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Improved maximum-norm a posteriori error estimates for linear and semilinear parabolic equations

Dedicated to Prof. Hans-Görg Roos on the occasion of his 65th birthday

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Abstract Linear and semilinear second-order parabolic equations are considered. For these equations, we give a posteriori error estimates in the maximum norm that improve upon recent results in the literature. In particular it is shown that logarithmic dependence on the time step size can be eliminated.

Semidiscrete and fully discrete versions of the backward Euler and of the Crank-Nicolson methods are considered. For their full discretizations, we use elliptic reconstructions that are, respectively, piecewise-constant and piecewise-linear in time. Certain bounds for the Green's function of the parabolic operator are also employed.

Keywords parabolic problems · maximum-norm a posteriori error estimates · backward Euler · Crank-Nicolson · elliptic reconstructions

Mathematics Subject Classification (2000) MSC 65M15 · 65M60

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1 Introduction

Residual-type a posteriori error estimates in the maximum norm for parabolic equations have been given in a number of works [2,5–7,11,12]. It appears that the error constants in all known error estimators of this type, both for semidiscrete in time and fully discrete methods, for linear and semilinear equations, exhibit logarithmic dependence on the local time step. By contrast, numerical results suggest that such logarithmic factors are an artefact of the analysis (see, e.g., [13]). The aim of this paper is to eliminate the logarithmic dependence on the time step, and hence obtain maximum-norm a posteriori error estimates that are sharper and in line with numerical experiments. This purpose is achieved by refining our recent analysis [12] (where all estimators still involve logarithmic factors); in particular, a more careful treatment of certain residual terms is introduced that is tailored to specific time discretizations.

Consider a semilinear parabolic equation in the form

$$Ku := \partial_t u + Lu + f(\cdot,\cdot,u) = 0 \qquad \text{in } Q := \Omega \times (0,T], \tag{1a}$$

with a second-order linear elliptic operator $L = L(t)$ in a spatial domain $\Omega \subset \mathbb{R}^n$ with Lipschitz boundary, and some function $f : \bar{\Omega} \times [0,T] \times \mathbb{R} \to \mathbb{R}$, subject to the initial condition

$$u(x,0) = u_0(x) \quad \text{for } x \in \bar{\Omega}, \tag{1b}$$

and the Dirichlet boundary condition

$$u(x,t) = 0 \quad \text{for } (x,t) \in \partial\Omega \times [0,T]. \tag{1c}$$

We assume that the intial and boundary data satify the zero-th order compatibility condition, i.e. $u_0|_{\partial\Omega} = 0$, and that u_0 is Hölder continuous in $\bar{\Omega}$. Under standard assumptions on f and L, problem (1) possesses a unique solution that is continuous on $\bar{\Omega} \times [0,T]$; see [14, Chapt. 5, Theorem 6.4].

Some restrictions have to be imposed on the operator L and on the non-linearity f to accommodate the analysis in the present paper. In particular, we assume that $f \in C(\bar{\Omega} \times [0,T] \times \mathbb{R})$ is differentiable in the third argument and, for some nonnegative constants ρ and $\bar{\rho}$, satisfies

$$\rho^2 \le \partial_z f(x,t,z) \le \bar{\rho}^2 \qquad \text{for} \quad (x,t,z) \in \bar{\Omega} \times [0,T] \times \mathbb{R}. \tag{2a}$$

Also, certain bounds on the parabolic Green's function must hold. These assumptions will be made precise in §2. For example, the results of this study apply to the frequently studied model equation

$$\partial_t u - \varepsilon^2 \Delta u + f(\cdot,\cdot,u) = 0 \tag{2b}$$

posed in a bounded polyhedral spatial domain $\Omega \subset \mathbb{R}^n$, $n = 1,2,3$, with a (possibly small) parameter $\varepsilon \in (0,1]$.

We consider the first-order backward Euler and the second-order Crank-Nicolson discretizations in time applied to problem (1), and obtain computable a posteriori error estimates in the maximum norm first for semi-discrete, and then for fully discrete methods. The analysis framework of [12] is partially followed; in particular, computed solutions are interpolated in time in a piecewise-constant and piecewise-linear manner, respectively, when dealing with the backward Euler method and the Crank-Nicolson methods. We also draw ideas from [5, 17] and employ elliptic reconstructions in the analysis of fully discrete methods.

