A Posteriori Error Estimates for Unsteady Convection–Diffusion–Reaction Problems and the Finite Volume Method

Nancy Chalhoub, Alexandre Ern, Tony Sayah, and Martin Vohralík

Abstract We derive a posteriori error estimates for the discretization of the unsteady linear convection–diffusion–reaction equation approximated with the cell-centered finite volume method in space and the backward Euler scheme in time. The estimates are based on a locally postprocessed approximate solution preserving the conservative fluxes and are established in the energy norm. We propose an adaptive algorithm which ensures the control of the total error with respect to a user-defined relative precision and refines the meshes adaptively while equilibrating the time and space contributions to the error. Numerical experiments illustrate the theory.

Key words: a posteriori estimate, unsteady convection–diffusion–reaction, cellcentered finite volumes, mesh adaptation **MSC2010:** 65N15, 76M12, 76S05

1 Introduction

We consider the time-dependent linear convection-diffusion-reaction equation

$$\partial_t u - \nabla \cdot (S \nabla u) + \nabla \cdot (\boldsymbol{\beta} u) + ru = f$$
 a.e. in $Q_T := \Omega \times (0, T),$ (1a)

$$u(\cdot,0) = u_0 \quad \text{a.e. in } \Omega, \tag{1b}$$

$$u = 0$$
 a.e. on $\partial \Omega \times (0, T)$. (1c)

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Here S is the diffusion–dispersion tensor, $\boldsymbol{\beta}$ is the velocity field, r is the reaction function, f is the source term, $\Omega \subset \mathbb{R}^d$, $d \ge 2$, is the space domain which we suppose polyhedral, and (0,T) is the time interval. We suppose that $S = (S_{i,j})$ with $S_{i,j} \in L^{\infty}(Q_T)$, $1 \le i, j \le d$, is a symmetric, bounded, and uniformly positive definite tensor (we suppose that $S_{i,j}$ are piecewise constant on space-time meshes defined below), $\boldsymbol{\beta} \in C^0([0,T]; [W^{1,\infty}(\Omega)]^d)$, $r \in L^{\infty}(Q_T)$, $f \in L^2(Q_T)$, and $u_0 \in L^2(\Omega)$.

Several works have studied a posteriori error estimates for the cell-centered finite volume method. Ohlberger derives in [7] estimates in the L^1 -norm. Nicaise [6] establishes a posteriori energy-norm estimates using Morley-type interpolants of the original piecewise constant finite volume approximation. Guaranteed flux-based estimates were established in [8] and extended in [3] to the parabolic case. Estimates for vertex-centered unsteady convection–diffusion–reaction problems were derived in [1] and [5].

The purpose of this work is to derive guaranteed a posteriori error estimates for the discretization of (1a)–(1c) by the cell-centered finite volume method in space and the backward Euler scheme in time. We allow for time-varying meshes.

2 Notation and Continuous Problem

2.1 Notation

We consider a strictly increasing sequence of discrete times $\{t^n\}_{0 \le n \le N}$ such that $t^0 = 0$ and $t^N = T$. For all $1 \le n \le N$, we define $\tau^n := t^n - t^{n-1}$ and $I^n := (t^{n-1}, t^n]$. On each time interval I^n , we consider partition \mathscr{T}^n of Ω such that $\overline{\Omega} = \bigcup_{K \in \mathscr{T}^n} K$. For simplicity, we assume that the meshes are simplicial and matching (in the sense that they do not contain hanging nodes). For $1 \le n \le N$, $\mathscr{T}^{n-1,n}$ is a common refinement of \mathscr{T}^{n-1} and \mathscr{T}^n . For all $0 \le n \le N$ and all $K \in \mathscr{T}^n$, h_K denotes the diameter of K. We denote by $c_{S,K}^n$ the smallest eigenvalue of S on K and by $c_{\beta,r,K}^n$ the essential minimum of $\frac{1}{2}\nabla \cdot \boldsymbol{\beta} + r$ on $K \times I^n$. We denote by \mathscr{E}_K the set of the sides of $K \in \mathscr{T}^n$, and we fix $\mathbf{n}_{K,\sigma}$ as the unit normal vector to a side σ outward to K.

