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Guaranteed and robust a posteriori error estimates for singularly perturbed reaction–diffusion problems

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Abstract

We derive a posteriori error estimates for singularly perturbed reaction–diffusion problems which yield a guaranteed upper bound on the discretization error and are fully and easily computable. Moreover, they are also locally efficient and robust in the sense that they represent local lower bounds for the actual error, up to a generic constant independent in particular of the reaction coefficient. We present our results in the framework of the vertex-centered finite volume method but their nature is general for any conforming method, like the piecewise linear finite element one. Our estimates are based on a $\mathbf{H}(\mathrm{div})$-conforming reconstruction of the diffusive flux in the lowest-order Raviart–Thomas space linked with mesh dual to the original simplicial one, previously introduced by the last author in the pure diffusion case. They also rely on elaborated Poincaré, Friedrichs, and trace inequalities-based auxiliary estimates designed to cope optimally with the reaction dominance. In order to bring down the ratio of the estimated and actual overall energy error as close as possible to the optimal value of one, independently of the size of the reaction coefficient, we finally develop the ideas of local minimizations of the estimators by local modifications of the reconstructed diffusive flux. The numerical experiments presented confirm the guaranteed upper bound, robustness, and excellent efficiency of the derived estimates.

Key words: vertex-centered finite volume/finite volume element/box method, singularly perturbed reaction–diffusion problem, a posteriori error estimates, guaranteed upper bound, robustness

AMS subject classifications: 65N15, 65N30, 76S05

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1 Introduction

We consider in this paper the model reaction–diffusion problem

$$-\Delta p + rp = f \quad \text{in } \Omega, \tag{1.1a}$$

$$p = 0 \quad \text{on } \partial\Omega, \tag{1.1b}$$

where $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, is a polygonal (polyhedral) domain (open, bounded, and connected set), $r \in L^\infty(\Omega)$, $r \geq 0$, is a reaction coefficient, and $f \in L^2(\Omega)$ is a source term. We denote respectively by $c_{r,S}$ and $C_{r,S}$ the best nonnegative constants such that $c_{r,S} \leq r \leq C_{r,S}$ a.e. on a given subdomain S of Ω. Our purpose is to derive optimal a posteriori error estimates for vertex-centered finite volume approximations of problem (1.1a)–(1.1b), with extensions to other conforming methods like the piecewise linear finite element one.

Averaging a posteriori error estimates like the Zienkiewicz–Zhu [23] one are quite popular for the purpose of adaptive mesh refinement in boundary value problems simulations but actually do not give a guaranteed upper bound on the error made in a numerical approximation. More severely, for problem (1.1a)–(1.1b) in particular, they are not robust in the sense that the ratio of the estimated and true energy errors blows up for high values of r. The improvement of the equilibrated residual method to singularly perturbed reaction–diffusion problems by Ainsworth and Babuška [1] does not have this drawback and yields robust estimates. It also gives a guaranteed upper bound but this bound is actually not computable, since it is based on a solution of an infinite-dimensional local problem on each mesh element. Approximations to these problems have to be used in practice, which rises the question of preservation of the guaranteed upper bound and even of the robustness. This question, along with a robust extension to anisotropic meshes, is treated by Grosman in [8]. By introducing suitable finite-dimensional approximations of the local infinite-dimensional problems, Grosman proves the robustness of the final practical estimate. Moreover, he also shows that these approximations yield an estimate which is equivalent with the original infinite-dimensional one up to an unknown constant, independent of the mesh size h and the reaction parameter r. He thus ensures the reliability of the final discrete version of the equilibrated residual method, the presented numerical results are excellent, but still the guaranteed upper bound property in the strict sense is lost, as one can notice it in [8, Table 1]. Moreover, this approach seems rather complicated and computationally quite expensive, although the evaluation cost remains linear.

Verfürth in [17] derived robust residual a posteriori error estimates for singularly perturbed reaction–diffusion problems which are explicitly and easily computable. Unfortunately, these estimates are not guaranteed in the sense that they contain various undetermined constants; they are suitable for adaptive mesh refinement but not for the actual error control. An extension of this result to anisotropic meshes is then given by Kunert [11]. Recently, Repin and Sauter [14] or Korotov [10] presented estimates which do give a guaranteed upper bound also for problem (1.1a)–(1.1b). However, for accurate error control, computational amount comparable to that necessary to the computation of the approximation itself is required and it is quite likely that this amount will grow for growing coefficient r, which does not match with the term robustness. Coincidently, no (local) efficiency is proved in these references. Guaranteed and locally computable estimators for problem (1.1a)–(1.1b) are also arrived at by Vejchodský [16], but, once again, no lower bound is proved and the estimate is not expected to be robust.

A family of "equilibrated fluxes" estimates was established recently for various numerical methods in [20, 19, 6, 21]. These estimates are explicitly and easily computable and yield a guaranteed upper bound together with local efficiency; the estimates of [21] for the pure diffusion case are moreover completely robust with respect to an inhomogeneous diffusion coefficient. In the conforming case, these estimates resemble ideas going back to the Prager–Synge equality [13].

The purpose of this paper is to extend the estimates of [21] to the singularly perturbed reaction–diffusion problem (1.1a)–(1.1b). We first in Section 3, after giving the necessary preliminaries in Section 2, present an abstract a posteriori error estimate for conforming (contained in $H_0^1(\Omega)$) approximations to problem (1.1a)–(1.1b). This estimate is shown to be optimal, i.e., equivalent to the energy error, and gives the basic framework for the further study. We start in Section 4 by presenting the ideas of the diffusive flux reconstruction in the lowest-order Raviart–Thomas space linked with the mesh dual to the original simplicial one and prove some important Poincaré, Friedrichs, and trace inequalities-based auxiliary estimates designed to cope optimally with the reaction dominance. Then the first main result, an a posteriori error estimate which is explicitly and easily computable and which gives a guaranteed upper bound on the overall energy error, is stated and proved. We present all these results in the framework of the vertex-centered finite volume method but their nature is general for any conforming method, like the piecewise linear finite element one. We finally in Section 5 present our second main result, the local efficiency and robustness, with respect to reaction (and also diffusion) dominance and also with respect to the spatial variation of r under the condition that r is piecewise constant on the dual mesh, of the derived a posteriori error estimates in the finite volume case. We there actually show that our estimates represent local lower bounds for those of Verfürth [17].

The numerical experiments of Section 6, using the package FreeFem++ [9], where our estimates are implemented, confirm all the theoretical results. The only element missing for perfection is that the effectivity index (the ratio of the estimated and actual error) is not as close to the optimal value of 1 as one would have wished (it ranges between 2 and 6 in the presented results). This phenomenon has been already observed in the pure diffusion case in [5] and [21]. A remedy to this has been proposed in these references, consisting in local minimizations of the estimators by local modifications of the reconstructed diffusive flux. In particular, an (approximate) full local minimization over the available degrees of freedom has been proposed and studied in [5]. Such a minimization leads to the solution of a local linear system for each vertex (of size equal to twice the number of sides sharing the given vertex); although the cost remains linear, the complexity is indeed slightly increased. The solution of local linear systems was completely avoided by the simplified minimization approach of [21, Section 7]. We extend in this paper the two approaches to the singularly perturbed reaction–diffusion problem (1.1a)–(1.1b). It turns out that the completely explicit simplified local minimization gives almost always the best results, so it can for its simplicity and efficiency be recommended for practical computations. In particular, with its use, the effectivity index in the presented results ranges between 1 and 3 for all the meshes from the coarsest to the finest and from uniformly to adaptively refined and for all values of the reaction coefficient r. We finally remark that the homogeneous Dirichlet boundary condition is considered only for simplicity of exposition. For inhomogeneous Dirichlet and Neumann boundary conditions in the present setting (with $r = 0$), we refer to [22].

2 Preliminaries

We set up in this section the considered meshes description and all notation and describe the continuous and discrete problems we shall work with.

2.1 Notation

We shall work in this paper with triangulations $\mathcal{T}_h$ which for all $h > 0$ consists of triangles K such that $\bar{\Omega} = \bigcup_{K \in \mathcal{T}_h} K$ and which are conforming, i.e., if $K, L \in \mathcal{T}_h, K \neq L$, then $K \cap L$ is either an empty set or a common face, edge, or vertex of K and L. Let h_K denote the diameter of K and

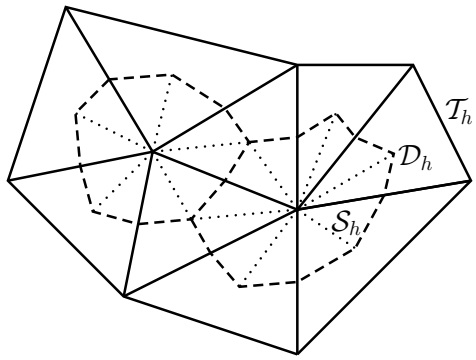

Figure 1: Original simplicial mesh $\mathcal{T}_h$, the associated dual mesh $\mathcal{D}_h$, and the fine simplicial mesh $\mathcal{S}_h$

let $h := \max_{K\in\mathcal{T}_h} h_K$. We next denote by $\mathcal{E}_h$ the set of all sides of $\mathcal{T}_h$, by $\mathcal{E}_h^{\text{int}}$ the set of interior, by $\mathcal{E}_h^{\text{ext}}$ the set of exterior, and by $\mathcal{E}_K$ the set of all the sides of an element $K \in \mathcal{T}_h$; h_σ stands for the diameter of $\sigma \in \mathcal{E}_h$. Finally, we denote by $\mathcal{V}_h$ ($\mathcal{V}_h^{\text{int}}$) the set of all (interior) vertices of $\mathcal{T}_h$ and define for $V \in \mathcal{V}_h$ and $\sigma \in \mathcal{E}_h$, respectively, $\mathcal{T}_V := \{L \in \mathcal{T}_h; L \cap V \neq \emptyset\}$, $\mathcal{T}_\sigma := \{L \in \mathcal{T}_h; \sigma \in \mathcal{E}_L\}$.

We shall next consider dual partitions $\mathcal{D}_h$ of Ω such that $\bar{\Omega} = \bigcup_{D\in\mathcal{D}_h} D$ and such that each $V \in \mathcal{V}_h$ is in exactly one $D_V \in \mathcal{D}_h$. The notation V_D stands inversely for the vertex associated with a given $D \in \mathcal{D}_h$. When $d = 2$, we construct $\mathcal{D}_h$ as follows. For each vertex V, we consider all the triangles $K \in \mathcal{T}_V$. Then, the dual volume D_V associated to V is the polygon which has these triangle barycenters and the midpoints of the edges passing trough V as vertices. An example of such a dual volume is shown in Figure 1. If $d = 3$, in each tetrahedron, face barycentres are first connected with face vertices and face edges midpoints. Then small tetrahedra are formed by the resulting triangles in each face and the tetrahedron barycentre. Finally, the union of all small tetrahedra sharing a given vertex V_D is the dual volume D. We use the notation $\mathcal{F}_h$ for all sides of $\mathcal{D}_h$, $\mathcal{F}_h^{\text{int}}$ ($\mathcal{F}_h^{\text{ext}}$) for all interior (exterior) sides of $\mathcal{D}_h$, and $\mathcal{D}_h^{\text{int}}$ ($\mathcal{D}_h^{\text{ext}}$) to denote the dual volumes associated with vertices from $\mathcal{V}_h^{\text{int}}$ ($\mathcal{V}_h^{\text{ext}}$).

Finally, in order to define our a posteriori error estimates, we need a second simplicial triangulation $\mathcal{S}_h$ of Ω. This is given by $\mathcal{S}_h := \cup_{D\in\mathcal{D}_h}\mathcal{S}_D$, where the local triangulation $\mathcal{S}_D$ of $D \in \mathcal{D}_h$ is given as shown in Figure 1 if $d = 2$ and by the "small" tetrahedra if $d = 3$. We will use the notation $\mathcal{G}_h$ for all sides of $\mathcal{S}_h$ and $\mathcal{G}_h^{\text{int}}$ ($\mathcal{G}_h^{\text{ext}}$, for all interior (exterior) sides of $\mathcal{S}_h$. Also, we will note $\mathcal{G}_D^{\text{int}}$ all $\sigma \in \mathcal{G}_h^{\text{int}}$ contained in the interior of a $D \in \mathcal{D}_h$.

