The effect of mesh modification in time on the error control of fully discrete approximations for parabolic equations

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\section{1. Introduction}

In recent years, a main approach towards the computation of solutions of Partial Differential Equations is based on self-adapted methods. In particular, methods utilizing self adjusted meshes have important benefits approximating PDEs with solutions that exhibit nontrivial characteristics. When appropriately chosen, they lead to efficient, accurate and robust algorithms. Adaptive algorithms are naturally related to error control. Appropriate analysis can provide guarantees on how accurate the approximate solution is through a posteriori estimates. Error control may lead to appropriate adaptive algorithms by identifying areas of large errors and adjusting the mesh accordingly. Error control and associated adaptive algorithms for time dependent problems is a challenging area, both for theory and computations. A key issue, often underestimated, is the need of spatial mesh modification (mesh movement) with time. In this paper we discuss the effect of mesh modification with time on the error control of fully discrete approximations of parabolic problems. The approximations are constructed by combining Crank–Nicolson (CN) time discretization with standard finite elements for the space discretization. The finite element spaces are allowed to change in different time nodes.

Roughly speaking, the main structure of an algorithm which permits mesh redistribution with time has the form: Given the approximation $u_n$ at the time step $n$, which belongs to a finite-dimensional space $V_n$ (reflecting the space discretization method)

\begin{enumerate}
  \item[(1a)] choose the next space $V_{n+1}$,
  \item[(1b)] project $u_n$ to the new space $V_{n+1}$ to get $\tilde{u}_n$,
  \item[(1c)] use $\tilde{u}_n$ as starting value to perform the evolution step in $V_{n+1}$ to obtain the new approximation $u_{n+1} \in V_{n+1}$.
\end{enumerate}

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Standard schemes involve only step (1c) (uniform or nonuniform mesh). The presence of (1a) and (1b) are in most of the cases neglected in the analysis. It should be noted though that, on one hand, such algorithms can accumulate the nodes of the computational mesh in the areas of interest, as expected, and on the other hand (1a) and (1b) have fundamental influence on the qualitative behavior of the schemes. Such influence becomes evident in pressure pollution in Navier–Stokes solvers. In fact, random mesh redistribution can pollute in a severe way the pressure approximation, see [5] where examples based on van Karman vortex shedding highlighting this effect are presented. On the positive side, in nonlinear hyperbolic problems geometric mesh redistribution can stabilize unstable schemes. Indeed, all stable schemes for these problems include terms inducing artificial numerical diffusion (upwinding). As it is well known, the right selection of such schemes is a nontrivial task. Recent results reported in e.g., [3,4] and their references, show that when steps (1a) and (1b) are based on geometric information on \(u_t\) then they effectively stabilize schemes even without additional terms reflecting artificial diffusion or upwinding. One has to mention the classical example of a divergent method through mesh modification due to Dupont [9]. For other studies related to mesh modification see also [7] and its references.

In the present paper, we investigate the influence of mesh change in the stability of fully discrete schemes based on Crank–Nicolson time discretizations, as well as its influence on the a posteriori error estimators. These estimators are derived in detail in [6] and are the first optimal order a posteriori estimates in \(L^\infty(L^2)\) for fully discrete Crank–Nicolson schemes allowing mesh modification. For completeness, we present the main ideas of the analysis here, but we focus mainly on the qualitative analytical and computational behavior of the schemes and the estimators. Our findings can be summarized as follows:

1. **Refinement can spoil Crank–Nicolson schemes.** Indeed, we present examples where recursive refinement of the mesh can spoil standard Crank–Nicolson schemes. This rather surprising conclusion was a consequence of our effort to understand the presence and the role in the a posteriori estimate of a term of the type \(\|\Delta^n - \Delta^{n-1}u_{n-1}\|\), here \(\Delta^n\) denotes the discrete Laplacian corresponding to the space \(V_n\), see below for precise definitions.

2. **We introduce a version of the Crank–Nicolson scheme consistent with mesh redistribution.** The definition of the new version of fully discrete CN scheme is motivated by the a posteriori analysis and the fact that the standard scheme is problematic when combined with mesh modification.

3. **Refinement can influence the a posteriori error estimators.** We present detailed computational experiments which show that the a posteriori estimators are of optimal order and include terms capturing separately the spatial and the temporal errors. We present a case study where refinement occurs at a given time level. In this case and when the solution is “fast” in the spatial variable, parts of the estimator become sensitive. This is a further indication that Crank–Nicolson fully discrete schemes should be used with great care during mesh change.

4. **Mesh change is related to known non-smooth data effects.** It is known that CN is a sensitive scheme and belongs to the border of stable time discretization methods for diffusion problems. Among its known properties is its lack of smoothing effect, see [14,19]. Smoothing is a desirable property for discretization schemes for parabolic problems and thus CN time discretization serves mostly as an interesting case study. We present computational results, as well as spectral arguments to show that this lack of smoothing of CN scheme is present and influences the behavior of the a posteriori estimators. This suggests, that nonstandard projections in the step (1b) of the above algorithm, might be desirable. This subtle issue requires further investigation.

Our estimators are based on the methodology developed in [16,12] for space discrete and fully discrete and in [1,2] for time discrete schemes. The key point is the definition of an auxiliary function which we call reconstruction of the approximation \(U\). As far as the time reconstruction is concerned we follow the approach of [2] which includes the reconstructions based on approximations on one time level (two point estimators) as in [1] as well as the reconstructions based on approximations on two time levels (three point estimators) as in [13]. The role of the elliptic reconstruction, [16], is also important for the derivation of the estimators.

Fully discrete a posteriori estimates for CN time discretization methods were derived previously in [13,21]. The estimators in [13] are valid only without mesh change and they are of optimal order in \(L^2(H^1)\) but not in \(L^\infty(L^2)\). The estimators in [21] are not second order in time, see [17]. Compared to existing results, apart from including the possibility of mesh-change, our analysis provides optimal order estimators in \(L^\infty(L^2)\) for higher order in time fully discrete schemes. Notice also that our approach is in principle applicable to other evolution problems, not necessarily of parabolic type. A posteriori bounds for Crank–Nicolson methods applied to the linear Schrödinger equation were derived by Dörfler [8]. Alternative estimators for the discretization–methods and the problem at hand based on the direct comparison of \(u\) and the numerical solution \(U\) could be derived using parabolic duality as in [11,10].

The rest of this article is organized as follows. In the remainder of this section we introduce the problem setting and define the CN discretization. In Section 2 we present the space–time reconstruction. Section 2.2 is concerned with a posteriori error estimates. In particular we emphasize on the use of two point and three point estimators. Then in Section 3 we discuss in detail numerical experiments highlighting in particular the stability of the scheme and the estimators with respect to data effects and mesh refinements. In Section 4 we summarize our findings.
1.1. The problem and its discretization

We consider the initial value problem for the heat equation: Find \( u \in L^\infty(0, T; H^1_0(\Omega)) \), with \( \partial_t u \in L^2(0, T; L^2(\Omega)) \), satisfying
\[
\begin{align*}
\{ (u_t, \phi) + a(u, \phi) &= (f, \phi), & \forall \phi \in H^1_0(\Omega), \\
(u(0) &= u^0, 
\end{align*}
\]  
(1.1)
where \( f \in L^2(0, T; L^2(\Omega)) \) and \( u^0 \in H^1_0(\Omega) \). Here \( \Omega \) is a bounded domain in \( \mathbb{R}^d \), \( d = 2, 3 \), and \( T > 0 \). We denote by \( \langle \cdot, \cdot \rangle \) the duality pairing between \( H^1_0(\Omega) \) and its dual \( H^{-1}(\Omega) \), and by \( a(\cdot, \cdot) \) the bilinear form in \( H^1_0(\Omega) \) defined as
\[
a(v, w) = \langle \nabla v, \nabla w \rangle, \quad \forall v, w \in H^1_0(\Omega).
\]  
(1.2)
For \( D \subset \mathbb{R}^d \) bounded we denote by \( \| \cdot \|_D \) the norm in \( L^2(D) \), by \( \| \cdot \|_{r, D} \) and by \( | \cdot |_{r, D} \) the norm and the semi-norm, respectively, in the Sobolev space \( H^r(D), r \in \mathbb{Z}^+ \). In view of the Poincaré inequality, we consider \( | \cdot |_{1, D} \) to be the norm in \( H^1_0(D) \) and denote by \( | \cdot |_{-1, D} \) the norm in \( H^{-1}(D) \). In the sequel, in order to simplify the notation, we shall omit the subscript \( D \) in the notation of function spaces and norms whenever \( D = \Omega \). In order to discretize the time variable in (1.1), we introduce the partition \( 0 = t^0 < t^1 < \cdots < t^N = T \) of \([0, T]\) and we denote by \( I_n := (t^{n-1}, t^n) \) the subintervals, by \( h_n := t^n - t^{n-1} \) the time steps, and by \( t^{n-1/2} \) the midpoints of \( I_n \). Moreover, for given sequence \( \{v^n\}_{n=0}^N \), we shall use the notation
\[
\partial v^n := \frac{v^n - v^{n-1}}{h_n} \quad \text{and} \quad v^{n-1/2} := \frac{v^{n-1} + v^n}{2}, \quad n = 1, \ldots, N.
\]  
(1.3)
We shall also denote by \( u^n(x) \) and \( f^n(x) \) the values \( u(x, t^n) \) and \( f(x, t^n) \), respectively, throughout the rest of the paper. In addition, we shall often drop the space dependence explicitly, e.g., we shall write \( u^n \) with reference to \( u^n(\cdot, t^n) \).

We use finite elements to discretize in space: Let \( (T_h)_{h>0} \) be a family of conforming shape-regular triangulations of the domain \( \Omega \), which corresponds to the time node \( t^n \). As emphasized earlier, we assume that the triangulations are allowed to change in time. We denote by \( h_n \) the local mesh-size function of each triangulation \( T_n \) defined by
\[
h_n(x) := h_K, \quad K \in T_n \text{ and } x \in K,
\]  
(1.4)
with \( h_K := \text{diam}(K) \). For each \( n \) and for each \( K \in T_n \), we let \( E_n(K) \) be the set of the sides of \( K \) (edges in \( d = 2 \) or faces in \( d = 3 \)) and \( E_n(\Omega) \subset E_n(K) \) be the set of the internal sides of \( K \); \( h_e \) denotes the diameter of the side \( e \). In addition, we introduce the sets \( E_n := \bigcup_{K \in T_n} E_n(K) \) and \( \Sigma_n := \bigcup_{K \in T_n} \Sigma_n(K) \). We shall also use the sets \( \Sigma_n := \Sigma_n \cap \Sigma_n^{-1} \) and \( \Sigma_n := \Sigma_n \cup \Sigma_n^{-1} \). With \( e \in E_n(K) \) we associate a unit vector \( \mathbf{n}_e \) orthogonal to \( e \) and denote by \( J[v]_e \) the jump of any function \( v \) across \( e \) in the direction of \( \mathbf{n}_e \).
\[
J[v]_e := \lim_{\delta \to 0^+} [v(x + \delta \mathbf{n}_e) - v(x - \delta \mathbf{n}_e)], \quad \text{for } x \in e.
\]  
(1.5)
The global function \( J[v] \) defined on \( \Sigma_n \) is just \( J[v]_e = J[v]_e \).