We denote by $(\cdot, \cdot)_S$ the $L^2(S)$ inner product, by $\|\cdot\|_S$ the associated norm (when $S = \Omega$, the index is dropped), and by |S| the Lebesgue measure of S. Next, we set $\mathbf{H}(\operatorname{div}, S) = \{\mathbf{v} \in \mathbf{L}^2(S); \nabla \cdot \mathbf{v} \in L^2(S)\}$. Moreover, we use the "broken Sobolev space" $H^1(\mathcal{T}^n) := \{\phi \in L^2(\Omega); \phi|_K \in H^1(K) \ \forall K \in \mathcal{T}^n\}$. Finally, we use the Raviart–Thomas–Nédélec space $\mathbf{RTN}^0(\mathcal{T}^n) := \{\mathbf{v}_h \in \mathbf{H}(\operatorname{div}, \Omega); \mathbf{v}_h|_K \in \mathbf{RTN}^0(K) \ \forall K \in \mathcal{T}^n\}$ where $\mathbf{RTN}^0(K) := [\mathbf{P}_0(K)]^d + \mathbf{xP}_0(K)$. For W, a vector space of functions defined on Ω , we define $\mathcal{P}^1_{\tau}(W)$ (respectively $\mathcal{P}^0_{\tau}(W)$) as the vector space of functions v defined on Q_T such that $v(\cdot, t)$ takes values in W and is continuous and piecewise affine (respectively constant) in time.

Because of the nonconformity of the cell-centered finite volume method, we introduce, for all $0 \le n \le N$, the broken gradient operator ∇^n such that for a function $v \in H^1(\mathcal{T}^n)$, $\nabla^n v \in [L^2(\Omega)]^d$ is defined as $(\nabla^n v)|_K := \nabla(v|_K)$ for all $K \in \mathcal{T}^n$. The broken gradient operator $\nabla^{n-1,n}$ on the mesh $\mathcal{T}^{n-1,n}$ is defined similarly.

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2.2 Continuous Problem

Let $X := L^2(0, T; H_0^1(\Omega)), X' = L^2(0, T; H^{-1}(\Omega))$, and $Y := \{v \in X; \partial_t v \in X'\}$. The weak solution *u* of the problem (1a)–(1c) is such that $u \in Y$ with $u(\cdot, 0) = u_0$. For a.e. $t \in (0, T)$ and for all $\varphi \in H_0^1(\Omega)$, there holds

$$\langle \partial_t u, \varphi \rangle(t) + (\mathsf{S}\nabla u, \nabla \varphi)(t) + (\nabla \cdot (\boldsymbol{\beta} u), \varphi)(t) + (ru, \varphi)(t) = (f, \varphi)(t), \qquad (2)$$

where $\langle \cdot, \cdot \rangle$ stands for the duality pairing between $H^{-1}(\Omega)$ and $H^{1}_{0}(\Omega)$.

For $y \in X$, we introduce the space-time energy norm $||y||_X^2 := \int_0^T |||y|||^2(t) dt$, where $|||y|||^2 := ||S^{\frac{1}{2}}\nabla y||^2 + ||(\frac{1}{2}\nabla \cdot \boldsymbol{\beta} + r)^{\frac{1}{2}}y||^2$. We extend the energy norm to discrete functions using the broken gradient.

3 The Cell-centered Finite Volume Schemes and Postprocessing

A general cell-centered finite volume scheme for the problem (1a)–(1c) can be written in the following form: for all $1 \le n \le N$, find $\overline{u}_h^n := (u_K^n)_{K \in \mathscr{T}^n}$, such that

$$\frac{1}{\tau^n}(\overline{u}_h^n - u_h^{n-1}, 1)_K + \sum_{\sigma \in \mathscr{E}_K} S_{K,\sigma}^n + \sum_{\sigma \in \mathscr{E}_K} W_{K,\sigma}^n + r_K^n (\overline{u}_h^n, 1)_K = f_K^n |K| \quad \forall K \in \mathscr{T}^n, (3)$$

where $f_K^n = \frac{1}{\tau^n} \int_{I^n} (f(\cdot,t), 1)_K / |K| dt$, $r_K^n = \frac{1}{\tau^n} \int_{I^n} (r(\cdot,t), 1)_K / |K| dt$, $S_{K,\sigma}^n$ and $W_{K,\sigma}^n$ are, respectively, the diffusive and convective fluxes through a side σ of an element K, and u_h^{n-1} is the postprocessed solution that we define below.