Next, for $K \in \mathcal{T}_h$, $\mathbf{n}$ always denotes its exterior normal vector and we employ the notation $\mathbf{n}_\sigma$ for a normal vector of a side $\sigma \in \mathcal{E}_h$, whose orientation is chosen arbitrarily but fixed for interior sides and coinciding with the exterior normal of Ω for exterior sides. For a function φ and a side $\sigma \in \mathcal{E}_h^{\text{int}}$ shared by $K, L \in \mathcal{T}_h$ such that $\mathbf{n}_\sigma$ points from K to L, we define the jump operator $[\![\cdot]\!]$ by

$$[\![\varphi]\!] := (\varphi|_K)|_\sigma - (\varphi|_L)|_\sigma. \tag{2.1}$$

We put $[\![\varphi]\!] := 0$ for any $\sigma \in \mathcal{E}_h^{\text{ext}}$. For $\sigma = \sigma_{K,L} \in \mathcal{E}_h^{\text{int}}$, we define the average operator $\{\!\{\cdot\}\!\}$ by

$$\{\!\{\varphi\}\!\} := \frac{1}{2}(\varphi|_K)|_\sigma + \frac{1}{2}(\varphi|_L)|_\sigma, \tag{2.2}$$

whereas for $\sigma \in \mathcal{E}_h^{\text{ext}}$, $\{\!\{\varphi\}\!\} := \varphi|_\sigma$. We use the same type of notation also for the meshes $\mathcal{D}_h$ and $\mathcal{S}_h$.

In what concerns functional notation, we denote by $(\cdot,\cdot)_S$ the L^2-scalar product on S and by $\|\cdot\|_S$ the associated norm; when $S = \Omega$, the index is dropped off. We denote by $|S|$ the Lebesgue measure of S, by $|\sigma|$ the $(d-1)$-dimensional Lebesgue measure of $\sigma \subset \mathbb{R}^{d-1}$, and in particular by $|\mathbf{s}|$ the

length of a segment $\mathbf{s}$. Next, $H^1(S)$ is the Sobolev space of functions with square-integrable weak derivatives and $H^1_0(S)$ is its subspace of functions with traces vanishing on ∂S. Finally, $\mathbf{H}(\mathrm{div}, S)$ is the space of functions with square-integrable weak divergences, $\mathbf{H}(\mathrm{div}, S) = \{\mathbf{v} \in \mathbf{L}^2(S); \nabla \cdot \mathbf{v} \in L^2(S)\}$, and $\langle \cdot, \cdot \rangle_{\partial S}$ stands for the appropriate duality pairing on ∂S.

2.2 Continuous and discrete problems

For problem (1.1a)–(1.1b), we define a bilinear form $\mathcal{B}$ by

$$\mathcal{B}(p, \varphi) := (\nabla p, \nabla \varphi) + (r^{1/2} p, r^{1/2} \varphi),$$

where $p, \varphi \in H^1_0(\Omega)$, and the associated energy norm by

$$|||\varphi|||^2 := \mathcal{B}(\varphi, \varphi). \tag{2.3}$$

The standard weak formulation for this problem is then to find $p \in H^1_0(\Omega)$ such that

$$\mathcal{B}(p, \varphi) = (f, \varphi) \qquad \forall \varphi \in H^1_0(\Omega). \tag{2.4}$$

For the approximation of problem (1.1a)–(1.1b), we will consider the vertex-centered finite volume method, also known as the finite volume element or the box method. It reads: find $p_h \in X^0_h$ such that

$$-\langle \nabla p_h \cdot \mathbf{n}, 1 \rangle_{\partial D} + (r p_h, 1)_D = (f, 1)_D \qquad \forall D \in \mathcal{D}^{\mathrm{int}}_h, \tag{2.5}$$

where

$$X^0_h := \left\{ \varphi_h \in H^1_0(\Omega);\ \varphi_h|_K \in \mathbb{P}_1(K) \quad \forall K \in \mathcal{T}_h \right\}$$

with $\mathbb{P}_1(K)$ the space of linear polynomials on $K \in \mathcal{T}_h$. This method for the approximation of problem (1.1a)–(1.1b) is very closely related to the piecewise linear finite element one, which consists in finding $p_h \in X^0_h$ such that

$$\mathcal{B}(p_h, \varphi_h) = (f, \varphi_h) \qquad \forall \varphi_h \in X^0_h.$$

In particular, for the considered dual meshes, the discretization of the diffusion term completely coincides, cf. [21, Lemma 3.8]. Similarly, if f is piecewise constant on $\mathcal{T}_h$, the discretization of the right-hand side again coincides, see [21, Lemma 3.11], whereas the discretization of the reaction term only differs by a numerical quadrature. We refer to [21] for the relations to other methods yielding an approximation in the space X^0_h.

3 Optimal abstract framework for a posteriori error estimation

In this section, we recall the basic results of [20, 6], giving an optimal abstract framework for a posteriori error estimation in problem (1.1a)–(1.1b).

3.1 Abstract estimate

The first result is the following abstract upper bound:

Theorem 3.1 (Abstract a posteriori error estimate)**.** *Let p be the weak solution of problem* (1.1a)–(1.1b) *given by* (2.4) *and let $p_h \in H^1_0(\Omega)$ be arbitrary. Then*

$$|||p - p_h||| \le \inf_{\mathbf{t} \in \mathbf{H}(\mathrm{div}, \Omega)} \sup_{\varphi \in H^1_0(\Omega),\, |||\varphi|||=1} \{(f - \nabla \cdot \mathbf{t} - r p_h, \varphi) - (\nabla p_h + \mathbf{t}, \nabla \varphi)\}. \tag{3.1}$$

Proof. We first notice that according to the definition of the energy norm by (2.3),

$$|||p - p_h||| = \mathcal{B}\left(p - p_h, \frac{p - p_h}{|||p - p_h|||}\right).$$

Here, as well as in the sequel, we treat the possible occurrence of 0/0 as 0 for the simplicity of notation. Next, as $\varphi := (p - p_h)/|||p - p_h||| \in H_0^1$, we have $\mathcal{B}(p, \varphi) = (f, \varphi)$ by (2.4). So, for any $\mathbf{t} \in \mathbf{H}(\mathrm{div}, \Omega)$, adding and subtracting $(\mathbf{t}, \nabla\varphi)$, we have

$$\begin{aligned} |||p - p_h||| &= (f, \varphi) - \mathcal{B}(p_h, \varphi) \\ &= (f, \varphi) - (\nabla p_h, \nabla\varphi) - (rp_h, \varphi) \\ &= (f, \varphi) - (\nabla p_h + \mathbf{t}, \nabla\varphi) - (rp_h, \varphi) + (\mathbf{t}, \nabla\varphi) \\ &= (f - \nabla\cdot\mathbf{t} - rp_h, \varphi) - (\nabla p_h + \mathbf{t}, \nabla\varphi), \end{aligned} \tag{3.2}$$

where we have lastly applied the Green theorem yielding $(\mathbf{t}, \nabla\varphi) = -(\nabla\cdot\mathbf{t}, \varphi)$. As $\mathbf{t} \in \mathbf{H}(\mathrm{div}, \Omega)$ was chosen arbitrarily and $|||\varphi||| = 1$, this concludes the proof. □

3.2 Efficiency of the abstract estimate

Concerning the efficiency of the above estimate, we have:

Theorem 3.2 (Global efficiency of the abstract estimate)**.** *Let p be the weak solution of problem* (1.1a)–(1.1b) *given by* (2.4) *and let $p_h \in H_0^1(\Omega)$ be arbitrary. Then*

$$\inf_{\mathbf{t}\in\mathbf{H}(\mathrm{div},\Omega)} \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{(f - \nabla\cdot\mathbf{t} - rp_h, \varphi) - (\nabla p_h + \mathbf{t}, \nabla\varphi)\} \le |||p - p_h|||.$$

Proof. We add and subtract the term (rp, φ), put $\mathbf{t} = -\nabla p$, and use the fact that p is the weak solution to obtain

$$\begin{aligned} &\inf_{\mathbf{t}\in\mathbf{H}(\mathrm{div},\Omega)} \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{(f - \nabla\cdot\mathbf{t} - rp_h, \varphi) - (\nabla p_h + \mathbf{t}, \nabla\varphi)\} \\ &\quad= \inf_{\mathbf{t}\in\mathbf{H}(\mathrm{div},\Omega)} \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{(f - \nabla\cdot\mathbf{t} - rp, \varphi) - (\nabla p_h + \mathbf{t}, \nabla\varphi) + (rp - rp_h, \varphi)\} \\ &\quad\le \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{(f + \Delta p - rp, \varphi) - (\nabla p_h - \nabla p, \nabla\varphi) + (rp - rp_h, \varphi)\} \\ &\quad= \sup_{\varphi\in H_0^1(\Omega),\, |||\varphi|||=1} \{(\nabla(p - p_h), \nabla\varphi) + (r(p - p_h), \varphi)\}. \end{aligned}$$

The proof is concluded by using the Cauchy–Schwarz inequality, the fact that $|||\varphi||| = 1$, and the definition of the energy norm (2.3). □

4 Guaranteed a posteriori error estimates

We derive here a locally computable version of the abstract a posteriori estimate of the previous section. The first step is to properly choose a reconstructed diffusive flux $\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ to be used as $\mathbf{t} \in \mathbf{H}(\mathrm{div}, \Omega)$ in Theorem 3.1. We next recall the Poincaré, Friedrichs, and trace inequalities and derive some auxiliary estimates that will turn out later as crucial in order to obtain robustness. We finally state our guaranteed a posteriori error estimates.

4.1 Diffusive flux reconstruction

We present here a particular diffusive flux reconstruction $\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ in the vertex-centered finite volume method (2.5), which will be crucial in our a posteriori error estimates. We define it in the lowest-order Raviart–Thomas–Nédélec space over the fine simplicial mesh $\mathcal{S}_h$ introduced in Section 2. The space $\mathbf{RTN}(\mathcal{S}_h)$ is a space of vector functions having on each $K \in \mathcal{S}_h$ the form $(a_K + d_K x, b_K + d_K y)^t$ if $d = 2$ and $(a_K + d_K x, b_K + d_K y, c_K + d_K z)^t$ if $d = 3$. Note that the requirement $\mathbf{RTN}(\mathcal{S}_h) \subset \mathbf{H}(\mathrm{div}, \Omega)$ imposes the continuity of the normal trace across all $\sigma \in \mathcal{G}_h^{\mathrm{int}}$ and recall that $\mathbf{v} \cdot \mathbf{n}_\sigma$ is constant on all $\sigma \in \mathcal{G}_h$ and that these side fluxes also represent the degrees of freedom of $\mathbf{RTN}(\mathcal{S}_h)$. For more details, we refer to Brezzi and Fortin [3] or Roberts and Thomas [15].