The paper is organized as follows. In §2, we introduce the parabolic Green's function and make a crucial assumption on its derivatives in time. §3 contains our findings for semidiscrete methods of backward Euler and Crank-Nicolson type, while in §4 we generalize these results to fully discrete methods. The semilinear case is addressed in §3.3 and §4.4. Numerical results are presented throughout §§3-4 to illustrate our theoretical findings and compare them with earlier results.

Distributions and left-continuity convention. Certain functions will be understood as distributions [9], which will be indicated. By contrast, if a certain function is Lebesgue-integrable in $\Omega\times(0,T)$, we shall refer to it as a regular function. Whenever we deal with a regular function, it will be understood as *left-continuous* for all $t\in(0,T]$. In particular, this convention will be applied to all piecewise-continuous temporal derivatives.

Further notation. The usual spaces $C(\bar\Omega)$ and $H_0^1(\Omega)$ are used, as well as the spaces $L_p(\Omega)$, $1\le p\le\infty$, with the norm $\|\cdot\|_{p,\Omega}$, and $L_\infty(Q)$ with the norm $\|\cdot\|_{\infty,Q}$ for some $Q\subset\Omega\times[0,T]$, while $\langle\varphi,\psi\rangle=\int_\Omega\varphi(x)\psi(x)\,\mathrm{d}x$ denotes the inner product in $L_2(\Omega)$. The $\bar{\ }$ and $\hat{\ }$ symbols (as in $\bar v$ and $\hat v$) will be used, respectively, for piecewise-constant and piecewise-linear interpolants in time (see (8) and (9) for more precise definitions).

2 The Green's function of the linearised parabolic operator

In this section we summarise our assumptions on the Green's function G associated with the linearisation of the parabolic operator K. With its help the error of a numerical approximation can be expressed in terms of its residual. For definitions and properties of fundamental solutions and Green's functions of parabolic operators the reader is referred to [8, Chap. 1 and §7 of Chap. 3].

Let w (a possible approximation of u) be a function that possesses at most a finite number of discontinuities in time, but is otherwise continuous on $\bar\Omega\times[0,T]$ and vanishes on $\partial\Omega$. Introducing the linearised operator $A:=\partial_t+L+a_{[w,u]}$ with

$$a_{[w,u]}(x,t):=\int_0^1\partial_z f\Big(x,t,\varsigma\big(w-u\big)(x,t)+u(x,t)\Big)\,\mathrm{d}\varsigma,\quad (x,t)\in\Omega\times(0,T],$$

we have $A(w-u)=Kw-Ku$. Then for any fixed $(\xi,s)\in\Omega\times[0,T]$, the Green's function $G(x,t;\xi,s)=:\Gamma(x,t)$ associated with A, satisfies

$$A\Gamma(x,t)=0\quad\text{for }(x,t)\in\Omega\times(s,T],\qquad \Gamma(x,s)=\delta(x-\xi)\quad\text{for }x\in\bar\Omega,$$

subject to $\Gamma(x,t)=0$ for $(x,t)\in\partial\Omega\times[s,T]$, where $\delta(\cdot)$ is the n-dimensional Dirac δ-distribution. Now, using G, the difference $w-u$ admits the representation

$$\big(w-u\big)(x,t)=\big\langle G(x,t;\cdot,0),\big(w-u\big)(\cdot,0)\big\rangle+\int_0^t\big\langle G(x,t;\cdot,s),\big(Kw\big)(\cdot,s)\big\rangle\,\mathrm{d}s. \quad (3)$$

where

$$\langle w,v\rangle:=\int_\Omega w(\xi)\,v(\xi)\,\mathrm{d}\xi.$$

Here Kw has to be understood as a distribution because w may have discontinuities. We shall discuss this in more detail later.

The analysis in this paper will be carried out under one of the following assumptions on the Green's function and its derivative.