For $1 \le n \le N$, we reconstruct a conforming convective flux $\boldsymbol{\psi}^n$ and a conforming diffusive flux $\boldsymbol{\theta}^n$ such that $\boldsymbol{\psi}^n$, $\boldsymbol{\theta}^n \in \mathbf{RTN}^0(\mathscr{T}^n)$ and verifying

$$\langle \boldsymbol{\psi}^n \cdot \mathbf{n}_{K,\sigma}, 1 \rangle_{\sigma} = W_{K,\sigma}^n \quad \forall K \in \mathscr{T}^n, \ \forall \sigma \in \mathscr{E}_K,$$
(4)

$$\langle \boldsymbol{\theta}^{n} \cdot \mathbf{n}_{K,\sigma}, 1 \rangle_{\sigma} = S_{K,\sigma}^{n} \quad \forall K \in \mathscr{T}^{n}, \, \forall \sigma \in \mathscr{E}_{K}.$$
 (5)

We refer to [4, 8] for more details on such construction. We define $\boldsymbol{\theta}$ and $\boldsymbol{\psi}$ in $\mathscr{P}^0_{\tau}(\mathbf{H}(\operatorname{div},\Omega))$ by $\boldsymbol{\theta}|_{I^n} := \boldsymbol{\theta}^n$ and $\boldsymbol{\psi}|_{I^n} := \boldsymbol{\psi}^n$.

Following [8], we introduce a piecewise quadratic approximation u_h^n for all $1 \le n \le N$ verifying for all $K \in \mathscr{T}^n$,

$$-\mathsf{S}\nabla u_h^n|_K = \boldsymbol{\theta}^n|_K,\tag{6}$$

$$(u_h^n, 1)_K = |K| u_K^n. (7)$$

When S = vId, u_h^n lies in the space $\mathbb{P}_{1,2}(\mathscr{T}^n)$ which is $\mathbb{P}_1(\mathscr{T}^n)$ enriched elementwise with $\sum_{i=1}^d x_i^2$. Finally, we set u_h^0 the L^2 -projection of u_0 onto $\mathbb{P}_{1,2}(\mathscr{T}^n)$.

Because of the nonconformity of u_h^n , i.e., of the fact that $u_h^n \in H^1(\mathscr{T}^n)$, $u_h^n \notin H_0^1(\Omega)$, we define an averaging interpolate $s^n = I_{av}(u_h^n) \in H_0^1(\Omega)$ of u_h^n that verifies

$$(s^n, 1)_K = (u_h^n, 1)_K \quad \forall K \in \mathscr{T}^{n, n+1}, \quad \forall 0 \le n \le N,$$
(8)

with the convention $\mathscr{T}^{N,N+1} := \mathscr{T}^N$. We refer to [3] for the details on such construction. Finally, we consider $u_{h,\tau} \in P_{\tau}^1(H^1(\mathscr{T}^n))$ and $s \in P_{\tau}^1(H_0^1(\Omega))$. They are defined by the values u_h^n and s^n for all $0 \le n \le N$. We set $\partial_t^n v = \partial_t v|_{I^n}$. An important consequence of this construction is the following, cf. [3],

$$(\partial_t^n s, 1)_K = (\partial_t^n u_{h,\tau}, 1)_K \quad \forall K \in \mathscr{T}^n.$$
(9)

4 A Posteriori Error Estimate

Our a posteriori estimate bounds the energy error between the weak solution u and the approximate solution $u_{h,\tau}$. We use the postprocessed solution instead of the original piecewise constant solution since the latter has a zero broken gradient and therefore is not suitable for energy norm estimates.

Let $1 \le n \le N$ and $K \in \mathcal{T}^n$. We define the *residual estimator* as

$$\eta_{\mathbf{R},K}^{n} := m_{K}^{n} \| \widetilde{f}^{n} - \partial_{t}^{n} s - \nabla \cdot \boldsymbol{\theta}^{n} - \nabla \cdot \boldsymbol{\psi}^{n} - r_{K}^{n} s^{n} \|_{K}.$$
(10)