Let us thus define $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$ by

$$\mathbf{t}_h \cdot \mathbf{n}_\sigma = -\{\!\{\nabla p_h \cdot \mathbf{n}_\sigma\}\!\} \qquad \forall \sigma \in \mathcal{G}_h, \tag{4.1}$$

where $\{\!\{\cdot\}\!\}$ is the average operator defined in Section 2. Note that $\mathbf{t}_h \cdot \mathbf{n}_\sigma$ is given directly by $-\nabla p_h \cdot \mathbf{n}_\sigma$ for such $\sigma \in \mathcal{G}_h$ where there is no jump in ∇p_h, i.e., on all the sides $\sigma \in \mathcal{G}_h$ which are in the interior of some $K \in \mathcal{T}_h$ or at the boundary of Ω. In the other cases, we may think of $\mathbf{t}_h$ as of a $\mathbf{H}(\mathrm{div}, \Omega)$-conforming smoothing of $-\nabla p_h$, which itself is not contained in $\mathbf{H}(\mathrm{div}, \Omega)$. The following important property holds for $\mathbf{t}_h$ constructed in this way:

Lemma 4.1 (Reconstructed diffusive flux)**.** *Let $p_h \in X_h^0$ be given by the vertex-centered finite volume method* (2.5) *and let $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$ be given by* (4.1)*. Then*

$$(\nabla \cdot \mathbf{t}_h + r p_h, 1)_D = (f, 1)_D \qquad \forall D \in \mathcal{D}_h^{\mathrm{int}}.$$

Proof. The local conservativity of the vertex-centered finite volume method (2.5) and the definition (4.1) of $\mathbf{t}_h$ imply that

$$\langle \mathbf{t}_h \cdot \mathbf{n}, 1 \rangle_{\partial D} + (r p_h, 1)_D = (f, 1)_D \qquad \forall D \in \mathcal{D}_h^{\mathrm{int}},$$

noticing that $\{\!\{\nabla p_h \cdot \mathbf{n}_\sigma\}\!\} = \nabla p_h \cdot \mathbf{n}_\sigma$ for all $\sigma \subset \partial D$, since all such sides lie in the interior of some $K \in \mathcal{T}_h$, where ∇p_h is constant. The assertion of the lemma now follows by the Green theorem. □

4.2 Poincaré, Friedrichs, and trace inequalities-based auxiliary estimates

In order to define our estimators, we will need the Poincaré, Friedrichs, and trace inequalities, which we recall below. We then prove several important auxiliary estimates, designed to cope optimally with the reaction dominance.

Let D be a polygon or a polyhedron. The Poincaré inequality states that

$$\|\varphi - \varphi_D\|_D^2 \le C_{\mathrm{P},D} h_D^2 \|\nabla \varphi\|_D^2 \qquad \forall \varphi \in H^1(D), \tag{4.2}$$

where φ_D is the mean of φ over D given by $\varphi_D := (\varphi, 1)_D / |D|$ and where the constant $C_{\mathrm{P},D}$ can for each convex D be evaluated as $1/\pi^2$, cf. [12, 2]. To evaluate $C_{\mathrm{P},D}$ for nonconvex elements D is more complicated but it still can be done, cf. Eymard *et al.* [7, Lemma 10.2] or Carstensen and Funken [4, Section 2].

The Friedrichs inequality states that

$$\|\varphi\|_D^2 \le C_{\mathrm{F},D,\partial\Omega} h_D^2 \|\nabla \varphi\|_D^2 \qquad \forall \varphi \in H^1(D) \text{ such that } \varphi = 0 \text{ on } \partial\Omega \cap \partial D \neq \emptyset. \tag{4.3}$$

As long as $\partial\Omega$ is such that there exists a vector $\mathbf{b} \in \mathbb{R}^d$ such that for almost all $\mathbf{x} \in D$, the first intersection of $\mathcal{B}_\mathbf{x}$ and ∂D lies in $\partial\Omega$, where $\mathcal{B}_\mathbf{x}$ is the straight semi-line defined by the origin $\mathbf{x}$ and

the vector $\mathbf{b}$, $C_{\mathrm{F},D,\partial\Omega} = 1$, cf. [18, Remark 5.8]. To evaluate $C_{\mathrm{F},D,\partial\Omega}$ in the general case is more complicated but it still can be done, cf. [18, Remark 5.9] or Carstensen and Funken [4, Section 3].

Finally, for a simplex K, the trace inequality states that

$$\|\varphi\|_\sigma^2 \le C_{\mathrm{t},K,\sigma}(h_K^{-1}\|\varphi\|_K^2 + \|\varphi\|_K\|\nabla\varphi\|_K) \qquad \forall\varphi \in H^1(K), \tag{4.4}$$

cf., e.g., Carstensen and Funken [4, Theorem 4.1]. For the value of $C_{\mathrm{t},K,\sigma}$ if $d = 2$, see Remark 4.3 below.

Lemma 4.2 (Auxiliary estimates on simplices)**.** *Let $K \in \mathcal{S}_h$, $\sigma \in \mathcal{E}_K$, $\varphi \in H^1(K)$, and $\varphi_K := (\varphi, 1)_K/|K|$. Then*

$$\|\varphi - \varphi_K\|_K \le m_K|||\varphi|||_K \tag{4.5}$$

with

$$m_K := \min\left\{C_{\mathrm{P},K}^{1/2}h_K, c_{r,K}^{-1/2}\right\}. \tag{4.6}$$

Moreover,

$$\|\varphi - \varphi_K\|_\sigma \le C_{\mathrm{t},K,\sigma}^{1/2}\widetilde{m}_K^{1/2}|||\varphi|||_K \tag{4.7}$$

with

$$\widetilde{m}_K := \min\left\{\left(C_{\mathrm{P},K} + C_{\mathrm{P},K}^{1/2}\right)h_K, c_{r,K}^{-1}h_K^{-1} + \frac{1}{2}c_{r,K}^{-1/2}\right\}. \tag{4.8}$$

Proof. We begin by the first assertion. As φ_K is the L^2 projection of φ over the constants, we have

$$\|\varphi - \varphi_K\|_K \le \|\varphi\|_K. \tag{4.9}$$

Now, using that

$$\|\varphi\|_K = \left\|\frac{r^{1/2}}{r^{1/2}}\varphi\right\|_K \le c_{r,K}^{-1/2}|||\varphi|||_K, \tag{4.10}$$

we obtain $\|\varphi - \varphi_K\|_K \le c_{r,K}^{-1/2}|||\varphi|||_K$. On the other hand, from the Poincaré inequality (4.2) and definition (2.3) of the energy norm, the estimate $\|\varphi-\varphi_K\|_K \le C_{\mathrm{P},K}^{1/2}h_K|||\varphi|||_K$ follows easily, whence we conclude (4.5).

In order to prove the second assertion, we use the trace inequality (4.4) for $\varphi - \varphi_K$. We have

$$\begin{aligned}
\|\varphi - \varphi_K\|_\sigma^2 &\le C_{\mathrm{t},K,\sigma}(h_K^{-1}\|\varphi - \varphi_K\|_K^2 + \|\varphi - \varphi_K\|_K\|\nabla(\varphi - \varphi_K)\|_K) \\
&\le C_{\mathrm{t},K,\sigma}(C_{\mathrm{P},K}h_K\|\nabla\varphi\|_K^2 + C_{\mathrm{P},K}^{1/2}h_K\|\nabla\varphi\|_K^2) \\
&\le C_{\mathrm{t},K,\sigma}\left(C_{\mathrm{P},K} + C_{\mathrm{P},K}^{1/2}\right)h_K|||\varphi|||_K^2,
\end{aligned}$$

using that $\nabla\varphi_K = 0$ and employing the Poincaré inequality (4.2) and definition (2.3) of the energy norm. Similarly,

$$\begin{aligned}
\|\varphi - \varphi_K\|_\sigma^2 &\le C_{\mathrm{t},K,\sigma}\left(h_K^{-1}\|\varphi\|_K^2 + \|\varphi\|_K\|\nabla\varphi\|_K\right) \\
&\le C_{\mathrm{t},K,\sigma}\left(c_{r,K}^{-1}h_K^{-1}|||\varphi|||_K^2 + c_{r,K}^{-1/2}\|r^{1/2}\varphi\|_K\|\nabla\varphi\|_K\right) \\
&\le C_{\mathrm{t},K,\sigma}\left(c_{r,K}^{-1}h_K^{-1}|||\varphi|||_K^2 + \frac{1}{2}c_{r,K}^{-1/2}|||\varphi|||_K^2\right),
\end{aligned}$$

using (4.9), (4.10), the inequality $2ab \le a^2+b^2$, and definition (2.3) of the energy norm, whence (4.7) follows. □

Remark 4.3 (Improved estimate on triangles)**.** *In two space dimensions, owing to the form of the trace inequality*

$$\|\varphi\|_\sigma^2 \le C_{\mathrm{t},K,\sigma}\left(h_K^{-1}\|\varphi\|_K^2 + \frac{2}{3}\|\varphi\|_K\|\nabla\varphi\|_K\right)$$

with

$$C_{\mathrm{t},K,\sigma} = \frac{3}{2}|\sigma|h_K|K|^{-1}, \tag{4.11}$$

which follows from Carstensen and Funken [4, Theorem 4.1], we can actually use the somewhat sharper bound

$$\widetilde{m}_K := \min\left\{\left(C_{\mathrm{P},K} + \frac{2}{3}C_{\mathrm{P},K}^{1/2}\right)h_K, c_{r,K}^{-1}h_K^{-1} + \frac{1}{3}c_{r,K}^{-1/2}\right\} \tag{4.12}$$

instead of (4.8) *in* (4.7)*.*

Lemma 4.4 (Auxiliary estimates on dual volumes)**.** *Let $D \in \mathcal{D}_h$, $\varphi \in H^1(D)$, and $\varphi_D := (\varphi, 1)_D/|D|$. Then,*

$$\begin{aligned}\|\varphi - \varphi_D\|_D &\le m_D|||\varphi|||_D, \quad D \in \mathcal{D}_h^{\mathrm{int}},\\ \|\varphi\|_D &\le m_D|||\varphi|||_D, \quad D \in \mathcal{D}_h^{\mathrm{ext}},\end{aligned}$$

where

$$m_D := \min\left\{C_{\mathrm{P},D}^{1/2}h_D, c_{r,D}^{-1/2}\right\}, \quad D \in \mathcal{D}_h^{\mathrm{int}}, \tag{4.13}$$

$$m_D := \min\left\{C_{\mathrm{F},D,\partial\Omega}^{1/2}h_D, c_{r,D}^{-1/2}\right\}, \quad D \in \mathcal{D}_h^{\mathrm{ext}}, \tag{4.14}$$

with $C_{\mathrm{P},D}$ the constant from the Poincaré inequality (4.2) *and $C_{\mathrm{F},D,\partial\Omega}$ that from the Friedrichs inequality* (4.3)*.*

Proof. The proof of the first statement is analogous to the proof of (4.5) in Lemma 4.2. For $D \in \mathcal{D}_h^{\mathrm{ext}}$, we use $\|\varphi\|_D \le c_{r,D}^{-1/2}|||\varphi|||_D$ (cf. (4.10)) and the Friedrichs inequality (4.3) to obtain the second statement. □

4.3 Guaranteed a posteriori error estimates

We define and prove here our a posteriori error estimates in a rather general form motivated by the diffusive flux reconstruction of Section 4.1:

Theorem 4.5 (Guaranteed a posteriori error estimate)**.** *Let p be the weak solution of problem* (1.1a)–(1.1b) *given by* (2.4) *and let $p_h \in H_0^1(\Omega)$ be arbitrary. Let next $\mathbf{t}_h \in \mathbf{H}(\mathrm{div},\Omega)$ be such that*

$$(\nabla\cdot\mathbf{t}_h + rp_h, 1)_D = (f, 1)_D \qquad \forall D \in \mathcal{D}_h^{\mathrm{int}}. \tag{4.15}$$

Define the residual estimator *by*

$$\eta_{\mathrm{R},D} := m_D\|f - \nabla\cdot\mathbf{t}_h - rp_h\|_D, \qquad D \in \mathcal{D}_h, \tag{4.16}$$

where m_D is given by (4.13)–(4.14)*, and the* diffusive flux estimator

$$\eta_{\mathrm{DF},D} := \min\left\{\eta_{\mathrm{DF},D}^{(1)}, \eta_{\mathrm{DF},D}^{(2)}\right\}, \qquad D \in \mathcal{D}_h, \tag{4.17}$$

where

$$\eta_{\mathrm{DF},D}^{(1)} := \|\nabla p_h + \mathbf{t}_h\|_D$$

and

$$\eta^{(2)}_{\mathrm{DF},D} := \left\{ \sum_{K\in S_D} \left(m_K \|\Delta p_h + \nabla\cdot \mathbf{t}_h\|_K + \widetilde{m}_K^{1/2} \sum_{\sigma\in\mathcal{E}_K} C^{1/2}_{\mathrm{t},K,\sigma} \|(\nabla p_h + \mathbf{t}_h)\cdot \mathbf{n}\|_\sigma \right)^2 \right\}^{1/2},$$

with m_K given by (4.6), and $\widetilde{m}_K^{1/2}$ and $C^{1/2}_{\mathrm{t},K,\sigma}$ respectively by (4.8) and (4.4) (or, more precisely, by (4.12) and (4.11) if $d = 2$). Then

$$|||p - p_h||| \le \left\{ \sum_{D\in\mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^2 \right\}^{1/2}. \tag{4.18}$$

