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Abstract

We present a unified framework for goal-oriented estimates for elliptic and parabolic problems that combines the dual-weighted residual method with equilibrated flux and potential reconstruction. These frameworks allow to analyze simultaneously different approximation schemes for the space discretization of the primal and the dual problems such as conforming or nonconforming finite element methods, discontinuous Galerkin methods, or the finite volume method. Our main contribution is twofold: first in a unified framework we prove the splitting of the error into a fully computable estimator η and a remainder, second this remainder is estimated by the product of the fully computable energy-based error estimators of the primal and dual problems. Some illustrative numerical examples that validate our theoretical results are finally presented.

AMS (MOS) subject classification: 65N30, 65N15, 65M15.

Key Words: goal-oriented estimates, quantity of interest, elliptic and parabolic problems.

1 Introduction

Many engineering problems require computing some quantities of interest, like the local or global mean value of the solution. These quantities of interest are usually linear functionals on a vector space that contains the solution of the considered boundary value problem. Error estimation on such functionals is called goal-oriented error estimation. The main ingredient for a such error estimation relies on the computation of the solution of the dual problem. Several approaches have been proposed for elliptic problems, namely: goal-oriented error estimates based on energy norm of the errors on the solutions of the primal and dual problems (combined with different a posteriori methods to estimate these errors) [39, 36, 2, 1, 18], the dual weighted residual method, for which the local information derived from the dual solution is used in the form of weights multiplied by local residuals [7, 8, 3, 29, 6, 13, 35], the constitutive relation error based on Saint-Venant's

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principle [22, 21, 40, 41], and the equilibrated flux and/or potential reconstruction method based on higher order approximation of the dual problem and the construction of equilibrated fluxes and/or potential reconstruction of the solutions [30, 26, 28, 37, 44]. Let us note that "potential reconstruction" is an *ad hoc* denomination used in the literature, which corresponds to a given reconstructed (more regular) field of a scalar quantity. To the best of our knowledge, there exist few papers concerning goal-oriented error estimation for parabolic problems [31, 32, 33], where the estimation is based on energy norm of the errors on the solutions of the primal and dual problems. Goal-oriented a posteriori analysis of nonlinear problems (under quasi-static conditions or not) and/or nonlinear quantities of interest are considered in [21, 14, 20, 23, 24, 25, 11, 5, 43], and we believe that our approach can be used in such situations but it is outside the scope of this paper.

The goal of this paper is to extend the equilibrium flux reconstruction method (combined with the dual-weighted residual method) by proposing a unified framework for the approximation of general reaction-diffusion problems and to parabolic problems. Indeed based on equilibrated flux and potential reconstructions, we furnish a decomposition of the error $\mathcal{E}$ on the quantity of interest in the form

$$\mathcal{E} = \eta_{QOI} + \mathcal{R}, \tag{1}$$

where $\eta_{QOI} = \sum_{j=1}^{J} \eta_j$, each term η_j being fully computable, with some positive integer J depending on the problem, is our proposed estimator on the quantity of interest, while the remainder term $\mathcal{R}$ may depend on the solution of the primal and dual problems but for which we have the bound

$$|\mathcal{R}| \leq C\eta\eta^*, \tag{2}$$

where C is a positive constant independent of the meshsize (and time step size) as explicit as possible, and η (resp. η^*) is an estimator of the error of the solution of the primal (resp. dual) problem using an approximation in a finite dimensional space V_h (resp. V_h^*) not necessarily included into the energy space. These two properties lead to the new estimate

$$|\mathcal{E}| \leq |\eta_{QOI}| + C\eta\eta^*, \tag{3}$$

that was not obtained before in our settings. As a consequence, one can choose as error estimator $|\eta_{QOI}| + C\eta\eta^*$ to implement an adaptive algorithm, this will be investigated in a forthcoming paper.

On the other hand, if we use a higher order approximation space V_h^* to approximate the dual problem, one may hope to obtain an efficient error estimator (effectivity index close to unity) [2, 30], if this is the case, the remainder term is negligible, hence it may be disregarded and the sole term $|\eta_{QOI}|$ can be used as error estimator. More precisely since the estimator η_{QOI} and the right-hand side of (2) are fully computable, we can estimate the ratio

$$\frac{\mathcal{R}}{\eta_{QOI}},$$

during a refinement procedure based on the use of η_{QOI} and check if it tends to zero or not. In the positive case, due to the identity (1) this means that the ratio

$$\frac{\mathcal{E}}{\eta_{QOI}}$$

tends to one and will validate the asymptotic exactness of the estimator $|\eta_{QOI}|$. Note that there are some exceptions to this general rule as the example from subsection 4.1.2 shows. It is worth noting that this point does not seem to have already been reported in the literature.

For a purely diffusion problem with piecewise constant diffusion tensor and piecewise polynomial righ-hand sides, this approach was successfully developed in [28]. We here extend their approach to reaction-diffusion problems and to parabolic problems. For a diffusion problem, the decomposition (1) is also obtained in [30], but with an a priori bound for the remainder, which is less interesting for adaptive purposes.

In many cases, the use of $|\eta_{QOI}|$ is sufficient to obtain an efficient error estimator, but it has been observed in [21, 22, 28] that it can overestimate the error. As we can compare all η_i and $\eta\eta^*$, we can improve the approximated value of the quantity of interest by adding the dominant term from η_{QOI}. For instance if η_1 reveals to be a dominant term, we can add η_1 to the approximated value of the quantity of interest and use $|\eta_{QOI} - \eta_1| + C\eta\eta^*$ as error estimator, see [22, Figure 10] and [28, Remark 4.7 and Theorem 4.8].

In summary, the developed approach is flexible and may be then adapted to the different situations to treat. Furthermore, unlike the majority of the papers mentioned above that treat specific approximation of the (primal and dual) particular elliptic problems, our unified framework applies to general reaction-diffusion and parabolic problems and to various finite element methods (conforming or not) as well as finite volume methods.

Let us introduce some notation used in the paper. In the whole paper $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}, d \geq 2$, is an open, bounded and connected domain with a Lipschitz and polyhedral boundary $\partial\Omega$. The usual norm and semi-norm of $H^s(\Omega)$ $(s \geq 0)$ are denoted by $\|\cdot\|_{s,\Omega}$ and $|\cdot|_{s,\Omega}$, respectively. In this paper we consider real valued function spaces. For $s = 0$ we drop the index s. Similarly, the inner product (resp. norm) in $L^2(\Omega)$ will be denoted by $(\cdot,\cdot)$ (resp. $\|\cdot\|$). The duality pairing between $H^{-1}(\Omega)$ (the dual space of $H_0^1(\Omega)$) and $H_0^1(\Omega)$ will be denoted by $\langle\cdot,\cdot\rangle$. By $a \lesssim b$, we mean that there exists a constant $C > 0$ independent of a, b, such that $a \leq Cb$.

The paper is organized as follows. Section 2 is devoted to the reaction-diffusion problem. The problem is defined in subsection 2.1 and the goal oriented functional as well as the adjoint problem are introduced in subsection 2.2. Then the discrete setting is defined in subsection 2.3 and the error representation given in subsection 2.4. The main results about the reaction-diffusion problem are obtained in Theorems 2.1 and 2.4. Similarly, section 3 is devoted to the parabolic problem and follows the same process from subsection 3.1 to subsection 3.4. The main results about the parabolic problem are obtained in Theorems 3.1 and 3.3. Finally, section 4 presents some numerical tests in order to illustrate the previous theoretical results.

2 The reaction-diffusion problem

2.1 Problem definition

In this section we consider the following reaction-diffusion problem

$$\begin{cases} -\operatorname{div}(D\nabla u) + ru = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases} \tag{4}$$

where $D \in L^\infty(\Omega; \mathbb{R}^{d\times d})$ is a diffusion tensor which is supposed to be a symmetric matrix-valued function such that

$$D(x)\xi \cdot \xi \gtrsim |\xi|^2, \ \forall\, \xi \in \mathbb{R}^d, \text{ and a.e. } x \in \Omega,$$

while $r \in L^\infty(\Omega)$ is the reaction function supposed to be nonnegative. The source term f is supposed to be in $L^2(\Omega)$.

By setting

$$B(u,v) = \int_\Omega (D\nabla u \cdot \nabla v + ruv)\, dx,\ \forall\, u, v \in H_0^1(\Omega), \tag{5}$$

and

$$F(v) = \int_\Omega fv\, dx,\ \forall\, v \in H_0^1(\Omega),$$

the variational formulation of problem (4) is

$$B(u,v) = F(v),\ \forall\, v \in H_0^1(\Omega), \tag{6}$$

that has a unique (weak) solution u in $H_0^1(\Omega)$.

2.2 Goal-oriented functional and the adjoint problem

We here consider the output functional that represents the physical quantity of interest [30, 28] given by

$$Q(v) = \int_\Omega qv\, dx,\ \forall\, v \in L^2(\Omega), \tag{7}$$

where $q \in L^2(\Omega)$ is a given function. As we want to have

$$Q(u) = B(u,u^*) = F(u^*), \tag{8}$$

where u^* is solution of the dual problem, we define the adjoint problem as

$$B(v,u^*) = Q(v),\ \forall\, v \in H_0^1(\Omega), \tag{9}$$

that has a unique (weak) solution u^* in $H_0^1(\Omega)$. Accordingly its strong formulation is

$$\begin{cases} -\operatorname{div}(D\nabla u^*) + ru^* = q & \text{in } \Omega, \\ u^* = 0 & \text{on } \partial\Omega. \end{cases} \tag{10}$$

Note finally that (9) is equivalent to

$$B(u^*,v) = Q(v),\ \forall\, v \in H_0^1(\Omega),$$

because B is here symmetric.

2.3 The discrete setting of the reaction-diffusion problem

To discretize problems (6) and (9), we suppose given a partition $\mathcal{T}$ of Ω into polygonal elements T that covers exactly Ω. For simplicity, we assume that the mesh is simplicial and matching (extensions to general polygonal and nonmatching meshes are possible). On such a mesh we introduce the so-called broken Sobolev space

$$H^1(\mathcal{T}) = \{v \in L^2(\Omega) \,|\, v_{|T} \in H^1(T),\ \forall\, T \in \mathcal{T}\}.$$

As in [17, 28], in order to analyse simultaneously different approximation schemes, the primal problem is approximated in a finite dimensional subspace V_h of $H^1(\mathcal{T})$, while the dual problem will be approximated in a finite dimensional subspace V_h^* of $H^1(\mathcal{T})$, that may be different from V_h. In other words, we suppose given an approximation $u_h \in V_h$ of the solution u of (6) and $u_h^* \in V_h^*$ of the solution u^* of (9). We further assume that a flux reconstruction θ_h is available (using u_h and the datum f), belongs to $H(\operatorname{div},\Omega)$ and satisfies the following conservation properties (compare with [17, identity (18)])

$$(\operatorname{div}\theta_h + ru_h - f, 1)_T = 0,\ \forall\, T \in \mathcal{T}. \tag{11}$$

In the same manner, we assume that a flux reconstruction θ_h^* can be constructed, belongs to $H(\mathrm{div},\Omega)$ and satisfies the following conservation properties

$$(\mathrm{div}\,\theta_h^* + ru_h^* - q, 1)_T = 0,\ \forall\, T \in \mathcal{T}. \tag{12}$$

Using θ_h and θ_h^*, in the spirit of [30] (see also [28]), let us show that the error $\mathcal{E} = Q(u) - Q(u_h)$ on the quantity of interest can be expressed into a fully computable expression and a remainder that will be estimated by a fully computable quantity (but is usually of higher order and can then be disregarded). Let us note that thanks to the linearity of Q, we also have $\mathcal{E} = Q(u - u_h)$.

2.4 The error representation of the reaction-diffusion problem

Theorem 2.1 *Let $s_h \in H_0^1(\Omega)$ be a potential reconstruction of u_h, then we have*

$$\mathcal{E} = Q(u - u_h) = \eta_{QOI} + \mathcal{R}, \tag{13}$$

where the estimator η_{QOI} is given by

$$\begin{aligned} \eta_{QOI} &= \int_\Omega q(s_h - u_h)\,dx \\ &+ \int_\Omega (f - \mathrm{div}\,\theta_h - ru_h)u_h^*\,dx \\ &+ \int_\Omega (\theta_h + D\nabla s_h)\cdot D^{-1}\theta_h^*\,dx \\ &- \int_\Omega ru_h^*(s_h - u_h)\,dx, \end{aligned} \tag{14}$$

while the remainder term $\mathcal{R}$ is defined by

$$\mathcal{R} = \mathcal{R}_1 + \mathcal{R}_2 + \mathcal{R}_3 \qquad \textit{with}$$

$$\begin{aligned} \mathcal{R}_1 &= \int_\Omega (f - \mathrm{div}\,\theta_h - ru_h)(u^* - u_h^*)\,dx, \\ \mathcal{R}_2 &= -\int_\Omega (\theta_h + D\nabla s_h)\cdot(D^{-1}\theta_h^* + \nabla u^*)\,dx, \\ \mathcal{R}_3 &= -\int_\Omega r(u^* - u_h^*)(s_h - u_h)\,dx. \end{aligned}$$

Proof. By the definition of the error and Green's formula we have

$$\mathcal{E} = F(u^*) - Q(u_h).$$

Introducing artificially s_h and using (9), this is equivalent to

$$\begin{aligned} \mathcal{E} &= F(u^*) - Q(u_h - s_h) \\ &- \int_\Omega (D\nabla u^*\cdot\nabla s_h + ru^* s_h)\,dx. \end{aligned} \tag{15}$$

Adding and subtracting the term

$$\int_\Omega \nabla u^*\cdot\theta_h\,dx$$

we find

$$\begin{aligned}\mathcal{E} &= F(u^*) - Q(u_h - s_h) \\ &- \int_\Omega \nabla u^* \cdot (D\nabla s_h + \theta_h)\, dx \\ &+ \int_\Omega (\nabla u^* \cdot \theta_h - r u^* s_h)\, dx.\end{aligned}$$

Using Green's formula in the fourth term of this right-hand side we find

$$\begin{aligned}\mathcal{E} &= F(u^*) - Q(u_h - s_h) \\ &- \int_\Omega \nabla u^* \cdot (D\nabla s_h + \theta_h)\, dx \\ &+ \int_\Omega u^* (-\operatorname{div} \theta_h - r s_h)\, dx.\end{aligned}$$

Replacing s_h by $s_h - u_h + u_h$ in this last term and recalling that $F(u^*) = \int_\Omega f u^*\, dx$, we obtain

$$\begin{aligned}\mathcal{E} &= -Q(u_h - s_h) \\ &- \int_\Omega \nabla u^* \cdot (D\nabla s_h + \theta_h)\, dx \\ &+ \int_\Omega u^* (f - \operatorname{div} \theta_h - r u_h)\, dx \\ &- \int_\Omega r u^* (s_h - u_h)\, dx.\end{aligned}$$

Writing $u^* = u_h^* + u^* - u_h^*$ and $D\nabla u^* = -\theta_h^* + D\nabla u^* + \theta_h^*$, we arrive at (13). ■

Note that we do not need the conservation properties (11) and (12) to obtain the splitting (13) from Theorem 2.1, but they are minimal assumptions to guarantee that θ_h (resp. θ_h^*) is a reasonable approximation of the continuous flux $-D\nabla u$ (resp. $-D\nabla u^*$).