Here $\tilde{f}^n = \frac{1}{\tau^n} \int_{I^n} f(\cdot, t) dt$ and $m_K^n := \min\{C_{\mathsf{P},K} h_K(c_{\mathsf{S},K}^n)^{-\frac{1}{2}}, (c_{\boldsymbol{\beta},r,K}^n)^{-\frac{1}{2}}\}$ is the constant from the inequality

$$\|\boldsymbol{\varphi} - \boldsymbol{\varphi}_{K}\|_{K} \leq m_{K}^{n} \|\|\boldsymbol{\varphi}\|\|_{K} \quad \forall K \in \mathscr{T}^{n}, \quad \forall \boldsymbol{\varphi} \in H^{1}(K),$$
(11)

shown in [8]. Here, $\varphi_K := (\varphi, 1)_K / |K|$ and $C_{P,K} := 1/\pi$ is the constant from the Poincaré inequality (recall that *K* are convex). We define the *flux estimator* as

$$\eta_{\mathrm{F},K}^{n}(t) := \|\mathsf{S}^{\frac{1}{2}}\nabla s + \mathsf{S}^{-\frac{1}{2}}\boldsymbol{\theta}^{n} - \mathsf{S}^{-\frac{1}{2}}\boldsymbol{\beta}s + \mathsf{S}^{-\frac{1}{2}}\boldsymbol{\psi}^{n}\|_{K}.$$
 (12)

Furthermore, we define the following nonconformity estimator

$$\eta_{\text{NC},K}^{n}(t) := |||u_{h,\tau} - s|||_{K}.$$
(13)

Let $\overline{m}^n := \min\{C_{F,\Omega}h_{\Omega}(c_{S,\Omega}^n)^{-\frac{1}{2}}, (c_{\boldsymbol{\beta},r,\Omega}^n)^{-\frac{1}{2}}\}$, where $C_{F,\Omega}$ is the Friedrichs inequality constant detailed in [5]. The quadrature estimator is given by

$$\eta_{\mathbf{Q},K}^{n}(t) := \overline{m}^{n} \| f - \widetilde{f}^{n} - rs + r_{K}^{n} s^{n} \|_{K}.$$
(14)

Finally, we define the *initial condition estimator* as

$$\eta_{\rm IC} := 2^{-\frac{1}{2}} \| s^0 - u^0 \|. \tag{15}$$

We now state and prove our main result concerning the error upper bound.

Theorem 1 (Energy norm a posteriori estimate). Let $\eta_{R,K}^n$, $\eta_{F,K}^n$, $\eta_{NC,K}^n$, $\eta_{Q,K}^n$, and η_{IC} be defined by (10) and (12)–(15). Then,

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$$\begin{split} \|u - u_{h,\tau}\|_{X} &\leq \eta := \left\{ \sum_{n=1}^{N} \int_{I^{n}} \sum_{K \in \mathscr{T}^{n}} \left(\eta_{R,K}^{n} + \eta_{F,K}^{n}(t) \right)^{2} dt \right\}^{\frac{1}{2}} + \eta_{IC} \\ &+ \left\{ \sum_{n=1}^{N} \int_{I^{n}} \sum_{K \in \mathscr{T}^{n}} (\eta_{Q,K}^{n}(t))^{2} dt \right\}^{\frac{1}{2}} + \left\{ \sum_{n=1}^{N} \int_{I^{n}} \sum_{K \in \mathscr{T}^{n}} (\eta_{NC,K}^{n}(t))^{2} dt \right\}^{\frac{1}{2}}. \end{split}$$

Proof. For $s \in Y$, we define $\mathscr{R}(s)$ in X' by $\langle \mathscr{R}(s), \varphi \rangle := \int_0^T \{(f - \partial_t s - \nabla \cdot (\boldsymbol{\beta} s) - rs, \varphi) - (S \nabla s, \nabla \varphi)\}(t) dt$, for all $\varphi \in X$. We obtain

$$\frac{1}{2} \|u - s\|^2(T) = \frac{1}{2} \|u^0 - s^0\|^2 + \int_0^T \langle \partial_t (u - s), u - s \rangle(t) dt$$

which yields

$$||u-s||_X^2 \le \frac{1}{2} ||u^0-s^0||^2 + \langle \mathscr{R}(s), u-s \rangle$$

Using the definition of the dual norm yields $||u-s||_X^2 \le ||\mathscr{R}(s)||_{X'} ||u-s||_X + \frac{1}{2} ||u^0 - s^0||^2$. Since $x^2 \le ax + b^2$ implies $x \le a + b$, (a, b > 0), we infer

$$\|u - s\|_{X} \le \|\mathscr{R}(s)\|_{X'} + 2^{-\frac{1}{2}} \|u^{0} - s^{0}\|.$$
(16)