Proof. Putting $\mathbf{t} = \mathbf{t}_h$ in (3.2) we have (with φ defined in the proof of Theorem 3.1)

$$|||p - p_h||| = (f - \nabla\cdot\mathbf{t}_h - rp_h, \varphi) - (\nabla p_h + \mathbf{t}_h, \nabla\varphi).$$

Next, multiplying (4.15) by $\varphi_D := (\varphi, 1)_D/|D|$, we come to

$$(f - \nabla\cdot\mathbf{t}_h - rp_h, \varphi_D)_D = 0 \qquad \forall D \in \mathcal{D}_h^{\mathrm{int}}.$$

Thus

$$\begin{aligned} |||p - p_h||| = &\sum_{D\in\mathcal{D}_h^{\mathrm{int}}} \{(f - \nabla\cdot\mathbf{t}_h - rp_h, \varphi - \varphi_D)_D - (\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D\} \\ &+ \sum_{D\in\mathcal{D}_h^{\mathrm{ext}}} \{(f - \nabla\cdot\mathbf{t}_h - rp_h, \varphi)_D - (\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D\}. \end{aligned} \tag{4.19}$$

Using the Cauchy–Schwarz inequality and Lemma 4.4, we have for $D \in \mathcal{D}_h^{\mathrm{int}}$

$$\begin{aligned} (f - \nabla\cdot\mathbf{t}_h - rp_h, \varphi - \varphi_D)_D &\le \|f - \nabla\cdot\mathbf{t}_h - rp_h\|_D \|\varphi - \varphi_D\|_D \\ &\le m_D \|f - \nabla\cdot\mathbf{t}_h - rp_h\|_D |||\varphi|||_D = \eta_{\mathrm{R},D} |||\varphi|||_D \end{aligned} \tag{4.20}$$

and for $D \in \mathcal{D}_h^{\mathrm{ext}}$

$$\begin{aligned} (f - \nabla\cdot\mathbf{t}_h - rp_h, \varphi)_D &\le \|f - \nabla\cdot\mathbf{t}_h - rp_h\|_D \|\varphi\|_D \\ &\le m_D \|f - \nabla\cdot\mathbf{t}_h - rp_h\|_D |||\varphi|||_D = \eta_{\mathrm{R},D} |||\varphi|||_D. \end{aligned} \tag{4.21}$$

In order to estimate the terms $-(\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D$, we can use Cauchy–Schwarz inequality and the definition (2.3) of the energy norm to obtain

$$-(\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D \le \|\nabla p_h + \mathbf{t}_h\|_D \|\nabla\varphi\|_D \le \eta^{(1)}_{\mathrm{DF},D} |||\varphi|||_D. \tag{4.22}$$

However, the estimate $\|\nabla\varphi\|_D \le |||\varphi|||_D$ is too strong if $r \gg 1$ and an a posteriori error estimate featuring only $\eta^{(1)}_{\mathrm{DF},D}$ would not be robust. We fortunately notice that there is another way of estimating the terms $-(\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D$. Using the fact that $\nabla\varphi_K = 0$ for $\varphi_K := (\varphi, 1)_K/|K|$ for all $K \in \mathcal{S}_D$ and the Green theorem, we obtain

$$\begin{aligned} -(\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D &= \sum_{K\in\mathcal{S}_D} -(\nabla p_h + \mathbf{t}_h, \nabla(\varphi - \varphi_K))_K \\ &= \sum_{K\in\mathcal{S}_D} \{-\langle(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}, \varphi - \varphi_K\rangle_{\partial K} + (\Delta p_h + \nabla\cdot\mathbf{t}_h, \varphi - \varphi_K)_K\}. \end{aligned} \tag{4.23}$$

We now estimate the terms of the last sum separately. Using the Cauchy–Schwarz inequality and estimate (4.7) from Lemma 4.2, the first terms of (4.23) can be estimated as

$$\begin{aligned} -\langle(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}, \varphi - \varphi_K\rangle_{\partial K} &\le \sum_{\sigma\in\mathcal{E}_K} \|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma \|\varphi - \varphi_K\|_\sigma \\ &\le \sum_{\sigma\in\mathcal{E}_K} \|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma C_{\mathrm{t},K,\sigma}^{1/2} \widetilde{m}_K^{1/2} |||\varphi|||_K . \end{aligned} \tag{4.24}$$

For the second terms of (4.23), we use the Cauchy–Schwarz inequality and estimate (4.5) from Lemma 4.2 in order to obtain

$$\begin{aligned} (\Delta p_h + \nabla\cdot\mathbf{t}_h, \varphi - \varphi_K)_K &\le \|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_K \|\varphi - \varphi_K\|_K \\ &\le \|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_K m_K |||\varphi|||_K . \end{aligned} \tag{4.25}$$

Putting inequalities (4.24) and (4.25) into (4.23), we obtain

$$\begin{aligned} &-(\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D \le \\ &\le \sum_{K\in S_D} \left(\widetilde{m}_K^{1/2} \sum_{\sigma\in\mathcal{E}_K} C_{\mathrm{t},K,\sigma}^{1/2} \|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma + m_K \|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_K \right) |||\varphi|||_K \\ &\le \eta_{\mathrm{DF},D}^{(2)} |||\varphi|||_D , \end{aligned} \tag{4.26}$$

employing finally the Cauchy–Schwarz inequality.

Now, using estimates (4.22) and (4.26), we have that

$$-(\nabla p_h + \mathbf{t}_h, \nabla\varphi)_D \le \eta_{\mathrm{DF},D} |||\varphi|||_D . \tag{4.27}$$

Hence, (4.19) with (4.20), (4.21), and (4.27), the Cauchy–Schwarz inequality, and the fact that $|||\varphi||| = 1$ yield

$$|||p - p_h||| \le \sum_{D\in\mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D}) |||\varphi|||_D \le \left\{ \sum_{D\in\mathcal{D}_h} (\eta_{\mathrm{R},D} + \eta_{\mathrm{DF},D})^2 \right\}^{1/2} .$$

□

Remark 4.6 (The estimate for the vertex-centered finite volume method (2.5))**.** *By Lemma 4.1,* $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$ *given by* (4.1) *for the vertex-centered finite volume method* (2.5) *satisfies* (4.15)*, whence it can directly be used in Theorem 4.5.*

Remark 4.7 (Extensions to other conforming methods)**.** *Using the general form of Theorem 4.5, extension of our a posteriori error estimates to other methods yielding a conforming approximation* p_h *consists only in finding an appropriate* $\mathbf{t}_h \in \mathbf{H}(\mathrm{div},\Omega)$ *satisfying* (4.15)*. For the pure diffusion case, we refer in this respect to [21].*

5 Local efficiency and robustness of the a posteriori error estimates

We prove in this section the local efficiency of the a posteriori error estimators of Theorem 4.5 for the vertex-centered finite volume method (2.5) and in particular their robustness, with respect to reaction (and also diffusion) dominance and also with respect to the spatial variation of r under the condition that r is piecewise constant on $\mathcal{D}_h$. We actually show that they represent local lower bounds for those of Verfürth [17].

Theorem 5.1 (Local efficiency and robustness of the a posteriori error estimate)**.** *Let the functions f and r be piecewise polynomials on $\mathcal{T}_h$ of degree m, let p be the weak solution of problem (1.1a)–(1.1b) given by (2.4), and let p_h be its vertex-centered finite volume approximation given by (2.5). Let next $\mathcal{T}_h$ be shape-regular, i.e., let $\min_{K\in\mathcal{T}_h}|K|/h_K^d \geq \kappa_{\mathcal{T}}$ for some positive constant $\kappa_{\mathcal{T}}$. Let finally the a posteriori error estimate be given by Theorem 4.5 with in particular $\mathbf{t}_h$ given by (4.1). Then, for each $D \in \mathcal{D}_h$, there holds*

$$\eta_{\mathrm{DF},D} + \eta_{\mathrm{R},D} \leq C|||p - p_h|||_D, \tag{5.1}$$

where the constant C depends only on the space dimension d, on the shape regularity parameter $\kappa_{\mathcal{T}}$, on the polynomial of degree m of f and r, on the constants $C_{\mathrm{P},D}$ if $D \in \mathcal{D}_h^{\mathrm{int}}$, $C_{\mathrm{F},D,\partial\Omega}$ if $D \in \mathcal{D}_h^{\mathrm{ext}}$, and $\max_{K\in\mathcal{S}_D}\max_{\sigma\in\mathcal{E}_K\cap\mathcal{G}_D^{\mathrm{int}}}\{C_{t,K,\sigma}\}$, and finally on the local variation of r through $C_{r,D}/c_{r,D}$.

Proof. Let $D \in \mathcal{D}_h$ be fixed. We first note that as $-\nabla p_h \cdot \mathbf{n}_\sigma = \mathbf{t}_h \cdot \mathbf{n}_\sigma$ for all $\sigma \subset \partial D$ by (4.1) and by the definition of the average operator, we may change the summation over $\sigma \in \mathcal{E}_K$ to the summation over $\sigma \in \mathcal{E}_K \cap \mathcal{G}_D^{\mathrm{int}}$ in the definition of $\eta_{\mathrm{DF},D}^{(2)}$. Then using the definition of the residual and diffusive flux estimators and the triangle inequality, we have

$$\begin{aligned}
\eta_{\mathrm{DF},D} + \eta_{\mathrm{R},D} &= \min\left\{\eta_{\mathrm{DF},D}^{(1)}, \eta_{\mathrm{DF},D}^{(2)}\right\} + \eta_{\mathrm{R},D} \leq \eta_{\mathrm{DF},D}^{(2)} + \eta_{\mathrm{R},D} \\
&\leq \left\{\sum_{K\in S_D}\left(m_K\|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_K + \widetilde{m}_K^{1/2}\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{G}_D^{\mathrm{int}}} C_{\mathrm{t},K,\sigma}^{1/2}\|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma\right)^2\right\}^{1/2} \\
&\quad + m_D\|f + \Delta p_h - r p_h\|_D + m_D\|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_D.
\end{aligned}$$

So, squaring the above estimate and applying the Cauchy–Schwarz inequality, we obtain

$$\begin{aligned}
C_1^{-1}(\eta_{\mathrm{DF},D} + \eta_{\mathrm{R},D})^2 \leq &\sum_{K\in S_D} m_K^2\|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_K^2 + \sum_{K\in S_D}\widetilde{m}_K\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{G}_D^{\mathrm{int}}} C_{\mathrm{t},K,\sigma}\|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma^2 + \\
&+ m_D^2\|f + \Delta p_h - r p_h\|_D^2 + m_D^2\|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_D^2
\end{aligned}$$

for some constant C_1 depending only on d and $\kappa_{\mathcal{T}}$.