Remark 2.2 *In the case where $u_h \in H_0^1(\Omega)$, then we take $s_h = u_h$, so that the first and the fourth terms arising in the right-hand side of* (14) *as well as $\mathcal{R}_3$ are equal to zero.*

Remark 2.3 (Comparison with earlier literature)
1. In the spirit of [30, Theorem 1 and Remark 1], our estimator η_{QOI} admits the decomposition

$$\eta_{QOI} = \eta_{\mathcal{O}} + \eta_{\nabla} + \eta_{\mathcal{H}},$$

where

$$\begin{aligned}\eta_{\mathcal{O}} &= \int_\Omega (f - \operatorname{div} \theta_h - r u_h) u_h^*\, dx, \\ \eta_{\nabla} &= \int_\Omega (\theta_h + D\nabla s_h) \cdot D^{-1} \theta_h^*\, dx \\ \eta_{\mathcal{H}} &= \int_\Omega q(s_h - u_h)\, dx - \int_\Omega r u_h^* (s_h - u_h)\, dx.\end{aligned}$$

Here $\eta_{\mathcal{O}}$ would represent the data oscillation with respect to the primal problem weighted by the dual approximate solution if $\operatorname{div} \theta_h + r u_h$ would be equal to the $L^2(\Omega)$-projection of f on the approximation space used to compute u_h (it slightly differs from the one from [30] because of our weaker assumption (11)), the flux estimator η_{∇} measures the deviation of $-D\nabla s_h$ from the reconstructed flux θ_h and $\eta_{\mathcal{H}}$ measures the deviation of u_h from $H_0^1(\Omega)$, these two last quantities also differ from the ones from [30] due to the use of the reconstructed field s_h.

2. We recover the splitting (4.13) from [28, Remark 4.7] if $r = 0$, D is constant and the data f and q are piecewise polynomials simply by replacing in the expression of η_∇ from (14) the factor θ_h^* by $-D\nabla s_h^*$, where $s_h^* \in H_0^1(\Omega)$ is a potential reconstruction of u_h^* and using the term

$$\int_\Omega (\theta_h + D\nabla s_h) \cdot D^{-1}(\theta_h^* + D\nabla s_h^*)\, dx,$$

in the remainder. More generally in the expression of η_∇, we may replace the factor θ_h^* by

$$\theta_h^{*,\alpha} = (1-\alpha)\theta_h^* - \alpha D\nabla s_h^*,$$

with $\alpha \in \mathbb{R}$ and plug the term

$$\int_\Omega (\theta_h + D\nabla s_h) \cdot D^{-1}(\theta_h^* - \theta_h^{*,\alpha})\, dx = \alpha \int_\Omega (\theta_h + D\nabla s_h) \cdot D^{-1}(\theta_h^* + D\nabla s_h^*)\, dx$$

in the remainder. For $\alpha = \frac{1}{2}$, we recover the splitting (4.17) from [28, Remark 4.7].

Let us now show that the remainder can be explicitly estimated using the error estimators for u and u^* obtained in [17, Theorem 7]. Namely denote by η (resp. η^*) the error estimator mainly obtained in this reference (for D diagonal and constant but easily extended to the case treated here) using the discrete spaces V_h (resp. V_h^*) to approximate the solution u of the primal problem (6) (resp. u^* of the dual problem (9)), so that

$$\|u - u_h\|_h \le \eta, \tag{16}$$
$$\|u^* - u_h^*\|_h \le \eta^*, \tag{17}$$

where the mesh-depending norm $\|\cdot\|_h$ is defined by

$$\|w\|_h^2 = \|D^{\frac{1}{2}}\nabla_h w\|^2 + \|r^{\frac{1}{2}} w\|^2,\ \forall\, w \in H_0^1(\Omega) \cup V_h,$$

where $\nabla_h w$ means the piecewise gradient of w, namely

$$\nabla_h w = \nabla w \text{ on } T,\ \forall\, T \in \mathcal{T},$$

and

$$\eta^2 = \sum_{T\in\mathcal{T}} (\eta_{NC,T}^2 + \eta_{R,T}^2 + \eta_{DF,T}^2),$$

with

$$\begin{aligned} \eta_{NC,T} &= \|u_h - s_h\|_{h,T}, \\ \eta_{R,T} &= m_T \|f - \operatorname{div}\theta_h + r u_h\|_T, \\ \eta_{DF,T} &= \|D^{-\frac{1}{2}}(\theta_h + D\nabla u_h)\|_T, \end{aligned}$$

recalling that

$$\|w\|_{h,T} = \int_T (D\nabla w \cdot \nabla w + r w^2)\, dx,\ \forall\, w \in H^1(T),$$
$$m_T := \min\{C_{P,T}\|D^{-\frac{1}{2}}\|_{\infty,T}, \|r^{-\frac{1}{2}}\|_{\infty,T}\},$$

and that $C_{P,T}$ is the Poincaré constant, namely the smallest positive constant such that

$$\|\varphi - \mathcal{M}_T\varphi\|_T \le C_{P,T}\|\nabla\varphi\|_T,\ \forall\, \varphi \in H^1(T), \tag{18}$$

where $\mathcal{M}_T\varphi$ is the mean of φ in T, namely

$$\mathcal{M}_T\varphi = |T|^{-1}\int_T \varphi(x)\,dx.$$

Let us note that since T is considered being a convex bounded Lipschitz domain, we can introduce the constant C_P such that $C_{P,T} = C_P\,h_T$, so that (18) is equivalent to

$$\|\varphi - \mathcal{M}_T\varphi\|_T \le C_P\,h_T\,\|\nabla\varphi\|_T,\ \forall\,\varphi\in H^1(T),$$

where C_P is no more dependent on T but satisfies $C_P \le \pi^{-1}$, see [4, Theorem 3.2] (see also [38]).

We further notice that by convention we set $\|r^{-\frac{1}{2}}\|_{\infty,T} = \infty$ if $\inf_{x\in T} r(x) = 0$. The expression of η^* is similar by replacing u_h by u_h^*, θ_h by θ_h^*, s_h by s_h^*, and f by q.

Theorem 2.4 *With η and η^* as defined before, we have*

$$|\mathcal{R}| \le 4\eta\eta^*. \tag{19}$$

Proof. We estimate each term of $\mathcal{R}$ separetely. For the first term, using the property (11), we have

$$\mathcal{R}_1 = \int_\Omega (f-\operatorname{div}\theta_h - ru_h)(u^*-u_h^*)\,dx = \sum_{T\in\mathcal{T}}\int_T (f-\operatorname{div}\theta_h - ru_h)\left((u^*-u_h^*) - \mathcal{M}_T(u^*-u_h^*)\right)\,dx.$$

By Cauchy-Schwarz's inequality, we find

$$|\mathcal{R}_1| \le \sum_{T\in\mathcal{T}} \|f-\operatorname{div}\theta_h - ru_h\|_T\|(u^*-u_h^*) - \mathcal{M}_T(u^*-u_h^*)\|_T. \tag{20}$$

Let us now show that

$$\|(u^*-u_h^*) - \mathcal{M}_T(u^*-u_h^*)\|_T \le m_T\|u^*-u_h^*\|_{h,T}. \tag{21}$$

Indeed first using the estimate (18), we find

$$\begin{aligned}\|(u^*-u_h^*) - \mathcal{M}_T(u^*-u_h^*)\|_T &\le C_{P,T}\,\|\nabla(u^*-u_h^*)\|_T\\ &\le C_{P,T}\,\|D^{-\frac{1}{2}}\|_{\infty,T}\|D^{\frac{1}{2}}\nabla(u^*-u_h^*)\|_T\\ &\le C_{P,T}\,\|D^{-\frac{1}{2}}\|_{\infty,T}\|u^*-u_h^*\|_{h,T}.\end{aligned}$$

This shows (21) if $\inf_{x\in T} r(x) = 0$. On the contrary if $\inf_{x\in T} r(x) > 0$, then we directly write

$$\|(u^*-u_h^*) - \mathcal{M}_T(u^*-u_h^*)\|_T \le \|u^*-u_h^*\|_T \le \|r^{-\frac{1}{2}}\|_{\infty,T}\|(r^{\frac{1}{2}}(u^*-u_h^*)\|_T.$$

In that case, this estimate combined with the previous one yield (21).

Coming back to (20) and using (21), we get

$$|\mathcal{R}_1| \le \sum_{T\in\mathcal{T}} \|f-\operatorname{div}\theta_h - ru_h\|_T m_T\|u^*-u_h^*\|_{h,T}.$$

By discrete Cauchy-Schwarz's inequality, the definition of the estimator η and the estimate (17), we find

$$|\mathcal{R}_1| \le \eta\eta^*. \tag{22}$$

For the second term, by Cauchy-Schwarz's inequality, we have

$$|\mathcal{R}_2| \le \|D^{-\frac{1}{2}}(\theta_h + D\nabla s_h)\|\|D^{-\frac{1}{2}}(\theta_h^* + D\nabla u^*)\|.$$

Replacing ∇u^* by $\nabla_h(u^* - u_h^*) + \nabla_h u_h^*$ and using the triangular inequality, one gets

$$|\mathcal{R}_2| \leq \|D^{-\frac{1}{2}}(\theta_h + D\nabla s_h)\|(\|D^{-\frac{1}{2}}(\theta_h^* + D\nabla_h u_h^*)\| + \|D^{\frac{1}{2}}\nabla_h(u^* - u_h^*)\|).$$

Using (17) and the definition of η and η^*, we obtain

$$|\mathcal{R}_2| \leq 2\eta\eta^*. \tag{23}$$

For the last term $\mathcal{R}_3$, again Cauchy-Schwarz's inequality yields

$$\begin{aligned} |\mathcal{R}_3| = \left| \int_\Omega r(u^* - u_h^*)(s_h - u_h)\, dx \right| &\leq \|r^{\frac{1}{2}}(u^* - u_h^*)\| \|r^{\frac{1}{2}}(s_h - u_h)\| \\ &\leq \eta\eta^*, \end{aligned}$$

again by (17) and the defintion of η.

This estimate and the estimates (22), (23) lead to the conclusion. ■

Remark 2.5 According to the observations from [22, Figure 10] (see also [28]), the flux estimator may overestimate the error due to the previous Theorem 2.4 and point 2 of Remark 2.3, therefore, if necessary, it may be added to the approximate quantity of interest.

Remark 2.6 Since the estimator η_{QOI} and the right-hand side of (19) are fully computable, we can estimate the ratio

$$\frac{\mathcal{R}}{\eta_{QOI}},$$

by computing $\dfrac{4\eta\eta*}{\eta_{QOI}}$, during a refinement procedure based on the use of η_{QOI} and check if it tends to zero or not. In the positive case, due to the identity (13) this means that the ratio

$$\frac{\mathcal{E}}{\eta_{QOI}}$$

tends to one and will validate the asymptotic exactness of the estimator η_{QOI}.

In any case, we can use the estimate

$$|\mathcal{E}| \leq |\eta_{QOI}| + 4\eta\eta^*, \tag{24}$$

that follows from (13) and (19), and then choose as estimator $|\eta_{QOI}| + 4\eta\eta^*$ to implement an adaptive algorithm.

Remark 2.7 As mentioned in the introduction, one may hope to obtain an effectivity index close to unity if we use a higher order approximation space V_h^* to approximate the dual problem [2, 30]. This fact is confirmed by the numerical tests from subsection 4.1. However approximating u^* by a higher order finite element scheme takes more CPU time, which limits the practical interest of such techniques. To overcome this issue, we can use a local higher order approximation of $u_h^* \in V_h$ as proposed in [8, p. 41], a local subproblems approach (each subproblem lives on a small subset of elements, that can be solved efficiently and in parallel using higher order finite elements) as proposed in [42, p. 196], or a reconstruction of $u_h \in V_h$ and $u_h^* \in V_h$ on a coarse mesh of size $2h$ with a higher order approximation as proposed in [42, p. 196]. These alternative solutions can be used as they enter in our framework, recalling that in our approach u_h^* is not necessarily a Galerkin approximation of the solution u^* of the dual problem and since V_h and V_h^* are not necessarily included into $H_0^1(\Omega)$.