Assumption 1 *There exist constants* κ_0, κ_1, $\kappa_2>0$ *and* κ_1', κ_2', $\gamma\geq 0$ *such that the Green's function* G *associated with the operator* K *satisfies*

$$\|G(x,t;\cdot,s)\|_{1,\Omega}\leq\kappa_0\,\mathrm{e}^{-\gamma^2(t-s)},\quad \|\partial_s^p G(x,t;\cdot,s)\|_{1,\Omega}\leq\left(\frac{\kappa_p}{(t-s)^p}+\kappa_p'\right)\mathrm{e}^{-\gamma^2(t-s)}, \quad (4)$$

for all $x\in\bar{\Omega}$, $0\leq s<t\leq T$, *and* $p=1,2$.

In the semilinear case, we shall employ a version of the above assumption.

Assumption 1* *There exist constants* κ_0, κ_1, $\kappa_2>0$ *and* κ_1', κ_2', $\gamma\geq 0$ *such that the Green's function* G *associated with the operator* K *satisfies the first bound in* (4)*, and furthermore, there is a function* $g(x,t;\xi,t)$ *such that* $\partial_s(G-g)$ *satisfies the second bound of* (4)*, while* $\int_0^T\|\partial_s g(x,t;\cdot,s)\|_{1,\Omega}\,\mathrm{d}s\leq\kappa_3$.

2.1 Problems that satisfy Assumption 1 or Assumption 1*

The first bound in (4) is easily established for problem (2), with $\rho\geq 0$, using the maximum principle (with $\kappa_0=1$ and $\gamma=\rho$). The second bound is for the time derivatives of G, and is certainly more challenging. A few results are available.

(i) For the heat equation $u_t-\Delta u=\varphi(x,t)$ in $\Omega\subset\mathbb{R}^n$, we have (4) with $\kappa_0=1$, $\kappa_p=p!\,18^{p-1}3^n\,2^{-(n/2+1)}$ and $\kappa_p'=\gamma=0$. For $p=1$, see [5, §2.2], [12, §12]. A similar argument (also using [3, Corollary 5]) yields the desired bound for $p=2$.

(ii) For the reaction-diffusion equation $u_t-\varepsilon^2\Delta u+r(x)u=\varphi(x,t)$ in $\Omega=(0,1)$, with $0<\varepsilon\ll 1$, $r\in C^{0,1}[0,1]$, $r\geq\rho^2$, $\rho>0$, the bounds of (4) hold true with $\gamma=\rho$, $\kappa_0=1$, $\kappa_1=\sqrt{2/(\pi\mathrm{e})}$ and $\kappa_1'=\kappa_0\|r\|_{\infty,[0,1]}+O(\varepsilon)$, $\varepsilon\to 0$; see [11, §2]. (In fact, here $O(\varepsilon)$ is bounded by $C\varepsilon(t-s)^q$ with some $q>0$ and C independent of ε, t or s.) A similar argument also yields

$$\kappa_2=\frac{4}{\sqrt{\pi}}\int_{\mathbb{R}}\left|4s^4-12s^2+3\right|\mathrm{e}^{-s^2}\,\mathrm{d}s+c_0\approx 0.70015+c_0,$$

with an arbitrary $c_0>0$, and $\kappa_2'=\|r\|^2_{\infty,[0,1]}(1+\kappa_1^2c_0^{-1})+O(\varepsilon)$.

(iii) For the reaction-diffusion equation $u_t - \varepsilon^2 \Delta u + r(x)u = \varphi(x,t)$ in $\Omega \subset \mathbb{R}^n$, with $\varepsilon \in (0,1]$, $r \in C^{0,1}(\bar{\Omega})$, $r \geq \rho^2 \geq 0$, one has (4) with $\gamma^2 = \rho^2/2$, $\kappa_0 = 1$, $\kappa_p = p!\,18^{p-1} 3^n 2^{-(n/2+1)}$ and $\kappa'_p = 0$; see [12, §12] for the case $p = 1$, and employ [3, Corollary 5] in a similar manner for $p = 2$.