Noticing that $m_D^2 \leq C_2 m_K^2$ for all $K \in S_D$, with a constant C_2 which depends only on $C_{\mathrm{P},D}$ if $D \in \mathcal{D}_h^{\mathrm{int}}$, $C_{\mathrm{F},D,\partial\Omega}$ if $D \in \mathcal{D}_h^{\mathrm{ext}}$, $\kappa_{\mathcal{T}}$, and $C_{r,D}/c_{r,D}$, we have from the last inequality

$$\begin{aligned}
(\eta_{\mathrm{DF},D} + \eta_{\mathrm{R},D})^2 \leq &C_1(1 + C_2)\sum_{K\in S_D} m_K^2\|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_K^2 \\
&+ C_1\sum_{K\in S_D}\widetilde{m}_K\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{G}_D^{\mathrm{int}}} C_{\mathrm{t},K,\sigma}\|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma^2 \\
&+ C_1C_2\sum_{K\in\mathcal{S}_D} m_K^2\|f + \Delta p_h - r p_h\|_K^2.
\end{aligned}$$

Recall now that for a simplex K and $\mathbf{v} \in \mathbf{RTN}(K)$, we have the inverse inequality $\|\nabla\cdot\mathbf{v}\|_K^2 \leq C_3 h_K^{-2}\|\mathbf{v}\|_K^2$, with C_3 depending only on d and $\kappa_{\mathcal{T}}$, and the estimate (cf., e.g. [6, Lemma 4.11])

$$\|\mathbf{v}\|_K^2 \leq C_4 h_K\sum_{\sigma\in\mathcal{E}_K}\|\mathbf{v}\cdot\mathbf{n}\|_\sigma^2,$$

with C_4 again depending only on d and $\kappa_{\mathcal{T}}$. Thus, as $\nabla p_h + \mathbf{t}_h \in \mathbf{RTN}(K)$,

$$\|\Delta p_h + \nabla\cdot\mathbf{t}_h\|_K^2 \leq C_3 h_K^{-2}\|\nabla p_h + \mathbf{t}_h\|_K^2 \leq C_3C_4 h_K^{-1}\sum_{\sigma\in\mathcal{E}_K\cap\mathcal{G}_D^{\mathrm{int}}}\|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma^2,$$

using also again the fact that $-\nabla p_h \cdot \mathbf{n}_\sigma = \mathbf{t}_h \cdot \mathbf{n}_\sigma$ for all $\sigma \subset \partial D$. Hence, putting $C_{t,K} := \max_{\sigma \in \mathcal{E}_K \cap \mathcal{G}_D^{\mathrm{int}}}\{C_{t,K,\sigma}\}$, we have the estimate

$$
\begin{aligned}
(\eta_{\mathrm{DF},D} + \eta_{\mathrm{R},D})^2 \leq & C_1 \sum_{K \in S_D} \left(\left((1+C_2)C_3C_4 m_K^2 h_K^{-1} + C_{t,K}\widetilde{m}_K\right) \sum_{\sigma \in \mathcal{E}_K \cap \mathcal{G}_D^{\mathrm{int}}} \|(\nabla p_h + \mathbf{t}_h)\cdot \mathbf{n}\|_\sigma^2 \right) \\
& + C_1 C_2 \sum_{K \in \mathcal{S}_D} m_K^2 \|f + \Delta p_h - r p_h\|_K^2 .
\end{aligned}
$$

Let us now recall that by definition (4.1) of $\mathbf{t}_h$, we have

$$
(\nabla p_h + \mathbf{t}_h)|_K \cdot \mathbf{n}_\sigma = (\nabla p_h \cdot \mathbf{n}_\sigma)|_K - \{\!\{\nabla p_h \cdot \mathbf{n}_\sigma\}\!\} = \frac{1}{2}\mathbf{n}_\sigma \cdot \mathbf{n} [\![\nabla p_h \cdot \mathbf{n}_\sigma]\!]
$$

if $\sigma \in \mathcal{E}_K \cap \mathcal{G}_D^{\mathrm{int}}$, where $\mathbf{n}_\sigma \cdot \mathbf{n} = \pm 1$ is used for sign alternation. Thus, we infer, for a constant C_5 only depending on the constants C_1–C_4, $\max_{K \in \mathcal{S}_D} C_{t,K}$, d, and $\kappa_{\mathcal{T}}$,

$$
(\eta_{\mathrm{DF},D} + \eta_{\mathrm{R},D})^2 \leq C_5 \sum_{K \in S_D} \left(m_K^2 \|f + \Delta p_h - r p_h\|_K^2 + (m_K^2 h_K^{-1} + \widetilde{m}_K) \sum_{\sigma \in \mathcal{E}_K \cap \mathcal{G}_D^{\mathrm{int}}} \|[\![\nabla p_h \cdot \mathbf{n}]\!]\|_\sigma^2 \right).
$$

We now show that $m_K^2 h_K^{-1} + \widetilde{m}_K \leq C_6 m_K$ with some constant C_6 only dependent on $C_{\mathrm{P},K}$ (recall that $C_{\mathrm{P},K} = 1/\pi^2$ as simplices are convex). Firstly, $m_K^2 h_K^{-1} \leq C_{\mathrm{P},K}^{1/2} m_K$ is obvious noticing that this statement is equivalent to $m_K \leq C_{\mathrm{P},K}^{1/2} h_K$, which follows from the definition (4.6) of m_K. Secondly, employing also this bound, we have

$$
\begin{aligned}
\widetilde{m}_K &\leq \min\left\{\left(C_{\mathrm{P},K} + C_{\mathrm{P},K}^{1/2}\right) h_K, c_{r,K}^{-1} h_K^{-1}\right\} + \min\left\{\left(C_{\mathrm{P},K} + C_{\mathrm{P},K}^{1/2}\right) h_K, \frac{1}{2} c_{r,K}^{-1/2}\right\} \\
&\leq \left(1 + C_{\mathrm{P},K}^{-1/2}\right) \min\left\{C_{\mathrm{P},K} h_K, c_{r,K}^{-1} h_K^{-1}\right\} + \left(1 + C_{\mathrm{P},K}^{1/2}\right) \min\left\{C_{\mathrm{P},K}^{1/2} h_K, c_{r,K}^{-1/2}\right\} \\
&= \left(1 + C_{\mathrm{P},K}^{-1/2}\right) m_K^2 h_K^{-1} + \left(1 + C_{\mathrm{P},K}^{1/2}\right) m_K \\
&\leq 2\left(1 + C_{\mathrm{P},K}^{1/2}\right) m_K,
\end{aligned}
$$

whence the assertion follows. Combining the previous bounds, we thus have

$$
(\eta_{\mathrm{DF},D} + \eta_{\mathrm{R},D})^2 \leq C_7 \sum_{K \in S_D} \left(m_K^2 \|f + \Delta p_h - r p_h\|_K^2 + m_K \sum_{\sigma \in \mathcal{E}_K \cap \mathcal{G}_D^{\mathrm{int}}} \|[\![\nabla p_h \cdot \mathbf{n}]\!]\|_\sigma^2 \right),
$$

for a constant C_7 depending only on C_5 and C_6. We now finally note from this estimate that our estimators represent a local lower bound for the residual a posteriori error estimators of Verfürth [17, Proposition 4.1] (for the case of r constant and on the mesh $\mathcal{S}_h$ instead of the mesh $\mathcal{T}_h$). Hence, in order to show their fully robust local efficiency, it is sufficient to use the results of this reference. In particular, applying the bubble function estimates (4.13) and (4.16) from this reference to a simplex $K \in \mathcal{S}_D$ and its side $\sigma \in \mathcal{G}_D^{\mathrm{int}}$ for r constant and f piecewise linear, we get

$$
\begin{aligned}
m_K \|f + \Delta p_h - r p_h\|_K &\leq C |||p - p_h|||_K, \\
m_K^{1/2} \|[\![\nabla p_h \cdot \mathbf{n}]\!]\|_\sigma &\leq C |||p - p_h|||_{\mathcal{S}_\sigma}
\end{aligned}
$$

(recall that $\mathcal{S}_\sigma$ are the two simplices sharing $\sigma \in \mathcal{G}_D^{\mathrm{int}}$), whence (5.1) follows. Finally, one can extend this result to general piecewise polynomial f and r, which gives the final dependencies of the constant C of (5.1) indicated in the announcement of the theorem. □

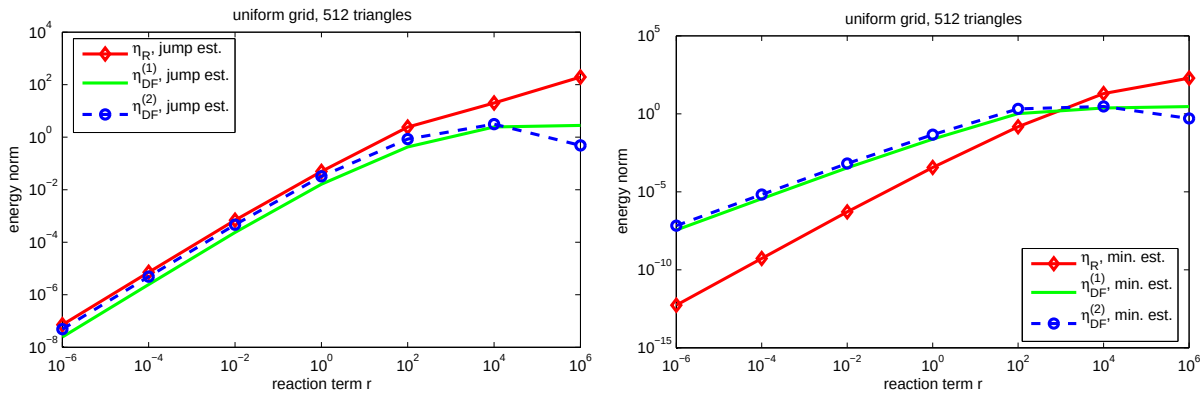

Figure 2: Comparison of the different estimators for the original jump estimate (4.18) with $\mathbf{t}_h$ given by (4.1) (left) and for the minimization estimate (C.1) (right) in dependence on r

6 Numerical experiments

We present in this section a series of numerical experiments which confirm the theoretical results of the paper. The a posteriori error estimate of Theorem 4.5 with the reconstructed diffusive flux $\mathbf{t}_h$ given by (4.1) gives a guaranteed upper bound on the overall energy error but the effectivity index is never close to the optimal value of one in our tests. For this reason, we also present results employing a local minimization procedure, consisting in modifications of the flux $\mathbf{t}_h$ in the interior of each $D \in \mathcal{D}_h$. This procedure is in detail described in the appendix below.

We perform our numerical experiments for problem (1.1a) with $\Omega = (0,1) \times (0,1)$, a constant reaction coefficient r, and $f = 0$. We prescribe the Dirichlet boundary condition by the exact solution

$$p(x,y) = e^{-r^{1/2}x} + e^{-r^{1/2}y},$$

as in [8]. This solution exhibits a boundary layer along the coordinate axes for high values of r. In order to carry out the tests, we have implemented our estimates into the FreeFem++ [9] package and all the results presented have been computed using FreeFem++. Finally, we shall in this section term estimate (4.18) of Theorem 4.5 with $\mathbf{t}_h$ given by (4.1) as the *jump estimate*, as this reconstructed diffusive flux $\mathbf{t}_h$ leads to estimators of the form $\|(\nabla p_h + \mathbf{t}_h)\cdot\mathbf{n}\|_\sigma = \|[\![\nabla p_h \cdot \mathbf{n}]\!]\|_\sigma/2$, and estimate (C.1) following from the local minimization strategy described in Appendix C below as the *minimization estimate*. We however note that in the majority of cases, it is the simple choice (B.1) which gives the minimum, so that very similar results may be presented with (B.1) instead of (C.1).