Remark 2.8 Our approach applies to the diffusion-reaction equation with mixed boundary conditions

$$\left\{\begin{array}{cc} -\operatorname{div}(D\nabla u) + ru = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ -D\nabla u \cdot \mathbf{n} = g_N & \text{on } \Gamma_N, \end{array}\right. \tag{25}$$

where Γ_D and Γ_N are two open parts of $\partial\Omega$ such that $\bar{\Gamma}_D \cap \bar{\Gamma}_N = \partial\Omega$, and $g_N \in L^2(\Gamma_N)$. Its variational formulation is (6) by replacing $H_0^1(\Omega)$, by

$$H^1_{\Gamma_D}(\Omega) = \{u \in H^1(\Omega) \mid u = 0 \text{ on } \Gamma_D\},$$

with B defined by (5) and

$$F(v) = \int_\Omega fv\,dx - \int_{\Gamma_N} g_N v\,d\sigma(x),\ \forall\, v \in H^1_{\Gamma_D}(\Omega),$$

while the weak formulation of the adjoint problem is still (9) by replacing $H_0^1(\Omega)$ by $H^1_{\Gamma_D}(\Omega)$.

For this problem, the flux reconstruction $\theta_h \in H(\operatorname{div},\Omega)$ has to satisfy (11) but furthermore

$$\int_e (\theta_h \cdot \mathbf{n} - g_N)\,d\sigma(x) = 0,\ \forall\, e \in \mathcal{E}_h \text{ s.t. } e \subset \bar{\Gamma}_N,$$

while the potential reconstruction s_h of u_h has to be in $H^1_{\Gamma_D}(\Omega) \cap V_h$ and to satisfy $\int_\Omega s_h\,dx = 0$ if meas $\Gamma_D = 0$ and $r = 0$ (a.e.). Similarly the flux reconstruction $\theta_h^* \in H(\operatorname{div},\Omega)$ has to satisfy (12) and

$$\int_e \theta_h^* \cdot \mathbf{n}\,d\sigma(x) = 0,\ \forall\, e \in \mathcal{E}_h \text{ s.t. } e \subset \bar{\Gamma}_N,$$

while s_h^* has to be in $H^1_{\Gamma_D}(\Omega)$ and $\int_\Omega s_h^*\,dx = 0$ if meas $\Gamma_D = 0$ and $r = 0$ (a.e.). With these slight modifications, Theorem 2.1 remains valid with the same definition for the estimator except for $\eta_{\mathcal{O}}$ which is here given by

$$\eta_{\mathcal{O}} = \int_\Omega (f - \operatorname{div}\theta_h - ru_h)u_h^*\,dx + \int_{\Gamma_N} (\theta_h \cdot \mathbf{n} - g_N)u_h^*\,d\sigma(x),$$

the remainder being modified accordingly. Further using the results from [15, 17], estimates like (16)-(17) are available, allowing to prove a result like Theorem 2.4.

Remark 2.9 Even if it is beyond the scope of this paper, our approach also applies to the convection-diffusion-reaction equation

$$\left\{\begin{array}{cc} -\operatorname{div}(D\nabla u - \mathbf{w}u) + ru = f & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{array}\right. \tag{26}$$

where $\mathbf{w} \in L^\infty(\Omega)^d$ is divergence-free. Its weak formulation is given by (6) with

$$B(u,v) = \int_\Omega ((D\nabla u - \mathbf{w}u)\cdot\nabla v + ruv)\,dx,\ \forall\, u,v \in H_0^1(\Omega),$$

while the weak formulation of the adjoint problem is given by (9). In this setting, Theorem 2.1 remains valid with a slight difference in the definition of η_∇ that here takes the form

$$\eta_\nabla = \int_\Omega (\theta_h + D\nabla s_h - \mathbf{w}s_h)\cdot D^{-1}(\theta_h^* + \mathbf{w}u_h^*)\,dx.$$

Further using the results from [15, 17], estimates like (16)-(17) are available, allowing to prove a result like Theorem 2.4.

Remark 2.10 *As in [28], the quantity of interest could be replaced by*

$$Q(v) = \int_\Omega qv\,dx + \langle D\nabla v \cdot \mathbf{n}, u_D^* \rangle,$$

for all $v \in H^1(\Omega)$ *such that* $\mathrm{div}(D\nabla v) \in L^2(\Omega)$*, where* $\mathbf{n}$ *is the outward unit normal vector along* $\partial\Omega$*,* u_D^* *is a fixed function in* $H^{1/2}(\partial\Omega)$ *and the bracket means the duality pair between* $H^{-1/2}(\partial\Omega)$ *and* $H^{1/2}(\partial\Omega)$*. In such a case, Theorem 2.1 remains valid by adding to* η_{QOI} *the term*

$$\langle (D\nabla u_h + \theta_h) \cdot \mathbf{n}, u_D^* \rangle$$

Moreover assuming that $s_h = u_D^*$ *on the boundary, then the estimate* (17) *remains valid (up to some multiplicative factors in the definition of the different terms of* η^**, see Lemma 7.1 of [45] and the proof of Theorem 2 of [17]); and consequently Thereom 2.4 remains also valid.*

3 The parabolic problem

3.1 Problem definition

We here consider the following heat type equation:

$$\begin{cases} \dfrac{\partial u}{\partial t} - \mathrm{div}(D\nabla u) = f & \text{in } C := \Omega \times I, \\ u(.,t) = 0 & \text{on } \partial\Omega \times I, \\ u(.,0) = u_0 & \text{in } \Omega, \end{cases} \tag{27}$$

where the time interval $I = (0,T)$, with a fixed time T, $D \in L^\infty(\Omega; \mathbb{R}^{d\times d})$ is a diffusion tensor satisfying the same assumptions than in section 2. The datum f is supposed to satisfy $f \in L^2(C)$ and the initial value $u_0 \in L^2(\Omega)$. Under these assumptions, problem (27) or equivalently

$$\langle \partial_t u(\cdot,t), v\rangle + (D\nabla u(\cdot,t), \nabla v) = (f(\cdot,t), v),\ \forall\, v \in H_0^1(\Omega),\ \forall\ \text{ a.e. } t \in I, \tag{28}$$

has a unique (weak) solution in $Y := \{y \in X := L^2(I; H_0^1(\Omega)) \,|\, \partial_t u \in X' = L^2(I; H^{-1}(\Omega))\}$. Note that Y is a Hilbert space with the norm

$$\|y\|_Y = \|y\|_X + \|\partial_t y\|_{X'},$$

where the space-time energy norm is given by

$$\|y\|_X^2 := \int_0^T \|D^{\frac{1}{2}}\nabla y\|^2\,dt,\ \forall\, y \in X.$$

Let us further notice that by [27, Theorem 3.4.1], Y is continuously embedded into $C(\bar{I}; L^2(\Omega))$, which gives a meaning to the initial condition in (27). For further purposes, we denote by C_Y the smallest positive constant such that

$$\|y\|_{C([0,T];L^2(\Omega))} \le C_Y \|y\|_Y,\ \forall\, y \in Y. \tag{29}$$

Note that an explicit upper bound on C_Y can be obtained, namely if we denote by C_Ω the smallest positive constant such that

$$\|u\|_\Omega \le C_\Omega \|D^{\frac{1}{2}}\nabla u\|,\ \forall\, u \in H_0^1(\Omega),$$

then one can show that

$$C_Y \le \frac{C_\Omega}{\sqrt{T}} + \sqrt{2},$$

see [12, p. 55]. Let us finally remark that $C_\Omega \le \|D^{\frac{1}{2}}\|_{\infty,\Omega}\frac{\sqrt{d}\pi}{d_\Omega}$, where d_Ω is the diameter of Ω, see [10, Theorem VI-3 and p. 301]

3.2 The goal oriented functional and the adjoint problem

We here consider the output functional that represents the physical quantity of interest given by (see [32, 33] for a similar choice)

$$Q(v) = \int_I (g(\cdot,t), v)\, dt + (u_T^*, v(\cdot,T)),\ \forall\ v \in C(\bar{I}, L^2(\Omega)), \tag{30}$$

where $g \in L^2(C)$ and $u_T^* \in L^2(\Omega)$ are given functions. As before the formulation of the adjoint problem is based on the fact that we want to have the identity (8), where u^* is solution of the dual problem. We therefore reformulate problem (28) in the space-time variables, by taking a test-function $v \in Y$ and integrating in I to find

$$B(u,v) = F(v),\ \forall v \in Y,$$

where

$$B(u,v) = \int_I \left(\langle \partial_t u(\cdot,t), v\rangle + (D\nabla u(\cdot,t), \nabla v)\right)\, dt + \int_\Omega u(x,0)v(x,0)\, dx,$$
$$F(v) = \int_I \int_\Omega f(x,t)v(x,t)\, dxdt + \int_\Omega u_0(x)v(x,0)\, dx.$$

Hence the adjoint problem consists in finding $u^* \in Y$ solution of

$$B(v,u^*) = Q(v),\ \forall v \in Y. \tag{31}$$

Indeed from the definition of B and Q, this problem is equivalent to

$$\int_I \left(\langle \partial_t v(\cdot,t), u^*\rangle + (D\nabla v(\cdot,t), \nabla u^*)\right)\, dt + \int_\Omega u(x,0)u^*(x,0)\, dx = \int_I (g(\cdot,t), v)\, dt + (u_T^*, v(\cdot,T)).$$

Due to the regularities of v and u^*, the following integration by parts formula is valid

$$\int_I \langle \partial_t v(\cdot,t), u^*(\cdot,t)\rangle\, dt = -\int_I \langle \partial_t u^*(\cdot,t), v(\cdot,t)\rangle\, dt + (v(\cdot,T), u^*(\cdot,T)) - (v(\cdot,0), u^*(\cdot,0)).$$

Inserting this identity into the previous one, we obtain

$$\int_I \left(-\langle \partial_t u^*(\cdot,t), v(\cdot,t)\rangle + (D\nabla u^*(\cdot,t), \nabla v) - (g,v)\right)\, dt + \int_\Omega (v(x,T)(u^*(x,T) - u_T^*(x))\, dx = 0,\ \forall v \in Y.$$

Taking appropriate test-functions v and using Green's formula, we find that u^* is solution of the backward heat type equation

$$\begin{cases} -\dfrac{\partial u^*}{\partial t} - \mathrm{div}(D\nabla u^*) = g & \text{in } C := \Omega \times I, \\ u^*(.,t) = 0 & \text{on } \partial\Omega \times I, \\ u^*(.,T) = u_T^* & \text{in } \Omega. \end{cases} \tag{32}$$

As before, its weak formulation is

$$-\langle \partial_t u^*(\cdot,t), v\rangle + (D\nabla u^*(\cdot,t), \nabla v) = (g(\cdot,t), v),\ \forall\ v \in H_0^1(\Omega),\ \forall\ \text{ a.e. } t \in I, \tag{33}$$

whose unique (weak) solution u^* has the same regularity than before, namely $u^* \in L^2(I; H_0^1(\Omega)) \cap C(\bar{I}; L^2(\Omega))$ with $\partial_t u^* \in L^2(I; H^{-1}(\Omega))$. Integrating (33) in time and using the arguments above, we see that this solution satisfies (31) and directly deduce that the identity (8) holds, which in particular yields

$$Q(u) = \int_I (f(\cdot,t), u^*(\cdot,t))\, dt + (u_0, u^*(0)). \tag{34}$$

3.3 The discrete setting of the parabolic problem

To discretize problem (27), we suppose given a sequence of discrete times $\{t^n\}_{n=0}^N$, with $N \in \mathbb{N}^*$ such that $t^0 = 0$, $t^N = T$ and $t^n < t^{n+1}$, for all $n = 0, \cdots, N-1$. For all $n = 1, \cdots, N$, we define $I_n = [t^{n-1}, t^n[$ and let $\tau^n = t^n - t^{n-1}$ be its length. For all $n = 0, \cdots, N$, we also suppose given a partition $\mathcal{T}^n$ of polygonal elements T that covers exactly Ω. As before for simplicity, we assume that the meshes are simplicial and matching. For all $n = 0, \cdots, N$, we set $h^n = \max_{T \in \mathcal{T}^n} h_T$.

In a standard a posteriori error analysis of the primal problem (27), the initial mesh $\mathcal{T}^0$ is used to approximate the initial data u_0, while for $n \geq 1$, $\mathcal{T}^n$ corresponds to a refinement or a coarsening of $\mathcal{T}^{n-1}$ as time evolves. Here the situation is more involved since our estimator is also based on the solution of the dual problem. Anyway, since we use an implicit scheme in time (for the primal and the dual problems), we suppose that for all $n = 1, \cdots, N$, $\mathcal{T}^{n-1}$ and $\mathcal{T}^n$ has a common refinement mesh $\mathcal{T}^{n-1,n}$.

For all $n = 0, \cdots, N$, we finally suppose given two finite-dimensional spaces V_h^n and $V_h^{*,n}$ of $H^1(\mathcal{T}^n)$.