We associate with each triangulation \( T_n \) the finite element spaces
\[
\mathbb{V}^n := \{ \phi \in H^1(\Omega); \forall K \in T_n : \phi|_K \in \mathbb{P}^l \} \quad \text{and} \quad \mathbb{V}^n := \mathbb{V}^n \cap H^1_0(\Omega),
\]  
(1.6)
where \( \mathbb{P}^l \) is the space of polynomials in \( d \) variables of degree at most \( l \).

1.2. The fully discrete scheme

The standard Crank–Nicolson Galerkin (GCN) finite element discretization is the following usual form of the fully discrete equations: let \( U^0 \) a given initial approximation of \( u^0 \) and for \( 1 \leq n \leq N \), find \( U^n \in \mathbb{V}^n \) such that
\[
\left( U^n - U^{n-1} \right) |_{h_n} + a \left( U^n + U^{n-1} \right) |_{h_n} = \left( f^{n-1/2} \right) |_{h_n} \quad \text{for all } \phi_n \in \mathbb{V}^n.
\]  
(1.7)
This scheme can be written in the point-wise form,
\[
\left( U^n - P^0_n U^{n-1} \right) |_{h_n} + \frac{1}{2} (-\Delta^n) U^n + \frac{1}{2} (-\Delta^n) U^{n-1} = P^0_n f^{n-1/2}.
\]  
(1.8)
Here \( P^0_n : L^2 \to \mathbb{V}^n \) is the \( L^2 \)-projection onto \( \mathbb{V}^n \) and \( \Delta^n \) is the discrete Laplacian corresponding to the finite element space \( \mathbb{V}^n \) defined by

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The discrete Laplacian $\Delta^n : H^1_0(\Omega) \to \mathcal{V}^n$ is the operator with the property
\[
\langle -\Delta^n v, \phi_n \rangle = a(v, \phi_n) \quad \forall \phi_n \in \mathcal{V}^n.
\] (1.9)

However, see [6], when changing the mesh, the term $\Delta^n U^{n-1}$ may cause problems. If for instance $T_n$ is a refinement of $T_{n-1}$, then the discrete Laplace operator on the finer mesh is applied to coarse grid functions leading to oscillatory behavior of the term $\Delta^n U^{n-1}$, see Fig. 1 for a computational example in 1d. There, the standard Galerkin Crank–Nicolson scheme (1.8) was applied for 20 time steps with global refinement each 6 time steps. Clearly the oscillatory behavior can be seen. Notice that this is particularly interesting since usually errors are not expected during refinement only, [18]. The a posteriori analysis of [6], has led to this unexpected finding. In fact, the final a posteriori estimate for the standard scheme (1.8) contains a term of the type, [6],
\[
\| (\Delta^{n-1} - \Delta^n) U^{n-1} \|
\]
which might grow without control (see Section 3.1, (3.6) for a discussion related to the actual computation of this term). This suggests that a possible solution that would resolve the oscillatory behavior of the classical scheme, is to consider the following modified Crank–Nicolson scheme:

For $n, 1 \leq n \leq N$ find $U^n \in \mathcal{V}^n$, $1 \leq n \leq N$, such that
\[
\frac{U^n - \hat{U}^n U^{n-1}}{k_n} + \frac{1}{2} \Pi^n (-\Delta^{n-1}) U^{n-1} + \frac{1}{2} (-\Delta^n) U^n = P^n_0 f^{n-1/2}.
\] (1.10)

Here, $\Pi^n, \hat{U}^n : \mathcal{V}^{n-1} \to \mathcal{V}^n$ denote suitable projections or interpolants to be chosen. For the computations of Fig. 1 we used $\hat{U}^n = \Pi^n = P^n_0$. The reason for introducing a further operator $\hat{U}^n$ is that we would like to study schemes and corresponding estimators including several possible choices for the projection step. Fig. 1 also displays computations with the scheme (1.10), which resolves the problem of this oscillatory behavior. The scheme (1.10) is in fact natural: One may think that the fact that the discrete Laplacian changes with time introduces an "artificial time dependence" of the form
\[
y_t + A(t)y = 0,
\]
say to the space discrete ode. An application of the Trapezoidal method to this problem will yield,
\[
\frac{y^n - y^{n-1}}{k_n} + \frac{1}{2} A(t^{n-1}) y^{n-1} + \frac{1}{2} A(t^n) y^n = 0,
\]
and the similarity to (1.10) is evident.

2. A posteriori error estimates in $L^{\infty}(L^2)$ norm

Towards error control the methodology developed in [16,12,12] summarized in [15] is used. It is based on the appropriate definition of an auxiliary function $\hat{U}$ which we call reconstruction of the approximation $\hat{U}$; here $\hat{U}$ is the piecewise linear in time interpolant of $U^n$. Then the error estimate relies on the separate control of $u - \hat{U}$ and $\hat{U} - U$. A key ingredient of this approach is the fact that $\hat{U}$ should satisfy the same PDE with the exact solution, but, perturbed with an a posteriori
term which we would like to have in the final estimate (terms which are not computable but can be bounded a posteriori are also allowed). The crucial and not trivial issue is to define appropriately the reconstruction \( \hat{U} \). For our case, following [6] we present the basic steps of this construction.

As it was observed first in the time discrete case in [1], \( U \) cannot lead to optimal order estimators using energy methods, see also [21,13,17]. As far as the time reconstruction is concerned we follow the approach of [2] which includes the reconstructions based on approximations on one time level (two point estimators) as in [1] as well as the reconstructions based on approximations on two time levels (three point estimators) as in [13]. We emphasize that in order to derive estimators of optimal order in \( L^\infty(0,T;L^2(\Omega)) \) we have to appropriately define \( \hat{U} \) by involving in its derivation the elliptic reconstruction operator [16].

### 2.1. The space–time reconstruction

We begin by introducing the piecewise linear approximation \( U : [0,T] \to H^1_0(\Omega) \) of \( u \) defined by linearly interpolating between the nodal values \( U^{n-1} \) and \( U^n \)

\[
U(t) := l^n_0(t)U^{n-1} + l^n_1(t)U^n, \quad t \in I_n, \tag{2.1}
\]

with

\[
l^n_0(t) := \frac{t-n}{k_n} \quad \text{and} \quad l^n_1(t) := \frac{t-n-1}{k_n}, \quad t \in I_n. \tag{2.2}
\]

In addition, let \( \Theta : [0,T] \to H^1_0(\Omega) \) be defined as

\[
\Theta(t) = l^n_0(t)l^n(\Delta^{-n-1})U^{n-1} + l^n_1(t)l^n(-\Delta^n)U^n, \quad t \in I_n. \tag{2.3}
\]

To proceed with the definition of the space–time reconstructions of the fully discrete approximate solution \( U^n, n = 0, \ldots, N \), defined in (1.10), we finally need to introduce the elliptic reconstruction operator \( \mathcal{R}^n \). Since its definition depends on the finite element space \( \mathcal{V}^n \), the operator \( \mathcal{R}^n \) changes also with \( n \).

**Definition 2.1 (Elliptic reconstruction).** For fixed \( v_h \in \mathcal{V}^n \), we define the elliptic reconstruction \( \mathcal{R}^n v_h \in H^1_0 \) of \( v_h \), as the solution of the following variational problem

\[
a(\mathcal{R}^n v_h, \psi) = \langle (-\Delta^n)\psi_h, \psi \rangle, \quad \forall \psi \in H^1_0. \tag{2.4}
\]

The elliptic reconstruction \( \mathcal{R}^n \) satisfies the Galerkin orthogonality property

\[
a(\mathcal{R}^n v_h - v_h, \chi_n) = 0, \quad \forall \chi_n \in \mathcal{V}^n. \tag{2.5}
\]

To define the space–time reconstruction it will be useful to rewrite our scheme (1.10) in the compact form

\[
\frac{U^n - \hat{U}^nU^{n-1}}{k_n} + F_0^{n-\frac{1}{2}} = 0, \tag{2.6}
\]

where

\[
F_0^{n-\frac{1}{2}} = \frac{1}{2}l^n(\Delta^{n-1})U^{n-1} + \frac{1}{2}(-\Delta^n)U^n - P_0^n f_0^{n-\frac{1}{2}}. \tag{2.7}
\]

Thus one can think that the scheme (1.10) is an application of the midpoint rule to a virtual function \( F \). According to [2] one should reconstruct in time \( F \) by a piecewise linear function. The situation in the fully discrete case is more involved:

**Definition 2.2 (Space–time reconstruction).** We define first the piecewise linear in time function \( \omega : [0,T] \to H^1_0 \) defined by linearly interpolating between the values \( \mathcal{R}^{n-1}U^{n-1} \) and \( \mathcal{R}^nU^n \)

\[
\omega(t) := l^n_0(t)\mathcal{R}^{n-1}U^{n-1} + l^n_1(t)\mathcal{R}^nU^n, \quad t \in I_n. \tag{2.8}
\]

with \( l^n_0 \) and \( l^n_1 \) defined in (2.2). Next, we define the space–time reconstruction, \( \hat{U} : [0,T] \to H^1_0 \), as follows

\[
\hat{U}(t) := \mathcal{R}^{n-1}U^{n-1} + \frac{\mathcal{R}^n\hat{F}U^nU^{n-1} - \mathcal{R}^{n-1}\hat{F}U^{n-1}}{k_n}(t - t^{n-1}) - \int_{t^{n-1}}^t \mathcal{R}^n\hat{F}(s)ds, \quad t \in I_n. \tag{2.9}
\]

Here \( \hat{F}(\cdot) \) is a piecewise linear function such that \( \hat{F}(\cdot)|_{I_n} \) is a linear polynomial interpolating \( F_0^{n-\frac{1}{2}} \):

\[
\hat{F}(t^{n-\frac{1}{2}}) = F_0^{n-\frac{1}{2}} = \frac{1}{2}(-\Delta^n)U^n + \frac{1}{2}l^n(-\Delta^{n-1})U^{n-1} - P_0^n f_0^{n-\frac{1}{2}}. \tag{2.10}
\]
It can be easily seen that the function \( \hat{U} \) interpolates the values \( R^{n-1}U^{n-1} \) and \( R^nU^n \). The first claim is obvious. Furthermore, evaluating the integral in (2.9) by the mid-point rule and recalling (1.10), we get

\[
\hat{U}(t^n) = R^n \hat{F}U^{n-1} - \int_{t^{n-1}}^{t^n} R^n \hat{F}(s) \, ds = R^n \{ \hat{F}U^{n-1} - k_n F(t^{n-\frac{1}{2}}) \} = R^n U^n.
\]

(2.11)

In addition, \( \hat{U} \) satisfies the following relation

\[
\hat{U}_t(t) + R^n \hat{F}(t) = \frac{R^n \hat{F}U^{n-1} - R^{n-1} U^{n-1}}{k_n}, \quad t \in I_n.
\]

(2.12)

The analysis in [6] is based on this particular choice of \( \hat{U} \) which incorporates the effect of the mesh change in a high order in time scheme. For Backward Euler the space–time reconstruction defined in [12] is different. A crucial point is the fact that the difference \( \hat{U} - \omega \) can be computed explicitly, and in fact is a second order in time term, see [6].