We first in the left part of Figure 2 show the different estimators of the original jump estimate (4.18) with $\mathbf{t}_h$ given by (4.1) on a fixed uniformly refined mesh with 512 elements in dependence on the reaction coefficient r, which we let vary between 10^{-6} and 10^6. We remark that the highest contribution is always given by the residual estimate $\eta_{\mathrm{R}} := \{\sum_{D\in\mathcal{D}_h} \eta_{\mathrm{R},D}^2\}^{\frac{1}{2}}$, whereas the contributions of the diffusive flux estimates $\eta_{\mathrm{DF}}^{(i)} := \{\sum_{D\in\mathcal{D}_h} (\eta_{\mathrm{DF},D}^{(i)})^2\}^{\frac{1}{2}}$ are smaller. Note also that although the estimate $\eta_{\mathrm{DF}}^{(1)}$ gives smaller values for moderate values of r, it gets eventually outperformed by the estimate $\eta_{\mathrm{DF}}^{(2)}$. We next in Figure 3 present, for two different (uniformly refined) grids, the corresponding effectivity indices. We can clearly see that they are bounded uniformly with respect to r which demonstrates the full robustness of our estimates. Unfortunately, in particular for smaller values of r, they are not too close to the optimal value of 1. This is the reason for

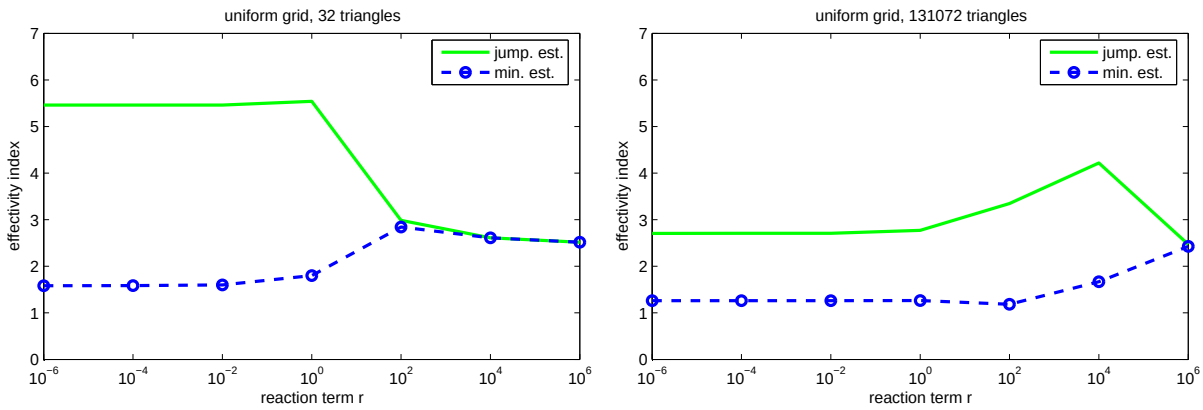

Figure 3: Effectivity indices for the original jump estimate (4.18) with $\mathbf{t}_h$ given by (4.1) and for the minimization estimate (C.1) in dependence on r for two different (uniformly refined) meshes

the introduction of a local minimization procedure which we have devised in [5] and [21, Section 7] in the pure diffusion case and which we adapt to the present case in the appendix below. The results using the minimization estimate (C.1) are then presented in the right part of Figure 2 and in Figure 3. We can see that for moderate values of r, the residual estimate has been decreased under the diffusive flux ones and consequently the effectivity index gets close to the optimal value of 1. In what follows, we present the results only for the minimization estimate (C.1).

Apart from overall error control, a posteriori error estimates are a key element for adaptive mesh refinement. We exploit for this purpose the capabilities of FreeFem++. We mark an element for refinement if the estimator exceeded 50% of the maximal element estimators but we recall that FreeFem++ actually generates a completely new mesh on the basis of this criterion and this new mesh is thus not a simple refinement of the previous one. In the adaptive refinement case, the elements marked for refinement were selected using the original jump estimators (4.18) with $\mathbf{t}_h$ given by (4.1). This approach seems to give better numerical results (better error decreasing with the number of elements) and is in coincidence with our theoretical results, since we prove the local efficiency for these original estimators in Theorem 5.1. We firstly plot, in the left parts of Figures 4 and 5, respectively, the estimated and actual errors against the number of elements in both uniformly and adaptively refined meshes for $r = 1$ and $r = 10^6$. In the first case, the solution posses no singularity, so the adaptive approach only leads to a slight improvement of the error attained for a given number of unknowns on coarse meshes, whereas this tendency is reversed for fine meshes. In the second case with a singular solution, the adaptive approach leads to an important improvement of the error attained for a given number of unknowns. The effectivity indices are then shown in the right parts of Figures 4 and 5, respectively. In the first case, they improve considerably with the mesh refinement and especially in the adaptive refinement mode they get very close to the optimal value of 1, whereas in the second one they are rather stable around the value of 2.4. Finally, to further promote the usability of our estimates for adaptive mesh refinement, we present in Figure 6 the excellently matching predicted and actual error distribution and the corresponding adaptively refined mesh as given by the jump estimator for $r = 10^6$.

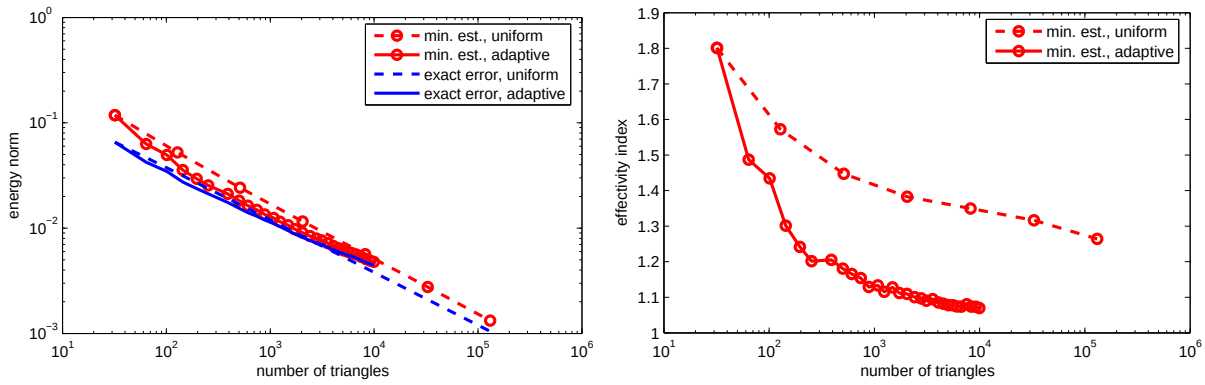

Figure 4: Estimated and actual error against the number of elements in uniformly/adaptively refined meshes (left) and corresponding effectivity indices (right) of the minimization estimator (C.1), $r = 1$

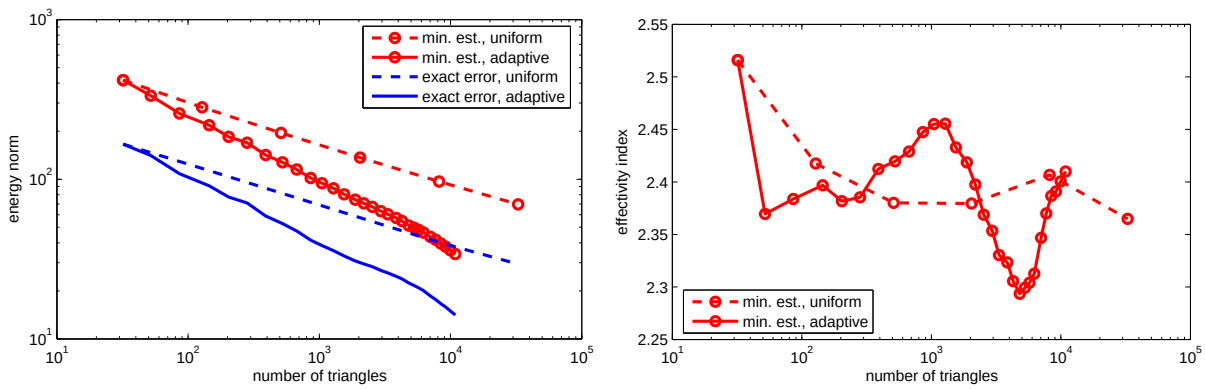

Figure 5: Estimated and actual error against the number of elements in uniformly/adaptively refined meshes (left) and corresponding effectivity indices (right) of the minimization estimator (C.1), $r = 10^6$

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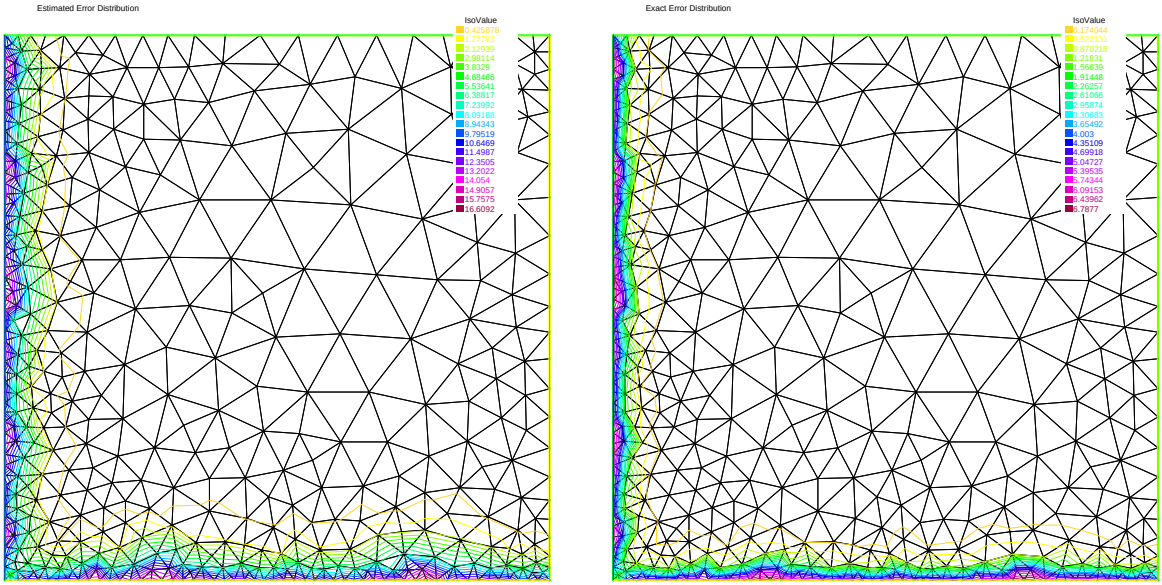

Figure 6: Estimated error (left) and exact error (right) distribution using the original jump estimate (4.18) with $\mathbf{t}_h$ given by (4.1) on an adaptively refined mesh for $r = 10^6$

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Appendix: Improvements by local minimization

In Sections 4 and 5, we have shown that a choice of $\mathbf{t}_h \in \mathbf{H}(\mathrm{div}, \Omega)$ in Theorem 4.5 for the vertex-centered finite volume method (2.5) leading to a guaranteed upper bound, local efficiency, and robustness is given by (4.1). However, it is not apparent at all whether this choice leads to the best upper bound. In particular, by closer investigation, it turns out that whereas in mixed finite element or discontinuous Galerkin (finite volume) methods, the residual estimator represents a higher-order term, as in these methods one has (with an appropriate $\mathbf{t}_h$) $(\nabla \cdot \mathbf{t}_h + rp_h, 1)_K = (f, 1)_K$ for all $K \in \mathcal{T}_h$, it is not the case here, as (4.15) is only true on a set of elements $\mathcal{S}_D$ of each interior

dual volume D and not on each element $K \in \mathcal{S}_D$. The numerical experiments for $\mathbf{t}_h$ given by (4.1) presented in Section 6 indeed show that the residual estimators $\eta_{\mathrm{R},D}$ represent a major contribution to the estimate.

A natural idea in order to decrease the estimate is to try to choose another $\mathbf{t}_h \in \mathbf{H}(\mathrm{div},\Omega)$ satisfying (4.15). Notice now that $\mathbf{t}_h \in \mathbf{RTN}(\mathcal{S}_h)$ given by (4.1) only for such $\sigma \in \mathcal{G}_h$ which are at the boundary of some $D \in \mathcal{D}_h^{\mathrm{int}}$ satisfies $\mathbf{t}_h \in \mathbf{H}(\mathrm{div},\Omega)$ and (4.15) and we can choose any value for the other edges. In particular, we can choose values that minimize the estimate. Moreover, as the estimator is build locally on each dual volume, we can perform this optimization process locally on each dual volume.