For a vector space W (of functions defined on Ω), and $k = 0$ or 1, we denote by

$$P_\tau^k(W) := \{v \in L^2(0,T,W) \,|\, v_{|I_n} \in \mathbb{P}^k(I_n, W),\ \forall\, n = 1, \cdots, N\},$$

where $\mathbb{P}^0(I_n, W)$ (resp. $\mathbb{P}^1(I_n, W)$) denotes the space of functions from I_n to W constant (resp. affine) in time. Note that any function $v \in P_\tau^1(W)$ is uniquely determined by its values $v^n := v(\cdot, t^n)$ at t^n, $n = 0, \cdots, N$. On the contrary, any function $v \in P_\tau^0(W)$ is uniquely determined by its values $v^n = v(\cdot, t)_{|I_n}$, $n = 1, \cdots, N$. Let us finally observe that the time derivative $\partial_t v$ of $v \in P_\tau^1(W)$ belongs to $P_\tau^0(W)$ and that

$$(\partial_t v)^n = \partial_t v_{|I_n} = \frac{v^n - v^{n-1}}{\tau^n},\ \forall\, n = 1, \cdots, N. \tag{35}$$

For shortness we set $\partial_t v^n = (\partial_t v)^n$.

Let us also introduce an approximation $\tilde{f} \in P_\tau^0(L^2(\Omega))$ of f defined by

$$\tilde{f}^n = \frac{1}{\tau_n} \int_{I_n} f(\cdot, t)\, dt,\ \forall\, n = 0, \cdots, N.$$

As in [16], we suppose given an approximation $u_{h\tau} \in P_\tau^1(L^2(\Omega))$ of the solution u of (28) such that $u_{h\tau}^n = u_{h\tau}(t^n) \in V_h^n$, for all $n = 0, \cdots, N$. Similarly, we suppose given an approximation $u_{h\tau}^* \in P_\tau^1(L^2(\Omega))$ of the solution u^* of (33) such that $u_{h\tau}^{*,n} = u_{h\tau}^*(t^n) \in V_h^{*,n}$, for all $n = 0, \cdots, N$.

We also assume that a flux reconstruction $\theta_{h\tau}$ and a potential reconstruction $s_{h\tau}$ are available and satisfy the following conservation properties. $\theta_{h\tau} \in P_\tau^0(H(\mathrm{div}, \Omega))$ and satisfies (compare with [16, identity (4.5)])

$$(\partial_t u_{h\tau}^n + \mathrm{div}\, \theta_{h\tau}^n - \tilde{f}^n, 1)_T = 0,\ \forall\, T \in \mathcal{T}^n, n = 1, \cdots, N. \tag{36}$$

On the other hand, $s_{h\tau} \in P_\tau^1(H_0^1(\Omega))$ and satisfies

$$(s_{h\tau}^n, 1)_{T'} = (u_{h\tau}^n, 1)_{T'},\ \forall\, T' \in \mathcal{T}^{n,n+1}, n = 0, \cdots, N. \tag{37}$$

A direct consequence of this property is that (see [16, Lemma 3.1])

$$(\partial_t s_{h\tau}^n, 1)_T = (\partial_t u_{h\tau}^n, 1)_T,\ \forall\, T \in \mathcal{T}^n, n = 1, \cdots, N, \tag{38}$$

holds.

Note further that (38) and (36) lead to

$$(\partial_t s_{h\tau}^n + \mathrm{div}\, \theta_{h\tau}^n - \tilde{f}^n, 1)_T = 0,\ \forall\, T \in \mathcal{T}^n, n = 1, \cdots, N. \tag{39}$$

In the same manner, we assume that a flux reconstruction $\theta^*_{h\tau}$ and a potential reconstruction $s^*_{h\tau}$ are available and satisfy the following conservation properties: $\theta^*_{h\tau} \in P^0_\tau(H(\mathrm{div},\Omega))$ and satisfies

$$(-\partial_t u^{*,n}_{h\tau} + \mathrm{div}\,\theta^{*,n}_{h\tau} - \tilde{g}^n, 1)_T = 0,\ \forall\, T \in \mathcal{T}^n, n = 0, \cdots, N-1. \tag{40}$$

As before, $s^*_{h\tau} \in P^1_\tau(H^1_0(\Omega)$ is such that

$$(s^{*,n}_{h\tau}, 1)_{T'} = (u^{*,n}_{h\tau}, 1)_{T'},\ \forall\, T' \in \mathcal{T}^{n-1,n}, n = 0, \cdots, N, \tag{41}$$

which yields

$$(\partial_t s^{*,n}_{h\tau}, 1)_T = (\partial_t u^{*,n}_{h\tau}, 1)_T,\ \forall\, T \in \mathcal{T}^n, n = 0, \cdots, N-1. \tag{42}$$

3.4 The error representation of the parabolic problem

The error on the quantity of interest is defined by

$$\mathcal{E} = Q(u) - Q(u_{h\tau}). \tag{43}$$

Inspired by section 2.3, we show that it can be decomposed into a fully computable expression and a remainder that will be estimated by a fully computable quantity.

Theorem 3.1 *With the previous notation, we have*

$$\mathcal{E} = \eta_{QOI} + \mathcal{R}, \tag{44}$$

where the estimator η_{QOI} is given by

$$\begin{aligned}
\eta_{QOI} &= (u_0 - s_{h\tau}(0), u^*_{h\tau}(0)) + (u^{*,N}_{h\tau}, s_{h\tau}(T) - u^N_{h\tau}) - \int_I (g(\cdot,t), u_{h\tau} - s_{h\tau})\,dt \\
&+ \int_I (f(\cdot,t) - \tilde{f}, u^*_{h\tau}(\cdot,t))\,dt \\
&+ \int_I (\tilde{f}(\cdot,t) - \mathrm{div}\,\theta_{h\tau}(\cdot,t) - \partial_t s_{h\tau}, u^*_{h\tau}(\cdot,t))\,dt \\
&+ \int_I \int_\Omega (\theta_{h\tau} + D\nabla s_{h\tau}) \cdot D^{-1}\theta^*_{h\tau}\,dxdt,
\end{aligned} \tag{45}$$

while the remainder term $\mathcal{R}$ is defined by

$$\begin{aligned}
\mathcal{R} &= (u_0 - s_{h\tau}(0), (u^* - u^*_{h\tau})(0)) + (u^*_T - u^{*,N}_{h\tau}, s_{h\tau}(T) - u^N_{h\tau}) \\
&+ \int_I (f(\cdot,t) - \tilde{f}, (u^* - u^*_{h\tau})(\cdot,t))\,dt \\
&+ \int_I (\tilde{f}(\cdot,t) - \mathrm{div}\,\theta_{h\tau}(\cdot,t) - \partial_t s_{h\tau}, (u^* - u^*_{h\tau})(\cdot,t))\,dt \\
&- \int_I \int_\Omega (\theta_{h\tau} + D\nabla s_{h\tau}) \cdot D^{-1}(D\nabla u^* + \theta^*_{h\tau})\,dxdt.
\end{aligned} \tag{46}$$

Proof. Using the definition (43) of the error and the identity (34), we have

$$\mathcal{E} = \int_I (f(\cdot,t), u^*(\cdot,t))\,dt + (u_0, u^*(0)) - \int_I (g(\cdot,t), u_{h\tau})\,dt - (u^*_T, u_{h\tau}(\cdot,T)).$$

Introducing artificially $s_{h\tau}$, we get

$$\mathcal{E} = \int_I (f(\cdot,t), u^*(\cdot,t))\,dt + (u_0, u^*(0)) - \int_I (g(\cdot,t), u_{h\tau} - s_{h\tau})\,dt - \int_I (g(\cdot,t), s_{h\tau})\,dt - (u^*_T, u_{h\tau}(\cdot,T)).$$

Using (32), this is equivalent to

$$\begin{aligned}\mathcal{E} &= \int_I (f(\cdot,t),u^*(\cdot,t))\,dt + (u_0,u^*(0)) - \int_I (g(\cdot,t),u_{h\tau}-s_{h\tau})\,dt \\ &+ \int_I (\partial_t u^* + \operatorname{div}(D\nabla u^*), s_{h\tau})\,dt - (u_T^*, u_{h\tau}(\cdot,T)).\end{aligned} \tag{47}$$

As $s_{h\tau}$ is in $H^1(I,H_0^1(\Omega))$ an integration by parts in space and in time leads to

$$\begin{aligned}\int_I (\operatorname{div}(D\nabla u^*), s_{h\tau})\,dt &= -\int_I\int_\Omega D\nabla u^*\cdot\nabla s_{h\tau}\,dxdt, \\ \int_I (\partial_t u^*, s_{h\tau})\,dt &= -\int_I (u^*,\partial_t s_{h\tau})\,dt + (u^*(T),s_{h\tau}(T)) - (u^*(0),s_{h\tau}(0)).\end{aligned}$$

Inserting these identities in (47) we find

$$\begin{aligned}\mathcal{E} &= (u_0 - s_{h\tau}(0),u^*(0)) + (u^*(T),s_{h\tau}(T)-u_{h\tau}^N) - \int_I (g(\cdot,t),u_{h\tau}-s_{h\tau})\,dt \\ &+ \int_I ((f(\cdot,t),u^*(\cdot,t)) - (u^*,\partial_t s_{h\tau}))\,dt \\ &- \int_I\int_\Omega D\nabla u^*\cdot\nabla s_{h\tau}\,dxdt.\end{aligned}$$

Adding and subtracting the term

$$\int_I\int_\Omega \nabla u^*\cdot\theta_{h\tau}\,dxdt,$$

we find

$$\begin{aligned}\mathcal{E} &= (u_0 - s_{h\tau}(0),u^*(0)) + (u^*(T),s_{h\tau}(T)-u_{h\tau}^N) - \int_I (g(\cdot,t),u_{h\tau}-s_{h\tau})\,dt \\ &+ \int_I (f(\cdot,t)-\partial_t s_{h\tau},u^*(\cdot,t))\,dt \\ &+ \int_I\int_\Omega \nabla u^*\cdot\theta_{h\tau}\,dxdt \\ &- \int_I\int_\Omega (\theta_{h\tau}+D\nabla s_{h\tau})\cdot\nabla u^*\,dxdt.\end{aligned}$$

Using Green's formula in the fourth term of this right-hand side we find

$$\begin{aligned}\mathcal{E} &= (u_0 - s_{h\tau}(0),u^*(0)) + (u^*(T),s_{h\tau}(T)-u_{h\tau}^N) - \int_I (g(\cdot,t),u_{h\tau}-s_{h\tau})\,dt \\ &+ \int_I (f(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau},u^*(\cdot,t))\,dt \\ &- \int_I\int_\Omega (\theta_{h\tau}+D\nabla s_{h\tau})\cdot\nabla u^*\,dxdt.\end{aligned}$$

Replacing f by $f-\tilde{f}+\tilde{f}$, we find

$$\begin{aligned}\mathcal{E} &= (u_0 - s_{h\tau}(0),u^*(0)) + (u^*(T),s_{h\tau}(T)-u_{h\tau}^N) - \int_I (g(\cdot,t),u_{h\tau}-s_{h\tau})\,dt \\ &+ \int_I (f(\cdot,t)-\tilde{f},u^*(\cdot,t))\,dt \\ &+ \int_I (\tilde{f}(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau},u^*(\cdot,t))\,dt \\ &- \int_I\int_\Omega (\theta_{h\tau}+D\nabla s_{h\tau})\cdot\nabla u^*\,dxdt\end{aligned}$$

Writing $u^* = u_{h\tau}^* + u^* - u_{h\tau}^*$ and $D\nabla u^* = -\theta_{h\tau}^* + D\nabla u^* + \theta_{h\tau}^*$, we arrive at (44). ■

Remark 3.2 As in Remark 2.3, our estimator η_{QOI} admits the decomposition

$$\eta_{QOI} = \eta_{\mathcal{O}} + \eta_{\nabla} + \eta_{\mathcal{H}},$$

where

$$\begin{aligned}
\eta_{\mathcal{O}} &= \int_I (f(\cdot,t) - \tilde{f}^n, u^*_{h\tau}(\cdot,t))\,dt \\
&+ \int_I (\tilde{f}(\cdot,t) - \operatorname{div}\theta_{h\tau}(\cdot,t) - \partial_t s_{h\tau}, u^*_{h\tau}(\cdot,t))\,dt, \\
\eta_{\nabla} &= \int_I \int_\Omega (\theta_{h\tau} + D\nabla s_{h\tau}) \cdot D^{-1}\theta^*_{h\tau}\,dxdt, \\
\eta_{\mathcal{H}} &= (u_0 - s_{h\tau}(0), u^*_{h\tau}(0)) + (u^{*,N}_{h\tau}, s_{h\tau}(T) - u^N_{h\tau}) - \int_I (g(\cdot,t), u_{h\tau} - s_{h\tau})\,dt.
\end{aligned}$$

As before $\eta_{\mathcal{O}}$ represents the data oscillation with respect to the primal problem weighted by the dual approximate solution, the flux estimator η_{∇} that measures the deviation of $-D\nabla s_{h\tau}$ from the reconstructed flux $\theta_{h\tau}$ and $\eta_{\mathcal{H}}$ that measures the deviation of $u_{h\tau}$ from $H^1_0(\Omega)$.