(iv) The semilinear reaction-diffusion equation (2) in $\Omega \subset \mathbb{R}^n$ satisfies Assumption 1^* with $\gamma^2 = \rho^2/2$, $\kappa_0 = 1$, $\kappa_1 = 3^n 2^{-(n/2+1)}$, $\kappa_p = p!\,18^{p-1} 3^n 2^{-(n/2+1)}$, $\kappa'_p = 0$, and some κ_3 independent of ε (and also of T if $\rho > 0$); combine [12, §12] with the bounds described in *(iii)*.

(v) The semilinear reaction-diffusion equation (2) in $\Omega = (0,1)$, with $0 < \varepsilon \ll 1$ and $\rho > 0$, satisfies Assumption 1^* with $\gamma = \rho$, $\kappa_0 = 1$, κ_p and κ'_p as in part (ii) (with $\|r\|_{\infty,[0,1]}$ replaced by ρ^2) and some κ_3 independent of ε (and also of T if $\rho > 0$); see [11, §12].

2.2 Test problems

The following **test problem**, which we shall later use to illustrate our theoretical findings, belongs to the above problem class (ii):

$$u_t - \varepsilon^2 u_{xx} + (1+x)u = \varphi(x,t) = 1 - \cos 10xt^2, \quad \text{in } (0,1) \times (0,T], \tag{5a}$$
$$u(x,0) = \sin \pi x, \qquad x \in [0,1], \tag{5b}$$
$$u(0,t) = u(1,t) = 0, \qquad t \in (0,T], \tag{5c}$$

Clearly, $\rho = 1$ and $\kappa'_1 = 2 + O(\varepsilon)$. Because $\varepsilon \ll 1$, we neglect the term $O(\varepsilon)$ and use $\kappa'_1 := 2$ in our numerical experiments.

We shall also consider a **semilinear test problem**, which belongs to the above problem class (iv):

$$u_t - \varepsilon^2 u_{xx} + \mathrm{e}^u = \cos 5x^2 t \tag{6}$$

is posed in the same domain as (5), subject to zero initial and boundary conditions.

3 Semidiscrete methods

Throughout the paper we consider an arbitrary nonuniform mesh

$$\omega_t : 0 = t_0 < t_1 < \cdots < t_M = T, \quad \tau_j := t_j - t_{j-1}, \quad j = 1, \ldots, M,$$

in the time direction. For any function v defined on Q that is continuous in time on $[0,T]$ we set $v^j(\cdot) := v(\cdot, t_j)$.

3.1 The backward Euler method

We discretize the abstract parabolic problem (1) in time on the mesh ω_t using the first-order backward Euler method as follows. We associate an approximate solution $U^j \in H_0^1(\Omega) \cap C(\bar{\Omega})$ with the time level t_j and require it to satisfy

$$\delta_t U^j + L^j U^j + f^j = 0 \quad \text{in } \Omega, \quad j = 1, \ldots, M; \quad U^0 = u_0, \tag{7}$$

where

$$\delta_t U^j := \frac{U^j - U^{j-1}}{\tau_j}, \quad L^j := L(t_j) \quad \text{and} \quad f^j := f(\cdot, t_j, U^j).$$

For any function v defined on ω_t, $t_j \mapsto v^j$, we define two interpolants: a piecewise linear interpolant $\hat{v}$ by

$$\hat{v}(\cdot, t) := \frac{t_j - t}{\tau_j} v^{j-1} + \frac{t - t_{j-1}}{\tau_j} v^j \quad \text{for } t \in [t_{j-1}, t_j], \quad j = 1, \ldots, M, \tag{8}$$

and a piecewise constant interpolant $\bar{v}$

$$\bar{v}(\cdot, t) := v^j \quad \text{for } t \in (t_{j-1}, t_j], \quad j = 1 \ldots, M; \quad \bar{v}(\cdot, 0) := v^0. \tag{9}$$

Set $\psi(\cdot, t) := \big(L\bar{U}\big)(\cdot, t) + f(\cdot, t, \bar{U}(\cdot, t))$ and $\vartheta := \psi - \bar{\psi}$. With this notation we have, by (7),

$$\psi - \vartheta = \bar{\psi} = L^j U^j + f^j = -\delta_t U^j = -\partial_t \hat{U} \quad \text{on } (t_{j-1}, t_j].$$