For $1 \le n \le N$, set $\langle \mathscr{R}^n(s), \varphi \rangle := T_{\mathrm{R}}^n(\varphi) + T_{\mathrm{F}}^n(\varphi) + T_{\mathrm{Q}}^n(\varphi)$ with

$$\begin{split} T^n_{\mathsf{R}}(\boldsymbol{\varphi}) &:= \sum_{K \in \mathscr{T}^n} (\widetilde{f}^n - \partial_t^n s - \nabla \cdot \boldsymbol{\theta}^n - \nabla \cdot \boldsymbol{\psi}^n - r_K^n s^n, \boldsymbol{\varphi})_K, \\ T^n_{\mathsf{F}}(\boldsymbol{\varphi}) &:= -(\mathsf{S}\nabla s + \boldsymbol{\theta}^n + \boldsymbol{\psi}^n - \boldsymbol{\beta}s, \nabla \boldsymbol{\varphi}), \\ T^n_{\mathsf{Q}}(\boldsymbol{\varphi}) &:= \sum_{K \in \mathscr{T}^n} (f - \widetilde{f}^n - rs + r_K^n s^n, \boldsymbol{\varphi})_K. \end{split}$$

First, we have $T_{R}^{n}(\varphi) = T_{R}^{n}(\varphi - \Pi_{0}\varphi)$, where $\Pi_{0}\varphi|_{K} := \varphi_{K}$ for all K, using $(\tilde{f}^{n} - \partial_{t}^{n}s - \nabla \cdot \boldsymbol{\theta}^{n} - \nabla \cdot \boldsymbol{\psi}^{n} - r_{K}^{n}s^{n}, 1)_{K} = 0$ from (3), (4), (5), and (7)–(9). Hence, $T_{R}^{n}(\varphi) \leq \sum_{K \in \mathscr{T}^{n}} \eta_{R,K}^{n} |||\varphi|||_{K}$ using the Cauchy–Schwarz inequality and (11). Moreover, $T_{F}^{n}(\varphi)$ is bounded by $\sum_{K \in \mathscr{T}^{n}} \eta_{F,K}^{n} |||\varphi|||_{K}$ using the Cauchy–Schwarz inequality, and $T_{Q}^{n}(\varphi)$ is bounded by $\left\{\sum_{K \in \mathscr{T}^{n}} (\eta_{Q,K}^{n})^{2}\right\}^{1/2} |||\varphi|||$ as in [5]. Using (16), the definition of $\mathscr{R}(s)$, and the Cauchy–Schwarz and triangle inequalities concludes the proof.

In order to make the calculation efficient, it is important to distinguish the space and time errors. To this purpose, the flux estimator $\eta_{F,K}^n(t)$ is split into two contributions using the triangle inequality. We define, for all $1 \le n \le N$,

$$\begin{aligned} &(\eta_{\rm sp}^n)^2 := 4 \sum_{K \in \mathscr{T}^n} \bigg\{ \tau^n (\eta_{\rm R,K}^n + \eta_{\rm F,1,K}^n)^2 + \int_{I^n} (\eta_{\rm NC,K}^n)^2(t) dt \bigg\}, \\ &(\eta_{\rm tm}^n)^2 := 4 \sum_{K \in \mathscr{T}^n} \bigg\{ \int_{I^n} \| \mathsf{S}^{\frac{1}{2}} \nabla(s - s^n) - \mathsf{S}^{-\frac{1}{2}} (\boldsymbol{\beta} s - \boldsymbol{\beta}^n s^n) \|_K^2(t) dt + \int_{I^n} (\eta_{\rm Q,K}^n(t))^2 dt \bigg\}. \end{aligned}$$

where $\boldsymbol{\beta}^n := \frac{1}{\tau^n} \int_{I^n} \boldsymbol{\beta}(\cdot, t) dt$ and $\eta_{F,1,K}^n := \|S^{\frac{1}{2}} \nabla s^n + S^{-\frac{1}{2}} \boldsymbol{\theta}^n - S^{-\frac{1}{2}} \boldsymbol{\beta}^n s^n + S^{-\frac{1}{2}} \boldsymbol{\psi}^n\|_K$. Proceeding as in [3], we obtain