Let us now show that the remainder can be explicitly estimated using the error estimators for u and u^* obtained in [16, Theorem 3.2]. Namely denote by η (resp. η^*) the estimator obtained in this reference using the discrete spaces V^n_h (resp. $V^{*,n}_h$) to approximate the solution u of the primal problem (28) (resp. u^* of the dual problem (33)), so that

$$\|u - u_{h\tau}\|_Y \le \eta + 3\|f - \tilde{f}\|_{X'}, \tag{48}$$

$$\|u^* - u^*_{h\tau}\|_Y \le \eta^* + 3\|g - \tilde{g}\|_{X'}, \tag{49}$$

where

$$\begin{aligned}
\eta &= 3\left\{\sum_{n=1}^N \int_{I_n} \sum_{T\in\mathcal{T}^n} (\eta^n_{R,T}(t) + \eta^n_{DF,T}(t))^2\,dt\right\}^{\frac12} + \eta_{IC} \\
&+ \left\{\sum_{n=1}^N \int_{I_n} \sum_{T\in\mathcal{T}^n} (\eta^n_{NC1,T}(t))^2\,dt\right\}^{\frac12} + \left\{\sum_{n=1}^N \tau^n \int_{I_n} \sum_{T\in\mathcal{T}^n} (\eta^n_{NC2,T}(t))^2\,dt\right\}^{\frac12},
\end{aligned}$$

with

$$\eta_{IC} = \sqrt{2}\|s^0_{h\tau} - u_0\|,$$

and for all $n = 1,\cdot,N$, $t \in I_n$ and $T \in \mathcal{T}^n$,

$$\begin{aligned}
\eta^n_{R,T}(t) &= \pi^{-1}\|D^{-\frac12}\|_{\infty,T} h_T \|\tilde{f} - \partial_t s_{h\tau} - \operatorname{div}\theta^n_{h\tau}\|_T, \\
\eta^n_{DF,T}(t) &= \|D^{-\frac12}(\theta_{h\tau} + D\nabla s_{h\tau})\|_T, \\
\eta^n_{NC1,T}(t) &= \|D^{\frac12}\nabla(s_{h\tau} - u_{h\tau})\|_T, \\
\eta^n_{NC2,T}(t) &= \pi^{-1}\|D^{-\frac12}\|_{\infty,T} h_T \|\partial_t(s_{h\tau} - u_{h\tau})^n\|_T.
\end{aligned}$$

The estimator η^* of the dual problem is defined similarly by replacing $u_{h\tau}$ by $u^*_{h\tau}$, $\theta_{h\tau}$ by $\theta^*_{h\tau}$, $s_{h\tau}$ by $s^*_{h\tau}$, $s^0_{h\tau}$ by $s^{*,0}_{h\tau}$, u_0 by u^*_T, f by q, and ∂_t by $-\partial_t$.

Theorem 3.3 *With η and η^* as defined before, we have*

$$\begin{aligned}
|\mathcal{R}| &\le D_Y\big(\eta + \|(s_{h\tau} - u_{h\tau})(T)\| + \|f - \tilde{f}\|_{X'}\big)\big(\eta^* + \|(s^*_{h\tau} - u^*_{h\tau})(0)\| + \|g - \tilde{g}\|_{X'}\big) \\
&+ \pi^{-1}h^n\|D^{-\frac12}\|_{\infty,\Omega}\|f(\cdot,t) - \tilde{f}\|_C\eta^*,
\end{aligned} \tag{50}$$

with $D_Y = \sqrt{2}\max\{1, 3C_Y\} + 11$.

Proof. We estimate each term of $\mathcal{R}$ separetely. For the first term, by Cauchy-Schwarz's inequality we have

$$|(u_0 - s_{h\tau}(0), (u^* - u^*_{h\tau})(0))| \leq \|u_0 - s_{h\tau}(0)\| \|(u^* - u^*_{h\tau})(0)\|. \tag{51}$$

Note that

$$\|u_0 - s_{h\tau}(0)\| \leq 2^{-1/2}\eta, \tag{52}$$

therefore it remains to estimate the second factor of the right-hand side of (51). But since $u^*_{h\tau}$ does not belong to Y, we write $(u^* - u^*_{h\tau})(0) = (u^* - s^*_{h\tau})(0) + (s^*_{h\tau} - u^*_{h\tau})(0)$, and use the triangular inequality to find

$$\|(u^* - u^*_{h\tau})(0)\| \leq \|(u^* - s^*_{h\tau})(0)\| + \|(s^*_{h\tau} - u^*_{h\tau})(0)\|. \tag{53}$$

For the first term of this right-hand side we use the continuous embedding $Y \hookrightarrow C([0,T]; L^2(\Omega))$ to find (see (29))

$$\|(u^* - s^*_{h\tau})(0)\| \leq C_Y \|u^* - s^*_{h\tau}\|_Y. \tag{54}$$

Then using the identity

$$\|u^* - s^*_{h\tau}\|_Y = \|\partial_t(u^* - s^*_{h\tau})\|_{L^2(0,T,H^{-1}(\Omega)} + \Big(\sum_{n=1}^{N} \int_{I_n} \sum_{T\in\mathcal{T}^{n-1,n}} \|D^{\frac{1}{2}}\nabla(u^* - s^*_{h\tau})(t)\|^2_T \, dt\Big)^{\frac{1}{2}},$$

inserting artificially $u^*_{h\tau}$ and using the triangular inequality, we find

$$\begin{aligned}
\|u^* - s^*_{h\tau}\|_Y &\leq \|\partial_t(u^* - u^*_{h\tau})\|_{L^2(0,T,H^{-1}(\Omega)} + \|\partial_t(u^*_{h\tau} - s^*_{h\tau})\|_{L^2(0,T,H^{-1}(\Omega)} \\
&+ \Big(\sum_{n=0}^{N-1} \int_{I_n} \sum_{T\in\mathcal{T}^{n-1,n}} \|D^{\frac{1}{2}}\nabla(u^* - u^*_{h\tau})(t)\|^2_T \, dt\Big)^{\frac{1}{2}} \\
&+ \Big(\sum_{n=0}^{N-1} \int_{I_n} \sum_{T\in\mathcal{T}^{n-1,n}} \|D^{\frac{1}{2}}\nabla(u^*_{h\tau} - s^*_{h\tau})(t)\|^2_T \, dt\Big)^{\frac{1}{2}}.
\end{aligned}$$

According to the definition of the norm Y for $u^* - u^*_{h\tau}$ and to the definition of η^*, we find

$$\begin{aligned}
\|u^* - s^*_{h\tau}\|_Y &\leq \|u^* - u^*_{h\tau}\|_Y + \eta^* \\
&+ \|\partial_t(u^*_{h\tau} - s^*_{h\tau})\|_{L^2(0,T,H^{-1}(\Omega)}.
\end{aligned} \tag{55}$$

For this last term, for all $t \in (0,T)$, we define the $H^{-1}(\Omega)$-norm by[1]

$$\|\partial_t(u^*_{h\tau} - s^*_{h\tau})(t)\|_{H^{-1}(\Omega)} = \sup_{\varphi\in H^1_0(\Omega), \varphi\neq 0} \frac{\left|\int_\Omega \partial_t(u^*_{h\tau} - s^*_{h\tau})(t)\varphi \, dx\right|}{\|D^{\frac{1}{2}}\nabla\varphi\|}. \tag{56}$$

Hence using (42), we may write

$$\int_\Omega \partial_t(u^*_{h\tau} - s^*_{h\tau})(t)\varphi \, dx = \sum_{T\in\mathcal{T}^n} \int_T \partial_t(u^*_{h\tau} - s^*_{h\tau})(t)(\varphi - \mathcal{M}_T\varphi) \, dx,$$

where $\mathcal{M}_T\varphi$ is the mean of φ on T. Therefore by the Poincaré inequality stating that

$$\|\varphi - \mathcal{M}_T\varphi\|_T \leq \pi^{-1} h_T |\varphi|_{1,T},$$

we find

$$\|\varphi - \mathcal{M}_T\varphi\|_T \leq \pi^{-1} h_T \|D^{-\frac{1}{2}}\|_{\infty,T} \|D^{\frac{1}{2}}\nabla\varphi\|_T,$$

[1] as D is bounded and positive definite this norm is equivalent to the usual one.

and hence

$$\left|\int_\Omega \partial_t(u^*_{h\tau}-s^*_{h\tau})(t)\varphi\,dx\right| \le \pi^{-1}\sum_{T\in\mathcal{T}^n} h_T\|D^{-\frac12}\|_{\infty,T}\|\partial_t(u^*_{h\tau}-s^*_{h\tau})(t)\|_T\|D^{\frac12}\nabla\varphi\|_T.$$

Using the discrete Cauchy-Schwarz's inequality and inserting this estimate in (56), we obtain

$$\|\partial_t(u^*_{h\tau}-s^*_{h\tau})(t)\|_{H^{-1}(\Omega)} \le \pi^{-1}\Big(\sum_{T\in\mathcal{T}^n} h_T^2\|D^{-\frac12}\|^2_{\infty,T}\|\partial_t(u^*_{h\tau}-s^*_{h\tau})(t)\|^2_T\Big)^{\frac12}.$$

Integrating the square of this estimate in $0,T)$ and using the definition of η^*, we arrive at

$$\|\partial_t(u^*_{h\tau}-s^*_{h\tau})(t)\|_{L^2(0,T,H^{-1}(\Omega))} \le \eta^*,$$

and using it into (55) yields

$$\|u^*-s^*_{h\tau}\|_Y \le \|u^*-u^*_{h\tau}\|^2_Y + 2\eta^*.$$

The estimate (49) then leads to

$$\|u^*-s^*_{h\tau}\|_Y \le 3(\eta^*+\|g-\tilde g\|_{X'}). \tag{57}$$

Combining this estimate with (54) leads to

$$\|(u^*-s^*_{h\tau})(0)\| \le 3C_Y(\eta^*+\|g-\tilde g\|_{X'}),$$

that can be used in (53) to find

$$\|(u^*-u^*_{h\tau})(0)\| \le \max\{1,3C_Y\}(\eta^*+\|(s^*_{h\tau}-u^*_{h\tau})(0)\|+\|g-\tilde g\|_{X'}). \tag{58}$$

Coming back to (51) and using this last estimate and (52), we finally find

$$|(u_0-s_{h\tau}(0),(u^*-u^*_{h\tau})(0))| \le 2^{-\frac12}\max\{1,3C_Y\}\eta(\eta^*+\|(s^*_{h\tau}-u^*_{h\tau})(0)\|+\|g-\tilde g\|_{X'}). \tag{59}$$

The second term is the symmetric of the first one by exchanging the rule of u and u^*, hence

$$|(u^*_T-u^{*,N}_{h\tau},s_{h\tau}(T)-u^N_{h\tau})| \le 2^{-\frac12}\max\{1,3C_Y\}(\eta+\|(s_{h\tau}-u_{h\tau})(T)\|+\|f-\tilde f\|_{X'})\eta^*. \tag{60}$$

Concerning the third term, we again introduce artificially $s^*_{h\tau}$ to get

$$\begin{aligned}\mathcal{R}_3 := \int_I (f(\cdot,t)-\tilde f,(u^*-u^*_{h\tau})(\cdot,t))\,dt &= \int_I (f(\cdot,t)-\tilde f,(u^*-s^*_{h\tau})(\cdot,t))\,dt\\ &\quad+\sum_{n=1}^N\int_{I_n}(f(\cdot,t)-\tilde f^n,(s^*_{h\tau}-u^*_{h\tau})(\cdot,t))\,dt,\end{aligned}$$

and by using a duality argument for the first term and Cauchy-Schwarz's inequality for the second one, we obtain

$$\begin{aligned}|\mathcal{R}_3| &\le \|f(\cdot,t)-\tilde f\|_{X'}\|u^*-s^*_{h\tau}\|_X\\ &+ \sum_{n=1}^N\int_{I_n}\sum_{T\in\mathcal{T}^{n,n-1}}\|f(\cdot,t)-\tilde f^n\|_T\|(s^*_{h\tau}-u^*_{h\tau})(\cdot,t)\|_T\,dt.\end{aligned}$$

Due to the property (41) and the Poincaré inequality, we find

$$\begin{aligned}|\mathcal{R}_3| &\le \|f(\cdot,t)-\tilde f\|_{X'}\|u^*-s^*_{h\tau}\|_X\\ &+ \pi^{-1}\sum_{n=1}^N\int_{I_n}\sum_{T\in\mathcal{T}^{n,n-1}}\|f(\cdot,t)-\tilde f^n\|_T h_T\|\nabla(s^*_{h\tau}-u^*_{h\tau}))(\cdot,t)\|_T\,dt.\end{aligned}$$

Using the definition of the broken gradient of $u^*_{h\tau}$ and the fact that $h_T \leq h^n$ for all $T \in \mathcal{T}^{n-1,n}$, we get

$$\begin{aligned}|\mathcal{R}_3| &\leq \|f(\cdot,t)-\tilde{f}\|_{X'}\|u^*-s^*_{h\tau}\|_X \\ &+ \pi^{-1}h^n\|D^{-\frac{1}{2}}\|_{\infty,\Omega}\sum_{n=1}^{N}\int_{I_n}\sum_{T\in\mathcal{T}^n}\|f(\cdot,t)-\tilde{f}^n\|_T\|D^{\frac{1}{2}}\nabla^{n-1,n}(s^*_{h\tau}-u^*_{h\tau}))(\cdot,t)\|_T\,dt.\end{aligned}$$

Hence using Cauchy-Schwarz's inequality, we find

$$|\mathcal{R}_3| \leq \|f(\cdot,t)-\tilde{f}\|_{X'}\|u^*-s^*_{h\tau}\|_X + \pi^{-1}h^n\|D^{-\frac{1}{2}}\|_{\infty,\Omega}\|f(\cdot,t)-\tilde{f}\|_C\eta^*.$$

Finally as by definition $\|u^*-s^*_{h\tau}\|_X \leq \|u^*-s^*_{h\tau}\|_Y$, the estimate (57) yields

$$|\mathcal{R}_3| \leq 3\|f(\cdot,t)-\tilde{f}\|_{X'}(\eta^*+\|g-\tilde{g}\|_{X'}) + \pi^{-1}h^n\|D^{-\frac{1}{2}}\|_{\infty,\Omega}\|f(\cdot,t)-\tilde{f}\|_C\eta^*. \tag{61}$$