The definition of the reconstruction when no mesh change in time is present is just

\[
\hat{U}(t) := R^n \left\{ U^{n-1} - \int_{t^{n-1}}^{t} \hat{F}(s) \, ds \right\}, \quad t \in I_n.
\]

One may view the above expression as the elliptic reconstruction operator applied to the time reconstruction constructed in the spirit of [12]. Then one can verify that \( \hat{U} \) would satisfy

\[
\{ \hat{U}_t(t), \psi \} + a(\hat{U}(t), \psi) = -\{ R^n \hat{F}(t) - \Theta(t), \psi \} + a(\hat{U}(t) - \omega(t), \psi), \quad t \in I_n.
\]

This simplified equation is the starting point of our analysis, since when compared to the equation for \( u \) it leads to the main error equation. Roughly speaking, the first term in the right-hand side will create spatial errors and the term \( a(\hat{U}(t) - \omega(t), \psi) \) temporal errors. When mesh modification is allowed the equation that \( \hat{U} \) satisfies is more involved since it will contain terms in the right-hand side accounting for mesh change, compare to the r.h.s. of (2.15) and (2.18).

### 2.2. Main error equation

Motivated by the discussion above we could hope that \( \hat{\rho} := u - \hat{U} \) satisfies the same PDE with the exact solution but with controllable (a posteriori) r.h.s. To this end we introduce some more notation: Let \( \epsilon := \omega - U \) be the elliptic reconstruction error, \( \hat{\rho} \) and \( \hat{\rho} \) be the parabolic errors defined by

\[
\rho := u - \omega \quad \text{and} \quad \hat{\rho} := u - \hat{U}.
\]

(2.13)

and \( \sigma := \hat{U} - \omega \) be the time reconstruction error. Then, the error \( e := u - U \) can be split as follows

\[
e = u - U = [u - \hat{U}] + [\hat{U} - U] = [u - \hat{U}] + [\hat{U} - \omega] + (\omega - U) = \hat{\rho} + [\sigma + \epsilon].
\]

(2.14)

The proof of the estimate relies on two main ingredients:

1. the direct estimation of \( \hat{U} - U \) via the estimate of \( \sigma \) and \( \epsilon \), and
2. the estimate of \( \hat{\rho} \) using PDE stability estimates.

Note that \( \sigma \) will account for the time discretization error, and \( \epsilon \), for the space discretization error. A crucial step in the proof is to establish the equation that \( \hat{\rho} \) satisfies, [6]: For each \( \psi \in H^1_0 \), we have

\[
\{ \hat{\rho}_t(t), \psi \} + a(\hat{\rho}(t), \psi) = \{ R^n \hat{F}(t) - \Theta(t), \psi \} + f_0(t)((\mathcal{P}^n - I)(-\Delta_{n-1})U^{n-1}, \psi) \]

\[
- k_n \{ R^n \hat{F}U^{n-1} - R^{n-1} U^{n-1}, \psi \} + \{ f(t), \psi \}, \quad t \in I_n.
\]

(2.15)

After a rearrangement of certain terms, we conclude

\[
\{ \hat{\rho}_t(t), \psi \} + a(\hat{\rho}(t), \psi) = \langle R_h, \psi \rangle, \quad \forall \psi \in H^1_0.
\]

(2.16)

where

\[
R_h := (\mathcal{P}^n - I)(\hat{F}(t) - F^{n-1/2}) + (\hat{F}(t) - \Theta(t)) - \frac{\hat{F}U^{n-1} - U^{n-1}}{k_n}
\]

\[
+ f_0(t)((\mathcal{P}^n - I)(-\Delta_{n-1})U^{n-1} - \frac{(\mathcal{P}^n - I)U^n - (\mathcal{P}^{n-1} - I)U^{n-1}}{k_n} + f(t).
\]

(2.17)

An examination of the above equation leads to the following conclusions:
Indeed, (2.16) yields
\[
\langle \hat{\rho}(t), \psi \rangle + a(\hat{\rho}(t), \psi) = (R_h, \psi) + a(\sigma(t), \psi), \quad \forall \psi \in H^1_0,
\]
(2.18)
since \( \hat{\rho}(t) - \rho(t) = -(\hat{U} - \omega) = -\sigma \). We keep \( a(\rho(t), \psi) \) in the left-hand side of (2.16) for technical reasons.

(ii) The terms in the r.h.s. of (2.18) are either direct a posteriori terms or involve spatial error operators of the form \( \mathcal{R}_j - 1 \).

Therefore, one can prove the following result. The estimators still depend on stationary finite element errors through \( \mathcal{R}_j - 1 \). These terms can be estimated using residual type a posteriori estimators, although other choices on the estimators are possible.

**Theorem 2.1 (Estimate in \( L^\infty(L^2) \) and \( L^2(H^1) \) for the parabolic error).** Let \( u \) be the exact solution of (1.1), and \( \omega \) and \( \hat{U} \) defined in (2.8) and (2.9) respectively. The following estimate holds
\[
\max_{t \in [0,T]} \left\{ \frac{\| \hat{\rho}(t) \|^2}{2} + \int_0^t \left( |\hat{\rho}(s)|^2 + |\rho(s)|^2 \right) ds \right\} \leq \| \hat{\rho}(\Theta) \|^2 + J_m,
\]
(2.19)
where \( J_m, m = 1, \ldots, N \), are defined by
\[
J_m := \sum_{n=1}^m \left( J_n^T + 2J_n^{S,1} + 2J_n^{S,2} + 2J_n^C + 2J_n^D \right),
\]
(2.20)
with
\[
J_n^T := \int_{t_n}^{t_n+1} |\sigma(s)|^2 \, ds,
\]
(2.21)
\[
J_n^{S,1} := \int_{t_n}^{t_n+1} |(\mathcal{R}^n - I)(\hat{F}(t) - F^{n-1/2})| \, ds,
\]
(2.22)
\[
J_n^{S,2} := \int_{t_n}^{t_n+1} \left| \left( \mathcal{R}^n - I \right) \left( U^n - (\mathcal{R}^{n-1} - I)U^{n-1} \right) \right| \, ds,
\]
(2.23)
\[
J_n^C := \int_{t_n}^{t_n+1} \left| (\mathcal{R}^n - I)(\hat{f}(t)(\Delta^n - 1)U^{n-1} - \frac{U^{n-1}}{k_n}) - \hat{\rho}(s) \right| \, ds,
\]
(2.24)
\[
J_n^D := \int_{t_n}^{t_n+1} \left| \hat{F}(s) - \Theta(s) + f(s) \hat{\rho}(s) \right| \, ds.
\]
(2.25)

In the next paragraphs we shall focus to two special choices of space–time reconstructions.

### 2.3. Specific choices for the reconstructions

To estimate of the terms appearing in the r.h.s. of the bound in Theorem 2.1, we need to specify the interpolation operator used in the definition of \( \hat{U} \). Depending on this choice we derive estimates involving one time interval (two point estimator) or estimates involving two time intervals (three point estimators), compare to [1,13].

#### 2.3.1. Choice of the interpolant: Two-point estimator

It is easily seen that the Crank–Nicolson method (1.10) can be written as follows
\[
\frac{U^n - \tilde{U}^nU^{n-1}}{k_n} + \omega(t^{n-\frac{1}{2}}) = \rho^n_\partial f(t^{n-\frac{1}{2}}).
\]
(2.26)
Let $F(t) := \Theta(t) - P^n_0 f(t)$ and let $\hat{I}$ be the piecewise linear interpolant chosen as

$$\hat{I}(v)|_{l_n} \in P_1(I_n), \quad \hat{I}(v)(t^{n-\frac{1}{2}}) = v(t^{n-\frac{1}{2}}), \quad \hat{I}(v)(t^{n-1}) = v(t^{n-1}).$$

(2.27)

Then, define $\hat{F} = \hat{I} F : I_n \to \mathbb{V}^n$ via

$$\hat{F}(t) = \hat{I}(\Theta(t) - P^n_0 f(t)) = \Theta(t) - P^n_0 \varphi(t)$$

(2.28)

where $\varphi(t) = \hat{I}(f(t))$. Then, there holds

$$\hat{F}(t^{n-\frac{1}{2}}) = \hat{I}(\Theta(t^{n-\frac{1}{2}}) - P^n_0 f(t^{n-\frac{1}{2}})) = F(t^{n-\frac{1}{2}}).$$

(2.29)

We shall now calculate the terms on the right-hand side in Theorem 2.1 depending on that special choice of $\hat{F}$.

**Lemma 2.1 (Calculation of $\hat{F}(t) - F^{n-1/2}$).** We have

$$\hat{F}(t) - F^{n-1/2} = 2(t - t^{n-1/2})w_n,$$

(2.30)

where $w_n$ is given by

$$w_n := \frac{1}{2} \frac{\partial_t \Theta(t) - P^n_0[f(t^{n-\frac{1}{2}}) - f(t^{n-1})]}{k_n}.$$ 

(2.31)

**Proof.** In view of (2.28), we have

$$\hat{F}(t) - F^{n-1/2} = \Theta(t) - \Theta(t^{n-1/2}) - P^n_0[\varphi(t) - \varphi(t^{n-1/2})].$$

(2.32)

Now, in view of (2.2), (2.3) and (2.2), it is easily seen that

$$\Theta(t) - \Theta(t^{n-1/2}) = P^n_0(t)\Pi^n(-\Delta^{n-1})U^{n-1} + P^n_1(t)(-\Delta^n)U^n - \frac{1}{2}(\Pi^n(-\Delta^{n-1})U^{n-1} + (-\Delta^n)U^n)
= \frac{1}{2}(P^n_1(t) - P^n_0(t))((-\Delta^n)U^n - \Pi^n(-\Delta^{n-1})U^{n-1})
= (t - t^{n-1/2})\frac{1}{k_n}((-\Delta^n)U^n - \Pi^n(-\Delta^{n-1})U^{n-1}).$$

(2.33)

The result claimed follows by combining the last two relations with the definition of $\varphi$. □

Furthermore, we have

$$\hat{F}(t) - \Theta(t) = - P^n_0 \varphi(t).$$

(2.34)

**2.3.2. Choice of the interpolant: Three-point estimator**

Our scheme (1.10) can be rewritten in the form

$$U^n - \hat{F}^{n-1} U^{n-1} = F^{n-1/2} - \frac{1}{k_n}.$$

(2.35)

