx}{\|\nabla\eta\|_{2,\Omega}}$$

is finite for almost all $t \in [0, T]$ and can be considered as a norm of this functional.

The terms I_1 and I_2 are estimated by the same method as has been used in the previous section. In view of (1.5), we have

$$I_3 = L(v, w) + \int\limits_\Omega (\widetilde{u}(x, T)w(x, T) - \widetilde{u}(x, 0)w(x, 0))\, dx,$$

where

$$L(v, w) := \int\limits_{Q_T} \left(\nabla v \cdot \nabla w + v_t w - fw\right)\, dx\, dt\,.$$

By following the lines of the previous section, we deduce the general estimate

$$\begin{aligned}(2-\delta)\|\nabla\widetilde{u}\|^2_{Q_T} + \left(1 - \frac{1}{\gamma}\right)\|\widetilde{u}(\cdot, T)\|^2_{2,\Omega} \le \gamma\|w(\cdot, T)\|^2_{2,\Omega} + \\ + \frac{1}{\delta}\int\limits_0^T \left((1+\beta)\|y^* - \nabla v + \nabla w\|^2_{2,\Omega} + \left(1 + \frac{1}{\beta}\right)[\![\mathcal{F}_t(v, w, y^*)]\!]^2_\Omega\right) dt + \\ + 2L(v, w) + \int\limits_\Omega \left(|\phi(x) - v(x, 0)|^2 - 2w(x, 0)(\phi(x) - v(x, 0))\right) dx,\end{aligned} \tag{3.1}$$

which is valid for any

$$w(x, t) \in W^1_{2,0}(Q_T)\,, \tag{3.2}$$

$$y^* \in Y^*(Q_T)\,, \tag{3.3}$$

$$\beta(t) \in \mathfrak{B}^\mu(0, T)\,, \tag{3.4}$$

$$\gamma \ge 1\,, \quad \delta \in (0, 2]. \tag{3.5}$$

As in the previous section, we find a majorant of the right-hand side of this estimate provided that

$$y^* \in Y^*_{\mathrm{div}}(Q_T). \tag{3.6}$$

This majorant is given by the functional

$$\begin{aligned}\widehat{\mathcal{M}}_{\gamma\delta}(v, w, y^*, \beta) := \gamma\|w(\cdot, T)\|^2_{2,\Omega} + \\ + \frac{1}{\delta}\int\limits_0^T \left((1+\beta)\|y^* - \nabla v + \nabla w\|^2_{2,\Omega} + \frac{C^2_\Omega(1+\beta)}{\beta}\|f - v_t - w_t + \mathrm{div} y^*\|^2_{2,\Omega}\right) dt + \\ + 2L(v, w) + \int\limits_\Omega \left(|\phi(x) - v(x, 0)|^2 - 2w(x, 0)(\phi(x) - v(x, 0))\right) dx\,.\end{aligned}$$

The theorem below states important properties of the quadratic functional $\widehat{\mathcal{M}}_{\gamma\delta}(v,w,y^*,\beta)$.

THEOREM 3. *Let the conditions* (2.1) , (2.2), *and* (3.5) *be satisfied. Then*

(*i*) *For any* β, w *and* y^* *subject to the conditions* (3.2) , (3.4), *and* (3.6) *the estimates*

$$\|\nabla\widetilde{u}\|^2_{2,Q_T} \leq \widehat{\mathcal{M}}_1(v,\ w,y^*,\beta)\,, \tag{3.7}$$

$$\max_{t\in[0,T]}\|\widetilde{u}(\cdot\,,t)\|^2_{2,\Omega} \leq \widehat{\mathcal{M}}_2(v,\ w,y^*,\beta) \tag{3.8}$$

hold.

(*ii*) *For any and* $\beta \in \mathfrak{B}^{\mu}(0\,,T)$, *the variational problem*

$$\inf_{\substack{v\in W^1_{2,0}(Q_T)\\ w\in W^1_{2,0}(Q_T)\\ y^*\in Y^*_{\rm div}(Q_T)}} \widehat{\mathcal{M}}_{\gamma\delta}(v,\ w,y^*,\beta) \tag{3.9}$$

has a solution. The exact lower bound of this problem is equal to zero and is attained if $v = u$, $w = 0$ *and* $y^* = \nabla u$.

PROOF. Estimates (3.7) and (3.8) directly follow from (3.1).

