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Error identities for parabolic equations with monotone spatial operators

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Abstract.

The article studies integral relations (error identities) that characterise distances between exact solutions of nonlinear evolutionary problems and functions considered as approximations. The restrictions imposed on such a function are minimal and actually come down to the condition that it belongs to the same functional class as the generalized solution of the problem under consideration. Functional identities of this type reflect the most general relations between deviations from exact solutions of parabolic initial boundary value problems and those data that can be observed in a numerical experiment. The identities contain no mesh dependent constants and are valid for any function in the admissible (energy) class regardless of the method by which it was constructed. Therefore, they can serve as basic tools for deriving fully reliable a posteriori estimates of approximation errors as well as for analysis of modeling errors. The corresponding examples are discussed in the paper.

Keywords.

parabolic equations, monotone operators, a posteriori error identities, a posteriori estimates of the functional type

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1 Introduction

Traditionally, accuracy of approximate solutions is studied by error estimates derived for certain error norms. A priori estimates operate with sequences of approximations and examine the question in an asymptotic sense, assuming that all calculations in solving finite-dimensional problems are performed absolutely exactly. A posteriori estimates follow another concept. They deal with a particular numerical solution and may be focused on estimation of guaranteed error bounds or on generation of suitable error indicators to be further used in mesh adaptive procedures. There is a fairly large freedom in choosing a measure by which the accuracy of the approximate solution is estimated. Some estimates operate with global (energy) norms while others use specially selected (goal oriented) quantities or may be aimed at comparing local errors in different areas. The choice of a measure depends on many factors and tasks posed by the researcher. However, there is a class of error measures that are defined by the problem itself. They emerge in the so–called error identities. Such an identity is derived by purely functional methods without using special features of approximations and exact solutions (e.g., Galerkin orthogonality or extra regularity). It holds for any function compared with the exact solution provided that the function belongs to an admissible functional class. A practically useful identity must satisfy a number of additional requirements.

Consider an abstract boundary value problem $\mathcal{A}u = f$ generated by a continuous bounded operator $\mathcal{A} : V \to V^*$ where V is a reflexive Banach space and V^* is its dual. Let $v \in V$ be an approximation compared with the exact solution u. The problem of controlling the accuracy of approximate solutions would be completely solved if we have the identity

$$\boldsymbol{\mu}(v, u) = \mathbb{F}(v, \mathcal{D}) \qquad \forall v \in V, \tag{1.1}$$

where $\boldsymbol{\mu}(v, u)$ is a suitable measure of the error (which tends to zero if v tends to u in V), $\mathcal{D}$ is the set of problem data (domain, coefficients, boundary conditions, known parameters etc.), and the functional $\mathbb{F}$ is computable. However, getting (1.1) with the above indicated properties may be a very difficult task. For example, the identity

$$\|\mathcal{A}e\|_V = \|\mathcal{R}(v)\|_{V^*}, \qquad \mathcal{R}(v) := \mathcal{A}v - f, \quad e := v - u \tag{1.2}$$

holds for a linear operator $\mathcal{A}$. The difficulty lies in the fact that the right side of (1.2) is represented by the norm, which may be practically incomputable. For example, if V is the Sobolev space $\overset{\circ}{H}{}^1(\Omega))$, then the space $V^* = H^{-1}(\Omega)$ has the norm defined as supremum over infinite amount of functions. Therefore, the identity (1.1) should be treated as a theoretical fact rather than a tool for direct computations.

Difficulties of another kind may appear if one tries to obtain easily computable identities and error estimates by changing V^* to a space containing more regular functions. They arise in connection with a quite natural requirement: the norm of $\mathcal{R}(v)$ used in error relations must be consistent with standard properties of approximation sequences (that follow from the classical a priori convergence theory, e.g., see [1, 3, 6]). This requirement imposes certain restrictions that "simple" relations often violate. An example of this kind gives the identity $\|\Delta e\|_\Omega = \|\Delta v + f\|$, which is easy to deduce for the problem $\Delta u + f = 0$ in a bounded Lipschitz domain Ω with the boundary condition $u = 0$ on $\partial\Omega$. Regrettably, for a sequence $\{v_k\}$ converging to u in the energy space $\overset{\circ}{H}{}^1(\Omega)$ such an identity is useless even if u and v_k possess extra differentiability. Analogous relations involving strong norm of the residual $\mathcal{R}(v)$ can be derived for various linear problems, e.g., for the parabolic heat equation. In this paper, we investigate computable error relations that hold for the widest possible class of approximate solutions, and therefore identities and estimates of such a type are excluded from the consideration. Instead, we try to keep a proper balance between the regularity and computability conditions.

There is one more reason why practically useful identities have forms that differ from (1.1). Modern numerical methods are often based on advanced posings of boundary value problems, where the solution is understood as a set of two (or more) functions. For example, mixed methods operate with a pair of functions $(u, p^*) \in V \times Y^*$, where Y^* is an (energy) space introduced for the second component. Thus, the solution consists of the primal and dual components u and p^*, respectively. Practically useful error identities must be well adapted to these and others advanced approximations of PDEs. Let $v \in V$ and $y^* \in Y^*$ are approximations of v and p^*, respectively. Then, instead of (1.1) we need the identity

$$\boldsymbol{\mu}(v, y^*; u, p^*) = \mathbb{F}(v, y^*, \mathcal{D}), \tag{1.3}$$

where $\boldsymbol{\mu}(v, y^*; u, p^*) \geq 0$ is a measure of the distance between (v, y^*) and (u, p^*). The functional $\mathbb{F}$ depends on the approximations v and y^* (which are supposed to be known) and problem data $\mathcal{D}$. The measure continuously depends on v and y^* (in the topology of V and Y^*, respectively) and vanishes if and only if $v = u$ and $y^* = p^*$. For elliptic boundary value problems error identities of the type (1.3) have been deduced for a class of variational problems

$$\inf_{v \in V} J(v), \qquad J(v) = G(\Lambda v) + F(v) \tag{1.4}$$

by the method suggested in [14, 15]. In (1.4), G and F are convex l.s.c. functionals and Λ is a bounded linear operator. The problem (1.4) includes a wide range of boundary value problems and variational inequalities of elliptic type. The corresponding error identity has the general form (2.19). The book [17] contains detailed analysis of error identities for elliptic boundary value problems and their applications to evaluation of modeling and approximation errors.

In the paper, we consider initial boundary value problems associated with the equation

$$u_t + \mathcal{A}(u) = f, \tag{1.5}$$

where $\mathcal{A}(u) = -\mathrm{div} p^* + \sigma$ and p^* and σ are defined as subdifferentials of certain convex potentials. In this case, $\mathcal{A}$ is a maximal monotone operator. Correctness of problems with monotone operators is based on the Browder–Minty theorem. For parabolic equations with monotone differential operators, existence of generalized solutions is well established (e.g., see [2, 4, 10, 18]). Our goal is to derive functional error identities for problems of the class (1.5) and study their implications.

In short, the outline of the paper is as follows. Section 2 contains preliminary results related to convex analysis and monotone operators. The main error identity is established in Section 3 (Theorem 1). Examples associated with various evolutionary problems are considered in Section 4. Here, together with error identities we also discuss estimates that follow from these identities. The next section 5 is devoted to numerical verification of identities and estimates. Numerical tests confirm that the identities hold for various approximations regardless of their origin and closeness to the exact solution. Finally, in section 6 we discuss applications of error identities to analysis of modeling errors generated by simplification of coefficients and changing the initial condition.

2 Preliminaries

2.1 Compound functionals

Let X be a reflexive Banach space and X^* denote the space conjugate to X with the product operation $< x^*, x > \in \mathbb{R}$ for $x \in X$ and $x^* \in X^*$. A convex l.s.c. functional $\Phi : X \to \mathbb{R}$ has a counterpart $\Phi^* : X^* \to \mathbb{R}$ defined by the relation

$$\Phi^*(x^*) := \sup_{x\in X} \{ < x^*, x > - \Phi(x) \},$$

which is called the Fenchel conjugate to Φ. The pair of functionals Φ and Φ^* generates the compound functional

$$\mathcal{D}_\Phi\,(x,x^*) := \Phi(x) + \Phi^*(x^*) - < x^*, x > .$$

It is easy to see that

$$\mathcal{D}_\Phi\,(x,x^*) \geq 0 \qquad \forall\, x\in X,\, x^*\in X^*. \tag{2.1}$$

An important property of this functional is (e.g., see [9])

$$\mathcal{D}_\Phi(x,x^*) = 0 \;\Leftrightarrow\; x^* \subset \partial\Phi(x) \text{ and } x \subset \partial\Phi^*(x^*). \tag{2.2}$$

If Φ (resp. Φ^*) is Gateaux differentiable, then the subdifferential inclusion in (2.2) is replaced by a simpler relation $x^* = \Phi'(x)$ (resp. $x = \Phi^{*\prime}(x^*)$), where prime denotes the derivative. If X is a Hilbert space and $\Phi(x) = \frac{1}{2}\|x\|^2_X$, then $\Phi^*(x^*) = \frac{1}{2}\|x^*\|^2_{X^*}$ and (since X and X^* are isomorphic) we may write the compound functional in the form $\mathcal{D}_\Phi(x,x^*) = \frac{1}{2}\|x-x^*\|^2_X$. Due to this fact squared norms play the role of natural error measures for many linear problems associated with Euler equations for quadratic energy functionals.