We shall need also the projected version of the same equation at the previous interval,

$$\pi^n U^{n-1} - \hat{F}^{n-1} U^{n-2} = \frac{\pi^n F^{n-1}}{k_{n-1}}.$$ 

(2.36)

Here $\pi^n$ is any projection to $\mathbb{V}^n$ at our disposal and

$$F^{n-1/2} = \frac{1}{2}(-\Delta^{n-1})U^{n-1} + \frac{1}{2}(\Pi^{n-2}(-\Delta^{n-2})U^{n-2} - P^{n-1}_0 f^{n-1/2}).$$

Then, we define the extended piecewise linear interpolant $\hat{F}$ as

$$\hat{F}(t) := I_{1/2}(t)F^{n-1/2} + I_{-1/2}(t)\pi^n F^{n-1/2}, \quad t \in I_n,$$

(2.37)

where

$$I_{1/2}(t) := \frac{2(t - t^{n-\frac{1}{2}})}{k_n + k_{n-1}}, \quad I_{-1/2}(t) := \frac{2(t^{n-\frac{1}{2}} - t)}{k_n + k_{n-1}}.$$ 

(2.38)
To motivate this choice one should compare to the simpler time discrete case discussed in [2, Example 4.6]. It is evident that by combining (2.35) and (2.36) one might create a second order in time difference based on $U^n$s as in [13]. Indeed, Lemma 2.2 below shows that this is the case. Next, observe that $\hat{F}(t) \in \mathbb{V}^n$ for each $t \in I_n$, $\hat{F}|_{I_n}$ is a linear function of $t$ and
\[ \hat{F}(t^n) = F(t^n). \] (2.39)
For the proof of the following two lemmata we refer to [6].

**Lemma 2.2 (Calculation of $\hat{F}(t) - F^{n-1/2}$).** We have
\[ \hat{F}(t) - F^{n-1/2} = 2(t - t^{n-1/2}) \tilde{w}_n, \] (2.40)
where $\tilde{w}_n$ is given by
\[ \tilde{w}_n := \frac{1}{k_n + k_{n-1}} \left( \left( \frac{U^n - \hat{F}^n U^{n-1}}{k_n} \right) - \pi^n \left( \frac{U^{n-1} - \hat{F}^{n-1} U^{n-2}}{k_{n-1}} \right) \right). \] (2.41)

**Lemma 2.3 (Calculation of $\hat{F}(t) - \Theta(t)$).** If we denote
\[ \hat{\phi}(t) := \frac{P_{1/2}^n(t) P_0^n f^{n-1/2}}{2} + \frac{P_{-1/2}^n(t) \pi^n P_0^n f^{n-3/2}}{2}, \quad t \in I_n, \] (2.42)
we have
\[ \hat{F}(t) - \Theta(t) = -\hat{\phi}(t) + \frac{P_{-1/2}^n(t)}{2} \left[ \frac{k_{n-1}}{k_n} (-\Delta^n) U^n \right. \]
\[ \left. - \left( 2I^n + \frac{k_{n-1}}{k_n} I^n - \pi^n \right) (-\Delta^{n-1}) U^{n-1} + \pi^n I^{n-1} (-\Delta^{n-2}) U^{n-2} \right]. \] (2.43)

### 2.4. Error estimate based on residual estimators

Using residual-based estimators estimating the spatial finite element errors we can conclude to the final error estimate for the modified Crank–Nicolson–Galerkin scheme. To this end we shall need the following definition. For functions defined in a piecewise sense we use the notation
\[ \| h^n_E (\Delta - \Delta^n) U^n \|_{T^n}^2 = \sum_{k \in T^n} \| h_k^n (\Delta - \Delta^n) U^n \|_k^2 \quad \text{and} \quad \| h^{3/2}_n J[\nabla U^n] \|_{\Sigma_n}^2 = \sum_{e \in \Sigma_n} \| h^{3/2}_n J[\nabla U^n] \|_e^2. \]

**Definition 2.3 ($L^\infty(L^2)$ error estimators).** Let $c_1$, $c_{i,j}$ be appropriate constants appearing in Clément type interpolation estimates. For $C_E$ being the elliptic regularity constant
\[ |\nabla|_2 \leq C_E \| \Delta v \|, \quad v \in H^2(\Omega) \cap H_0^1(\Omega), \]
we denote
\[ C_{j,2} = C_E c_{j,2}. \]
For $n = 1, \ldots, N$, we define: The **elliptic reconstruction error estimator** appearing in definition of both two- and three-point estimators
\[ \varepsilon_n = C_{1,2} \| h^n_E (\Delta - \Delta^n) U^n \|_{T^n} + C_{2,2} \| h^{3/2}_n J[\nabla U^n] \|_{\Sigma_n}, \] (2.44)
Let $\hat{h}_n := \max(h_n, h_{n-1})$: the **space-mesh error estimator** that appears also in both two- and three-point estimators
\[ \gamma_n = C_{1,2} \| h^n_E k^{-1}_n (\Delta - \Delta^n) U^n - k^{-1}_n (\Delta - \Delta^{n-1}) U^{n-1} \|_{T^n} \]
\[ + C_{2,2} \| h^{3/2}_n J[\nabla U^n - \nabla U^{n-1}] \|_{\Sigma_n} + C_{3,2} \| h^{3/2}_n J[\nabla U^n - \nabla U^{n-1}] \|_{\Sigma_n \setminus \Sigma_n}. \] (2.45)
Let $w_n$ and $\tilde{w}_n$ be as in Lemmas 2.2 and 2.3, respectively. We define the **time reconstruction error estimator** that corresponds to the two-point reconstruction by
\[ \delta_n := \frac{k^2}{4} \left( \| w_n \| + C_{1,2} \| h^n_E (\Delta - \Delta^n) w_n \|_{T^n} + C_{2,2} \| h^{3/2}_n J[\nabla w_n] \|_{\Sigma_n} \right), \] (2.46)
and to the three-point reconstruction by
\[
\delta_n := \frac{k_n^2}{4} \left( \| \tilde{w}_n \| + C_{1.2} \| h_n^2 (\Delta - \Delta^n) \tilde{w}_n \|_{\mathcal{F}_n} + C_{2.2} \| h_n^{3/2} J[\nabla \tilde{w}_n] \|_{\Sigma_n} \right).
\]

Further we define: The space error estimator corresponding to the two-point reconstruction
\[
\eta_n := k_n \left( C_{1.2} \| h_n^2 (\Delta - \Delta^n) w_n \|_{\mathcal{F}_n} + C_{2.2} \| h_n^{3/2} J[\nabla w_n] \|_{\Sigma_n} \right),
\]
and to the three-point reconstruction
\[
\tilde{\eta}_n := k_n \left( C_{1.2} \| h_n^2 (\Delta - \Delta^n) \tilde{w}_n \|_{\mathcal{F}_n} + C_{2.2} \| h_n^{3/2} J[\nabla \tilde{w}_n] \|_{\Sigma_n} \right).
\]
The time error estimator in case of the two-point reconstruction
\[
\theta_n := \frac{k_n^2}{30} \left( C_{1.1} \| w_n \| + C_{1.1} \| h_n (\Delta^n) w_n \| \right),
\]
and in case of three-point reconstruction
\[
\tilde{\theta}_n := \frac{k_n^2}{30} \left( C_{1.1} \| \tilde{w}_n \| + C_{1.1} \| h_n (\Delta^n) \tilde{w}_n \| \right).
\]
The coarsening error estimator
\[
\beta_n := \left\| (P^n - I)(-\Delta^{n-1})U^{n-1} \right\| + \left\| (P^n - I)k_n^{-1}U^{n-1} \right\|,
\]
and the data approximation estimators
\[
\xi_{n,1} := \frac{1}{k_n} \int_{t^{n-1}}^{t^n} \| f(s) - \varphi(s) \| \, ds,
\]
\[
\xi_{n,2} := 2C_{1.1} \max \left\{ \| h_n(I - P_0^n)f^{n-1} \|, \| h_n(I - P_0^n)f^{-1/2} \| \right\}
\]
and
\[
\xi_{n,1} := \frac{1}{k_n} \int_{t^{n-1}}^{t^n} \| f(s) - \tilde{\varphi}(s) \| \, ds.
\]
In case of the three-point estimator the following additional estimator appears
\[
\tilde{\xi}_n := \frac{k_n}{4(k_n + k_{n-1})} \left( k_{n-1} (\Delta^n) U^n - \left( \frac{2k_n + k_{n-1}}{k_n} P^n - \pi^n \right) (\Delta^{n-1}) U^{n-1} + \pi^n P^n U^{n-1} (\Delta^{n-2}) U^{n-2} \right).
\]
The a posteriori bounds are summarized in the following theorem.

**Theorem 2.2 (Complete $L^\infty(L^2)$ a posteriori error estimates).** For the reconstruction defined in Section 2.3 and for $m = 1, \ldots, N$, the following two level estimate holds
\[
\max_{t \in [0, t^m]} \| u(t) - U(t) \| \leq \sqrt{2} \| u^0 - R^0 u^0 \| + \left( 2 \sum_{n=1}^{m} k_n \delta_n^2 \right)^{1/2} + \left( \varepsilon_{m,1}^2 + \varepsilon_{m,2}^2 \right)^{1/2} + \max_{0 \leq n \leq m} \delta_n + \max_{0 \leq n \leq m} \varepsilon_n,
\]
where
\[
\varepsilon_{m,1} := \sum_{n=1}^{m} k_n \left( \eta_n + \gamma_n + \beta_n + \xi_{n,1} \right), \quad \varepsilon_{m,2} := \left( \sum_{n=1}^{m} k_n \xi_{n,2}^2 \right)^{1/2}.
\]
Alternatively, if we use the reconstruction defined in Section 2.4 the following three level estimate holds for $m = 1, \ldots, N$,
\[
\max_{t \in [0, t^m]} \| u(t) - U(t) \| \leq \sqrt{2} \| u^0 - R^0 u^0 \| + \left( 2 \sum_{n=1}^{m} k_n \delta_n^2 \right)^{1/2} + \tilde{\varepsilon}_{m,1} + \max_{0 \leq n \leq m} \tilde{\delta}_n + \max_{0 \leq n \leq m} \varepsilon_n,
\]
where
\[
\tilde{\varepsilon}_{m,1} := \sum_{n=1}^{m} k_n (\tilde{\eta}_n + \gamma_n + \beta_n + \tilde{\xi}_{n,1} + \tilde{\delta}_n).
\]
The proof of the theorem uses Theorem 2.1. For completeness, in the rest of the section we present the basic steps taken in [6] to prove Theorem 2.2. We consider the case of the two point estimator only here. Thus one can associate the estimators appearing in Theorem 2.2 (and thus in Definition 2.3) to the bounds in Theorem 2.1. For the complete analysis we refer to [6].