For the fourth term again inserting artificially $s^*_{h\tau}$ we get

$$\begin{aligned}\mathcal{R}_4 &:= \sum_{n=1}^{N}\int_{I_n}\sum_{T\in\mathcal{T}^n}(\tilde{f}^n(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau},(u^*-u^*_{h\tau})(\cdot,t))_T\,dt \\ &= \sum_{n=1}^{N}\int_{I_n}\sum_{T\in\mathcal{T}^n}(\tilde{f}^n(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau},(u^*-s^*_{h\tau})(\cdot,t))_T\,dt \\ &+ \sum_{n=1}^{N}\int_{I_n}\sum_{T\in\mathcal{T}^n}(\tilde{f}^n(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau},(s^*_{h\tau}-u^*_{h\tau})(\cdot,t))_T\,dt.\end{aligned}$$

For the first term using (39), we can replace $u^*-s^*_{h\tau}$ by $u^*-s^*_{h\tau}-\mathcal{M}_T(u^*-s^*_{h\tau})$ on $T\in\mathcal{T}^n$, while for the second term we reorganize the summation on the triangulation $\mathcal{T}^{n-1,n}$ and then find

$$\begin{aligned}\mathcal{R}_4 = &\sum_{n=1}^{N}\int_{I_n}\sum_{T\in\mathcal{T}^n}(\tilde{f}^n(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau},(u^*-s^*_{h\tau})(\cdot,t)-\mathcal{M}_T(u^*-s^*_{h\tau}))_T\,dt \\ &+\sum_{n=1}^{N}\int_{I_n}\sum_{T'\in\mathcal{T}^{n-1,n}}(\tilde{f}^n(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau},(s^*_{h\tau}-u^*_{h\tau})(\cdot,t))_{T'}\,dt.\end{aligned}$$

Using Poincaré inequality for each term of this right-hand side (recalling the property (41)), we find

$$\begin{aligned}|\mathcal{R}_4| \leq\ &\pi^{-1}\sum_{n=1}^{N}\int_{I_n}\sum_{T\in\mathcal{T}^n}h_T\|D^{-\frac{1}{2}}\|_{\infty,T}\|\tilde{f}^n(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau}\|_T\|D^{\frac{1}{2}}\nabla(u^*-s^*_{h\tau})(\cdot,t)\|_T\,dt \\ &+\pi^{-1}\sum_{n=1}^{N}\int_{I_n}\sum_{T'\in\mathcal{T}^{n-1,n}}h_{T'}\|D^{-\frac{1}{2}}\|_{\infty,T'}\|\tilde{f}^n(\cdot,t)-\operatorname{div}\theta_{h\tau}(\cdot,t)-\partial_t s_{h\tau}\|_{T'}\|D^{\frac{1}{2}}\nabla(s^*_{h\tau}-u^*_{h\tau})\|_{T'}\,dt.\end{aligned}$$

Using Cauchy-Schwarz's inequality and reorganizing the summation in the second term (using the fact that $h_{T'}\leq h_T$, for all $T'\in\mathcal{T}^{n-1,n}$ such that $T'\subset T\in\mathcal{T}^n$), we get

$$|\mathcal{R}_4| \leq \eta(\|u^*-s^*_{h\tau}\|_Y+\eta^*).$$

As before the estimate (57) yields

$$|\mathcal{R}_4| \leq 3\eta(\eta^*+\|g-\tilde{g}\|_{X'})+\eta\eta^*. \tag{62}$$

It remains the last term that can be transformed as

$$\begin{aligned}\mathcal{R}_5 &:= \int_I \int_\Omega (\theta_{h\tau} + D\nabla s_{h\tau}) \cdot D^{-1}(D\nabla u^* + \theta^*_{h\tau})\, dxdt \\ &= \int_I \int_\Omega (\theta_{h\tau} + D\nabla s_{h\tau}) \cdot \nabla(u^* - s^*_{h\tau})\, dxdt \\ &+ \int_I \int_\Omega (\theta_{h\tau} + D\nabla s_{h\tau}) \cdot D^{-1}(D\nabla s_{h\tau} + \theta^*_{h\tau})\, dxdt.\end{aligned}$$

Hence Cauchy-Schwarz's inequality directly yields

$$|\mathcal{R}_5| \leq \eta(\|u^* - s^*_{h\tau}\|_Y + \eta^*).$$

With the help of the estimate (57) we again obtain

$$|\mathcal{R}_5| \leq 3\eta(\eta^* + \|g - \tilde{g}\|_{X'}) + \eta\eta^*. \tag{63}$$

The conclusion follows from the estimates (59), (60), (61) (62), and (63). ■
Note that Remark 2.6 remains valid for our parabolic problem (27). ,

4 Numerical examples

In this section, we present some illustrative numerical examples that validate our theoretical results. Before going on, let us notice that all numerical simulations are realized by the free scientific computing software FreeFem++ [19].

4.1 Diffusion-reaction problems

In this subsection, we aim to illustrate the theoretical results obtained for diffusion problems, and specifically Theorems 2.1 and 2.4. These tests are performed in the case $u_h \in H^1_0(\Omega)$, so that we always take $s_h = u_h$.

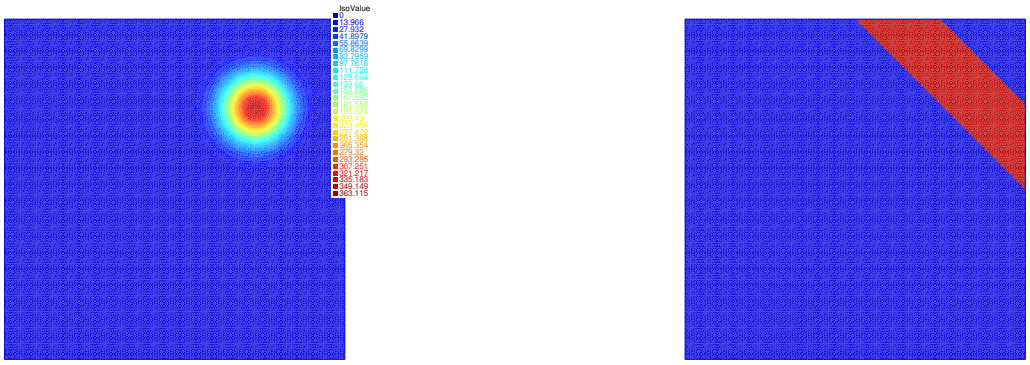
4.1.1 Diffusion problem : regular solution

We first consider the same benchmark as the one proposed in [30], section 8 and [28], section 6.1. The primal problem (4) is defined with $d = 2$, $\Omega =]0,1[^2$, $D = I_{\mathbb{R}^2}$ [2] and $r = 0$. The exact solution is chosen equal to $u(x,y) = 10^4 x(1-x)y(1-y)e^{-100(\rho(x,y))^2}$ with $\rho(x,y) = ((x-0.75^2)+(y-0.75)^2)^{1/2}$ (see Figure 1(a)), and the right-hand side f is computed accordingly. The dual problem is defined by (10) with $q = \mathbb{1}_\omega$ and $\omega = \{(x,y) \in \Omega : 1.5 \leq x + y \leq 1.75\}$ (see Figure 1(b)).

The approximation u_h of u solution of the primal problem is made using standard conforming $\mathbb{P}_1$ finite elements on regular meshes made of triangles (see Figure 2 for the first three refinements), and the corresponding flux reconstruction θ_h is approximated using some standard $\mathbb{RT}_1$ finite elements (Raviart-Thomas finite elements of degree 2 on each triangle). The approximation u^*_h of u^* solution of the dual problem is made using standard conforming $\mathbb{P}_2$ finite elements on the same meshes, and the corresponding flux reconstruction θ^*_h is approximated using some standard $\mathbb{RT}_2$ finite elements (Raviart-Thomas finite elements of degree 3 on each triangle).

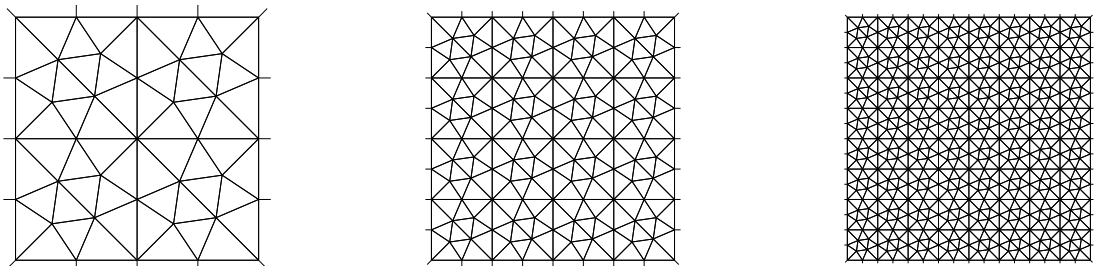
For each mesh, the value of $\mathcal{E} = Q(u - u_h)$ defined by (7) is computed, as well as the one of η_{QOI} defined by (14). We plot on Figure 3(a) the values of $\mathcal{E}$ as well as the ones of η_{QOI} and $4\eta\eta^*$ as a function of h in a log-log scale. Using (13), we also plot the value of $|\mathcal{R}|$ which can be

[2] here and below, $I_{\mathbb{R}^2}$ means the 2×2 identity matrix



(a) (b)

Figure 1: Diffusion problem with regular solution: (a) exact solution; (b) loading term q in dual problem.



Mesh 1 - $h = 1/4$ Mesh 2- $h = 1/8$ Mesh 3 - $h = 1/16$

Figure 2: Unstructured regular meshes, first three refinements.

computed by $\mathcal{R} = Q(u - u_h) - \eta_{QOI}$.

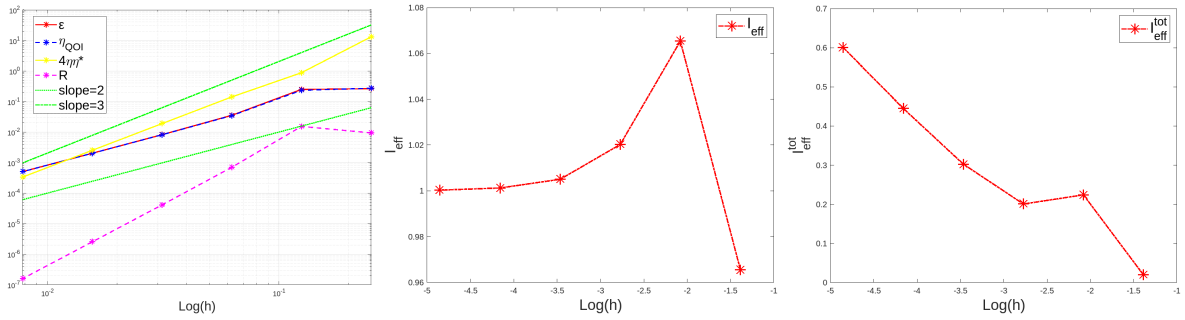
First of all, we remark that $\mathcal{E}$ goes towards zero at the order $O(h^2)$, which is the expected behaviour since $u \in H^2(\Omega)$ and u_h is approximated by $\mathbb{P}_1$ finite elements. Moreover, the estimator η_{QOI} converges towards zero also in $O(h^2)$, while the remainder $\mathcal{R}$ superconverges. Figure 3(b) displays the effectivity index I_{eff} defined by

$$I_{eff} = |\mathcal{E}/\eta_{QOI}|. \tag{64}$$

Whatever the value of h, the effectivity index I_{eff} is always nearly equal to one, what illustrates on this benchmark the asymptotically exactness of the estimator η_{QOI}. Coming back to Figure 3(a), we observe that the value of $4\eta\eta^*$ goes towards zero faster than $\mathcal{E}$ and η_{QOI}, while remaining quite larger for coarse meshes. Let us now introduce the total effectivity index I^{tot}_{eff} defined by

$$I^{tot}_{eff} = |\mathcal{E}|/(|\eta_{QOI}| + 4\eta\eta^*). \tag{65}$$

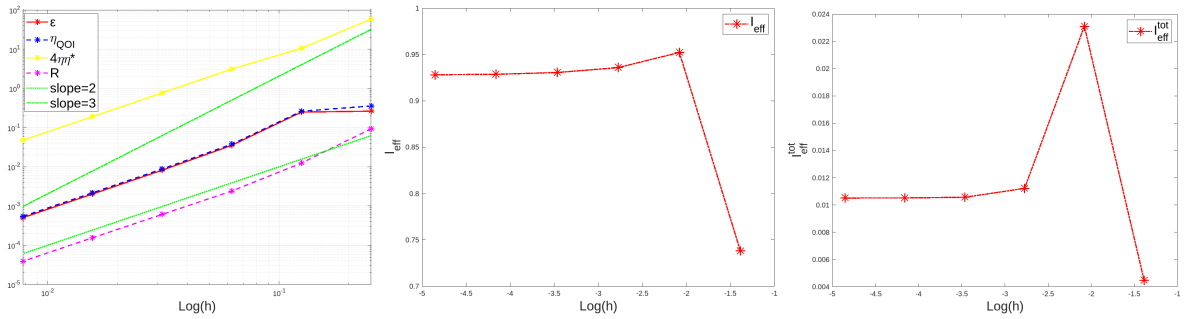
We see in Figure 3(c) that I^{tot}_{eff} is smaller than one as theoretically expected (see (24)). But thanks to the superconvergence of $4\eta\eta^*$, it is also expected to converge towards one when h goes towards zero.



(a) (b) (c)

Figure 3: Diffusion problem, $D = I_{\mathbb{R}^2}$, regular solution: (a) rates of convergence; (b) effectivity index I_{eff}; (c) total effectivity index I^{tot}_{eff}.