Lemma 1 Let Φ and $\widehat{\Phi}_{\ell^*}$ be two convex functionals that differ by a linear functional $\ell^*\in X^*$, i.e.

$$\widehat{\Phi}(x) = \Phi(x) + < \ell^*, x > \qquad \forall\, x\in X.$$

Then for any $x\in X$ and $x^*\in X^*$, it holds

$$\mathcal{D}_{\widehat{\Phi}}(x,x^*) = \mathcal{D}_\Phi(x, x^* - \ell). \tag{2.3}$$

Proof. We have

$$\widehat{\Phi}(x^*) = \sup_x \{ < (x^* - \ell^*), x > - \Phi(x)\} = \Phi^*(x^* - \ell^*).$$

Hence

$$\mathcal{D}_{\widehat{\Phi}}(x,x^*) = \widehat{\Phi}(x) + \widehat{\Phi}^*(x^*) - < x^*, x > = \Phi(x) + \Phi^*(x^*-\ell^*) - < x^*-\ell^*, x > = \mathcal{D}_\Phi(x, x^*-\ell^*).$$

□

Lemma 2 Let $\eta\in X$ and $\eta^*\in X^*$ satisfy the relation $\mathcal{D}_\Phi(\eta,\eta^*) = 0$. Then for any $x\in X$ and $x^*\in X^*$ it holds

$$\mathcal{D}_\Phi(x,x^*) = \mathcal{D}_\Phi(x,\eta^*) + \mathcal{D}_\Phi(\eta,x^*) + < \eta^* - x^*, x-\eta > . \tag{2.4}$$

Proof. Using (2.4), we can rewrite $\mathcal{D}_\Phi(x,x^*)$ as follows:

$$\begin{aligned}
\mathcal{D}_\Phi(x,x^*) &= \Phi(x) + \Phi^*(x^*) - < x, x^* > \\
&= \Phi(\eta) + \Phi^*(x^*) - < x^*, \eta > + \Phi(x) + \Phi^*(\eta^*) - < \eta^*, x > + < x^*, \eta > \\
&\quad + < \eta^*, x > - < \eta, \eta^* > - < x, x^* > \\
&= \mathcal{D}_\Phi(\eta, x^*) + \mathcal{D}_\Phi(x,\eta^*) + < \eta^* - x^*, x - \eta > .
\end{aligned}$$

□

2.2 Notation and nomenclature

Throughout the paper Ω denotes a bounded set in $\mathbb{R}^d$ $(d \geq 1)$ with a Lipshitz boundary Γ, $V(\Omega)$ denotes a reflexive Banach space of functions defined in Ω, and V_0 is a subspace of V containing the functions vanishing on Γ. It is assumed that $V \subset \mathcal{V}$, where $\mathcal{V}$ is a Banach space with the norm $\|\cdot\|_{\mathcal{V}}$ and V is compactly embedded in $\mathcal{V}$. The spaces V^* and $\mathcal{V}^*$ are dual to V_0 and $\mathcal{V}$, respectively. We assume that the norms $\|\cdot\|_{\mathcal{V}}$ and $\|\cdot\|_{\mathcal{V}^*}$ are of integral type (computable). If $\zeta^* \in \mathcal{V}^* \subset V^*$ then the product $\langle \zeta^*, \zeta \rangle$ can be expressed by the integral $\int\limits_\Omega \zeta^* \zeta dx$.

For vector valued functions, we introduce another triple of spaces $Y \subset U \subset Y^*$, where Y^* is the corresponding dual space and $U := L^2(\Omega, \mathbb{R}^d)$. In particular, Y contains ∇v for any $v \in V$. The pairing of y and y^* is denoted by $(\cdot, \cdot)_\Omega$. It can be also written as the integral $\int\limits_\Omega y \cdot y^* \, dx$ provided that the components possess necessary integrability. The operator of spatial divergence is defined as an element of V^* such that

$$(y^*, \nabla w)_\Omega + \langle \mathrm{div} y^*, w \rangle = 0 \qquad \forall w \in V_0. \tag{2.5}$$

Let the operator $\mathcal{A}$ be defined by the identity

$$\langle \mathcal{A}(u), w \rangle = (p^*, \nabla w)_\Omega + \langle \sigma, w \rangle \qquad \forall w \in V_0, \tag{2.6}$$

where p^* and σ satisfy the relations

$$\mathcal{D}_G(\nabla u, p^*) \;=\; G(\nabla u) + G^*(p^*) - (p^*, \nabla u)_\Omega = 0, \tag{2.7}$$

$$\mathcal{D}_R(u, \sigma) \;=\; R(u) + R^*(\sigma) - \langle \sigma, u \rangle = 0 \tag{2.8}$$

and the functionals $G : Y \to \mathbb{R}$ and $R : \mathcal{V} \to \mathbb{R}$ have the form

$$G(y) = \int\limits_\Omega g(y) dx \quad \text{and} \quad R(u) := \int\limits_\Omega \rho(u) dx, \tag{2.9}$$

where g and ρ are convex functions and $G(y) \to +\infty$ as $\|y\|_Y \to +\infty$. Henceforth, we assume that

$$\|w\|_{\mathcal{V}} \leq C(\Omega) \|\nabla w\|_Y \qquad \forall w \in V_0, \tag{2.10}$$

where $C(\Omega) > 0$, so that the functional $G(\nabla w)$ is coercive on $V_0(\Omega)$.

For simplicity we assume that g and ρ do not depend on t, so that the operator $\mathcal{A}$ also do not depend on t. However, this restriction is not related to principal difficulties and the results discussed below can be extended to a wider class of problems with time–dependent coefficients.

It is easy to see that (2.7) defines a constitutive relation that relates ∇u and the flux p^* (cf. (2.2)). Indeed, since $g(\nabla u) + g^*(p^*) - \nabla u \cdot p^* \geq 0$ (2.7) means that

$$g(\nabla u) + g^*(p^*) - \nabla u \cdot p^* = 0 \quad \text{for a.e. } x \in \Omega. \tag{2.11}$$

If g is differentiable, then (2.11) amounts $p^* = g'(\nabla u)$. In particular, if $g(y) = \frac{1}{2}|y|^2$, then we arrive at the linear model with the simplest diffusion law $p^* = \nabla u$.

Analogously, the condition (2.8) defines properties of the lower term, which in physical models often reflects generated by chemical reactions. It means that $\sigma \in \partial \rho(u)$, if ρ is differentiable, then (2.8) yields the relation $\sigma = \rho'(u)$.

Lemma 3 Let $u_1, u_2 \in V$, $\sigma_1, \sigma_2 \in V^*$, and $p_1^*, p_2^* \in Y^*$ satisfy the relations

$$\mathcal{D}_G(\nabla u_i, p_i^*) = 0 \quad \text{and} \quad \mathcal{D}_R(u_i, \sigma_i) = 0 \quad i = 1, 2. \tag{2.12}$$

Then

$$\langle \mathcal{A}(u_1) - \mathcal{A}(u_2), u_1 - u_2 \rangle = \mathcal{D}_G(\nabla u_1, p_2^*) + \mathcal{D}_G(\nabla u_2, p_1^*) + \mathcal{D}_R(u_1, \sigma_2) + \mathcal{D}_R(u_2, \sigma_1). \tag{2.13}$$

Proof. We have

$$\langle \mathcal{A}(u_1) - \mathcal{A}(u_2), u_1 - u_2 \rangle = (p_1^* - p_2^*, \nabla(u_1 - u_2))_\Omega + \langle \sigma_1 - \sigma_2, u_1 - u_2 \rangle . \tag{2.14}$$

In view of (2.12), the right hand side of (2.14) has the form

$$\int\limits_\Omega (g(\nabla u_1) + g^*(p_1^*) + g(\nabla u_2) + g^*(p_2^*) - \nabla u_1 \cdot p_2^* - \nabla u_2 \cdot p_1^*) dx$$
$$+ \int\limits_\Omega (\rho(u_1) + \rho^*(\sigma_1) + \rho(u_2) + \rho^*(\sigma_2) - u_1\sigma_2 - u_2\sigma_1) dx$$

and coincides with the right hand side of (2.13). The relation (2.13) shows that the operator $\mathcal{A}$ is monotone (cf. (2.1)). □

2.3 Error identities for nonlinear elliptic problems

Error identities of the type (1.3) have beed deduced for a class of variational problems

$$\inf_{v \in V} J(v), \qquad J(v) = G(\Lambda v) + F(v) \tag{2.15}$$

generated by convex l.s.c. functionals G and F (see [14, 15, 17]). It includes a wide range of boundary value problems and variational inequalities of elliptic type. The corresponding dual problem has the form

$$\sup_{y^* \in Y^*} I^*(y^*), \qquad I^*(y^*) = -G^*(y^*) - F^*(\Lambda^* y^*). \tag{2.16}$$

If u and p^* are the solutions of (2.15) and (2.16), respectively, then $J(u) = I^*(p^*)$ and (e.g., see [9])

$$G(\Lambda u) + G^*(p^*) - (p^*, \Lambda u)_\Omega = 0, \tag{2.17}$$
$$F(u) + F^*(-\Lambda^* p^*) + \langle \Lambda^* p^*, u \rangle = 0. \tag{2.18}$$

For this class of problems, the identity (1.3) is known (see [14] and Chapter 3 of the book [17]). For example, if $\Lambda v := \nabla v$ and $\Lambda^* y^* = -\mathrm{div} y^*$, then the identity is

$$\boldsymbol{\mu}(v, u) + \boldsymbol{\mu}^*(y^*, p^*) = \mathcal{D}_G(\nabla v, y^*) + \mathcal{D}_F(v, \mathrm{div} y^*). \tag{2.19}$$

where

$$\boldsymbol{\mu}(v, u) := \mathcal{D}_G(\nabla v, p^*) + \mathcal{D}_F(v, \mathrm{div} p^*) \quad \text{and} \quad \boldsymbol{\mu}^*(y^*, p^*) := \mathcal{D}_G(\nabla u, y^*) + \mathcal{D}_F(u, \mathrm{div} y^*).$$

are nonnegative measures that vanish if $v = u$ and $y^* = p^*$ (this fact follows from (2.17) and (2.18)). The converse is also true.

Lemma 4 If $\boldsymbol{\mu}(v,u)=0$, then v is a minimizer of (2.15). If $\boldsymbol{\mu}^*(y^*,p^*)=0$ then p^* is a maximizer of (2.16).

Proof. If $\boldsymbol{\mu}(v,u)=0$, then

$$0=G(\nabla v)+G^*(p^*)-(p^*,\nabla v)=G(\nabla v)-G(\nabla u)-(p^*,\nabla(v-u))_\Omega, \tag{2.20}$$
$$0=F(v)+F^*(\mathrm{div}p^*)-\langle \mathrm{div}p^*,v\rangle=F(v)-F(u)-\langle \mathrm{div}p^*,v-u\rangle\,. \tag{2.21}$$

Adding (2.20) and (2.21), we find that

$$G(\nabla u)+F(u)=G(\nabla v)+F(v),$$

i.e., v is a minimizer.

Analogously, the condition $\boldsymbol{\mu}^*(y^*,\nabla u)=0$ implies the identities

$$0=G^*(y^*)-G^*(p^*)-(y^*-p^*,\nabla u), \tag{2.22}$$
$$0=F(u)+F^*(\mathrm{div}y^*)-\langle \mathrm{div}y^*,u\rangle=F^*(\mathrm{div}y^*)-F^*(\mathrm{div}p^*)-\langle \mathrm{div}(y^*-p^*),u\rangle\,. \tag{2.23}$$

From (2.22) and (2.23) it follows that $G^*(p^*)+F^*(\mathrm{div}p^*)=G^*(y^*)+F^*(\mathrm{div}y^*)$. Taking into account (2.16), we conclude that y^* is a maximizer of (2.16). $\square$

Lemma 4 shows that $\boldsymbol{\mu}(v,u)+\boldsymbol{\mu}^*(y^*,p^*)$ can be viewed is a natural measure of the distance between the pair of approximations (v,y^*) and the pair of exact solutions (u,p^*). The identity (2.19) holds for any $v\in V$ and $y^*\in Y^*$ and its right hand side contains only known data and approximations v and y^*. Below we deduce similar identities for evolutionary problems generated by monotone spatial operators.