2.4.1. Elliptic estimators

Using approximation properties of the Clément-type interpolants it can be proved by applying standard techniques in a posteriori error analysis for elliptic problems, cf., e.g., [20], the following estimate for the elliptic reconstruction error.

**Lemma 2.4.** For any \( \varphi_n \in \mathbb{V}^n \) there holds

\[
\| (R^n - I) \varphi_n \| \leq C_{1.2} h_n^2 (\Delta - \Delta^n) \varphi_n \| \mathcal{J}_n + C_{2.2} h_n^{3/2} J [\nabla \varphi_n] \Sigma_n. \tag{2.60}
\]

In particular for \( m = 1, \ldots, N \), the following estimate holds

\[
\max_{t \in [0,tn^{\text{end}}]} \| \epsilon(t) \| \leq \max_{0 \leq n \leq m} \epsilon_n. \tag{2.61}
\]

2.4.2. Main time estimator

The main time reconstruction error is due to \( \sigma \). Its estimate is based on the expression

\[
\sigma(t) = \dot{U}(t) - \omega(t) = (t - t^{n-1})(t^n - t)R^n w_n, \quad t \in I_n. \tag{2.62}
\]

Then,

\[
\max_{t \in [0,tn^{\text{end}}]} \| \sigma(t) \| \leq \max_{1 \leq n \leq m} \delta_n. \tag{2.63}
\]

The proof hinges on

\[
\| \sigma(t) \| \leq |(t - t^{n-1})(t^n - t)\| (R^n - I) w_n \| + \| w_n \|. \tag{2.64}
\]

Next, one can bound the similar term \( \mathcal{J}_n^T \) in Theorem 2.1 by first noticing

\[
|\sigma(t)|^2 = a(\sigma(t), \sigma(t)) = (t - t^{n-1})(t^n - t)a(R^n w_n, \sigma(t)). \tag{2.65}
\]

One can conclude in this case that

\[
\mathcal{J}_n^T \leq k_n \delta_n^2. \tag{2.66}
\]

2.4.3. Spatial error estimate

In order to estimate the term \( \mathcal{J}_n^{S.1} \) in Theorem 2.1, which accounts for the space discretization error, we use (2.60) and the expression for \( IF(t) - F^{n-1/2} \) to obtain

\[
\mathcal{J}_n^{S.1} \leq C_k \max_{s \in [0,tn^{\text{end}}]} \| \hat{\rho}(s) \| \eta_n. \tag{2.67}
\]

2.4.4. Space estimator accounting for mesh changing

The estimate of the term \( \mathcal{J}_n^{S.2} \) in Theorem 2.1 is based on the orthogonality properties of \( R_n - R_{n-1} \) on \( \mathbb{V}^{n-1} \cap \mathbb{V}^n \). The final estimate in this case is

\[
\mathcal{J}_n^{S.2} \leq k_n \max_{t \in [0,tn^{\text{end}}]} \| \hat{\rho}(t) \| \gamma_n. \tag{2.68}
\]

2.4.5. Coarsening error estimate

The term \( \mathcal{J}_n^C \) in Theorem 2.1 can be obviously bounded as follows

\[
\mathcal{J}_n^C \leq k_n \max_{t \in [0,tn^{\text{end}}]} \| \hat{\rho}(t) \| \beta_n. \tag{2.69}
\]
2.4.6. Estimation of the term $J_n^D$

This term can be written as

$$J_n^D = \int_{t_{n-1}}^{t_n} \left\| \left( f(s) - P_0^n \Psi(s), \dot{\rho}(t) \right) \right\| ds,$$

(2.70)

and it can be estimated

$$J_n^D \leq k_n \max_{0 \leq t \leq t_n} \left\| \dot{\rho}(t) \right\| \xi_{n,1} + k_n^{1/2} \xi_{n,2} \left( \int_{t_{n-1}}^{t_n} |\dot{\rho}(s)|^2 \right)^{1/2}.$$

(2.71)

3. Behavior of the estimators

In this section we study the behavior of the error estimators. In particular, we start with the influence of the non-smooth initial data on the error indicators and compare this influence with the known non-smooth data effects of the Crank–Nicolson method (Section 3.1). Next, we study the asymptotic behavior of the error estimators of Section 2 and compare this behavior with the true error on four model problems, where the one of them is chosen such that the right-hand side $f$ to satisfy non-zero boundary conditions (Section 3.2). Finally, we investigate how refinement can influence the a posteriori error estimators. In particular we consider a computational case study where refinement occurs at a given time level and compare the behavior of the estimators (Section 3.3). All the error estimators were implemented in a C code that uses the adaptive finite element library ALBERTA [18].

For our purpose, we consider the heat equation (1.1) on the unit square, $\Omega = [0, 1]^2$, and $T = 1$ and the exact solution $u$ be one of the following:

- case (1): $u(x, y, t) = \sin(\pi t) \sin(\pi x) \sin(\pi y)$;
- case (2): $u(x, y, t) = \sin(15\pi t) \sin(\pi x) \sin(\pi y)$ (fast in time);
- case (3): $u(x, y, t) = \sin(0.5\pi t) \sin(10\pi x) \sin(10\pi y)$ (fast in space).

In addition we consider the following tests

- case (4): $u(x, y, t) = \sin(\pi t)(x^4 - 2x^3 + x^2)(4y^3 - 6y^2 + 2y)$ ($u_0 = 0$, $f \neq 0$ on $\partial \Omega$);
- case (5): $u(x, y, t) = \exp(-2\pi^2 t) \sin(\pi t) \sin(\pi x) \sin(\pi y)$ ($u_0(x, y) = \sin(\pi x) \sin(\pi y)$, $f = 0$).

The right-hand side $f$ of each problem is calculated by applying the pde to the corresponding $u$. Note that in cases (1) and (4) the error is due to both space and time discretization, in cases (2) and (5) the error comes mainly from the time discretization and in case (3) mainly from the space discretization. The initial conditions vanish in the first four cases and is $\sin(\pi t) \sin(\pi y)$ in the last. Finally, in cases (1), (2), (3) and (5) the right-hand side $f$ is equal to zero on $\partial \Omega$ and in case (4) $f$ satisfies non-zero boundary conditions.

3.1. Practical implementation of the estimators

As we mentioned, we used the finite element library ALBERTA for the computations. In ALBERTA, the sequence of the triangulations is constructed as follows: An initial triangulation of the domain is given (macro triangulation); based on an appropriate procedure which assures mesh conformity and conserves shape regularity, some simplexes are first refined by bisection and, after several refinements, some other simplexes may be coarsened. The mesh is represented as a binary tree whose nodes represent the simplexes. The children of each simplex (parent) are the two sub-simplexes obtained by bisection. During coarsening the children of a simplex are coarsened to get their parent. The leaves of the tree represent the simplexes of the current mesh.

In this paragraph we shall shortly describe a practical implementation of the parts of the estimators which involve finite element functions corresponding to two successive meshes $T_{n-1}$ and $T_n$. Let $\tilde{T}_n$ be the finest intermediate triangulation between $T_{n-1}$ and $T_n$, that is

$$T_{n-1} \xrightarrow{\text{refine}} \cdots \xrightarrow{\text{refine}} \tilde{T}_n \xrightarrow{\text{coarsen}} \cdots \xrightarrow{\text{coarsen}} T_n$$

(3.1)

(note that if the new mesh $T_n$ has been generated using non-nested refinement the implementation is more involved).

We shall first describe how inner products of the form

$$\langle W_{n-1}, W_n \rangle, \quad W_{n-1} \in \mathbb{V}^{n-1}, \quad W_n \in \mathbb{V}^n$$

(3.2)

can be computed exactly. We note that, when the grid is only refined, that means $\mathbb{V}^{n-1} \subset \mathbb{V}^n$, the expression (3.2) can be calculated exactly on the new grid, since $w_{n-1}$ belongs also to $\mathbb{V}^n$. Thus, no information during refinement is lost. On the
other hand, when $T_n$ comes only from coarsening of $T_{n-1}$, information is usually lost, since $w_{n-1}$ cannot be represented exactly on the coarsest mesh $T_n$. However, also in that case, we can calculate expression (3.2) exactly by working as follows: Let $\{\psi_j\}$ be the basis functions of $V^{n-1}$ and $\{\phi^n_i\}$ be the basis function of $V^n$. We can compute expressions of the form $\langle w_{n-1}, \psi_j \rangle$ exactly on the finest grid $T_{n-1}$, and then, by using the representation of the basis functions $\{\psi_j\}$ by the basis functions $\{\phi^n_i\}$, the data can be transformed during coarsening (from the children to their parent) such that $\langle w_{n-1}, \phi^n_i \rangle$ is calculated also exactly. If

$$w_n = \sum_{i=1}^{N} \alpha_i \phi^n_i$$

(3.3)

is the representation of $w_n$ in terms of the basis $\{\phi^n_i\}$, then we have

$$\langle w_{n-1}, w_n \rangle = \sum_i \alpha_i \langle w_{n-1}, \phi^n_i \rangle,$$

(3.4)

and this computation is exact. Notice that the coefficients in coarsening are exactly the ones appearing in the representation of functions with respect to the “hierarchical basis”, see [22]. In general case when $T_n$ comes from both refinement and coarsening of $T_{n-1}$, we may work as follows: Let $\{\tilde{\psi}_j\}$ be any basis of the finite element space $V^n$ with respect to $T_n$. We compute $\langle w_{n-1}, \tilde{\psi}_j \rangle$ for all basis functions $\tilde{\psi}_j \in V^n$, on the finest grid $T_n$, and then continue as described above in case of coarsening. We proceed with the exact computation of quantities of the form

$$\| w_{n-1} - w_n \|_{T_{n-1} \cup T_n}, \quad w_{n-1} \in V^{n-1}, \quad w_n \in V^n.$$

(3.5)

By applying the Pythagorean Theorem, we obtain that

$$\| w_{n-1} - w_n \|_{T_{n-1} \cup T_n}^2 = \| w_{n-1} \|_{T_{n-1} \cup T_n}^2 + \| w_n \|_{T_{n-1} \cup T_n}^2 - 2 \langle w_{n-1}, w_n \rangle_{T_{n-1} \cup T_n}.$$

(3.6)

The first term on the right-hand side is calculated on the intermediate grid $\tilde{T}_n$ and the result is transformed during coarsening in such a way that no information is lost. The second term is computed after refinement and coarsening on the new mesh $T_n$. For the exact calculation of the last term we proceed as described above.

3.2. Data effects

In this section, we shall study the behavior of the estimators in case of non-zero initial data $u_0$. Since the Crank–Nicolson method requires further regularity assumptions on the data in order to be second order accurate, [14,19], we are interested in studying the influence of the smoothness of the data on the error estimators. Here we refer to the smoothness of the discrete approximations of $u^n$ and not on the smoothness of $u^0$ per se. Indeed we distinguish three cases for starting the fully discrete scheme. The first is the “non-smooth” choice. The last which is the “smoothest” choice was suggested already in [14] as a remedy for CN scheme to have the smoothing property and hence to be second order accurate even with $L^2$ data. In particular the initial approximation $U^0$ is chosen to be

- the interpolant $I^0 u^0$ of the initial data $u^0$;
- the elliptic projection $P^0_I u^0$ of $u^0$, namely the solution of the system

$$a(P^0_I u^0, \phi) = \langle -\Delta u^0, \phi \rangle, \quad \forall \phi \in V^0;$$

(3.7)

- the approximation given by performing two steps of the Backward Euler with the half time-step.