Therefore, $\partial_t \hat{U} + \psi = \vartheta$ in Q, and

$$K\bar{U} = \partial_t \bar{U} + \psi = \partial_t \big(\bar{U} - \hat{U}\big) + \vartheta \quad \text{in } Q. \tag{10}$$

Remark 1 Here the temporal derivative $\partial_t \bar{U}$ is to be understood as a distribution, while $\partial_t \hat{U}$ is a regular function, equal to $\delta_t U^j$ in $(t_{j-1}, t_j]$ (in agreement with our left-continuity convention).

Alternatively, one may think of $\bar{U}$ being the limit, for $\nu \to 0^+$, of the continuous piecewise-linear function $\bar{U}_\nu$ on $[0, T]$ with

$$\bar{U}_\nu(\cdot, t) = U^j \quad \text{for } t \in [t_{j-1} + \nu, t_j], \; j = 1, \ldots, M, \quad 0 < \nu < \min_{j=1,\ldots,M} \tau_j,$$

see Fig. 1.

Next we use (3) with $w := \bar{U}$ to obtain a presentation for the error in (x, t_m), $x \in \Omega$, $m \le M$. To this end let $\Gamma := G(x, t_m; \cdot, \cdot)$. Then, by (10)

$$\begin{aligned} U^m(x) - u(x, t_m) &= \big(\bar{U} - u\big)(x, t_m) \\ &= \int_0^{t_m} \left\langle \Gamma(\cdot, s), \big(\partial_s \big(\bar{U} - \hat{U}\big) + \vartheta\big)(\cdot, s) \right\rangle \mathrm{d}s \\ &= \sum_{j=1}^m \int_{t_{j-1}}^{t_j} \left\langle -\partial_s \Gamma(\cdot, s), \big(\bar{U} - \hat{U}\big)(\cdot, s) \right\rangle \mathrm{d}s + \int_0^{t_m} \langle \Gamma(\cdot, s), \vartheta(\cdot, s) \rangle \, \mathrm{d}s, \end{aligned} \tag{11}$$

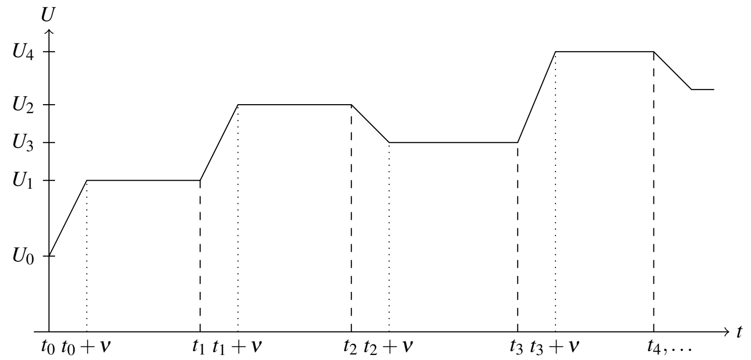

Fig. 1 $\bar{U}$ as limit (as $\nu \to 0^+$) of a continuous piecewise linear function $\bar{U}_\nu$.

where we have used integration by parts and $\big(\bar{U}-\hat{U}\big)(\cdot,s)=0$ for $s=t_0,t_m$. Next, note that

$$\big(\bar{U}-\hat{U}\big)(\cdot,s)=\big(t_j-s\big)\delta_t U^j \quad \text{for } s\in(t_{j-1},t_j]. \tag{12}$$

Alternatively, setting $W^j := \frac{1}{2}\big[(U^j-U^{j-1})-(U^m-U^{m-1})\big]$ for $j=0,\ldots,m$, we get

$$\big(\bar{U}-\hat{U}\big)(\cdot,s)=\tfrac{1}{2}\tau_m\delta_t U^m+\bar{W}+\big(t_{j-1/2}-s\big)\delta_t U^j \quad \text{for } s\in(t_{j-1},t_j].$$