We describe in this appendix two ways of a local minimization. In the pure diffusion case, the first one was devised in [5] and consists in true local minimization for the given degrees of freedom, leading to a small linear system solution for each vertex. The second, simplified one, was proposed in [21, Section 7] and avoids any local linear system solution. We adapt them here to the reaction–diffusion case; our exposition will be given in two space dimensions but a similar development can be done in three space dimensions. For the sake of simplicity, we assume henceforth that f and r are piecewise constant on $\mathcal{T}_h$.

A A full local minimization strategy

We outline here the generalization of the "full minimization strategy" of [5] to the reaction–diffusion case.

A.1 Notation and previous results

Let $D \in \mathcal{D}_h$ be the dual volume corresponding to a vertex V_D as in Figure 7; D is decomposed into a subdivision $\mathcal{S}_D$ of n subtriangles $K_0, \dots, K_{n-1}$, numbered in the counter-clockwise direction. On each subtriangle K_i, the vertex 0 is the center of the volume D, the other vertices are numbered in the counter-clockwise direction, and we call σ_j^i the edge opposite to the vertex j and $\mathbf{n}_{\sigma_j^i}$ the exterior normal vector of the edge σ_j^i. Let next $\boldsymbol{\psi}_j^i$, $j = 0, 1, 2$, be the basis function of $\mathbf{RTN}(K_i)$ corresponding to the vertex j, i.e., $\boldsymbol{\psi}_j^i = \frac{1}{d|K_i|}(\mathbf{x} - V_j^i)$, where V_j^i is vertex j of the triangle K_i. On K_i, $\mathbf{t}_h$ can consequently be written as $\mathbf{t}_h|_{K_i} = \alpha_0^i \boldsymbol{\psi}_0^i + \alpha_1^i \boldsymbol{\psi}_1^i + \alpha_2^i \boldsymbol{\psi}_2^i$.

The values of the external fluxes over ∂D are prescribed by (4.1) in the same way as before: for any dual volume $D \in \mathcal{D}_h$, $\alpha_0^i = -|\sigma_0^i| \nabla p_h \cdot \mathbf{n}_{\sigma_0^i}$, $i = 0, \dots, n-1$; if $D \in \mathcal{D}_h^{\mathrm{ext}}$, then in addition $\alpha_2^0 = -|\sigma_2^0| \nabla p_h \cdot \mathbf{n}_{\sigma_2^0}$ and $\alpha_1^{n-1} = -|\sigma_1^{n-1}| \nabla p_h \cdot \mathbf{n}_{\sigma_1^{n-1}}$. The internal fluxes, given by the coefficients α_1^i and α_2^i, have to first fulfill the continuity of the normal trace across the edges, which imposes

- if $D \in \mathcal{D}_h^{\mathrm{int}}$,
$$\alpha_1^i + \alpha_2^{i+1} = 0,\ i = 0, \dots, n-1 \text{ with } \alpha_2^n = \alpha_2^0; \tag{A.1}$$
- if $D \in \mathcal{D}_h^{\mathrm{ext}}$,
$$\alpha_1^i + \alpha_2^{i+1} = 0,\ i = 0, \dots, n-2. \tag{A.2}$$

Therefore, there are n degrees of freedom $\mathbf{X} = (\alpha^0, \dots, \alpha^{n-1})^t$ if $D \in \mathcal{D}_h^{\mathrm{int}}$ and $n-1$ degrees of freedom $\mathbf{X} = (\alpha^0, \dots, \alpha^{n-2})^t$ if $D \in \mathcal{D}_h^{\mathrm{ext}}$ left and these can be chosen in order to minimize the estimator; from now on, the local estimator $\eta_D(\mathbf{X}) = \eta_{\mathrm{DF},D}(\mathbf{X}) + \eta_{\mathrm{R},D}(\mathbf{X})$ will be considered as a function of them. Later on, we will also employ the notation $\eta_D(\mathbf{t}_h) = \eta_{\mathrm{DF},D}(\mathbf{t}_h) + \eta_{\mathrm{R},D}(\mathbf{t}_h)$.

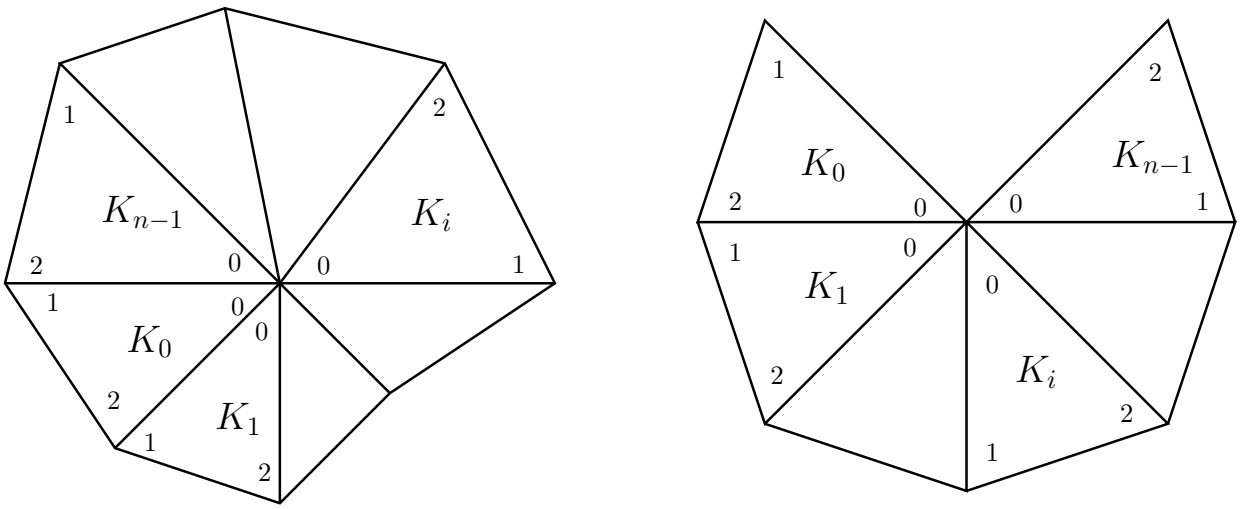

Figure 7: Dual volume and its subdivision $\mathcal{S}_D$. Left: interior dual volume; right: boundary dual volume

It has been in particular shown in [5, Section 3] that the square of the first diffusive flux estimator $\eta^{(1)}_{\mathrm{DF},D}$ on a dual volume $D \in \mathcal{D}_h$ is a quadratic form with respect to $\mathbf{X}$ of the form

$$\left(\eta^{(1)}_{\mathrm{DF},D}\right)^2(\mathbf{X}) = a^{(1)}_{\mathrm{DF}} - \left(\mathbf{B}^{(1)}_{\mathrm{DF}}\right)^t \mathbf{X} + \frac{1}{2}\mathbf{X}^t \mathbb{A}^{(1)}_{\mathrm{DF}}\mathbf{X}; \tag{A.3}$$

we refer to this reference for the precise form of the entries. Similarly, by a slight modification of the approach of this reference, one can derive that

$$\eta^2_{\mathrm{R},D}(\mathbf{X}) = a_{\mathrm{R}} - \mathbf{B}^t_{\mathrm{R}}\mathbf{X} + \frac{1}{2}\mathbf{X}^t \mathbb{A}_{\mathrm{R}}\mathbf{X}. \tag{A.4}$$

We now accomplish a similar task for the diffusive flux estimator $\eta^{(2)}_{\mathrm{DF},D}$.

A.2 Diffusive flux estimator $\eta^{(2)}_{\mathrm{DF},D}$

By the definition, the square of the second diffusive flux estimator $\eta^{(2)}_{\mathrm{DF},D}$ on a dual volume $D \in \mathcal{D}_h$ is not a quadratic form with respect to the degrees of freedom $\mathbf{X}$ as the other ones. As our purpose is to improve the estimator without increasing too much the computational cost, we choose not to minimize $\left(\eta^{(2)}_{\mathrm{DF},D}\right)^2$ directly, but an upper bound instead: we have

$$\begin{aligned}\left(\eta^{(2)}_{\mathrm{DF},D}\right)^2 \quad \leq \quad & 2\sum_{K\in\mathcal{S}_D}\left(m_K^2||\nabla\cdot\mathbf{t}_h||_K^2 + 2\widetilde{m}_K\left(C_{\mathrm{t},K,\sigma_1}\|(\nabla p_h+\mathbf{t}_h)\cdot\mathbf{n}\|^2_{\sigma_1}\right.\right.\\ & \left.\left.+C_{\mathrm{t},K,\sigma_2}\|(\nabla p_h+\mathbf{t}_h)\cdot\mathbf{n}\|^2_{\sigma_2}\right)\right),\end{aligned}$$

using the inequality $(a+b)^2 \leq 2(a^2+b^2)$ and the fact that on the edge σ_0 of each subtriangle K, $\mathbf{t}_h$ is prescribed such that $(\nabla p_h + \mathbf{t}_h)|_K \cdot \mathbf{n}_{\sigma_0} = 0$. We denote by $\left(\eta^{(3)}_{\mathrm{DF},D}\right)^2$ this upper bound and study it separately for interior and exterior dual volumes.

A.2.1 Interior dual volumes

Let $D \in \mathcal{D}_h^{\text{int}}$ and $\mathcal{S}_D = \{K_0, \dots, K_{n-1}\}$ be its subtriangulation. Using the definition of $\boldsymbol{\psi}_j^i$ and (A.1), we have

$$\begin{aligned} \mathbf{t}_h|_{K_0} &= \tfrac{1}{d|K_0|}\left(\alpha_0^0(\mathbf{x}-V_0^0) + \alpha^0(\mathbf{x}-V_1^0) - \alpha^{n-1}(\mathbf{x}-V_2^0)\right), \\ \mathbf{t}_h|_{K_i} &= \tfrac{1}{d|K_i|}\left(\alpha_0^i(\mathbf{x}-V_0^i) + \alpha^i(\mathbf{x}-V_1^i) - \alpha^{i-1}(\mathbf{x}-V_2^i)\right), \quad i = 1, \dots, n-1 \end{aligned} \tag{A.5}$$

and consequently

$$\begin{aligned} \|\nabla \cdot \mathbf{t}_h\|_{K_0}^2 &= \tfrac{1}{|K_0|}(\alpha_0^0 + \alpha^0 - \alpha^{n-1})^2, \\ \|\nabla \cdot \mathbf{t}_h\|_{K_i}^2 &= \tfrac{1}{|K_i|}(\alpha_0^i + \alpha^i - \alpha^{i-1})^2, \quad i = 1, \dots, n-1. \end{aligned}$$

Using (A.5) and the fact that the normal components of the basis functions $\boldsymbol{\psi}_j^i$ are constant over the edges, we have

$$\begin{aligned} \|(\nabla p_h + \mathbf{t}_h)\cdot \mathbf{n}_{\sigma_1^i}\|_{\sigma_1^i}^2 &= |\sigma_1^i|\left(\nabla p_h \cdot \mathbf{n}_{\sigma_1^i} + \tfrac{1}{|\sigma_1^i|}\alpha^i\right)^2, \quad i = 0, \dots, n-1, \\ \|(\nabla p_h + \mathbf{t}_h)\cdot \mathbf{n}_{\sigma_2^0}\|_{\sigma_2^0}^2 &= |\sigma_2^0|\left(\nabla p_h \cdot \mathbf{n}_{\sigma_2^0} - \tfrac{1}{|\sigma_2^0|}\alpha^{n-1}\right)^2, \\ \|(\nabla p_h + \mathbf{t}_h)\cdot \mathbf{n}_{\sigma_2^i}\|_{\sigma_2^i}^2 &= |\sigma_2^i|\left(\nabla p_h \cdot \mathbf{n}_{\sigma_2^i} - \tfrac{1}{|\sigma_2^i|}\alpha^{i-1}\right)^2, \quad i = 1, \dots, n-1. \end{aligned}$$