Remark 4.1 *If we solve the same problem, but this time using conforming $\mathbb{P}_1$ finite elements for the computation of u^*_h and $\mathbb{RT}_1$ finite elements for the computation of θ^*_h (in other words, the same finite element spaces for the dual problem than for the primal one), then the results are not the same. Figure 4 displays the same quantities as the ones in Figure 3. As previoulsy, it can be observed in Figure 4(a) that the error $\mathcal{E}$ and the estimator η_{QOI} both converge towards zero at the order $O(h^2)$. Nevertheless, the remainder $\mathcal{R}$ does not superconverge anymore, even if it remains here very small compared to $\mathcal{E}$ and η_{QOI}. It explains the fact that I_{eff} is slightly worse (around 0.93 instead of 1 for the smallest values of h, see Figure 4(b)). Moreover, it can also be seen in Figure 4(a) that $4\eta\eta^*$ is no more superconvergent. It remains larger than $\mathcal{E}$ and η_{QOI}, converging towards zero at the same order. That is why the value of I^{tot}_{eff} converges towards a constant significantly smaller than one. This test illustrates the fact that for a regular solution, if the dual problem is approximated by the same spaces than the ones used for the resolution of the primal problem, then the remainder term $\mathcal{R}$ (or its bound $4\eta\eta^*$) is not necessarily negligible, and that the asymptotic exactness can be lost. Nevertheless, it is clear that I^{tot}_{eff} always remains bounded by one, and that the estimator $|\eta_{QOI}| + 4\eta\eta^*$ is always an upper bound for the error $|\mathcal{E}|$, as theoretically expected from* (24).



(a) (b) (c)

Figure 4: Diffusion problem, $D = I_{\mathbb{R}^2}$, regular solution with same finite element spaces for primal and dual problems: (a) rates of convergence; (b) effectivity index I_{eff}; (c) total effectivity index I^{tot}_{eff}.

4.1.2 Diffusion problem : singular solution

This time we consider a singular case. The primal problem (4) is defined with $d = 2$, $\Omega =]-1,1[^2$ and $r = 0$. The diffusion coefficient D is piecewise constant in Ω and defined by $D = d_i\, I_{\mathbb{R}^2}$ in Ω_i, $1 \leq i \leq 4$, with $\Omega_1 = (0,1)\times(0,1)$, $\Omega_2 = (-1,0)\times(0,1)$, $\Omega_3 = (-1,0)\times(-1,0)$ and $\Omega_4 = (0,1)\times(-1,0)$, $0 < d_1 = d_3 = a < 1$ and $d_2 = d_4 = 1$. Defining the singular exponent $\alpha = \dfrac{4}{\pi}\arctan(\sqrt{a})$, the exact solution as shown in Figure 5(a) is given by

$$u(x,y) = p(x,y)\, S(x,y),$$

where $p(x,y) = (1-x^4)(1-y^4)$ is a truncation function and $S(x,y) = \rho^\alpha v(\theta)$ with

$$\rho = \sqrt{x^2+y^2} \quad , \quad \theta = \begin{cases} \arctan(y/x) & \text{in} \quad \Omega_1 \cup \Omega_4, \\ \pi + \arctan(y/x) & \text{in} \quad \Omega_2 \cup \Omega_3, \end{cases}$$

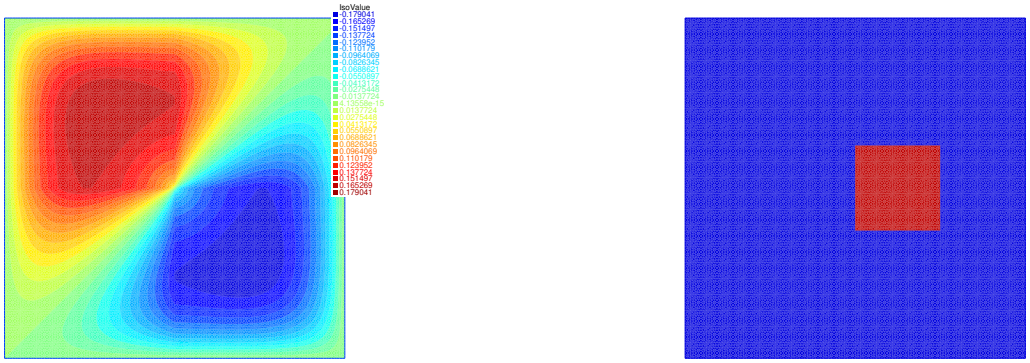
and

$$v(\theta) = \begin{cases} \sin\left(\alpha\left(\theta - \dfrac{\pi}{4}\right)\right) & \text{in} \quad \Omega_1, \\ \sqrt{a}\cos\left(\alpha\left(\dfrac{3\pi}{4} - \theta\right)\right) & \text{in} \quad \Omega_2, \\ \sin\left(\alpha\left(\dfrac{5\pi}{4} - \theta\right)\right) & \text{in} \quad \Omega_3, \\ -\sqrt{a}\cos\left(\alpha\left(\dfrac{\pi}{4} + \theta\right)\right) & \text{in} \quad \Omega_4. \end{cases}$$

The right-hand side f is computed accordingly. Let us note that in such a configuration, for any $\varepsilon > 0$ we have $u \in H^{1+\alpha-\varepsilon}(\Omega)$ (see e.g. the appendix of [9] for a similar configuration).

The dual problem is defined by (10) with $q = \mathbb{1}_\omega$ and $\omega = (0, 0.5)\times(-0.25, 0.25)$ (see Figure 5(b)). All the spatial discretizations are done similarly to the regular case of section 4.1.1.

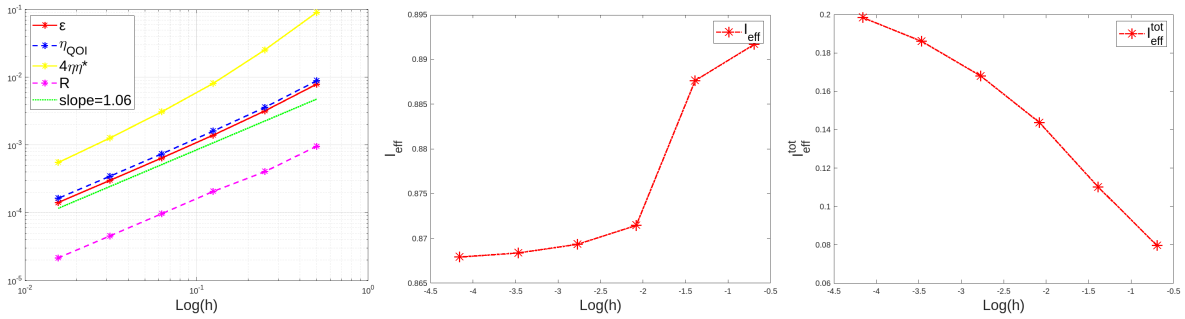
The obtained results are respectively displayed in Figures 6 and 7 for $a = 1/5$ and $a = 1/20$, respectively leading to the values of $\alpha \approx 0.53$ and $\alpha \approx 0.28$. From these figures, we may notice that the error, the estimator η_{QOI} and $4\eta\eta^*$ all converge towards zero with order $O(h^{2\alpha})$. In both cases, I_{eff} remains in the order of unity but is no more close to one. The remainder $\mathcal{R}$ seems to be no more superconvergent. Moreover, $4\eta\eta^*$ significantly overestimates the value of $|\mathcal{R}|$, leading to the convergence of I^{tot}_{eff} towards values less than one. This means that for such problems with



(a) (b)

Figure 5: Diffusion problem with singular solution: (a) exact solution; (b) loading term q in dual problem.

singular solutions, an adaptive algorithm should be based on the sum of the estimator $|\eta_{QOI}|$ and of the product $4\eta\eta^*$, since they have the same rate of convergence, even with a higher order approximation of the dual problem.



(a) (b) (c)

Figure 6: Diffusion problem, singular solution, $a = 1/5$: (a) rates of convergence; (b) effectivity index I_{eff}; (c) total effectivity index I_{eff}^{tot}.

4.1.3 A boundary layer problem

Now, we investigate the behaviour of the estimator in the case of a solution with a boundary layer, in order to test the robustness of the estimator in this configuration. For an arbitrary $\varepsilon \in \mathbb{R}_+$, we consider the problem (4) with $d = 2$, $\Omega =]0,1[^2$, $D = \varepsilon^2 I_{\mathbb{R}^2}$ and $r = 1$. We choose

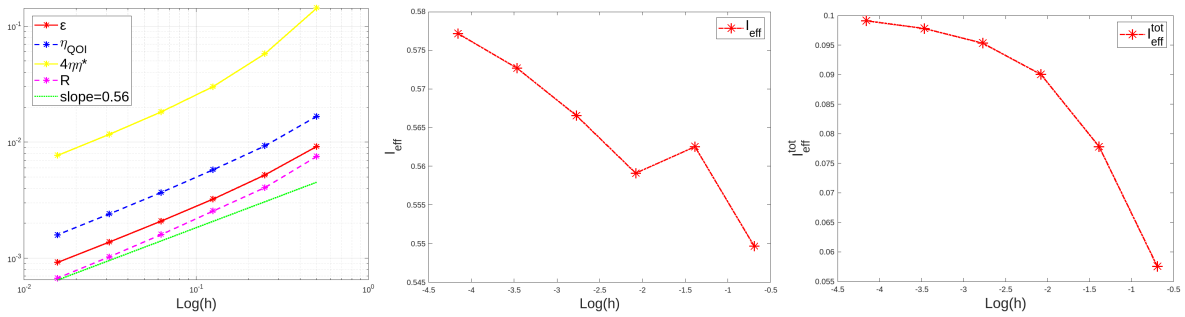
$$f(x,y) = 2\varepsilon^2 v_\varepsilon(x) + y(1-y),\ \forall (x,y) \in \Omega,$$

with

$$v_\varepsilon(x) = 1 + \alpha_\varepsilon e^{-\frac{x}{\varepsilon}} - (1+\alpha_\varepsilon)e^{\frac{x}{\varepsilon}},\ \forall x) \in (0,1), \quad \text{and} \quad \alpha_\varepsilon = \frac{1 - e^{\frac{1}{\varepsilon}}}{2\sinh\frac{1}{\varepsilon}},$$

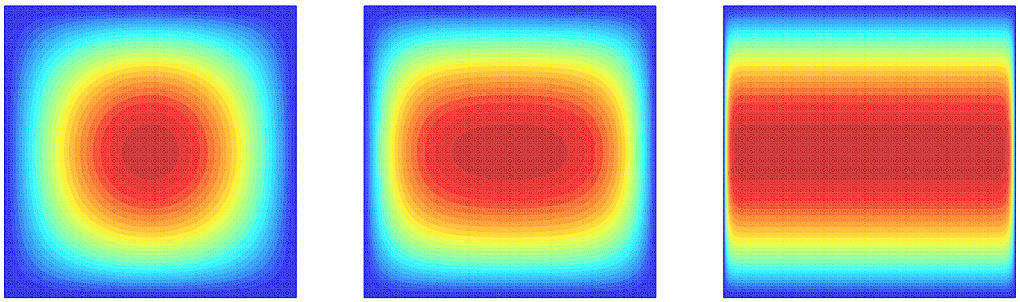
so that the exact solution u_ε is given by $u_\varepsilon(x,y) = v_\varepsilon(x)y(1-y)$. Clearly we have $u_\varepsilon = 0$ on $\partial\Omega$, and a boundary layer appears in the vicinity of the boundaries $x = 0$ and $x = 1$ when ε tends towards zero (see Figure 8).

Like in section 4.1.1, the dual problem is defined by (10) with $q = \mathbb{1}_\omega$ and $\omega = \{(x,y) \in \Omega : 1.5 \leq x + y \leq 1.75\}$ (see Figure 1(b)). Figures 9, 10 and 11 display the rates of convergence and the effectivity index, similarly to Figure 3, respectively for $\varepsilon = 1$, $\varepsilon = 10^{-1}$ and $\varepsilon = 10^{-2}$.



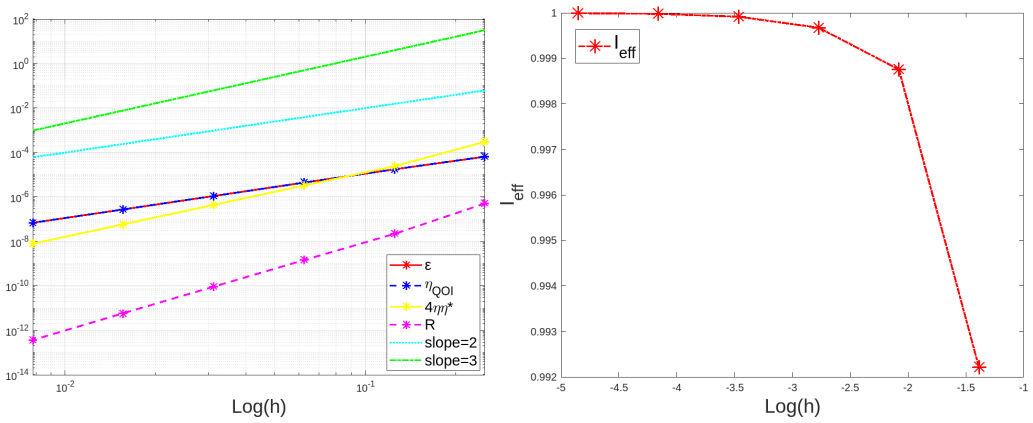
(a) (b) (c)

Figure 7: Diffusion problem, singular solution, $a = 1/20$: (a) rates of convergence; (b) effectivity index I_{eff}; (c) total effectivity index I^{tot}_{eff}.