3 Error identities for a class of evolutionary problems

3.1 The problem

Consider the following class of initial boundary value problems:

$$u_t+\mathcal{A}(u)=f \text{ in } Q_T, \tag{3.1}$$
$$u(x,t)=0 \qquad \text{on } S_T, \tag{3.2}$$
$$u(x,0)=u_0(x). \tag{3.3}$$

Here $Q_T:=(0,T)\times\Omega$ is the space–time cylinder, $S_T:=(0,T)\times\Gamma$, and the spatial operator $\mathcal{A}$ is defined by the relations (2.6), (2.7), and (2.8). For the functions in Q_T, we use the following Bochner spaces

$$\mathbb{V}(Q_T):=L^q((0,T);V(\Omega)), \qquad \mathbb{V}_0(Q_T):=L^q((0,T);V_0(\Omega)),$$
$$\mathbb{V}^*(Q_T):=L^{q^*}((0,T);V^*(\Omega)), \qquad \widetilde{\mathbb{V}}^*(Q_T):=L^{q^*}((0,T);\mathcal{V}^*)\subset\mathbb{V}^*(Q_T),$$

where $q>1$ and $q^*=\frac{q}{q-1}$. For fluxes, we introduce the space

$$\mathbb{Y}^*(Q_T):=\{y^*=L^{q^*}((0,T),Y^*(\Omega))\mid \mathrm{div}y^*\in\mathbb{V}^*(Q_T)\}$$

and its subspace

$$\widetilde{\mathbb{Y}}^*(Q_T):=\{y^*\in L^{q^*}((0,T),Y^*(\Omega))\mid \mathrm{div}y^*\in\widetilde{\mathbb{V}}^*(Q_T)\}.$$

Multiplying (3.1) by the test function and recalling (2.6), we define a generalised solution of the problem (3.1)–(3.3) as the function $u \in \mathbb{V}(Q_T)$, $u_t \in \mathbb{V}^*(Q_T)$ such that

$$\int_0^T (\langle u_t, w\rangle + (p^*, \nabla w)_\Omega + \langle \sigma - f, w\rangle)dt = 0 \qquad \forall w \in \mathbb{V}_0(Q_T), \tag{3.4}$$

which holds together with the relations (2.7) and (2.8). Using them, and (3.4) with $w = u$, we obtain the evolutional variational inequality

$$\int_0^T \Big(\langle u_t, w-u\rangle + G(\nabla w) - G(\nabla u) + R(w) - R(u)\Big)dt \geq \int_0^T \langle f, w-u\rangle\, dt \qquad \forall w \in \mathbb{V}_0(Q_T), \tag{3.5}$$

where $u(x,t)$ is subject to the initial condition (3.3).

Evolutionary problems with monotone spatial operators are well studied (e.g., see [2, 7, 10, 12, 18]) Henceforth, we assume that the problem (3.5) has a unique solution $u \in \mathbb{V}_0(Q_T)$ and the relations (2.7) and (2.8) uniquely define $p^* \in \mathbb{Y}^*(Q_T)$ and $\sigma \in \mathbb{V}^*(Q_T)$.

3.2 The main error identity

Theorem below presents the main error identity that holds for approximations v, y^*, and τ of u, p^*, and σ, respectively.

Theorem 1 For $(v, y^*, \tau) \in \mathcal{H}(Q_T) := \mathbb{V}_0(Q_T) \times \mathbb{Y}^*(Q_T) \times \mathbb{V}^*(Q_T)$ it holds

$$\int_0^T \Big(\boldsymbol{\mu}(v, y^*, \tau; u, p^*, \sigma) + \langle e_t, e\rangle\Big)dt = \int_0^T \Big(\mathcal{D}_G(\nabla v, y^*) + \mathcal{D}_R(v, \tau) - \langle \mathcal{R}(y^*, \tau, v),\, e\rangle\Big)dt, \tag{3.6}$$

where

$$\mathcal{R}(y^*, \tau, v) := \mathrm{div} y^* - \tau + f - v_t$$

and

$$\boldsymbol{\mu}(v, y^*, \tau; u, p^*, \sigma) := \mathcal{D}_G(\nabla u, y^*) + \mathcal{D}_G(\nabla v, p^*) + \mathcal{D}_R(u, \tau) + \mathcal{D}_R(v, \sigma).$$

Proof. In view of Lemma 2,

$$\int_0^T \mathcal{D}_G(\nabla v, y^*)dt = \int_0^T \Big(\mathcal{D}_G(\nabla v, p^*) + \mathcal{D}_G(\nabla u, y^*) + (p^* - y^*, \nabla(v-u))_\Omega\Big)dt \tag{3.7}$$

and

$$\int_0^T \mathcal{D}_R(v, \tau)dt = \int_0^T \Big(\mathcal{D}_R(v, \sigma) + \mathcal{D}_R(u, \tau) + \langle \sigma - \tau, v-u\rangle\Big)dt. \tag{3.8}$$

Consider the integral

$$I(e) := \int_0^T ((p^* - y^*), \nabla e)_\Omega + \langle \sigma - \tau, e\rangle\, dt.$$

Since $e \in \mathbb{V}_0(Q_T)$, we use (3.4) and find that

$$\int\limits_0^T \Big((p^*, \nabla e)_\Omega + \langle \sigma, e \rangle \Big) dt = \int\limits_0^T \langle f - u_t, e \rangle \, dt.$$

By this relation and (2.5), we reform the integral as follows:

$$I(e) = \int\limits_0^T \langle \mathrm{div} y^* - \tau + f - v_t, e \rangle \, dt + \int\limits_0^T \langle e_t, e \rangle \, dt. \tag{3.9}$$

Summation of (3.7) and (3.8) yields

$$\int\limits_0^T \mathcal{D}_G(\nabla v, y^*) dt + \int\limits_0^T \mathcal{D}_R(v, \tau) dx dt = \boldsymbol{\mu}(v, y^*, \tau; u, p^*, \sigma) + I(e).$$

and using (3.9) we get (3.6). $\square$

Theorem 1 presents the most general form of the identity. Let $f \in \widetilde{\mathbb{V}}^*(Q_T)$ and other data of the problem be sufficiently regular so that

$$\sigma, u_t \in \widetilde{\mathbb{V}}^*(Q_T), \quad p^* \in \widetilde{\mathbb{Y}}^*(Q_T). \tag{3.10}$$

Consider approximations that possess the same properties, i.e., $\tau, v_t \in \widetilde{\mathbb{V}}^*(Q_T)$ and $y^* \in \widetilde{\mathbb{Y}}^*(Q_T)$. In this case, the product $\langle \mathcal{R}(y^*, \tau, v), e \rangle$ is expressed via the integral $\int\limits_\Omega \mathcal{R}(y^*, \tau, v) \, e \, dx$ and

$$\int\limits_0^T \langle e_t, e \rangle \, dt = \int\limits_0^T \int\limits_\Omega e_t \, e \, dx dt.$$

Since $e_t \in \widetilde{\mathbb{V}}^*(Q_T)$ we have

$$\int\limits_{Q_T} |e_t \, e| \, dx dt \leq \|e_t\|_{\widetilde{\mathbb{V}}^*} \|e\|_{\widetilde{\mathbb{V}}} < +\infty.$$

Hence using the Fubini's theorem, we find a more transparent presentation of the term

$$\int\limits_0^T \langle e_t, e \rangle \, dt = \int\limits_0^T \int\limits_\Omega e_t e \, dx dt$$

$$= \int\limits_\Omega \int\limits_0^T \frac{1}{2} \frac{d}{dt} e^2 \, dx dt - \frac{1}{2} \Big[\|e(\cdot, T)\|^2_\Omega - \|e(\cdot, 0)\|^2_\Omega \Big] =: \frac{1}{2} [\![\, \|e\|^2_\Omega \,]\!]_0^T .$$

Now the main error identity (3.6) is written in terms of Lebesgue integrals:

$$\int_0^T \boldsymbol{\mu}(v,y^*,\tau;u,p^*,\sigma)dt + \frac{1}{2}[\![\, \|e\|^2_\Omega \,]\!]_0^T$$

$$= \int_0^T \Big(\mathcal{D}_G(\nabla v, y^*) + \mathcal{D}_R(v,\tau)\Big)dt - \int_\Omega \mathcal{R}(y^*,\tau,v)e\,dxdt. \quad (3.11)$$

The last integral in (3.11) can be excluded if we set

$$\tau = \tau_f := \mathrm{div} y^* + f - v_t.$$

Then, the error identity reads

$$\int_0^T \Big(\mathcal{D}_G(\nabla u, y^*) + \mathcal{D}_G(\nabla v, p^*) + \mathcal{D}_R(u,\tau_f) + \mathcal{D}_R(v,\sigma)\Big)dt + \frac{1}{2}[\![\, \|e\|^2_\Omega \,]\!]_0^T$$

$$= \int_0^T (\mathcal{D}_G(\nabla v, y^*) + \mathcal{D}_R(v,\tau_f))dt, \quad (3.12)$$

where

$$\mathcal{D}_R(v,\tau_f) = \int_\Omega (\rho(v) + \rho^*(\mathrm{div} y^* + f - v_t) - v(\mathrm{div} y^* + f - v_t))dx.$$

Notice that the right hand side of (3.12) contains only approximations and known data and, therefore, is directly computable. It vanishes if

$$\mathrm{div} y^* + f - v_t \in \partial\rho(v) \quad \text{for a.e. } t \in [0,T] \quad \text{and } \mathcal{D}_G(\nabla v, y^*) = 0,$$

what implies $v = u$ and $y^* = p^*$.

3.3 Comments

1. For $v = 0$, $y^* = 0$, and $\tau = 0$, (3.11) is reduced to the identity

$$\int_0^T \Big(G(\nabla u) + G^*(p^*) + R(u) + R^*(\sigma)\Big)dxdt + \frac{1}{2}[\![\, \|u\|^2_\Omega \,]\!]_0^T = \int_\Omega fu\,dxdt.$$

Using (2.7) and (2.8) we rewrite it in the form

$$\int_{Q_T} \Big(p^* \cdot \nabla u + \sigma u\Big)dxdt + \frac{1}{2}[\![\, \|u\|^2_\Omega \,]\!]_0^T = \int_\Omega fu\,dxdt. \quad (3.13)$$

Since $p^* = p^*(u)$ and $\sigma = \sigma(u)$ this is a form of the energy balance identity for the exact solution u. For example, if p^* and σ are defined by (4.1) and (4.2), then we arrive at the identity

$$\int_{Q_T} \Big(A\nabla u \cdot \nabla u + u\rho'(u)\Big)dxdt + \frac{1}{2}[\![\, \|u\|^2_\Omega \,]\!]_0^T = \int_\Omega fu\,dxdt,$$

which is the well known energy balance relation (e.g., see §3 of Ch. 3 in [11]). The identity, (3.6) reflects a more general form of balance that holds for all energy admissible deviations from the exact solution. It implies (3.13) as a rather special case.