Therefore, we find that $\left(\eta_{\text{DF},D}^{(3)}\right)^2$ is a quadratic form with respect to $\mathbf{X} = (\alpha^0, \dots, \alpha^{n-1})^t$:

$$\left(\eta_{\text{DF},D}^{(3)}\right)^2(\mathbf{X}) = a_{\text{DF}}^{(3)} - \left(\mathbf{B}_{\text{DF}}^{(3)}\right)^t \mathbf{X} + \frac{1}{2}\mathbf{X}^t \mathbb{A}_{\text{DF}}^{(3)}\mathbf{X}, \tag{A.6}$$

where $a_{\text{DF}}^{(3)} = \sum_{i=0}^{n-1} E_0^i$ and

$$\mathbf{B}_{\text{DF}}^{(3)} = -\begin{pmatrix} E_1^0 + E_2^1 \\ \vdots \\ E_1^{n-1} + E_2^0 \end{pmatrix}, \quad \mathbb{A}_{\text{DF}}^{(3)} = \begin{pmatrix} 2(E_4^0 + E_5^1) & E_3^1 & & & E_3^0 \\ E_3^1 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & E_3^{n-1} \\ E_3^0 & & & E_3^{n-1} & 2(E_4^{n-1} + E_5^0) \end{pmatrix}.$$

Here

$$\begin{aligned} E_0^i &= 2m_{K_i}^2 \tfrac{(\alpha_0^i)^2}{|K_i|} + 4\widetilde{m}_{K_i}(C_{\text{t},K_i,\sigma_1^i}|\sigma_1^i|(\nabla p_h \cdot \mathbf{n}_{\sigma_1^i})^2 + C_{\text{t},K_i,\sigma_2^i}|\sigma_2^i|(\nabla p_h \cdot \mathbf{n}_{\sigma_2^i})^2), \\ E_1^i &= 4m_{K_i}^2 \tfrac{\alpha_0^i}{|K_i|} + 8C_{\text{t},K_i,\sigma_1^i}\widetilde{m}_{K_i}\nabla p_h \cdot \mathbf{n}_{\sigma_1^i}, \\ E_2^i &= -4m_{K_i}^2 \tfrac{\alpha_0^i}{|K_i|} - 8C_{\text{t},K_i,\sigma_2^i}\widetilde{m}_{K_i}\nabla p_h \cdot \mathbf{n}_{\sigma_2^i}, \\ E_3^i &= -4\tfrac{m_{K_i}^2}{|K_i|}, \\ E_4^i &= 2\tfrac{m_{K_i}^2}{|K_i|} + 4\tfrac{C_{\text{t},K_i,\sigma_1^i}\widetilde{m}_{K_i}}{|\sigma_1^i|}, \\ E_5^i &= 2\tfrac{m_{K_i}^2}{|K_i|} + 4\tfrac{C_{\text{t},K_i,\sigma_1^i}\widetilde{m}_{K_i}}{|\sigma_2^i|}. \end{aligned}$$

A.2.2 Boundary dual volumes

Let $D \in \mathcal{D}_h^{\text{ext}}$ be a boundary dual volume. In the general case $n > 2$, using the conditions (A.2), we find that $\left(\eta^{(3)}_{\text{DF},D}\right)^2$ is a quadratic form of the form (A.6), where $a^{(3)}_{\text{DF}} = \tilde{E}^0_0 + \sum_{i=1}^{n-3} E^i_0 + \tilde{E}^{n-2}_0$ and

$$\mathbf{B}^{(3)}_{\text{DF}} = -\begin{pmatrix} \tilde{E}^0_1 + E^1_2 \\ E^1_1 + E^2_2 \\ \vdots \\ E^{n-3}_1 + E^{n-2}_2 \\ \tilde{E}^{n-2}_1 \end{pmatrix}, \quad \mathbb{A}^{(3)}_{\text{DF}} = \begin{pmatrix} 2(E^0_4 + E^1_5) & E^1_3 & & & \\ E^1_3 & \ddots & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & 2(E^{n-3}_4 + E^{n-2}_5) & E^{n-2}_3 \\ & & & E^{n-2}_3 & 2\tilde{E}^{n-2}_4 \end{pmatrix}.$$

Here E^i_0, E^i_1, E^i_2, E^i_3, E^i_4, E^i_5, $i = 0, \ldots, n-2$ are defined as for interior dual volumes, and we introduce

$$\begin{aligned} \tilde{E}^0_0 &= E^0_0 - E^0_2\alpha^0_2 + E^0_5(\alpha^0_2)^2, \\ \tilde{E}^0_1 &= E^0_1 - E^0_3\alpha^0_2, \\ \tilde{E}^{n-2}_0 &= E^{n-2}_0 + E^{n-1}_0 + E^{n-1}_1\alpha^{n-1}_1 + E^{n-1}_4(\alpha^{n-1}_1)^2, \\ \tilde{E}^{n-2}_1 &= E^{n-2}_1 + E^{n-1}_2 + E^{n-1}_3\alpha^{n-1}_1, \\ \tilde{E}^{n-2}_4 &= E^{n-2}_4 + E^{n-1}_5. \end{aligned}$$

In the limit case $n = 2$, we find (A.6) with the scalar entries

$$\begin{aligned} a^{(3)}_{\text{DF}} &= E^0_4 + E^1_5, \\ \mathbf{B}^{(3)}_{\text{DF}} &= E^0_1 + E^1_2 - E^0_3\alpha^0_2 + E^1_3\alpha^1_1, \\ \mathbb{A}^{(3)}_{\text{DF}} &= E^0_0 + E^1_1\alpha^0_1 - E^0_2\alpha^0_2 + E^0_5(\alpha^0_2)^2 + E^1_4(\alpha^1_1)^2. \end{aligned}$$

A.3 Minimization

Given a dual volume $D \in \mathcal{D}_h$, we would like to find the vector of degrees of freedom $\mathbf{X}_0$ such that $\eta_D(\mathbf{X}_0) = \min_{\mathbf{X}} \eta_D(\mathbf{X})$ in order to improve the estimator. However, as we want to make this improvement with a computational cost as small as possible, we choose not to minimize directly η_D, but rather quadratic forms; precisely, we minimize $\eta^2_{\text{R},D} + \min\left\{\left(\eta^{(1)}_{\text{DF},D}\right)^2, \left(\eta^{(3)}_{\text{DF},D}\right)^2\right\}$, i.e,

$$\min\left\{\min_{\mathbf{X}}\left\{\eta^2_{\text{R},D}(\mathbf{X}) + \left(\eta^{(1)}_{\text{DF},D}\right)^2(\mathbf{X})\right\}, \min_{\mathbf{X}}\left\{\eta^2_{\text{R},D}(\mathbf{X}) + \left(\eta^{(3)}_{\text{DF},D}\right)^2(\mathbf{X})\right\}\right\}.$$

Using definitions (A.3), (A.4), and (A.6), this amounts to find the minima of two quadratic forms:

$$\mathbf{X}_1 = \text{argmin}_{\mathbf{X}}\left(a^{(1)} - \left(\mathbf{B}^{(1)}\right)^t\mathbf{X} + \frac{1}{2}\mathbf{X}^t\mathbb{A}^{(1)}\mathbf{X}\right),$$

where $a^{(1)} = a_{\text{R}} + a^{(1)}_{\text{DF}}$, $\mathbf{B}^{(1)} = \mathbf{B}_{\text{R}} + \mathbf{B}^{(1)}_{\text{DF}}$, and $\mathbb{A}^{(1)} = \mathbb{A}_{\text{R}} + \mathbb{A}^{(1)}_{\text{DF}}$, and

$$\mathbf{X}_2 = \text{argmin}_{\mathbf{X}}\left(a^{(3)} - \left(\mathbf{B}^{(3)}\right)^t\mathbf{X} + \frac{1}{2}\mathbf{X}^t\mathbb{A}^{(3)}\mathbf{X}\right),$$

where $a^{(3)} = a_{\text{R}} + a^{(3)}_{\text{DF}}$, $\mathbf{B}^{(3)} = \mathbf{B}_{\text{R}} + \mathbf{B}^{(3)}_{\text{DF}}$, and $\mathbb{A}^{(3)} = \mathbb{A}_{\text{R}} + \mathbb{A}^{(3)}_{\text{DF}}$.

The matrices $\mathbb{A}_{\mathrm{R}}$ and $\mathbb{A}_{\mathrm{DF}}^{(1)}$ are positive, and so is $\mathbb{A}^{(1)}$; it is also definite: one can easily prove that $\mathbf{X}^t\mathbb{A}_{\mathrm{R}}\mathbf{X}$ and $\mathbf{X}^t\mathbb{A}_{\mathrm{DF}}^{(1)}\mathbf{X}$ cannot be zero at the same time except if $\mathbf{X}=0$. Thus, finding $\mathbf{X}_1$ is reduced to computing the unique solution of the linear system $\mathbb{A}^{(1)}\mathbf{X}=\mathbf{B}^{(1)}$. This is also true for $\mathbf{X}_2$. Then we define the local estimator as

$$\eta_D^{\mathrm{min,full}} := \min\left\{\eta_D(\mathbf{X}_1), \eta_D(\mathbf{X}_2), \eta_D(\mathbf{t}_h)\right\}. \tag{A.7}$$

Here $\mathbf{t}_h$ is given by (4.1) and we include the term $\eta_D(\mathbf{t}_h)$ for the sake of security, as, having minimized the quadratic forms, we are not sure to have found the minimum. Once again, we stress that this minimization process is local and the size of the matrices is small: it corresponds to the number of subtriangles of the dual volume, which is generally of the order of 10. Thus, the computational cost of the estimator does not increase excessively and remains linear.

B A simplified local minimization strategy

We generalize here one part of the "simplified minimization strategy" of [21, Section 7] to the reaction–diffusion case.

Let $D \in \mathcal{D}_h$ be fixed. We construct $\mathbf{t}_D \in \mathbf{RTN}(\mathcal{S}_D)$ given by (4.1) only for such $\sigma \in \mathcal{G}_h$ contained in D which are at the boundary of some $E \in \mathcal{D}_h^{\mathrm{int}}$ and such that $(\nabla\cdot\mathbf{t}_D + rp_h, 1)_K = (f,1)_K$ for all $K \in \mathcal{S}_D$. Note that as $(\nabla\cdot\mathbf{t}_D + rp_h, 1)_D = (f,1)_D$ when $D \in \mathcal{D}_h^{\mathrm{int}}$, this can be done without any (local) linear system solution by choosing the flux over one interior side and a sequential construction as $\sum_{K\in\mathcal{S}_D}(f,1)_K = (f,1)_D$. If $D \in \mathcal{D}_h^{\mathrm{ext}}$, this argument is then replaced by the fact that we are free to choose the fluxes over the exterior sides. We thus can define a local estimator

$$\eta_D^{\mathrm{min,loc}} := \min\left\{\eta_D(\mathbf{t}_D), \eta_D(\mathbf{t}_h)\right\}, \tag{B.1}$$

where $\mathbf{t}_h$ is given by (4.1). We remark that in [21, Section 7], a parameter α such that $\eta_D(\alpha\mathbf{t}_h + (1-\alpha)\mathbf{t}_D)$ was (approximately) minimal was searched in addition and the value $\eta_D(\alpha\mathbf{t}_h + (1-\alpha)\mathbf{t}_D)$ was included in the above minimum. We do not perform here such an additional minimization since the above extremely simple choice already works very well.

C A minimization strategy used in the numerical experiments

In the numerical experiments of this paper, we finally use the minimization estimate of the form

$$|||p-p_h||| \le \left\{\sum_{D\in\mathcal{D}_h}(\eta_D^{\mathrm{min}})^2\right\}^{1/2}, \qquad \eta_D^{\mathrm{min}} := \min\left\{\eta_D^{\mathrm{min,full}}, \eta_D^{\mathrm{min,loc}}\right\}, \tag{C.1}$$

where $\eta_D^{\mathrm{min,full}}$ is given by (A.7) and $\eta_D^{\mathrm{min,loc}}$ by (B.1). As however noted in the text, in the majority of the cases, it is the simple choice (B.1) which gives the minimum.