Let $\omega(s):=(t_j-s)(s-t_{j-1})$, $s\in[t_{j-1},t_j]$, so that $(t_{j-1/2}-s)=-\frac{1}{2}\omega'(s)$. Then integration by parts yields

$$\begin{aligned} U^m(x)-u(x,t_m) &= \big(\bar{U}-u\big)(x,t_m)\\ &= \int_0^{t_m}\langle\Gamma(\cdot,s),\vartheta(\cdot,s)\rangle\,\mathrm{d}s-\int_{t_{m-1}}^{t_m}\langle\partial_s\Gamma(\cdot,s),(t_m-s)\delta_t U^m\rangle\,\mathrm{d}s\\ &\quad -\sum_{j=1}^{m-1}\int_{t_{j-1}}^{t_j}\Big\{\big\langle\partial_s\Gamma(\cdot,s),\tfrac{1}{2}\tau_m\delta_t U^m+\bar{W}\big\rangle\,\mathrm{d}s+\big\langle\partial_{ss}\Gamma(\cdot,s),\tfrac{1}{2}\omega(s)\delta_t U^j\big\rangle\Big\}\,\mathrm{d}s. \end{aligned}$$

We apply Hölder's inequality and obtain

$$\begin{aligned} \|U^m-u(\cdot,t_m)\|_{\infty,\Omega} \le & \sum_{j=1}^{m}\|\vartheta\|_{\infty,\Omega\times(t_{j-1},t_j)}\int_{t_{j-1}}^{t_j}\|\Gamma(\cdot,s)\|_{1,\Omega}\,\mathrm{d}s\\ &+\|\delta_t U^m\|_{\infty,\Omega}\int_{t_{m-1}}^{t_m}\|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,(t_m-s)\,\mathrm{d}s\\ &+\frac{\tau_m}{2}\|\delta_t U^m\|_{\infty,\Omega}\Big(\|\Gamma(\cdot,0)\|_{1,\Omega}+\|\Gamma(\cdot,t_{m-1})\|_{1,\Omega}\Big)\\ &+\sum_{j=1}^{m-1}\big\|W^j\big\|_{\infty,\Omega}\int_{t_{j-1}}^{t_j}\|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,\mathrm{d}s\\ &+\sum_{j=1}^{m-1}\big\|\delta_t U^j\big\|_{\infty,\Omega}\int_{t_{j-1}}^{t_j}\|\partial_{ss}\Gamma(\cdot,s)\|_{1,\Omega}\,\frac{\omega(s)}{2}\,\mathrm{d}s. \end{aligned} \tag{13}$$

We bound the integrals on the right-hand side that involve the Green's function and its derivatives based on Ass. 1:

$$\int_{t_{j-1}}^{t_j} \|\Gamma(\cdot,s)\|_{1,\Omega}\,\mathrm{d}s \le \kappa_0\tau_j\beta_{m,j} \quad \text{with} \quad \beta_{m,j} := \mathrm{e}^{-\gamma^2(t_m-t_j)}.$$

We also use

$$\int_{t_{m-1}}^{t_m} \|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,(t_m-s)\,\mathrm{d}s \le \tau_m\left(\kappa_1+\kappa_1'\frac{\tau_m}{2}\right),$$

$$\int_{t_{j-1}}^{t_j} \|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,\mathrm{d}s \le \left\{\kappa_1\int_{t_{j-1}}^{t_j}\frac{\mathrm{d}s}{t_m-s}+\kappa_1'\tau_j\right\}\beta_{m,j} =: \nu_{m,j}, \tag{14}$$

and

$$\int_{t_{j-1}}^{t_j} \|\partial_{ss}\Gamma(\cdot,s)\|_{1,\Omega}\,\frac{\omega(s)}{2}\,\mathrm{d}s \le \beta_{m,j}\int_{t_{j-1}}^{t_j}\left[\frac{\kappa_2}{(t_m-s)^2}+\kappa_2'\right]\frac{\omega(s)}{2}\,\mathrm{d}s =: \zeta^{\mathrm{E}}_{m,j}.$$