2. It is worth discussing the identity (3.12) from one more side. Adaptive approaches to solving boundary value problems arose as a successful computational technology (e.g., see [8]) whose effectiveness has been confirmed by a huge number of experiments. At present, the adaptivity concept is increasingly acquiring the form of a complete mathematical theory (a unified approach and many related references can be found in [5]). Error identities naturally fit this concept and generate error indicators to be used in adaptive computations. Indeed, the integrand of the right side of (3.12) is a function of x and t. Since (3.12) is an identity, this is exactly the function that should be used as an error indicator if the goal is to minimize the measure in the left side of (3.12). In other words, correct error indicators automatically follow from (3.12) and its particular forms (4.5), (4.11), and (4.19). Examples of using this type error indicators are presented in [13], where error identities and related a posteriori estimates are discussed in the context of IgA approximations of parabolic problems.

3. If $\rho = 0$, then the reaction term vanishes, so that formally $\sigma = 0$. Error identities for this case has been earlier derived and studied in [16]. Also, they follow from Theorem 1. Notice that $\mathcal{D}_R(v, \tau) = 0$ if $\tau = 0$ and $\mathcal{D}_R(v, \tau) = +\infty$ in all other cases. Hence both sides of (3.11) are finite provided that $\tau = 0$ and we arrive at the identity

$$\int\limits_0^T \Big(\mathcal{D}_G(\nabla u, y^*) + \mathcal{D}_G(\nabla v, p^*)\Big) dt + \frac{1}{2} [\![\, \|e\|^2_\Omega \,]\!]_0^T \\ = \int\limits_0^T \Big(\mathcal{D}_G(\nabla v, y^*) - \int\limits_\Omega (\mathrm{div} y^* + f - v_t) e \, dx\Big) dt. \quad (3.14)$$

Using Lemma 1, we can rewrite (3.12) in terms of the functional $F(u) := R(u) - \langle f, u \rangle$. Since

$$D_R(v, \tau_f) = D_F(v, \tau_f - f) \quad \text{and} \quad D_R(u, \tau_f) = D_F(u, \tau_f - f),$$

we have

$$\int\limits_0^T \Big(\mathcal{D}_G(\nabla u, y^*) + \mathcal{D}_G(\nabla v, p^*) + \mathcal{D}_F(u, \mathrm{div} y^* - v_t) + \mathcal{D}_F(v, \mathrm{div} p^* - u_t)\Big) dt \\ + \frac{1}{2} [\![\, \|e\|^2_\Omega \,]\!]_0^T = \int\limits_0^T \Big(\mathcal{D}_G(\nabla v, y^*) + \mathcal{D}_F(v, \mathrm{div} y^* - v_t)\Big) dt. \quad (3.15)$$

This identity can be regarded as a natural generalization of (2.19) to the class of initial boundary value problems.

4 Examples

1. Linear diffusion problem with nonlinear reaction term. Let $f \in L^2(\Omega)$, $g(y) = \frac{1}{2} A y \cdot y$, where A is a symmetric positive definite matrix with bounded coefficients $a_{ij}(x)$ such that

$$c_1 |\zeta|^2 \leq |\zeta|^2_A := A\zeta \cdot \zeta \leq c_2 |\zeta|^2 \qquad \forall \zeta \in \mathbb{R}^d$$

for some $c_2 \geq c_1 > 0$. Next, let ρ be a convex function such that $\rho(0) = 0$ and $\rho(v) \leq \gamma_1 |v|^\nu + \gamma_2$, where $\nu \in [1, \frac{2d}{d-2})$, $\gamma_1, \gamma_2 \in \mathbb{R}$, and $\gamma_1 > 0$. This choice of g and ρ leads to a problem with linear diffusion and nonlinear reaction. If ρ is a differentiable function, then (3.1)–(3.3) reads

$$u_t - \mathrm{div} p^* + \rho'(u) = f, \tag{4.1}$$

$$p^* = A\nabla u, \tag{4.2}$$

$$u(x,t) = 0 \text{ on } S_T, \qquad u(x,0) = u_0(x). \tag{4.3}$$

In this case, $V = H^1(\Omega)$, $\mathcal{V} = L^2(\Omega)$, $V^* = H^{-1}(\Omega)$, $\mathbb{V}(Q_T) = L^2((0,T); V)$, $\mathbb{V}^*(Q_T) = L^2((0,T); H^{-1}(\Omega))$, and $\widetilde{\mathbb{V}}^*(Q_T) = L^2((0,T), \mathcal{V}(\Omega))$. Let $\tau, v_t \in \widetilde{\mathbb{V}}^*(Q_T)$ and $y^* \in \widetilde{\mathbb{Y}}^*(Q_T)$. Then

$$\mathcal{D}_G(\nabla v, p^*) = \frac{1}{2} \int\limits_\Omega |\nabla(v-u)|_A^2 dx, \qquad \mathcal{D}_G(\nabla u, y^*) = \frac{1}{2} \int\limits_\Omega |\nabla(v-u)|_{A^{-1}}^2 dx,$$

and the identity (3.11) reads

$$\int\limits_{Q_T} \Big(\frac{1}{2}|\nabla e|_A^2 + \frac{1}{2}|e^*|_{A^{-1}}^2 + D_\rho(v,\sigma) + D_\rho(u,\tau) \Big) dxdt + \frac{1}{2} [\![\, \|e\|_\Omega^2 \,]\!]_0^T$$
$$= \int\limits_{Q_T} \Big(\frac{1}{2}|y^* - A\nabla v|_{A^{-1}}^2 + D_\rho(v,\tau) - \mathcal{R}(y^*,\tau,v) e dx \Big) dxdt, \tag{4.4}$$

where $D_\rho(v,\tau) := \rho(v) + \rho^*(\tau) - v\tau$. The first and the second terms in the right hand side of (4.4) are directly computable, but the last term contains unknown function e. This difficulty can be overcome by different methods.

If we set $\tau = \tau_f := \mathrm{div} y^* + f - v_t$, then $\mathcal{R}(y^*, \tau_f, v) = 0$ and (4.4) is transformed into the identity

$$\int\limits_{Q_T} \Big(\frac{1}{2}|\nabla e|_A^2 + \frac{1}{2}|e^*|_{A^{-1}}^2 + D_\rho(v,\sigma) + D_\rho(u,\tau_f) \Big) dxdt + \frac{1}{2} [\![\, \|e\|_\Omega^2 \,]\!]_0^T$$
$$= \int\limits_{Q_T} \Big(\frac{1}{2}|y^* - A\nabla v|_{A^{-1}}^2 + D_\rho(v,\tau_f) \Big) dxdt, \tag{4.5}$$

whose right hand side is directly computable.

Another option is to use the estimate

$$2 \left| \int\limits_\Omega \mathcal{R}(y^*,\tau,v) e dx \right| \leq \int\limits_\Omega \left(\frac{1}{\beta(t)} \frac{C_\Omega^2}{c_1} |\mathcal{R}(y^*,\tau,v)|^2 + \beta(t) |\nabla e|_A^2 \right) dx \tag{4.6}$$

with a positive function $\beta(t)$. Then (4.4) implies fully computable two sided estimates

$$\int\limits_{Q_T} \Big((1-\beta)\, |\nabla e|_A^2 + |e^*|_{A^{-1}}^2 + 2D_\rho(v,\sigma) + 2D_\rho(u,\tau) \Big) dxdt + [\![\, \|e\|_\Omega^2 \,]\!]_0^T$$
$$\leq \int\limits_{Q_T} \Big(|y^* - A\nabla v|_{A^{-1}}^2 + 2D_\rho(v,\tau) + \frac{C_\Omega^2}{c_1 \beta} |\mathcal{R}(y^*,\tau,v)|^2 \Big) dxdt \tag{4.7}$$

and

$$\int\limits_{Q_T}\Big((1+\beta)\,|\nabla e|^2_A+|e^*|^2_{A^{-1}}+2D_\rho(v,\sigma)+2D_\rho(u,\tau)\Big)dxdt+[\![\,\|e\|^2_\Omega\,]\!]_0^T$$

$$\geq \int\limits_{Q_T}\Big(|y^*-A\nabla v|^2_{A^{-1}}+2D_\rho(v,\tau)-\frac{C^2_\Omega}{c_1\beta}|\mathcal{R}(y^*,\tau,v)|^2\Big)dxdt \quad (4.8)$$

In (4.7) $0<\beta\leq 1$ and in (4.8) β is any positive function. The freedom to choose this function can be used to optimize the estimates.

2. Obstacle problem Another example is related to the problem $u_t-\mathrm{div}A\nabla u=f$ with two obstacles. Let $\varphi(x)$ and $\psi(x)$ be two given functions in $H^2(\Omega)$ such that

$$\psi(x)>\varphi(x),\quad \varphi(x)\leq 0,\quad \psi(x)\geq 0\quad \forall\, x\in\Omega.$$

We set $V=H^1(\Omega)$, $V_0=\overset{\circ}{H}{}^1(\Omega)$, $\mathcal{V}=L^2(\Omega)$, and define

$$K_{\varphi\psi}:=\{v\in \mathbb{V}_0(Q_T)\ \mid\ \varphi(x)\leq v(x,t)\leq\psi(x)\}.$$

In this case, the functionals R and R^* have the forms

$$R(v):=\left\{\begin{array}{cc} 0 & \text{if } v\in K_{\varphi\psi},\\ +\infty & \text{else}\end{array}\right.,\qquad R^*(\tau)=\int\limits_\Omega\Big((\tau)_+\,\psi\ -\ (\tau)_-\,\varphi\Big)dx,$$

where $(\tau)_+:=\max\{0,\tau\}$ and $(\tau)_-:=-\min\{0,\tau\}$ and (3.5) is reduced to the parabolic variational inequality

$$\int\limits_{Q_T}\Big(u_t(w-u)+A\nabla u\cdot\nabla(w-u)\Big)dxdt\geq\int\limits_{Q_T}f(w-u)dxdt\quad \forall w\in K_{\varphi\psi}. \quad (4.9)$$

Since $\tau v=\Big((\tau)_+-(\tau)_-\Big)v$, we find that

$$\mathcal{D}_R(v,\tau)=\left\{\begin{array}{ll}\int\limits_\Omega D_{\varphi\psi}(v,\tau)dx & \text{if } v\in K_{\varphi\psi},\\ \qquad +\infty & \text{if } v\notin K_{\varphi\psi},\end{array}\right.\qquad D_{\varphi\psi}(v,\tau):=(\tau)_+(\psi-v)+(\tau)_-(v-\varphi).$$

Notice that $\mathcal{D}_R(v,\tau)\geq 0$ and the relation $\mathcal{D}_R(v,\tau)=0$ means that τ and $v\in K_{\varphi\psi}$ satisfy the relations:

$$\begin{array}{rl}\tau=0 & \text{if } (x,t)\in Q^v_{T,0}:=\{(x,t)\in Q_T\ \mid\ \varphi(x)<v(x,t)<\psi(x)\},\\ (\tau)_+=0 & \text{if } (x,t)\in Q^v_{T,\varphi}:=\{(x,t)\in Q_T\ \mid\ \varphi(x)=v(x,t)\},\\ (\tau)_-=0 & \text{if } (x,t)\in Q^v_{T,\psi}:=\{(x,t)\in Q_T\ \mid\ \psi(x)=v(x,t)\}.\end{array}$$

Here $Q^v_{T,\varphi}$ and $Q^v_{T,\psi}$ are the upper and lower coincidence sets defined by the function $v(x,t)$. If v is the solution u, then they coincide the exact coincidence sets.