Following the analysis in [19] for the Crank–Nicolson method applying to linear parabolic equations with non-smooth data, we shall next study the behavior of $w_n$ and $\tilde{w}_n$, which appear in the definitions of the error estimators, in case of uniform time meshes. In parallel we show the computational behavior of these terms for the test problem (5) which are in agreement to the different behavior found in the spectral bounds of these terms, in this section the spaces $V^n = V_h$ remain the same for all $n$ and $-\Delta_h = -\Delta^h$ is the corresponding discrete Laplacian, see Definition 1.1.

We consider the homogeneous heat equation with $u^0 \neq 0$. Let $(\lambda_j^h)_{j=1}^N$ be the eigenvalues of the discrete Laplacian $-\Delta_h$ and $(e_j^h)_{j=1}^N$ be a corresponding basis of orthonormal eigenvectors. Then, any function $v \in V^0 = V_h$ can be written as

$$v = \sum_{j=1}^{N} \langle v, e_j^h \rangle e_j^h.$$

(3.8)

The approximate solution $U^n$ may be written in the recursive form

$$U^n = r_1 (k(-\Delta_h)) U^{n-1},$$

(3.9)
where \( r_1 \) is the rational function appearing in the Crank–Nicolson method,
\[
r_1(\lambda) := \frac{1 - \lambda}{1 + \frac{k}{2}},
\]
(3.10)

It is easily seen that
\[
\sup_{\lambda \in \sigma(-k\Delta h)} |r_1(\lambda)| \leq 1 \quad \text{and} \quad \lim_{\lambda \to +\infty} |r_1(\lambda)| = 1.
\]
(3.11)

According to (3.32), we have
\[
w_n = \frac{1}{2k} \left( (-\Delta h)U^n - (-\Delta h)U^{n-1} \right) = \frac{1}{2k} (-\Delta h)r_1(-k\Delta h)^{n-1}(r_1(-k\Delta h) - 1)U^0.
\]
(3.12)

Hence, \( w_n \) can be written in the following spectral representation form [19],
\[
w_n = \frac{1}{2k} \sum_{j=1}^{N} \lambda_j r_1(k\lambda_j)^{n-1} (r_1(k\lambda_j) - 1)U^0, e_j e_j.
\]
(3.13)

Similarly, we have
\[
\tilde{w}_n = \frac{1}{2k} \sum_{j=1}^{N} r_1(k\lambda_j)^{n-2} (r_1(k\lambda_j) - 1)^2 U^0, e_j e_j.
\]
(3.14)

The following spectral bounds for \( w_n, \tilde{w}_n \) as well as the associated numerical experiments serve the purpose of comparing the effect of the three different choices for the initial approximations. In particular we provide spectral bounds for the quantities
\[
\|w_n\|, \quad \|h(-\Delta h)w_n\| \quad \text{and} \quad \|\tilde{w}_n\|, \quad \|h(-\Delta h)\tilde{w}_n\|.
\]

We observe that in the last (“smoothest”) case 3.2.3 for the initial data, the undesirable term \( \lambda_{\max} \) term is not present in the spectral bounds of all the above terms. In addition, the computations show that they decay fast with \( t \), see Figs. 6, 7. This, however, is not the case in the “non-smooth” case 3.2.1. We can conclude that the discrete regularity of data, which affects the order of convergence of the Crank–Nicolson method, affects also the behavior of the estimators. Further, when comparing \( w_n \) to \( \tilde{w}_n \) in all cases below, it follows that the three point estimator is less sensitive to the discrete smoothness of the data. A fact which is reflected in the spectral estimates, in the way which the undesirable term \( \lambda_{\max} \) appears and in the computations by checking whether or not the above terms decay with \( t \), compare Figs. 2–7. We conclude therefore that the three point estimator shows a more robust behavior with respect to this criterion, which, we believe, partially explains its better behavior under refinement observed in Section 3.4. At the end of the paragraph we provide an additional argument for this purpose by expressing both \( w_n \) and \( \tilde{w}_n \) in a comparable form. It turns out that \( \tilde{w}_n \) contains an additional “Backward Euler” smoothing step compared to \( w_n \).

### 3.2.1. Starting with \( U^0 = I^0 u^0 \)

Two-point estimator. In view of Parseval’s identity and (3.13), we get
\[
\|w_n\|^2 = \frac{1}{4k^2} \sum_{j=1}^{N} \lambda_j r_1(k\lambda_j)^{n-1} (r_1(k\lambda_j) - 1)\|I^0 u^0, e_j\|^2.
\]
(3.15)
Fig. 3. Test problem of case (5) \((u_0 \neq 0 \text{ and } f = 0)\) and \(U^0 = P^0_1 u_0\). The non-smooth initial data influences the behavior of \(\|h(-\Delta_h)\tilde{w}_n\|\) and \(\|\nabla \tilde{w}_n\|\), which are included in the definition of the three-point estimator.

Fig. 4. Test problem of case (5) \((u_0 \neq 0 \text{ and } f = 0)\) and \(U^0 = P^0_1 u_0\): Compared to Fig. 2, we can observe an improvement on the results. The quantity \(\|w_n\|\) decreases with respect to time as \(Ce^{-2\pi^2 t}\). Moreover, the quantities \(\|w_n\|, |w_n|, |h(-\Delta_h)w_n|\) show a similar behavior compared to the quantities \(\|\tilde{w}_n\|, |\tilde{w}_n|, \|h(-\Delta_h)\tilde{w}_n\|\) in Fig. 3.

Fig. 5. Test problem of case (5) \((u_0 \neq 0 \text{ and } f = 0)\) and \(U^0 = P^0_1 u_0\): Compared to Fig. 3, we can notice an improvement on the results. The norms \(\|w_n\|\) and \(|w_n|\) decrease with respect to time as \(Ce^{-2\pi^2 t}\).

Fig. 6. Test problem of case (5) \((u_0 \neq 0 \text{ and } f = 0)\) and starting with Backward Euler: Compared to Fig. 2 and Fig. 4, the norms \(\|w_n\|, |w_n|\) and \(\|h(-\Delta_h)w_n\|\) decrease with respect to time as \(Ce^{-2\pi^2 t}\).
Fig. 7. Test problem of case (5) \((u_0 \neq 0 \text{ and } f = 0)\) and starting with Backward Euler: the norms \(\|\tilde{w}_n\|, |\tilde{w}_n|_1\), and \(\|h(-\Delta h)\tilde{w}_n\|\), decrease with respect to time as \(Ce^{-2\pi^2 t}\).


given, we obtain

\[
\|w_n\| \leq \frac{1}{2k^2} \sup_{\lambda_j \in \sigma(-\Delta h)} |(k\lambda_j)r_1(k\lambda_j)^{n-1}(r_1(k\lambda_j) - 1)| \|I^0u_0\|.
\]

(3.16)

where

\[
|(k\lambda_j)r_1(k\lambda_j)^{n-1}(r_1(k\lambda_j) - 1)| \leq 2k\lambda_{\text{max}}.
\]

Hence,

\[
\|w_n\| \leq \frac{k\lambda_{\text{max}}}{k^2} \|I^0u_0\|.
\]

(3.17)

3.2.1.1. Three-point estimator  
According to Parseval’s relation and (3.14), it follows that

\[
\|\tilde{w}_n\| \leq \frac{1}{k^2} \sup_{\lambda_j \in \sigma(-\Delta h)} r_1(k\lambda_j)^{n-2}(r_1(k\lambda_j) - 1)^2 \|I^0u_0\|.
\]

(3.18)

But,

\[
|r_1(k\lambda_j)^{n-2}(r_1(k\lambda_j) - 1)^2| \leq 4.
\]

Hence,

\[
\|\tilde{w}_n\| \leq \frac{4}{k^2} \|I^0u_0\|.
\]

(3.19)

On the other hand, we have

\[
\|h(-\Delta h)\tilde{w}_n\|^2 = \frac{h}{k^2} \sum_{j=1}^N |\lambda_jr_1(k\lambda_j)^{n-2}(r_1(k\lambda_j) - 1)^2 \langle I^0u_0, e_j \rangle |^2,
\]

(3.20)

and

\[
|(k\lambda_j)r_1(k\lambda_j)^{n-2}(r_1(k\lambda_j) - 1)^2| \leq 4k\lambda_{\text{max}}.
\]

Thus, we have

\[
\|h(-\Delta h)\tilde{w}_n\| \leq \frac{4h\lambda_{\text{max}}}{k^2} \|I^0u_0\|.
\]

(3.21)

Hence, \(\lambda_{\text{max}}\) is present in (3.21) although not in (3.19). In the “smoother” case 3.2.2 below \(\lambda_{\text{max}}\) is not present even in the bound of \(\|h(-\Delta h)\tilde{w}_n\|\).

3.2.2. Starting with \(U^0 = P_1^0u_0\)

Next, we consider the case of the elliptic projection, namely we choose \(U^0 = P_1^0u_0\).
Thus, hence, \(3.2.2.2.\) **Three-point estimator**

Since
\[
(-\Delta u^0, \varphi) = (\nabla P^0_1u^0, \nabla \varphi) = (-\Delta h P^0_1u^0, \varphi)
\]
for all \(\varphi \in V^0\),

the discrete function \(w_n\) appearing in the definition of the two-point estimator may now be written as follows
\[
w_n = \frac{1}{2k} (-\Delta h) r_1 (-k\Delta h)^{n-1} (r_1 (-k\Delta h) - 1) (-\Delta h)^{-1} P^0_0 \Delta u^0.
\]
(3.22)

The Parseval relation implies
\[
\|w_n\|^2 = \frac{1}{4k^2} \sum_{j=1}^{N} |r_1(k\lambda_j)^{n-1} (r_1(k\lambda_j) - 1) (P^0_0 \Delta u^0, e_j)|^2.
\]

Thus it follows
\[
\|w_n\| \leq \frac{1}{2k} \sup_{\lambda_j \in \sigma(-\Delta h)} |r_1(k\lambda_j)^{n-1} (r_1(k\lambda_j) - 1)| \|P^0_0 \Delta u^0\|.
\]
where
\[
|r_1(k\lambda_j)^{n-1} (r_1(k\lambda_j) - 1)| \leq 2.
\]

Hence,
\[
\|w_n\| \leq \frac{1}{k} \|P^0_0 \Delta u^0\|.
\]
(3.23)