Theorem 2 (A posteriori estimate distinguishing the space and time errors). There holds

$$\|u-u_{h,\tau}\|_{X} \leq \left\{\sum_{n=1}^{N} \left\{ (\eta_{\rm sp}^{n})^{2} + (\eta_{\rm tm}^{n})^{2} \right\} \right\}^{1/2} + \eta_{\rm IC}.$$

5 A Space-time Adaptive Time-marching Algorithm

We present here an adaptive algorithm based on our a posteriori error estimates which ensures that the relative energy error between the exact and the approximate solutions is below a prescribed tolerance ε . At the same time, it intends to equilibrate the space and time estimators η_{sp}^n and η_{tm}^n . Recalling Theorem 2 and neglecting η_{IC} we aim at achieving

$$\frac{\sum_{n=1}^{N} \{(\eta_{\rm sp}^{n})^{2} + (\eta_{\rm tm}^{n})^{2}\}}{\sum_{n=1}^{N} \|u_{h,\tau}\|_{X(t^{n-1},t^{n})}^{2}} \le \varepsilon^{2}.$$
(17)

On a given time level t^{n-1} , we set $\mathbf{Crit} := \varepsilon \frac{\|u_{h,\tau}\|_{X(t^{n-1},t^n)}}{\sqrt{2}}$ and we choose the space mesh \mathscr{T}^n and the time step τ^n such that $\eta_{sp}^n \leq \mathbf{Crit}$ and $\eta_{tm}^n \leq \mathbf{Crit}$. For practical implementation purposes and because of computer limitations, we introduce maximal refinement level parameters N_{sp} and N_{tm} . The actual algorithm is as follows:

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Choose an initial mesh \mathscr{T}^0, an initial time step \tau^0, and set t^0 = 0

Set n = 1 and t^1 = t^0 + \tau^0

Loop in time: While t^n \leq T

Set \mathscr{T}^{n\star} := \mathscr{T}^{n-1}

Do

Solve u_h^{n\star} = \operatorname{Sol}(u_h^{n-1}, \tau^{n-1}, \mathscr{T}^{n\star})

Estimate \eta_{sp}^n and \eta_{tm}^m

Refine the elements K \in \mathscr{T}^{n\star} where \eta_{sp,K}^n \geq \operatorname{Ref} \eta_{sp}^n and such

that their level of refinement is less than N_{sp}

While \{\eta_{sp}^n \geq \operatorname{Crit} or \eta_{sp}^n is much larger than \eta_{tm}^n\}

If \{\eta_{tm}^n \geq \operatorname{Crit} or \eta_{tm}^n is much larger than \eta_{sp}^n and when

the level of time refinement is less than N_{tm}\}

Set t^n = t^n - \tau^{n-1} and \tau^{n-1} = \tau^{n-1}/2

Else

Save the approximate solution u_h^n := u_h^{n\star}, the mesh \mathscr{T}^n := \mathscr{T}^{n\star},

and the time step \tau^n, and set n = n + 1
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In this version we are only refining the elements and time steps where the estimated error is large. In a later version, we will also coarsen elements and time steps where the estimated error is small.

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6 Numerical Experiments

We consider (1a)–(1c) on $\Omega = (0,3) \times (0,3)$ with $S = \nu Id$, $\boldsymbol{\beta} = (\beta_1, \beta_2)$, r = 0, and f = 0, where $\nu > 0$ determines the amount of diffusion. The initial condition u_0 , as well as the Dirichlet boundary condition, are given by the exact solution

$$u(x,y,t) = \frac{1}{200vt+1} e^{-50\frac{(x-x_0-\beta_1 t)^2 + (y-y_0-\beta_2 t)^2}{200vt+1}}$$