For $v\in K_{\varphi\psi}$ the identity (3.11) reads

$$\int\limits_{Q_T}\Big(\frac12|\nabla e|^2_A+\frac12|e^*|^2_{A^{-1}}+D_{\varphi\psi}(u,\tau)+D_{\varphi\psi}(v,\sigma)\Big)dxdt+\frac12[\![\,\|e\|^2_\Omega\,]\!]_0^T$$

$$=\int\limits_{Q_T}\Big(|A\nabla v-y^*|^2_{A^{-1}}+D_{\varphi\psi}(v,\tau)-\mathcal{R}(y^*,\tau,v)e\Big)dxdt. \quad (4.10)$$

Setting $\tau = \tau_f := \mathrm{div} y^* + f - v_t = 0$ in (4.10), we obtain the identity

$$\int\limits_{Q_T} \Big(\frac{1}{2}|\nabla e|_A^2 + \frac{1}{2}|e^*|_{A^{-1}}^2 + D_{\varphi\psi}(u,\tau_f) + D_{\varphi\psi}(v,\sigma)\Big) dxdt + \frac{1}{2} [\![\, \|e\|_\Omega^2 \,]\!]_0^T$$
$$= \int\limits_{Q_T} \Big(|A\nabla v - y^*|_{A^{-1}}^2 + D_{\varphi\psi}(v,\tau_f)\Big) dxdt, \quad (4.11)$$

which is a form of (3.12) for the obstacle problem. The left hand side of (4.11) consists of nonnegative quantities and the right hand side contains only know functions and, therefore, it is computable. Assume that the right hand side is equal to zero. Then

$$y^* = A\nabla v \quad \text{and} \quad D_{\varphi\psi}(v,\tau_f) = 0.$$

The latter equality means that

$$\begin{aligned} \mathrm{div} y^* + f - v_t &= 0 \qquad \text{if } (x,t) \in Q_{T,0}^v, \\ \mathrm{div} y^* + f - v_t &\geq 0 \qquad \text{if } (x,t) \in Q_{T,\psi}^v, \\ \mathrm{div} y^* + f - v_t &\leq 0 \qquad \text{if } (x,t) \in Q_{T,\varphi}^v. \end{aligned}$$

Hence for any $w \in K_{\varphi\psi}$

$$\int\limits_{Q_T} (v_t - \mathrm{div} y^* - f)(w - v) dxdt = \int\limits_{Q_{T,\psi}^v} (v_t - \mathrm{div} y^* - f)(w - \psi) dxdt + \int\limits_{Q_{T,\varphi}^v} (v_t - \mathrm{div} y^* - f)(w - \varphi) dxdt \geq 0,$$

so that v satisfies the variational inequality (4.9). We see that the right hand side of (4.11) vanishes if and only if v coincides with u.

If τ is not chosen in a special way, but is considered as a function from $\widetilde{\mathbb{V}}^*$, then an estimate can be deduced from (4.10). Using (4.6) and same reasoning as before, we obtain a computable upper bound

$$\int\limits_{Q_T} \Big((1-\beta) \, \|\nabla e\|_A^2 + |e^*|_{A^{-1}}^2 + 2D_{\varphi\psi}(v,\sigma) + 2D_{\varphi\psi}(u,\tau)\Big) dxdt + [\![\, \|e\|_\Omega^2 \,]\!]_0^T$$
$$\leq \int\limits_{Q_T} \Big(|y^* - A\nabla v|_{A^{-1}}^2 + 2D_{\varphi\psi}(v,\tau) + \frac{C_\Omega^2}{c_1\beta} |\mathcal{R}(y^*,\tau,v)|^2\Big) dxdt. \quad (4.12)$$

A lower bound is quite analogous to (4.8). It is easy to see that the right hand side of (4.12) vanishes if and only if $v = u$, $y^* = p^*$ and $\tau = \sigma := \mathrm{div} p^* + f - u_t$.

3. Parabolic equation with nonlinear Laplacian operator. Consider the problem with nonlinear diffusion, where

$$g(\nabla u) = \frac{1}{\alpha}|\nabla u|^\alpha \quad \text{and} \qquad g^*(p^*) = \frac{1}{\alpha^*}|p^*|^{\alpha^*}, \qquad \alpha > 1,\ \alpha^* = \frac{\alpha}{\alpha - 1}. \quad (4.13)$$

In this case, ∇u and p^* are joined by the relations

$$p^* = |\nabla u|^{\alpha-2}\nabla u, \qquad \nabla u = |p^*|^{\frac{2-\alpha}{\alpha-1}} p^*, \quad (4.14)$$

and (1)–(3) is reduced to the Cauchy problem

$$u_t - \mathrm{div}|\nabla u|^{\alpha-2}\nabla u + \rho'(u) = f \text{ in } Q_T, \tag{4.15}$$

$$u(x,t) = 0 \qquad \text{on } S_T, \tag{4.16}$$

$$u(x,0) = u_0(x). \tag{4.17}$$

Let $V = W^{1,\alpha}(\Omega)$, $V_0 = \overset{\circ}{W}{}^{1,\alpha}(\Omega)$, $\mathcal{V} = L^\alpha(\Omega)$, $\mathcal{V}^* = L^{\alpha^*}(\Omega)$, $V^* = W^{-1,\alpha^*}(\Omega)$, $Y^* = L^{\alpha^*}(\Omega,\mathbb{R}^d)$. Taking into account (4.14), we have

$$\mathcal{D}_G(\nabla v, p^*) = \int\limits_\Omega (\frac{1}{\alpha}|\nabla v|^\alpha + \frac{1}{\alpha^*}|\nabla u|^\alpha - \nabla v\cdot\nabla u|\nabla u|^{\alpha-2})dx =: \boldsymbol{\mu}_\alpha(v,u),$$

$$\mathcal{D}_G(\nabla u, y^*) = \int\limits_\Omega (\frac{1}{\alpha^*}|y^*|^{\alpha^*} + \frac{1}{\alpha}|p^*|^{\alpha^*} - p^*\cdot y^*|p^*|^{\alpha^*-2})dx =: \boldsymbol{\mu}^*_{\alpha^*}(y^*,p^*).$$

The quantities $\boldsymbol{\mu}_\alpha(v,u)$ and $\boldsymbol{\mu}^*_{\alpha^*}(y^*,p^*)$ are nonlinear measures of the distance from v to u and from y^* to p^*, respectively. Now the identity (3.6) reads

$$\int\limits_0^T (\boldsymbol{\mu}_\alpha(v,u) + \boldsymbol{\mu}^*_{\alpha^*}(y^*,p^*))dt + \int\limits_{Q_T} (D_\rho(v,\sigma) + D_\rho(u,\tau))\,dxdt + [\![\, \|e\|^2_\Omega \,]\!]_0^T$$
$$= \int\limits_0^T \left(\int\limits_\Omega (\frac{1}{\alpha}|\nabla v|^\alpha + \frac{1}{\alpha^*}|y^*|^{\alpha^*} - \nabla v\cdot y^*)dx - \langle \mathcal{R}(y^*,\tau,v), e\rangle \right) dt + \int\limits_{Q_T} D_\rho(v,\tau)dxdt. \tag{4.18}$$

Setting $\tau = \tau_f$, we obtain a form of (4.18)

$$\int\limits_0^T (\boldsymbol{\mu}_\alpha(v,u) + \boldsymbol{\mu}^*_{\alpha^*}(y^*,p^*))dt + \int\limits_{Q_T} (D_\rho(v,\sigma) + D_\rho(u,\tau_f))\,dxdt + [\![\, \|e\|^2_\Omega \,]\!]_0^T$$
$$= \int\limits_0^T \mathcal{D}_G(\nabla v, y^*)dt + \int\limits_{Q_T} D_\rho(v,\tau_f)dxdt \tag{4.19}$$

whose right hand side is fully defined by the functions v and y^*.

There measures $\boldsymbol{\mu}_\alpha(v,u)$ and $\boldsymbol{\mu}^*_{\alpha^*}(y^*,p^*)$ can be bounded from below by norms in the standard Lebesgue spaces L^α and L^{α^*}. Let $\mu_\alpha : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}_+$ be defined by the relation

$$\mu_\alpha(a,b) := \frac{1}{\alpha}|a|^\alpha + \frac{1}{\alpha^*}|b|^\alpha - a\cdot b|b|^{\alpha-2}.$$

In [16] it was proven that for $\alpha \geq 2$ it holds

$$\mu_\alpha(a,b) \geq c_\alpha|a-b|^\alpha \qquad \forall a,b\in\mathbb{R}^d, \tag{4.20}$$

where $c_\alpha = \frac{\alpha-1}{\alpha}(1+\lambda_0)^{2-\alpha}$ and λ_0 is defined by the equation $\lambda_0^{\alpha-1} + \lambda_0(1-\alpha) = \alpha - 2$ (e.g., $c_{2.5} \approx 0.3072$, $c_3 \approx 0.1953$, and $c_4 \approx 0.0833$).

From (4.20) it follows that

$$\boldsymbol{\mu}_\alpha(v,u) \geq c_\alpha \|\nabla(v-u)\|^\alpha_{\alpha,Q_T} \qquad \text{if } \alpha \geq 2,$$
$$\boldsymbol{\mu}^*_{\alpha^*}(v,u) \geq c_{\alpha^*} \|y^* - p^*\|^{\alpha^*}_{\alpha^*,Q_T} \qquad \text{if } \alpha^* \geq 2.$$

Hence the right hand side of (4.19) provides a guaranteed bound for the corresponding Lebesque norms of either gradients or fluxes.