In addition, we have
\[
\|h(-\Delta h) w_n\|^2 = \frac{h^2}{4k^2} \sum_{j=1}^{N} (k\lambda_j)^2 (k\lambda_j)^{n-1} (r_1(k\lambda_j) - 1) (P^0_0 \Delta u^0, e_j)|^2.
\]

Now,
\[
|k\lambda_j r_1(k\lambda_j)^{n-1} (r_1(k\lambda_j) - 1)| \leq 2k\lambda_{max}.
\]

Therefore,
\[
\|h(-\Delta h) w_n\| \leq \frac{h\lambda_{max}}{k} \|P^0_0 \Delta u^0\|.
\]

**3.2.2.2. Three-point estimator** In this case, in view of Parseval's identity and (3.14), we obtain
\[
\|\tilde{w}_n\| \leq \frac{1}{k} \sup_{\lambda_j \in \sigma(-\Delta h)} |r_1(k\lambda_j)^{n-2} (r_1(k\lambda_j) - 1)^2 (k\lambda_j)^{-1}| \|P^0_0 \Delta u^0\|.
\]
(3.24)

with
\[
|r_1(k\lambda_j)^{n-2} (r_1(k\lambda_j) - 1)^2 (k\lambda_j)^{-1}| \leq 4.
\]

Hence,
\[
\|\tilde{w}_n\| \leq \frac{4}{k} \|P^0_0 \Delta u^0\|.
\]
(3.25)

On the other hand, we have
\[
\|h(-\Delta h) \tilde{w}_n\|^2 = \frac{h^2}{k^2} \sum_{j=1}^{N} \lambda_j (k\lambda_j)^{n-2} (r_1(k\lambda_j) - 1)^2 \lambda_j^{-1} (P^0_0 \Delta u^0, e_j)|^2,
\]
and
\[
|r_1(k\lambda_j)^{n-2} (r_1(k\lambda_j) - 1)^2| \leq 4.
\]
Thus,
\[
\|h(-\Delta h) \tilde{w}_n\| \leq \frac{4h}{k^2} \|P^0_0 \Delta u^0\|.
\]
(3.26)
3.2.3. Starting with two steps of Backward Euler method

3.2.3.1. Two-point estimator In the case where we start the Crank–Nicolson method by first performing two steps of Backward Euler with the half time-step, the discrete function $w_n$ is written

$$w_n = (-\Delta h) r_1 (-k\Delta h)^{n-2} (r_1 (-k\Delta h) - l) r_0 \left(-\frac{k}{2} \Delta h\right)^2 l^0 u^0,$$

(3.27)

where $r_0$ is the rational function of the Backward Euler method,

$$r_0(\lambda) := \frac{1}{1 + \lambda}.$$

(3.28)

By Parseval’s relation, we obtain

$$\|w_n\| \lesssim \frac{1}{2k^2} \sup_{\lambda_j \in \sigma(-\Delta h)} \left| (k\lambda_j) r_1 (k\lambda_j)^{n-2} (r_1 (k\lambda_j) - 1) r_0 \left(\frac{k}{2} \lambda_j\right)^2 \right| \|l^0 u^0\|,$$

where

$$\left| (k\lambda_j) r_1 (k\lambda_j)^{n-2} (r_1 (k\lambda_j) - 1) r_0 \left(\frac{k}{2} \lambda_j\right)^2 \right| \leq 4.$$

In addition, we have

$$\|h(-\Delta h) w_n\|^2 = \frac{h^2}{4k^6} \sum_{j=1}^{N} \left( (k\lambda_j)^2 r_1 (k\lambda_j)^{n-2} (r_1 (k\lambda_j) - 1) r_0 \left(\frac{k}{2} \lambda_j\right)^2 \right) \|l^0 u^0, e_j\|^2.$$

Now

$$\left| (k\lambda_j)^2 r_1 (k\lambda_j)^{n-2} (r_1 (k\lambda_j) - 1) r_0 \left(\frac{k}{2} \lambda_j\right)^2 \right| \leq 8.$$

Thus,

$$\|h(-\Delta h) w_n\| \lesssim \frac{h}{2k^3} \|l^0 u^0\|.$$

(3.29)
Fig. 9. Test problem of case (1). On first and third row we plot the logs of each quantity and below the corresponding EOC. The elliptic reconstruction estimator \( \max_n \delta_n \) and the space-mesh estimator \( \sum_n k_n \gamma_n \) decrease with second order. Both the time reconstruction estimators \( \max_n \delta_n \), \( \max_n \tilde{\delta}_n \) and both the time estimators \( \left( \sum_n k_n \theta^2_n \right)^{1/2} \), \( \left( \sum_n k_n \tilde{\theta}^2_n \right)^{1/2} \), are of optimal order. The space estimator \( \sum_n k_n \eta_n \) is of second order, while \( \sum_n k_n \tilde{\eta}_n \) superconverges.

3.2.3.2. Three-point estimator  Similarly, we get

\[
\| \tilde{\bar{w}}_n \| \leq \frac{1}{k^2} \sup_{\lambda_j \in \sigma(\Delta_h)} \left| r_1(k^2 \lambda_j)^{n-3} \left( r_1(k^2 \lambda_j) - 1 \right)^2 \left( \frac{k\lambda_j}{2} \right)^2 \right| \| L^0 u^0 \| \leq \frac{4}{k^2} \| L^0 u^0 \|. \tag{3.30}
\]

since

\[
\left| r_1(k^2 \lambda_j)^{n-3} \left( r_1(k^2 \lambda_j) - 1 \right)^2 \left( \frac{k\lambda_j}{2} \right)^2 \right| \leq 4.
\]

Finally,
Fig. 10. Test problem of case (1). The last part of the three-point estimator, which we can see here, decreases also with optimal order with respect to both time and spatial variables.

Fig. 11. Numerical results for the problem with exact solution the one of case (2). On top we plot the logs of the errors and the estimators and below their EOC or the effectivity index. We observe that the $L^\infty(L^2)$ error is $O(h^2 + k^2)$, the $L^2(H^1)$ error is $O(h + k^2)$. See Figs. 12 and 13 to verify that both the estimators decrease with second order with respect to time and space.

$$\|h(-\Delta_h)\hat{w}_n\|^2 = \frac{h^2}{K^{\delta}} \sum_{j=1}^{N} \left| k\lambda_j r_1(k\lambda_j)^{n-2}(r_1(k\lambda_j) - 1)^2 r_0 \left( \frac{k\lambda_j}{2} \right)^2 \langle I_0 u_0, e_j \rangle \right|^2,$$

and

$$\left| (k\lambda_j)r_1(k\lambda_j)^{n-2}(r_1(k\lambda_j) - 1)^2 r_0 \left( \frac{k\lambda_j}{2} \right)^2 \right| \leq 8.$$

Therefore

$$\|h(-\Delta_h)\hat{w}_n\| \leq \frac{8h}{K^\delta} \| I_0 u_0 \|. \quad (3.31)$$

3.2.4. Direct comparison of two and three-point estimators

We will use the recursive relation

$$U^n = r_1(k(-\Delta_h))U^{n-1},$$

and the definition of the scheme to directly compare $w_n$ and $\hat{w}_n$ in the case of constant time step and constant in time finite element mesh. Recall that
Fig. 12. Numerical results for the problem with exact solution the one of case (2) (fast in time). On the first and third rows we plot the logs of estimators and below them the corresponding EOCs. We observe that all the estimators decrease with at least second order with respect to time- and space-step. Moreover, in both cases the time error estimator and the time reconstruction dominate all other estimators. Again the space estimator $\sum k_n \tilde{\eta_n}$ superconverges.

\[
w_n = \frac{1}{2k} \left[ (\Delta h) U^n - (\Delta h) U^{n-1} \right]
\]

(3.32)

and

\[
\tilde{w}_n = \frac{1}{k^2} \left( U^n - 2U^{n-1} + U^{n-2} \right).
\]

(3.33)

Using the definition of the scheme, it turns out that

\[
\tilde{w}_n = - \frac{1}{2k} \left[ (\Delta h) U^n - (\Delta h) U^{n-2} \right].
\]

(3.34)
Fig. 13. Test problem of case (2); This part of the three-point estimator decreases also with optimal.

Fig. 14. Numerical results for the problem with exact solution the one of case (3) (fast in space). We observe that the $L^\infty(L^2)$ error is $O(h^2 + k^2)$, the $L^2(H^1)$ error is $O(h + k^2)$. As before all the estimators decrease with second order with respect to time and space (EOC for each estimator are not included).

Hence, modulo a constant factor the only difference between $w_n$ and $\tilde{w}_n$ is the fact that $w_n$ involves the difference $U^n - U^{n-1}$ while $\tilde{w}_n$ involves the difference $U^n - U^{n-2}$. It turns out that this exactly is the source of the smoother behavior of $\tilde{w}_n$ in certain cases. Indeed,

$$
\tilde{w}_n = -\frac{1}{2k}(-\Delta_h)r_1(-k\Delta_h)^{n-2}(r_1(-k\Delta_h)^2 - l)U^0 \\
= -\frac{1}{2k}(-\Delta_h)r_1(-k\Delta_h)^{n-2}(r_1(-k\Delta_h) - l)(r_1(-k\Delta_h) + l)U^0 \\
= -\frac{1}{k}(-\Delta_h)r_1(-k\Delta_h)^{n-2}(r_1(-k\Delta_h) - l)r_0\left(-\frac{k}{2}\Delta_h\right)U^0.
$$

(3.35)

Where we used the fact $r_1(\lambda) + 1 = 2r_0(\lambda/2)$, where $r_0$ is the rational function of the Backward Euler method $r_0(\lambda) = \frac{1}{\lambda+\tau}$. The corresponding expression for $w_n$ is

$$
w_n = \frac{1}{2k}(-\Delta_h)r_1(-k\Delta_h)^{n-1}(r_1(-k\Delta_h) - l)U^0.
$$

(3.36)

Therefore modulo a constant factor the main difference between $w_n$ and $\tilde{w}_n$ is that $\tilde{w}_n$ contains an additional “Backward Euler” smoothing step compared to $w_n$. 