Theorem 1 *Let U^m be the approximation of $u(\cdot,t_m)$ obtained by the semidiscrete backward Euler method* (7) *on the mesh ω_t. Then, under Assumption 1, one has*

$$\|U^m-u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^{\mathrm{E}} := \eta^{\mathrm{E}}_{\mathrm{osc}}+\eta^{\mathrm{E}}_{\mathrm{t}}+\eta^{\mathrm{E}}_{\mathrm{t},\dagger}+\eta^{\mathrm{E}}_{\mathrm{t,W}},$$

where

$$\eta^{\mathrm{E}}_{\mathrm{osc}} := \kappa_0\sum_{j=1}^{m}\beta_{m,j}\tau_j\,\|\psi-\bar\psi\|_{\infty,\Omega\times(t_{j-1},t_j]}, \quad \eta^{\mathrm{E}}_{\mathrm{t}} := \sum_{j=1}^{m-1}\zeta^{\mathrm{E}}_{m,j}\,\|\delta_t U^j\|_{\infty,\Omega},$$

$$\eta^{\mathrm{E}}_{\mathrm{t},\dagger} := \tau_m\mu^{\mathrm{E}}_m\,\|\delta_t U^m\|_{\infty,\Omega}, \quad \eta^{\mathrm{E}}_{\mathrm{t,W}} := \sum_{j=1}^{m-1}\nu_{m,j}\,\|W^j\|_{\infty,\Omega}$$

with $\psi = L\bar U + f(\cdot,\cdot,\bar U)$, its piecewise constant interpolation $\bar\psi$, and the quantities $\beta_{m,j}$, $\nu_{m,j}$, and $\zeta^{\mathrm{E}}_{m,j}$ defined above and $\mu^{\mathrm{E}}_m := \kappa_1+\kappa_1'\frac{\tau_m}{2}+\frac{\kappa_0}{2}(\beta_{m,0}+\beta_{m,m-1})$.

Remark 2 Under Assumption 1 (with $p \le 1$), a version of [12, Theorem 4.1] (obtained in a similar manner, but using (12) only) gives the a posteriori error bound

$$\begin{aligned}\|U^m-u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^{\mathrm{E}}_{[12]} &:= \kappa_0\sum_{j=1}^{m}\beta_{m,j}\,\tau_j\,\|\psi-\bar\psi\|_{\infty,\Omega\times(t_{j-1},t_j]}+2\kappa_0\tau_m\,\|\delta_t U^m\|_{\infty,\Omega}\\ &+\kappa_1\ln\left(\frac{t_m}{\tau_m}\right)\max_{j=1,\dots,m-1}\beta_{m,j}\tau_j\,\|\delta_t U^j\|_{\infty,\Omega}+\frac{\kappa_1'}{2}\sum_{j=1}^{m-1}\beta_{m,j}\,\tau_j^2\,\|\delta_t U^j\|_{\infty,\Omega},\end{aligned} \tag{15}$$

which involves the logarithmic factor $\ln(t_m/\tau_m)$.

			Theorem 1		[12]		
M	$\|u-U\|_{\infty,\Omega}$	rate	η^{E}	C_{eff}	$\eta^{\mathrm{E}}_{[12]}$	C_{eff}	$\frac{C_{\mathrm{eff}}}{\ln(T/\tau_M)+5}$
2^{10}	3.254e-04	1.00	1.572e-03	4.83	4.085e-03	12.55	1.05
2^{11}	1.627e-04	1.00	7.862e-04	4.83	2.159e-03	13.27	1.05
2^{12}	8.135e-05	1.00	3.932e-04	4.83	1.138e-03	13.98	1.05
2^{13}	4.068e-05	1.00	1.966e-04	4.83	5.977e-04	14.69	1.05
2^{14}	2.034e-05	1.00	9.833e-05	4.83	3.133e-04	15.40	1.05
2^{15}	1.017e-05	1.00	4.917e-05	4.83	1.639e-04	16.11	1.05
2^{16}	5.085e-06	—	2.458e-05	4.83	8.554e-05	16.82	1.05

Table 1 Maximum-norm error at final time $t_M = T = 1/2$ for problem (5), $\varepsilon = 10^{-6}$. Semidiscrete backward Euler, uniform mesh in time. Comparison of the error estimators from Theorem 1 and [12] (in the form of (15)).