Remark 1 The measure $\mu_\alpha(a,b)$ is not symmetric. Let $\mu^{\rm s}_\alpha(a,b) := \frac{1}{2}(\mu_\alpha(a,b) + \mu_\alpha(b,a))$ denote the symmetrization of $\mu_\alpha(a,b)$. It is easy to see that for $\alpha \geq 2$

$$\mu^{\rm s}_\alpha(a,b) := \tfrac{|a|^\alpha + |b|^\alpha}{2} - a\cdot b \tfrac{|a|^{\alpha-2}+|b|^{\alpha-2}}{2} \geq c_\alpha |a-b|^\alpha \qquad \text{if } \alpha \geq 2, \tag{4.21}$$

However, the constant in (4.21) can be improved. The exact constant in (4.21) is $c^{\rm s}_\alpha = 2^{1-\alpha} \geq c_\alpha$.

5 Numerical verification of error identities

In the tests below, error identities are verified for different functions g and $\rho(v)$ and various approximations $v \in \mathbb{V}_0(Q_T)$ and $y^* \in \widetilde{\mathbb{Y}}^*(Q_T)$. The approximations are generated randomly so that some of them are very close to u and p^* while others may be essentially different. The functions $v(x,t)$ satisfy the boundary conditions but may not satisfy the initial condition. The tests show that the identities hold for any v and y^*. Also, we verify the efficiency of error estimates that follow from them. In the examples, $\Omega = (0,1)$ and $T = 3$. We consider exact solutions of three different types: $u_1(x,t) = \sin(\pi x)\frac{t}{t^2+1}$ (decreasing with respect to t), $u_2(x,t) = x(x-1)\sin(3\pi t)$ (oscillating), and $u_3(x,t) = \sin(2\pi x)(t-1) + \sin(\pi x)t^{3/2}$ (growing with respect to t). These functions are depicted in Fig. 1.

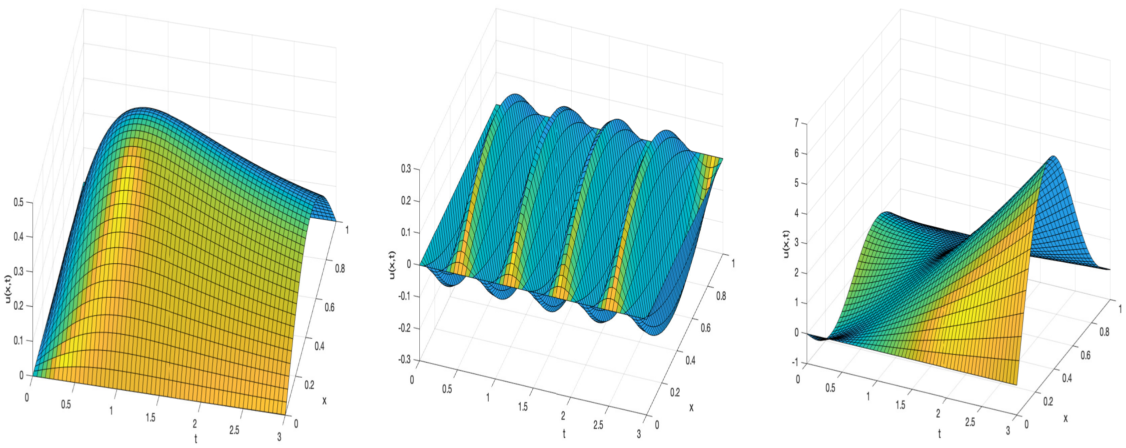

Figure 1: The functions u_1 (left), u_2 (center), and u_3 (right).

Example 1. First, we consider the problem (4.1)–(4.3) with the unit matrix A, and reaction term $\rho(v) = \frac{\delta}{2}|v|^2$, $\delta > 0$. Then, $D_\rho(v,\tau) = \frac{1}{2\delta}|\tau - \delta v|^2$, $\sigma = \delta u$, and $\tau_v := \delta v$. The functions v and y^*

are chosen randomly in the vicinity of u and p^*, and the distance to the exact solution gradually increases with the test number. Thus, numerical tests verify the identities (4.4) and (4.5) and the estimates (4.7) and (4.8) for both good and rough approximations. In the first series of tests T1.1, it was taken $\delta = 1$, $u = u_1$, and τ was also selected randomly at the vicinity of the exact function σ. In the series T1.2, $u = u_2$, $\delta = 0.01$, and $\tau = \tau_v$. The series T1.3 corresponds to the choice $u = u_3$, $\delta = 0.1$, and $\tau = \tau_f$, where $\tau_f - \sigma = \operatorname{div} y^* + f - v_t - \sigma = \operatorname{div} e^* - e_t$. In the latter case, the identity (4.5) reads

$$\int_0^T \Big(\|\nabla e\|_A^2 + \delta \|e\|^2 + \|e^*\|_{A^{-1}}^2 + \frac{1}{\delta} \|\operatorname{div} e^* - e_t\|^2 \Big) dt + \|e(\cdot, T)\|_\Omega^2$$
$$= \|e(\cdot, 0)\|_\Omega^2 + \int_0^T \Big(\|y^* - A\nabla v\|_{A^{-1}}^2 + \frac{1}{\delta} \|\tau_f - \delta v\|^2 \Big) dt. \quad (5.1)$$

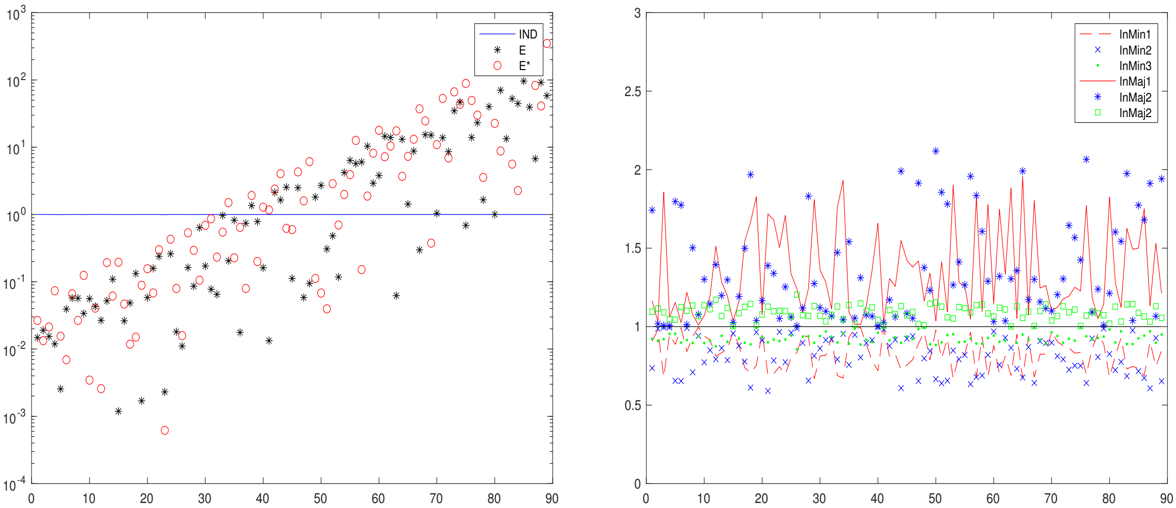

Figure 2: The identity (5.1) in the test T1.3 (left) and the estimates (4.7) and (4.8) in the tests T1.1, T1.2, and T1.3(right).

Blue line in Fig. 2 (left) shows the ratio IND$=\frac{r.h.s.(5.1)}{l.h.s.(5.1)}$ in different tests (test number is indicated on the x-axis). In all the tests IND is equal to 1 (up to very small errors caused by numerical integration). The symbols $*$ and $\circ$ mark the quantities $E := \|\nabla(v - u)\|^2$ and $E^* := \|y^* - p^*\|^2$, respectively, which are quite different in different tests. The picture shows that the identity holds for any pair of functions (v, y^*) regardless of the proximity to (u, p^*).

Fig. 2 (right) shows the ratio between the right and left parts of (4.4) (blue line) and behaviour of the estimates (4.7) and (4.8) (that follow from (4.4)). Here InMaj1$=\frac{r.h.s.(4.7)}{l.h.s.(4.7)}$ and InMin1$=\frac{r.h.s.(4.8)}{l.h.s.(4.8)}$ in the test series T1.1. The same quantities for T1.2 and T1.3 are denoted by InMaj2, InMin2 and InMaj3, InMin3, respectively.

Example 2. These examples are related to problems with nonlinear reaction term. In the test series T2.1 and T2.2, ρ is a function with power growth: $\rho = \frac{\delta}{\mu}|v|^{\mu}$, $\mu > 1$ ($\mu = 3$ and $\delta = 0.1$ in T2.1, $\mu = 1.5$ and $\delta = 2$ in T2.2). In T2.3, we consider the case, where ρ is a linear growth function

$$\rho(v) = \begin{cases} \frac{1}{2}|v|^2 & \text{if } |v| \le 1, \\ v - \frac{1}{2} & \text{if } v > 1, \\ -v - \frac{1}{2} & \text{if } v < -1, \end{cases} \qquad \rho'(v) = \begin{cases} v & \text{if } |v| \le 1, \\ 1 & \text{if } v > 1, \\ -1 & \text{if } v < -1, \end{cases} \qquad \rho^*(\tau) = \begin{cases} \frac{1}{2}|\tau|^2 & \text{if } |\tau| \le 1, \\ +\infty & \text{if } |\tau| > 1. \end{cases}$$

This type nonlinearity may arise in certain variants of the reaction law with saturation.

As before, the tests verify the main identity and the estimates for various randomly selected v, y^*. In T2.1 and T2.3, the function τ was selected randomly and in T2.2 $\tau = \tau_v$, where $\tau_v = v$ if $|v| \le 1$ and $\tau_v = 1$ if $|v| > 1$. In the latter case, $D_\rho(v, \tau_v) = 0$. Fig. 3 (left) exposes the results related to the

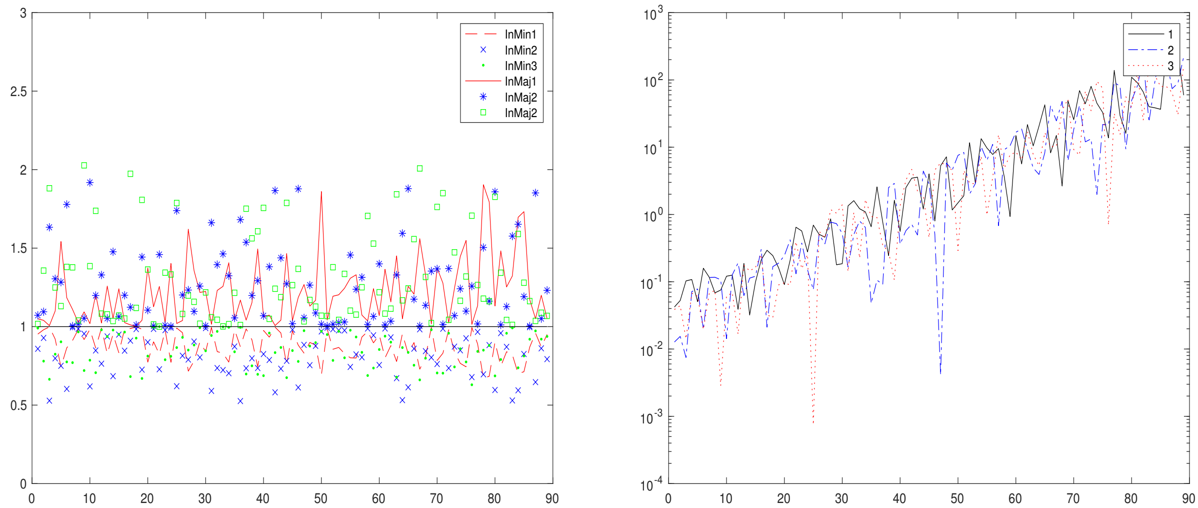

Figure 3: efficiency of the estimates (4.7) and (4.8) in the tests T2.1, T2.2, and T2.3 (left) and values of error measures (right).

estimates (4.7) and (4.8) (with $\beta = 0.5$). It shows that the estimates well represent the corresponding error measures. The right part of Fig. 3 depicts values of the error measure in (forming the left side of (4.7)) in different tests. Line 1 is related to T2.1, line 2 to T2.2, and line 3 to T2.3. Fig. 3 shows that the corresponding majorants and minorants efficiently estimate values of the error measure in the diapason from 10^{-3} to 10^2.