Since $\widehat{\mathcal{M}}_{\gamma\delta}(v,\ w,y^*,\beta) > 0$ and $\widehat{\mathcal{M}}_{\gamma\delta}(u;\,0\,,\nabla u\,,\beta) = 0$, we see that $(u\,,0\,,\nabla u)$ is a minimizer. □

3.2. *Equivalence of the deviation and majorant.*

Let us now focus on another property of the majorant. Assume that v is a given approximation of u. From (3.1), we find that the estimate

$$[\widetilde{u}]^2_{(\gamma',\delta')} \leq \widehat{\mathcal{M}}_{\gamma\delta}(v,\ w,y^*,\beta)\,, \quad \gamma' = 1 - \frac{1}{\gamma}\,,\ \delta' = 2-\delta \tag{3.10}$$

holds for any $\beta \in \mathfrak{B}^{\mu}(0\,,T)$, $w \in W^1_{2,0}(Q_T)$, and $y^* \in Y^*_{\rm div}(Q_T)$. However, to obtain a rigorous upper bound one should minimize the majorant over the above defined sets. This procedure gives the quantity

$$\widehat{\mathcal{M}}^{\oplus}_{\gamma\delta}(v) := \inf_{\substack{\beta\in\mathfrak{B}^{\mu}(0,T)\\ w\in W^1_{2,0}(Q_T)\\ y^*\in Y^*_{\rm div}(Q_T)}} \widehat{\mathcal{M}}_{\gamma\delta}(v,\ w,y^*,\beta)\,,$$

which is the desired upper bound. We are aimed to show that this bound is realistic, *i.e.* it does not lead to large overestimation of the actual value of the deviation. Since

$u \in W^{\Delta,1}_{2,0}(Q_T)$, we may set $y^* = \nabla u \in Y^*_{\rm div}(Q_T)$. Then

$$\mathcal{M}^{\oplus}_{\gamma\delta}(v) \leq \widehat{\mathcal{M}}_{\gamma\delta}(v,\ u-v, \nabla u, \beta) = \frac{4}{\delta}\int\limits_0^T (1+\beta)\|\nabla\widetilde{u}\|^2_{2,\Omega}\,dt +$$

$$+\gamma\|\widetilde{u}(\cdot\,,T)\|^2_{2,\Omega} - 2\int\limits_{Q_T}(|\nabla\widetilde{u}|^2 + \widetilde{u}_t\widetilde{u})dxdt +$$

$$+2\int\limits_{Q_T}(\nabla u\cdot\nabla(u-v) + u_t(u-v) - f(u-v))dxdt +$$

$$-\|\phi - v(\cdot\,,0)\|^2_{2,\Omega} = \int\limits_0^T\left(4\frac{1+\beta}{\delta} - 2\right)\|\nabla\widetilde{u}\|^2_{2,\Omega}\,dt +$$

$$+(\gamma-1)\|\widetilde{u}(\cdot\,,T)\|^2_{2,\Omega} + \|\widetilde{u}(\cdot\,,0)\|^2_{2,\Omega} - \|\phi - v(\cdot\,,0)\|^2_{2,\Omega}.$$

Hence, we obtain

$$\widehat{\mathcal{M}}^{\oplus}_{\gamma\delta}(v) \leq \frac{2}{\delta}(\delta' + 2\mu)\|\nabla\widetilde{u}\|^2_{2,Q_T} + (\gamma-1)\|\widetilde{u}(\cdot\,,T)\|^2_{2,\Omega}.$$

Thus, for any $v \in W^1_{2,0}(Q_T)$,

$$[u-v]^2_{(\gamma',\delta')} \leq \widehat{\mathcal{M}}^{\oplus}_{\gamma\delta}(v) \leq [u-v]^2_{(\gamma'',\delta'')}\,, \tag{3.11}$$

where $\delta'' = \frac{2}{\delta}(\delta' + 2\mu)$ and $\gamma'' = \gamma - 1$. This relation means that the quantity $\mathcal{M}^{\oplus}_{\gamma\delta}(v)$ is equivalent to a certain measure of deviation $\widetilde{u}$. In particular, if set $\delta = 1$ and $\gamma = 1$, then this double inequality comes in the form

$$\|\nabla(u-v)\|^2_{2,Q_T} \leq \widehat{\mathcal{M}}^{\oplus}_{1,1}(v) \leq 2(1+2\mu)\|\nabla(u-v)\|^2_{2,Q_T}\,,$$

which shows that $\widehat{\mathcal{M}}^{\oplus}_{1,1}(v)$ is equivalent to a certain measure of deviation.