Here $x_0 = 0.33$, $y_0 = 1.125$, $\beta_1 = 0.8$, and $\beta_2 = 0.4$. We set T = 0.6. We use the DDFV method detailed in [2]. We neglect the additional error from the inhomogeneous Dirichlet boundary condition. We consider two cases v = 0.1 and v = 0.001. We start from an initial time step $\tau = 0.05$ and an initial mesh of 336 triangles and we refine uniformly by dividing the time step by 2 and each triangle into 4 subelements. Tables 1 and 2 show the actual and estimated energy error where η is the upper bound from Theorem 1, as well as the contribution of each estimator to the upper bound. Specifically, we define the global-intime and global-in-space version of the estimators, $(\eta_R)^2 := \sum_{n=1}^N \tau^n \sum_{K \in \mathcal{F}^n} (\eta_{R,K}^n)^2$, $(\eta_{NC})^2 := \sum_{n=1}^N \int_{I^n} \sum_{K \in \mathcal{F}^n} (\eta_{NC,K}^n(t))^2 dt$ and $(\eta_F)^2 := \sum_{n=1}^N \int_{I^n} \sum_{K \in \mathcal{F}^n} (\eta_{F,K}^n(t))^2 dt$.

Table 1 Convergence results with uniform refinement in the case v = 0.1

$\ u-u_{h,\tau}\ _X$	η	η_R	$\eta_{\rm F}$	η_{NC}	$\frac{\eta}{\ u-u_{h,\tau}\ _X}$
0.0625	0.2070	0.0420	0.0910	0.0600	3.3102
0.0366	0.1299	0.0242	0.0613	0.0327	3.5464
0.0199	0.0662	0.0065	0.0328	0.0179	3.3182
0.0104	0.0335	0.0017	0.0167	0.0095	3.2104

Table 2 Convergence results with uniform refinement in the case v = 0.001

$\ u-u_{h,\tau}\ _X$	η	η_R	η_{F}	η_{NC}	$\frac{\eta}{\ u-u_{h,\tau}\ _X}$
0.0342	1.6490	0.3894	1.0875	0.0101	48.2496
0.0286	1.2341	0.2175	0.8354	0.0091	43.2175
0.0221	0.7992	0.0701	0.5541	0.0083	36.1332
0.0158	0.4773	0.0226	0.3312	0.0076	30.2736

We next compare the uniform and adaptive refinement strategies. We note that the refinement maintains the conformity of the mesh. Figure 1 shows that we obtain a better precision in the adaptive strategy for much fewer space-time unknowns. Figure 2 depicts the approximate solution at the final time for v = 0.001 obtained with adaptive refinement for $N_{sp} = N_{tm} = 2$, and $N_{sp} = N_{tm} = 4$. We can see that in the second case the approximate solution better approximates the exact solution.



Fig. 1 Energy error in adaptive and uniform refinement for $\nu = 0.1$ (left) and $\nu = 0.001$ (right)



Fig. 2 Approximate solution with adaptive refinement: $N_{sp} = N_{tm} = 2$ (left), $N_{sp} = N_{tm} = 4$ (right)

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References

- Amaziane, B. and Bergam, A. and El Ossmani, M. and Mghazli, Z.: A posteriori estimators for vertex centred finite volume discretization of a convection-diffusion-reaction equation arising in flow in porous media. Internat. J. Numer. Methods Fluids 59, 259–284, (2009)
- Domelevo, K. and Omnes, P.: A finite volume method for the Laplace equation on almost arbitrary two-dimensional grids. M2AN Math. Model. Numer. Anal. 39, 1203–1249 (2005)
- Ern, A. and Vohralík, M.: A posteriori error estimation based on potential and flux reconstruction for the heat equation. SIAM J. Numer. Anal. 48, 198–223 (2010)
- 4. Eymard, R. and Gallouët, T. and Herbin, R.: Finite volume approximation of elliptic problems and convergence of an approximate gradient. Appl. Numer. Math. **37**, 31–53 (2001)
- Hilhorst, D. and Vohralík, M.: A posteriori error estimates for combined finite volume–finite element discretizations of reactive transport equations on nonmatching grids. Comput. Methods Appl. Mech. Engrg. 200, 597–613 (2011)
- Nicaise, S.: A posteriori error estimations of some cell centered finite volume methods for diffusion-convection-reaction problems. SIAM J. Numer. Anal. 44, 949–978 (2006)
- Ohlberger, M.: A posteriori error estimate for finite volume approximations to singularly perturbed nonlinear convection-diffusion equations. Numer. Math. 87, 737–761 (2001)
- Vohralík, M.: Residual flux-based a posteriori error estimates for finite volume and related locally conservative methods. Numer. Math. 11, 121–158 (2008)

The paper is in final form and no similar paper has been or is being submitted elsewhere.