Fig. 4 (left) shows results of numerical verification of the identity (4.4) in the example T2.3, where D_ρ is generated by a linear growth function. As before, the computations confirm correctness of the identity.

We note another interesting observation. Analysis of a large number of tests leads to the conclusion that $\mathcal{D}_G(\nabla v, y^*)$ and $\mathcal{D}_R(v, \tau)$ well reflect the values of $\mathcal{D}_G(\nabla u, y^*) + \mathcal{D}_G(\nabla v, p^*)$ and $\mathcal{D}_R(u, \tau) + \mathcal{D}_R(v, \sigma)$, respectively. Fig. 4 (right) shows the corresponding data. Here

$$\mathrm{IR} := \frac{\mathcal{D}_R(u,\tau) + \mathcal{D}_R(v,\sigma)}{\mathcal{D}_R(v,\tau)} \quad \text{and} \quad \mathrm{IG} := \frac{\mathcal{D}_G(u,\tau) + \mathcal{D}_G(v,\sigma)}{\mathcal{D}_G(v,\tau)}.$$

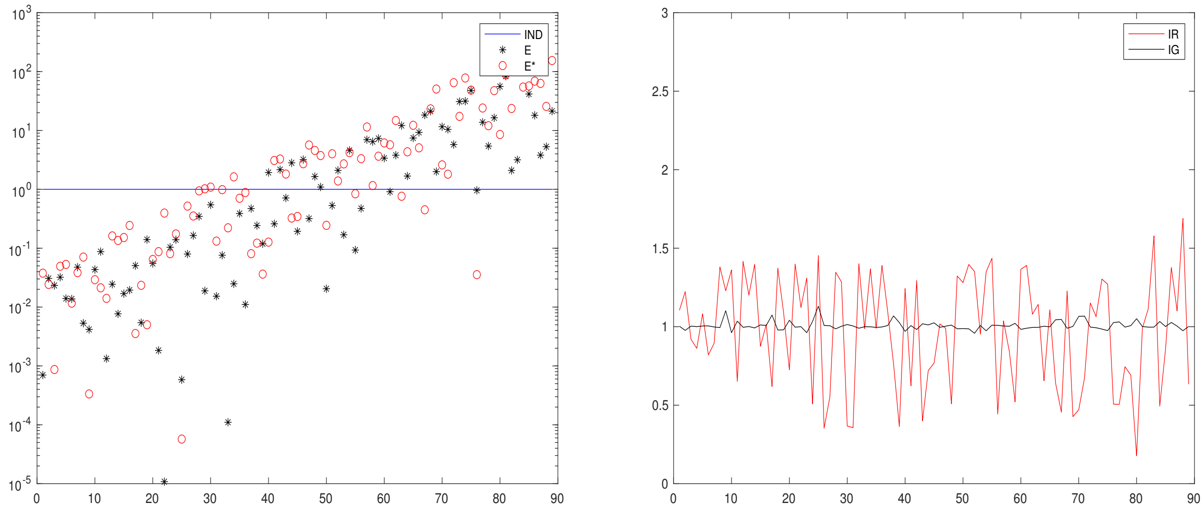

Figure 4: The identity (5.1) (left) and the values IR and ID (right) in the test T2.3.

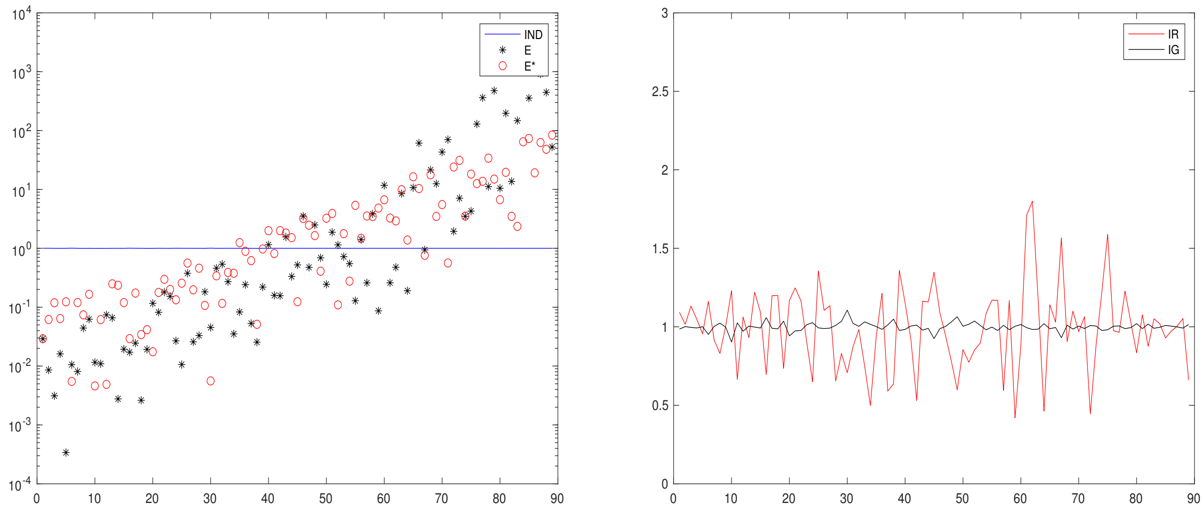

Figure 5: The identity (4.19) (left) and the values IR and ID (right) in the test T3.1.

We cannot say that the quantity $\mathcal{D}_R(v,\tau)$ (which is directly computable) is a majorant (or a minorant) of the quantity $\mathcal{D}_R(u,\tau) + \mathcal{D}_R(v,\sigma)$. However, in the vast majority of cases $\mathcal{D}_R(v,\tau)$ gives a correct presentation on this sum of measures (red line). To an even greater extent, this statement is true for the computable quantity $\mathcal{D}_G(\nabla v, y^*)$, which efficiently represents the measure $\mathcal{D}_G(\nabla u, y^*) + \mathcal{D}_G(\nabla v, p^*)$ (black line). Additional results that confirm this observation are presented

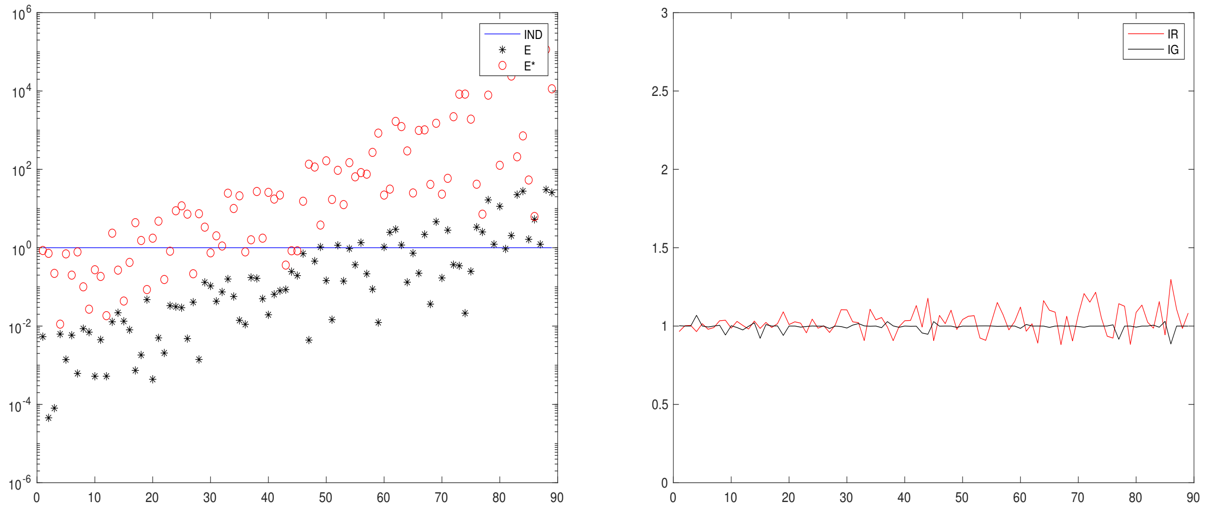

Figure 6: The identity (4.19) (left) and the values IR and ID (right) in the test T3.2.

in Figs. 5 and 6 below.

Example 3. Now we consider the problem (4.15) – (4.17) and verify numerically the identities (4.18) and (4.19). As in previous examples, the calculations confirmed that the identities hold. Here are some results.

In the test T3.1, we set $\alpha = 3$, $\rho(v) = \frac{1}{\mu}|v|^{\mu}$, $\mu = 1.5$, and $u = u_2$. Fig. 5 (left) shows the quantity IND:$=\frac{r.h.s.(4.19}{l.h.s.(4.19})$ in the tests.

In the series of examples T3.2, we set $\mu = 4$, $\alpha = 1.3$, and $u = u_3$. As before the identities (4.18) and (4.19) hold in all tests. Fig. 6 exposes the results, which are quite similar to those in Fig. 5.

6 Estimates of modeling errors

Since the identities (and respective estimates) were obtained by purely functional methods without using special properties of approximations, they can also be used to analyse errors of mathematical models. Next, we will look at two cases. In the first case, we compare the exact solutions of evolutionary problems that differ in the initial data and in the second case compare solutions with different spatial operators.