3.3. *On the justification of the method of Runge.*

Finally, we briefly comment on possible applications of the estimates derived. In the numerical analysis, it is widely used a heuristic method originally proposed for ordinary differential equations by C. Runge. In this method, the accuracy of an approximate solution obtained on the mesh with mesh-size H is controlled by comparing it with another solution obtained on a finer mesh h (*e.g.* $h = H/2$). Subsequently, such a heuristic approach was often applied to partial differential equations solved by finite difference or finite element methods. The estimates obtained in this paper provide a quantitative basis for the method of Runge. Really, let $U_{\mathcal{T}H}$ be an approximate solution of the heat equation computed on the mesh with mesh-size $\mathcal{T}$ for time variable and H for spatial variables. Let $u_{\tau h}$ be another approximate solution computed on a finer mesh $(\tau\,, h)$. Then, estimates (2.15), (2.16), (2.20), (2.21), (3.7), (3.8), (3.10), and (3.11) can be directly used for measuring computational errors. For example, by applying the estimates (2.21) and (3.10), we obtain

$$[u - U_{\mathcal{T}H}]^2_{(1,\delta')} \leq \widehat{\mathcal{M}}_\delta(U_{\mathcal{T}H}, \mathcal{R}(\nabla u_{\tau h}), \beta), \tag{3.12}$$

$$[u - U_{\mathcal{T}H}]^2_{(\gamma',\delta')} \leq \widehat{\mathcal{M}}_{\gamma\delta}(U_{\mathcal{T}H}, u_{\tau h} - U_{\mathcal{T}H}, \mathcal{R}(\nabla u_{\tau h}), \beta), \tag{3.13}$$

where $\mathcal{R}$ is an appropriate smoothing operator mapping vector-valued functions to $Y^*_{\rm div}(Q_T)$. To make these estimates sharper one may minimize their right-hand sides with respect to $\beta \in \mathfrak{B}^\mu(0, T)$ by using a suitable minimization procedure.

Acknowledgements

The author expresses deep gratitude to O. Ladyzhenskaya for advises and attention to his work.

References

[1] O.A. Ladyzhenskaya - V.A. Solonnikov - N.N. Uraltseva, *Linear and Quasilinear Equations of Parabolic Type*. Nauka, Moscow 1967.

[2] M. Ainthworth - J.T. Oden, *A posteriori error estimation in finite element analysis*. Wiley, 2000.

[3] I. Babuška - T. Strouboulis, *The finite element method and its reliability*. Clarendon Press, Oxford 2001.

[4] R. Verfürth, *A review of a posteriori error estimation and adaptive mesh-refinement techniques*. Wiley, Teubner, New York 1996.

[5] Ph. Clément, *Approximations by finite element functions using local regularization*. RAIRO Anal. Numér., 9, 1975, R-2, 77-84.

[6] C. Carstensen - S.A. Funcen, *Costants in Clement's-interpolation error and residual based a posteriori error estimates in finite element methods*. East-West J. Numer. Anal., 8, 2000, n. 3, 153-175.

[7] C. Johnson - A. Szepessy, *Adaptive finite element methods for conservation laws based on a posteriori error estimates*. Commun. Pure and Appl. Math., vol. XLVIII, 1995, 199-234.

[8] O.A. Ladyzhenskaya, *The boundary value problems of mathematical physics*. Springer, New York 1985.

[9] S. Repin, *A posteriori error estimation for nonlinear variational problems by duality theory*. Zapiski Nauchnych Seminarov POMI, 243, 1997, 201-214.

[10] S. Repin, *A posteriori error estimation for variational problems with uniformly convex functionals*. Math. Comput., v. 69, 230, 2000, 481-500.

[11] S. Repin, *A unified approach to a posteriori error estimation based on duality error majorants*. Mathematics and Computers in Simulation, 50, 1999, 313-329.

[12] S. Repin, *Estimates of the accuracy of two-dimensional models in elasticity theory*. Probl. Mat. Anal., v. 22, 2001, 178-196 (in Russian).

[13] S. Repin, *Two-sided estimates of deviations from exact solutions of uniformly elliptic equations*. Trudi St.-Petersburg Mathematickal Society, v. 9, 2001, 148-179.

[14] S. Repin, *A posteriori estimates of the accuracy of variational methods for problems with nonconvex functionals*. Algebra i Analiz, 11, 1999, n. 4, 151-182 (in Russian, translated in St.-Petersburg Mathematical Journal, v. 11, n. 4, 2000).

Pervenuta il 4 marzo 2002,
in forma definitiva il 29 aprile 2002.

V.A. Steklov Institute of Mathematics in St.-Petersburg
Fontanka, 27 - 191011 Sankt-Petersburg (Russia)
repin@pdmi.ras.ru