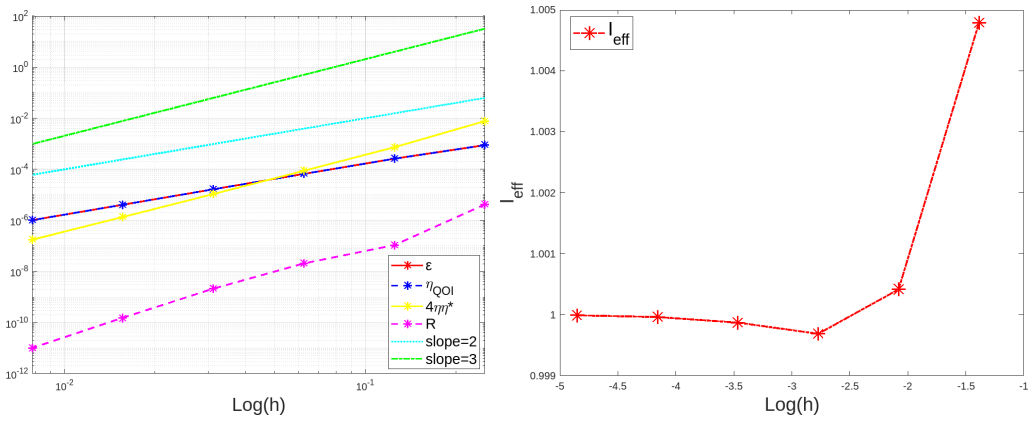
$\varepsilon = 1$ $\varepsilon = 10^{-1}$ $\varepsilon = 10^{-2}$

Figure 8: Reaction-diffusion problem with a boundary layer solution: isovalues of u_ε.



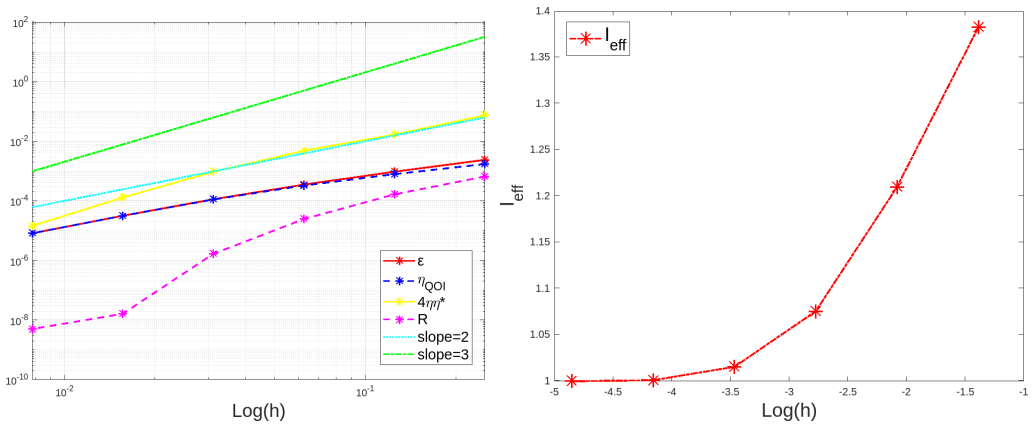
(a) (b)

Figure 9: A boundary layer problem, $\varepsilon = 1$: (a) rates of convergence; (b) effectivity index I_{eff}.



(a) (b)

Figure 10: A boundary layer problem, $\varepsilon = 10^{-1}$: (a) rates of convergence; (b) effectivity index I_{eff}.



(a) (b)

Figure 11: A boundary layer problem, $\varepsilon = 10^{-2}$: (a) rates of convergence; (b) effectivity index I_{eff}.

Whatever the value of ε, the conclusions are the same as the ones of section 4.1.1 devoted to the pure diffusion regular problem : $\mathcal{E}$ as well as η_{QOI} go towards zero at the order $O(h^2)$. I_{eff} tends towards one when h goes towards zero. Finally, the value of $4\eta\eta^*$ goes towards zero faster than $\mathcal{E}$. Consequently, in accordance with the theory, the estimation is robust in ε.

4.2 Parabolic problems

In this subsection, we aim to illustrate the theoretical results obtained for parabolic problems, and specifically Theorems 3.1 and 3.3. These tests are performed in the case $u_{h\tau}^n \in H_0^1(\Omega)$, so that we always take $s_{h\tau} = u_{h\tau}$.

4.2.1 The heat equation

We start to propose a simple problem, defining the primal problem by (27) with $d = 2$, $\Omega =]0,1[^2$, $T = 1.0$ and $D = I_{\mathbb{R}^2}$. We choose the exact solution being equal to $u(x,y,t) = x^2y^2(x-1)^2(y-1)^2\sin(t)$ and compute the right-hand side f accordingly. The dual problem is defined by (32), where we choose $g = 0$ and $u_T^* = e^{-\frac{\rho(x,y)^2}{32\ln 10}}$ with $\rho(x,y) = ((x-0.5)^2 + (y-0.5)^2)^{1/2}$.

Concerning the time approximation, we use the definition of $(\partial_t u)^n$ given in (35) to compute an implicit-Euler time integration for the computation of the approximated solution of the primal problem, where u^n is the approximation of $u(t_n,\cdot)$ and solution of the elliptic problem:

$$\begin{cases} \dfrac{u^n - u^{n-1}}{\tau} - \operatorname{div}(D\nabla u^n) = \tilde{f}^n & \text{in } \Omega, \\ u^n = 0 & \text{on } \partial\Omega, \\ u^0 = u_0 & \text{in } \Omega. \end{cases} \tag{66}$$

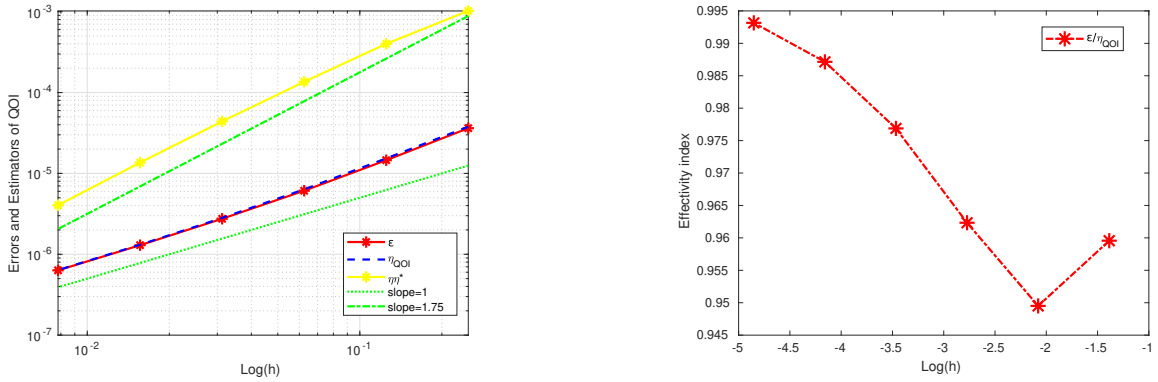
Since the scheme is fully implicit in time, there is no need to impose any stability condition linking h and τ. For accuracy reasons, we choose $\tau = h$. Similarly to the stationary tests, the spatial approximation u_h^n of u^n is made using standard $\mathbb{P}_1$ finite elements and the corresponding flux reconstruction θ_h is approximated using some standard $\mathbb{RT}_1$ finite elements. The time integration of the dual problem is also done using an implicit-Euler scheme (with $\tau = h$), where $u^{*,n}$ is the approximation of $u^*(t_n,\cdot)$ and solution of:

$$\begin{cases} -\dfrac{u^{*,n} - u^{*,n-1}}{\tau} - \operatorname{div}(D\nabla u^{*,n-1}) = g & \text{in } \Omega, \\ u^{*,n-1} = 0 & \text{on } \partial\Omega, \\ u^{*,N} = u_T^* & \text{in } \Omega. \end{cases} \tag{67}$$

The spatial approximation $u_h^{*,n}$ of $u^{*,n}$ is made using standard $\mathbb{P}_2$ finite elements on the same meshes, and the corresponding flux reconstruction θ_h^* is approximated using some standard $\mathbb{RT}_2$ finite elements.

For each mesh, we compute the value of $\mathcal{E} = Q(u - u_h)$ defined by (43) as well as the one of η_{QOI} defined by (45). We plot on Figure 12(a) the values of $\mathcal{E}$ as well as the ones of η_{QOI} and $\eta\eta^*$ as functions of h in a log-log scale. First of all, we remark that the error $\mathcal{E}$ goes towards zero at the order $O(h)$, which is the expected behaviour since even if u is regular enough and u_h is approximated by $\mathbb{P}_1$ finite elements, the time integration is of order one and the choice of $\tau = h$ leads to a global rate of convergence equal to one. Moreover, the estimator η_{QOI} converges towards zero at the same rate of convergence. Figure 12(b) displays the effectivity index $I_{eff} = \mathcal{E}/\eta_{QOI}$ as a function of h. As for the stationary tests with regular solutions, it is always nearly equal to one and converges towards one. Consequently the estimator η_{QOI} is asymptotically exact. Finally, coming back to Figure 12(a), we see that the value of $\eta\eta^*$ goes

towards zero faster than $\mathcal{E}$ (here around the order $O(h^{1.75})$), what illustrates the fact that $\mathcal{R}$ is clearly superconvergent (see (50)).



(a) (b)

Figure 12: Heat equation: (a) rates of convergence; (b) asymptotical exactness.

4.2.2 A moving Gaussian

Finally we consider a more difficult test coming from [34]. This time, the primal problem is defined by (27) with $d = 2$, $\Omega =]0,1[^2$, $T = 1.0$ and $D = I_{\mathbb{R}^2}$. We choose the exact solution being equal to $u(x,y,t) = \beta(t)\, e^{-50(r(x,y,t))^2}$ with $r(x,y,t) = ((x-0.4t-0.3)^2 + (y-0.4t-0.3)^2)^{1/2}$ and $\beta(t)$ defined by:

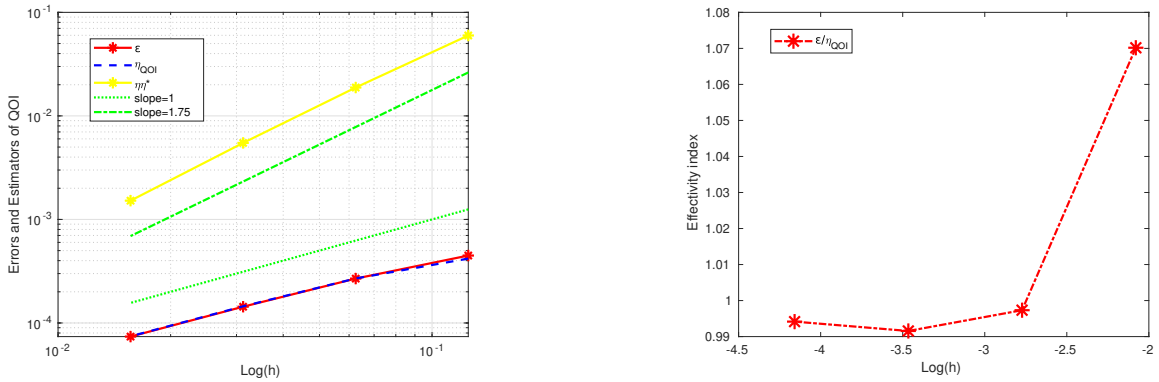
$$\beta(t) = \begin{cases} 1 - e^{-50(0.98t+0.01)^2} & \text{if } t \leq 0.5, \\ 1 - e^{-50(1-0.98t+0.01)^2} & \text{else.} \end{cases}$$

It consists in a moving Gaussian from the position $(0.3, 0.3)$ to the position $(0.7, 0.7)$ at a non constant speed. As usual, the right-hand side f is computed accordingly. The dual problem is defined by (32), where we choose $g = 0$ and $u_T^* = e^{-\frac{\rho(x,y)^2}{32 \ln 10}}$ with $\rho(x,y) = ((x-0.7)^2 + (y-0.7)^2)^{1/2}$.

For the numerical simulation, we set $\tau = h/10$, all the other numerical parameters are the same as the ones of section 4.2.1. We can see in Figure 13(a) that once again, the estimator η_{QOI} converges towards zero at the order $O(h)$ as theoretically expected, whereas the product $\eta\,\eta^*$ goes faster towards zero (in the order $O(h^{1.75})$). As expected by Theorems 3.1 and 3.3, Figure 13(b) illustrates the asymptotic exactness of the estimator since the effectivity index $I_{eff} = \mathcal{E}/\eta_{QOI}$ goes towards 1 when h goes towards zero.

5 Conclusion

In this paper, we have performed goal-oriented a posteriori error estimations for conforming and nonconforming discretizations of elliptic and parabolic problems. It is based on $H(\mathrm{div})$-conforming flux reconstructions and H^1-conforming potential reconstructions. Our main novelty is a decomposition of the error into a fully computable error estimator and a remainder, this remainder being bounded by the product of the estimators of the direct and dual problems, up to an explicit multiplicative factor (see Theorems 2.1 and 2.4 for reaction-diffusion problems and Theorems 3.1 and 3.3 for parabolic problems). Various numerical results illustrate that the error in the quantity of interest is estimated precisely by the error estimator, with an effectivity index of order 1. Nevertheless, in some particular cases, we have observed that this asymptotic exactness does not hold and that the use of the additional term, namely the product of the



(a) (b)

Figure 13: Moving Gaussian: (a) rates of convergence; (b) asymptotical exactness.

estimators of the direct and dual problems (that we prove that it bounds the remainder), should be required in adaptive algorithms.

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