6.1 Errors generated by initial data

Let the functions $\widetilde{u}$ and $\widetilde{p^*}$ solve the problem (4.1), (4.2), and (4.3) with the initial condition $\widetilde{u}_0(x)$ instead of $u_0(x)$. Then, we can use (3.6) to estimate the difference between two solutions. We have

$$\mathcal{D}_G(\nabla\widetilde{u}, \widetilde{p^*}) = 0 \quad \text{and} \quad \mathcal{D}_R(\widetilde{u}, \widetilde{\sigma}) = 0.$$

Besides, it holds the equation $\operatorname{div}\widetilde{p^*} + f - \widetilde{\sigma} - \widetilde{u}_t = 0$. Therefore, the right hand side of (3.6) vanishes and we obtain

$$\int_0^T \boldsymbol{\mu}(\widetilde{u}, \widetilde{p^*}, \widetilde{\sigma}; u, p^*, \sigma)dx + \frac{1}{2}\|(\widetilde{u} - u)(\cdot, T)\|_\Omega^2 = \frac{1}{2}\|\widetilde{u}_0 - u_0\|_\Omega^2. \tag{6.1}$$

Notice that for any interval $(t, t + \Delta)$, $\Delta > 0$, the quantity $\mathbf{m}_{t,t+\Delta} := \int_t^{t+\Delta} \boldsymbol{\mu}(\widetilde{u}, \widetilde{p^*}, \widetilde{\sigma}; u, p^*, \sigma)dx$ is nonnegative, so that the first integral in (6.1) is a non–decreasing function of T. Since the right hand side does not depend on T, the norm $\|(\widetilde{u} - u)(\cdot, T)\|_\Omega$ is a bounded and non-increasing function of T. Thus, we conclude that

$$\mathbf{m}_{t,t+\Delta} \to 0 \quad \text{as } t \to +\infty. \tag{6.2}$$

The asymptotic relation (6.2) can be viewed as a form of the stabilization property well known for parabolic problems with monotone operators (e.g., see [7, 18]).

Using properties of g and g^* associated with a concrete class of problems one can deeper investigate convergence of $\widetilde{u}$ to u by estimating the first term in (6.1). Consider the functions g and g^* defined by (4.13). The identity (4.18) reads

$$\int_0^T (\boldsymbol{\mu}_\alpha(\widetilde{u}, u) + \boldsymbol{\mu}^*_{\alpha^*}(\widetilde{p^*}, p^*))dt + \frac{1}{2}\|(\widetilde{u} - u)(\cdot, T)\|_\Omega^2 = \frac{1}{2}\|\widetilde{u}_0 - u_0\|_\Omega^2. \tag{6.3}$$

Consider the case $\alpha > 2$. Since $\widetilde{u}$ and $\widetilde{p^*}$ satisfy (4.14), we have

$$\boldsymbol{\mu}_\alpha(\widetilde{u}, u) = \int_\Omega \left(\frac{1}{\alpha}|\nabla u|^\alpha + \frac{1}{\alpha^*}|\nabla\widetilde{u}|^\alpha - \nabla\widetilde{u}\cdot\nabla u|\nabla\widetilde{u}|^{\alpha-2}\right)dx,$$

$$\boldsymbol{\mu}^*_{\alpha^*}(\widetilde{p^*}, p^*) = \int_\Omega \left(\frac{1}{\alpha}|\nabla\widetilde{u}|^\alpha + \frac{1}{\alpha^*}|\nabla u|^\alpha - \nabla\widetilde{u}\cdot\nabla u|\nabla u|^{\alpha-2}\right)dx.$$

Therefore,

$$\int_0^T (\boldsymbol{\mu}_\alpha(\widetilde{u}, u) + \boldsymbol{\mu}^*_{\alpha^*}(\widetilde{p^*}, p^*))dt = \int_{Q_T} \left(|\nabla\widetilde{u}|^\alpha + |\nabla u|^\alpha - \nabla\widetilde{u}\cdot\nabla u(|\nabla u|^{\alpha-2} + |\nabla\widetilde{u}|^{\alpha-2})\right)dxdt$$

$$= 2\int_{Q_T} \mu^{\mathrm{s}}_\alpha(\nabla u, \nabla\widehat{u})dxdt \geq 2c^{\mathrm{s}}_\alpha\|\nabla e\|^\alpha_{Q_T}.$$

Hence (6.3) implies the estimate

$$2c^{\mathrm{s}}_\alpha\|\nabla e\|^\alpha_{\alpha,Q_T} + \frac{1}{2}\|e(\cdot, T)\|_\Omega^2 \leq \frac{1}{2}\|\widetilde{u}_0 - u_0\|_\Omega^2, \tag{6.4}$$

which shows that the norm $\|\nabla e\|_{\alpha,Q_T}$ is uniformly bounded with respect to T and, therefore, $\int_t^{t+\Delta} \|\nabla e\|^\alpha_\Omega dt$ must tend to zero as $t \to +\infty$.

Assume that $1 < \alpha < 2$. In this case, $\alpha^* > 2$ and it is convenient to rewrite the error identity in terms of fluxes. Using the relation $\nabla\widetilde{u} = |\widetilde{p^*}|^{\frac{2-\alpha}{\alpha-1}}\widetilde{p^*}$, we find that

$$\boldsymbol{\mu}_\alpha(\widetilde{u}, u) = \int\limits_{Q_T} (\frac{1}{\alpha}|\widetilde{p^*}|^{\alpha^*} + \frac{1}{\alpha^*}|p^*|^{\alpha^*} - p^* \cdot \widetilde{p^*}|\widetilde{p^*}|^{\alpha^*-2})dx,$$

$$\boldsymbol{\mu}_{\alpha^*}(\widetilde{p^*}, p^*) \int\limits_{Q_T} (\frac{1}{\alpha^*}|\widetilde{p^*}|^{\alpha^*} + \frac{1}{\alpha}|p^*|^{\alpha^*} - p^* \cdot \widetilde{p^*}|p^*|^{\alpha^*-2})dx$$

and

$$\int\limits_0^T (\boldsymbol{\mu}_\alpha(\widetilde{u}, u) + \boldsymbol{\mu}^*_{\alpha^*}(\widetilde{p^*}, p^*))dt = \int\limits_{Q_T} \Big(|y^*|^{\alpha^*} + |p^*|^{\alpha^*} - p^* \cdot y^*(|y^*|^{\alpha^*-2} + |p^*|^{\alpha^*-2})\Big)dxdt$$

$$= 2\int\limits_{Q_T} \mu^{\rm s}_{\alpha^*}(p^*, \widehat{p^*})dxdt \geq\ 2c^{\rm s}_{\alpha^*}\|e^*\|^{\alpha^*}_{\alpha^*,Q_T}. \quad (6.5)$$

From (6.1) and (6.5), we deduce the estimate

$$2c^{\rm s}_{\alpha^*}\|e^*\|^{\alpha}_{\alpha,Q_T} + \frac{1}{2}\|e(\cdot,T)\|^2_\Omega \leq \frac{1}{2}\|\widetilde{u}_0 - u_0\|^2_\Omega, \quad (6.6)$$

which shows that $\|e^*\|_{\alpha^*,Q_T}$ tends to zero as $T \to +\infty$ so that $\int\limits_t^{t+\Delta} \|e^*\|^{\alpha^*}_\Omega dt$ must tend to zero as $t \to +\infty$. Notice that the estimates (6.4) and (6.6) characterise the stabilization phenomenon quantitatively.

6.2 Errors generated by simplification

Identities (3.6), (3.11), (3.12), and (3.15) can be used to compare solutions of different mathematical models. For example, the problem (4.1)–(4.3) contains the matrix A whose entries are functions of x. We replace it by a simpler matrix $\widehat{A}$. Analogously, let $\widehat{\rho}$ and $\widehat{f}$ be certain simplifications of ρ and f, respectively. Thus, we arrive at the problem

$$\widehat{u}_t - {\rm div}\widehat{p^*} + \widehat{\rho}'(\widehat{u}) = \widehat{f}, \quad (6.7)$$

$$\widehat{p^*} = \widehat{A}\nabla\widehat{u}, \quad (6.8)$$

$$\widehat{u}(x,t) = 0 \text{ on } S_T, \qquad \widehat{u}(x,0) = u_0(x), \quad (6.9)$$

which is a simplified version of (4.1)–(4.3). Techniques of this kind (the so–called defeaturing of a model) are used in modern computer simulation methods. Simplifying the model by discarding irrelevant parts often allows us to get a good approximation at a significantly lower cost. However, in this case, it is important to evaluate the arising error caused by simplification. In [17] this question is discussed in the context of elliptic boundary value problems. Below we shortly consider it in connection with parabolic problems.

In view of (6.8), the identity (4.4) reads as follows:

$$\int_{Q_T} (|\nabla(\widehat{u} - u)|_A^2 + |\widehat{p^*} - p^*|_{A^{-1}}^2 + 2D_\rho(\widehat{u}, \sigma) + 2D_\rho(u, \widehat{\sigma}))dxdt$$

$$= \int_{Q_T} (B\nabla\widehat{u} \cdot \nabla\widehat{u} + D_\rho(\widehat{u}, \widehat{\sigma}) - 2(f - \widehat{f})e)dxdt, \qquad B := (\widehat{A} - A)A^{-1}(\widehat{A} - A). \quad (6.10)$$

It is natural to assume that simplification of f does not change integral values, so that $\int_\Omega (f - \widehat{f})dx = 0$ for all $t \in [0, T]$. Then,

$$\int_\Omega (f - \widehat{f})edx \leq \frac{C_P}{c_1} \|\nabla e\|_A \|f - \widehat{f}\|_\Omega, \quad (6.11)$$

where C_P is a constant in the Poincare inequality for the finctions having zero mean in Ω. We use (6.11) and the relation $\widehat{\rho}(\widehat{u}) + \widehat{\rho}^*(\widehat{\sigma}) - \widehat{\sigma}\,\widehat{u} = 0$ to represent (6.10) in the form

$$\int_{Q_T} \Big((1 - \beta(t))|\nabla(\widehat{u} - u)|_A^2 + |\widehat{p^*} - p^*|_{A^{-1}}^2 + 2(\widehat{\sigma}(\widehat{u}) - \sigma(u))(\widehat{u} - u)\Big)dxdt$$

$$= \int_{Q_T} (B\nabla\widehat{u} \cdot \nabla\widehat{u} + D_\rho(\widehat{u}, \widehat{\sigma}))dxdt + \int_0^T \frac{C_P^2}{c_1^2 \beta^2(t)} \|f - \widehat{f}\|_\Omega^2 dt, \quad (6.12)$$

where $\beta(t) \in (0, 1]$. Notice that and the norm $\|f - \widehat{f}\|_\Omega$ and the "deflection" matrix B are directly computable and the term $(\widehat{\sigma}(\widehat{u}) - \sigma(u))(\widehat{u} - u)$ is nonnegative. Therefore, the right hand side of (6.12) contains only known data and solution of the simplified problem (6.7)–(6.9). It provides a guaranteed upper bound of the modeling error.

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