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3.3. Experimental order of convergence (EOC)

In this section, we study the asymptotic behavior of the estimators. Since we are interested in understanding the asymptotic behavior of the estimators, we conduct tests on uniform meshes with uniform time steps. Linear Lagrange elements are used for the spatial discretization. The computed quantities here and in the next sections are:

- The error in the $L^\infty(0, t^m; L^2(\Omega))$ norm
  \[
  \max_{0 \leq n \leq m} \|e^n\| := \max_{0 \leq n \leq m} \|u(t^n) - U^n\|
  \]
  and the total error which is dominated by the $L^2(0, t^m; H^1(\Omega))$ error
  \[
  \epsilon_{\text{total}}(t^m) := \max_{0 \leq n \leq m} \left( \|e^n\|^2 + \sum_{n=1}^m k_n \|\nabla e^n\|^2 \right)^{1/2}.
  \]
- The elliptic reconstruction and the space-mesh error estimators:
  \[
  \max_{0 \leq n \leq m} \tilde{\epsilon}_n \quad \text{and} \quad \sum_{n=1}^m k_n \gamma_n.
  \]
- The time reconstruction error estimators:
  \[
  \max_{1 \leq n \leq m} \delta_n \quad \text{and} \quad \max_{0 \leq n \leq m} \tilde{\delta}_n.
  \]
- The space error estimators:
  \[
  \sum_{n=1}^m k_n \eta_n \quad \text{and} \quad \sum_{n=1}^m k_n \tilde{\eta}_n.
  \]
- The time error estimators:
  \[
  \left( \sum_{n=1}^m k_n \theta_n^2 \right)^{1/2} \quad \text{and} \quad \left( \sum_{n=1}^m k_n \tilde{\theta}_n^2 \right)^{1/2}.
  \]
Fig. 16. Test problem of case (4); On first and third rows we plot the logs of each quantity and below them the corresponding EOC. The elliptic reconstruction estimator $\max_n \delta_n$ and the space-mesh estimator $\sum_n k_n \gamma_n$ decrease with second order. Both the time reconstruction estimators $\max_n \tilde{\delta}_n$, $\max_n \tilde{\gamma}_n$ and both the time estimators $\left( \sum_n k_n \theta_n^2 \right)^{1/2}$, $\left( \sum_n k_n \tilde{\theta}_n^2 \right)^{1/2}$ are of optimal order. The space estimators $\sum_n k_n \eta_n$ and $\sum_n k_n \tilde{\eta}_n$ superconverge.

- The estimator appearing only in case of the three-point reconstruction:
  $$\sum_{n=1}^m k_n \tilde{\zeta}_n.$$
- The two-point estimator defined as
  $$E_m := \left( 2 \sum_{n=1}^m k_n \theta_n^2 \right)^{1/2} + 2 \sum_{n=1}^m k_n (\eta_n + \gamma_n) + \max_{0 \leq n \leq m} \delta_n + \max_{0 \leq n \leq m} \epsilon_n.$$
Fig. 17. Test problem of case (4): The last part of the three-point estimator, which we can see here, decreases also with optimal order with respect to both time and spatial variables.

Fig. 18. Test problem of case (5): We plot the EOCs of all the estimators in case that the starting value $U^0$ of the Crank–Nicolson method is chosen to be the approximation given by two-steps of Backward Euler. All the estimators decrease with optimal order.

and the three-point estimator defined as

$$\tilde{E}_m := \left( \frac{2 \sum_{n=1}^{m} k_n \tilde{e}_n^2}{2 \sum_{n=1}^{m} k_n^2 (\tilde{\eta}_n + \gamma_n + \tilde{\zeta}_n) + \sum_{0 \leq n \leq m} \delta_n + \max_{0 \leq n \leq m} \varepsilon_n} \right)^{1/2} + \sum_{n=1}^{m} k_n \tilde{e}_n.$$

- The corresponding effectivity indices defined as

$$E1(t^m) := \frac{\xi_m}{\varepsilon_{total}(t^m)} \quad \text{and} \quad \tilde{E}1(t^m) := \frac{\tilde{\xi}_m}{\varepsilon_{total}(t^m)}.$$

For quantities of interest we look at their experimental order of convergence (EOC). The EOC is defined as follows: for a given finite sequence of successive runs (indexed by $i$), the EOC of the corresponding sequence of quantities of interest $E(i)$ (estimator or part of an estimator), is itself a sequence defined by

$$\text{EOC}(E(i)) = \frac{\log(E(i+1)/E(i))}{\log(h(i+1)/h(i))}.$$

where $h(i)$ denotes the meshsize of the run $i$.

Each curve of the plots in Figs. 8–21 corresponds to a given run (or an EOC of a quantity of interest) performed with equal time and spatial mesh sizes. The most coarse grid, corresponds to $k = h = 0.125$ (curve with the largest error) and the finest grid corresponds to $k = h = 0.0078125$ (curve with the smallest error). The time and spatial mesh sizes are divided.
Fig. 19. Test problem of case (1). The space estimator $\sum_n k_n \tilde{\eta}_n$ corresponding to the three-point reconstruction jumps at the time level of refinement ($t = 0.125$). (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

by two while moving from the highest to the lowest curve. On odd rows of each figure we plot the logs of the errors and the estimators and below them the corresponding EOC. The values of EOC of a given estimator indicates its order.

Remark 3.1. By comparing the estimators $E_m$ and $\tilde{E}_m$ to the corresponding estimators in Theorem 2.2 we notice that in the computational experiments we do not include the estimators for data approximation (approximation of $u^0$ and $f$). It is clear however by standard estimates that these terms are of optimal order and thus do not contain interesting information for our purposes. In a real adaptive computation these terms should be included in the estimator since they might lead to specialized refinement. In addition, the coarsening error estimator $\beta_n$ is not included in the estimators $E_m$ and $\tilde{E}_m$ since in our experiments (same mesh or refinement) this term is zero. Indeed, in the case of refinement, Section 3.4, $\mathcal{V}^{m-1} \subset \mathcal{V}^m$, thus for $\varphi_{n-1} \in \mathcal{V}^{m-1}$, there holds $(1 - \Pi^n)\varphi_{n-1} = 0$ for any projection $\Pi^n$ into $\mathcal{V}^m$.

Since, the finite element spaces consist of linear Lagrange elements and the Crank-Nicolson method is second order accurate, the error in $L^\infty(0, T; L^2(\Omega))$ norm is $O(k^2 + h^2)$. The main conclusion of this paragraph is that all the error estimators, in both cases of time-reconstruction, decrease with optimal order with respect to time and spatial variable, Figs. 8–17. Notice that also in the forth problem where the right-hand side $f$ satisfies non-zero boundary condition, the error estimators decrease still with optimal order, Fig. 18.

3.4. Behavior of the estimators under refinement

We present here some numerical results regarding the error norms, the estimators and their EOC under mesh modification. To this end, we chose the most “harmless” mesh modification, namely refinement. More precisely, the following geometric refinement is performed: at time level $t = 0.125$, we mark each element $K$ with at least one of the coordinates of the barycenter $(x_K, y_K)$ less than 0.25 or greater than 0.75 to be refined, Figs. 19–21.
The time mesh-size remains constant in all of the experiments of this paragraph. Each curve of the plots corresponds to runs that start with equal time and spatial mesh sizes. The most coarse grid corresponds to $k = h = 0.03125$ (green color) and the finest grid corresponds to $k = h = 0.00039625$ (black color). The time and spatial mesh sizes are divided by two while moving from the highest to the lowest curve.

We observe that, when the exact solution of the heat equation is “fast” in the space variable, both the two- and three-point estimators jump under the refinement procedure described above (see Fig. 21). In particular, both space error estimators, $\sum_n k_n \eta_n$ and $\sum_n k_n \tilde{\eta}_n$, both time-estimators, $(\sum_n k_n \theta_n^2)^{1/2}$ and $(\sum_n k_n \tilde{\theta}_n^2)^{1/2}$, and both time reconstruction error estimators, $\max_n \delta_n$ and $\max_n \tilde{\delta}_n$, jump at the time level of refinement. Nevertheless the global three point estimator is only marginally affected. Notice that the previous mentioned estimators, and only them, depend on the discrete functions $w_n$ and $\tilde{w}_n$. In case that the exact solution of the problem changes faster in time, the influence of the given refinement on the behavior of the estimators is very small or non-existent (see Figs. 19 and 20).

4. Conclusions

In the present paper we have verified that CN is a sensitive scheme for diffusion problems when it is to be combined with self adjusted meshes. This sensitivity is related to mesh change with time, the behavior of the a posteriori error estimators as well as, as expected, its dependence on the smoothness of the data.

In Section 1 we have found that refinement can spoil Crank–Nicolson schemes and we have suggested a modified scheme which is natural and more robust with respect to mesh change. This finding is of particular interest since up to now refinement during mesh change was considered an error free procedure [12,18].

In Section 2 we have presented the main steps of the a posteriori analysis and the resulting error estimators; detailed analysis is presented in [6]. In Section 3 we have studied the behavior of the estimators from different perspectives. First, in
Section 3.1, with respect to the discrete smoothness of the data. It is well known that the Crank–Nicolson method requires further regularity assumptions on the data in order to be second order accurate, [14,19]. Our main conclusion is that the smoothness of the data can have significant affect on the behavior of the error estimators. Here we refer to the smoothness of the discrete approximations of $u_0$ and not on the smoothness of $u_0$ per se. Indeed we provide spectral arguments as well as computations to support this claim. We distinguish three cases for starting the fully discrete scheme: the interpolant (the “non-smooth” choice), the elliptic projection as well as the approximation given by performing two steps of the Backward Euler with the half time-step, [14]. We can conclude that the discrete regularity of data affects the behavior of the estimators. We have compared also the two and three point estimators with respect to this criterion. It follows that the three point estimator is less sensitive to the discrete smoothness of the data. A fact which is reflected in the spectral estimates in the way which the maximum eigenvalue of the discrete Laplacian appears.

At the end of the paragraph we provide an additional argument for this purpose by expressing the leading terms of the two point estimator $w_n$ and that of the three point estimator $\tilde{w}_n$ in a comparable form. It turns out that $\tilde{w}_n$ contains an additional “Backward Euler” smoothing step compared to $w_n$, a fact that explains this difference in the behavior. It is interesting to note that we have found that the only difference between these terms is the fact that $w_n$ involves the difference $U^n - U^{n-1}$ while $\tilde{w}_n$ involves the difference $U^n - U^{n-2}$. Hence, one may conclude that in a posteriori estimators equivalent terms in order corresponding to discrete derivatives are independent objects with possibly different behavior.

Next, we have presented detailed computational experiments which show that the a posteriori estimators are of optimal order and include terms capturing separately the spatial and the temporal errors.

Finally, in Section 3.4, we chose the most “harmless” mesh modification, namely refinement. We have presented a case study where refinement occurs at a given time level. We observe that, when the exact solution of the heat equation is “fast” in the space variable, both the two- and three-point estimators jump under the selected refinement procedure. Nevertheless
the global three point estimator is only marginally affected. Notice that the previous mentioned estimators, and only them, depend on the discrete functions \( w_n \) and \( w_{n+1} \). In case that the exact solution of the problem changes faster in time, the influence of the given refinement on the behavior of the estimators is very small or non-existent.

One may conclude that the mesh change procedure is in some way related to data effects discussed in Section 3.1. In this light, the smoother performance of the three point estimator observed in Section 3.4 is related to the comparison in Section 3.1.4. In addition, nonstandard projections in the step (1b) of the basic algorithm of Section 1, might be desirable since they may provide additional smoothness. This subtle issue requires further investigation.

Overall, at this point, we conclude that mesh modification should be used with great care when combined with Crank-Nicolson time discretization for diffusion problems. In addition, the a posteriori error control and the investigation of the behavior of higher order schemes than Backward Euler time discretization schemes for parabolic problems seems particularly interesting.

References