Numerical test. Let us consider the test problem (5) to illustrate the superiority of Theorem 1 over the result in [12]. We use P_1-FEM on a very fine layer-adapted Bakhvalov mesh [1] to solve (7), so the errors from the spatial discretisation can be neglected (as the extremely fine spatial mesh is also a priori adapted to the solution singularities; the parameters in all Bakhvalov meshes that we use are chosen as in [13]). Furthermore, for our test the operator L is independent of time. Therefore,

$$\|\psi-\bar{\psi}\|_{\infty,\Omega\times(t_{j-1},t_j]} = \left\|\varphi-\varphi^j\right\|_{\infty,\Omega\times(t_{j-1},t_j]}, \quad j=1,\ldots,M.$$

This term captures the data oscillations and has to be estimated by evaluating $\varphi-\varphi^j$ at suitable points.

The constants that appear in the estimator are described in §2.1. In addition, we replaced $\kappa_2(t-s)^{-2}+\kappa_2'$ in the bound of $\partial_s^2 G$ in (4), and hence in the definition of $\zeta^{\mathrm{E}}_{m,j}$, by a sharper bound $\kappa_2(t-s)^{-2}+\tilde{\kappa}_2'(t-s)^{-1}+\kappa_2'$, where κ_2 uses $c_0=0$, while $\tilde{\kappa}_2 = 2\kappa_1\|r\|_{\infty,[0,1]}$ and $\kappa_2' = \|r\|^2_{\infty,[0,1]} + O(\varepsilon)$.

Table 1 contains the results of our numerical tests for $\varepsilon = 10^{-6}$. For each error estimator, we also compute its efficiency index C_{eff} (estimator divided by error). The error estimator of Theorem 1 clearly gives sharper error bounds than the one from [12]. Crucially, for the former, we do not witness any logarithmic dependence on the time-step size.

3.2 The Crank-Nicolson method

We continue using the notation introduced in the previous section and discretize the abstract parabolic problem (1) in time using the second-order Crank-Nicolson method as follows. We associate an approximate solution $U^j \in H_0^1(\Omega)\cap C(\bar{\Omega})$ with the time level t_j and require it to satisfy

$$\delta_t U^j + \tfrac{1}{2}\left(L^{j-1}U^{j-1} + L^j U^j\right) + \tfrac{1}{2}\left(f^{j-1}+f^j\right) = 0 \quad \text{in } \Omega, \quad j=1,\ldots,M; \qquad (16)$$
$$U^0 = u_0.$$

Let $\psi(\cdot,t) := \big(L\hat{U}\big)(\cdot,t) + f(\cdot,t,\hat{U}(\cdot,t))$ and $\vartheta := \psi - \hat{\psi}$. Then, by (16)

$$\partial_t \hat{U} = \delta_t U^j = -\tfrac{1}{2}\big(\psi^j + \psi^{j-1}\big), \quad \text{in } (t_{j-1},t_j).$$

Therefore,

$$K\hat{U} = \psi - \tfrac{1}{2}\big(\psi^j + \psi^{j-1}\big) = \vartheta + \hat{\psi} - \tfrac{1}{2}\big(\psi^j + \psi^{j-1}\big), \quad \text{in } (t_{j-1},t_j).$$

Furthermore,

$$\hat{\psi}(\cdot,s) = \tfrac{1}{2}\big(\psi^j + \psi^{j-1}\big) + \big(s - t_{j-1/2}\big)\frac{\psi^j - \psi^{j-1}}{\tau_j}, \quad s \in (t_{j-1},t_j).$$

Thus

$$\hat{\psi}(\cdot,s) - \tfrac{1}{2}\big(\psi^j + \psi^{j-1}\big) = \big(s - t_{j-1/2}\big)\delta_t \psi^j, \quad s \in (t_{j-1},t_j).$$

Recall that $\omega(s) := (t_j - s)(s - t_{j-1})$, $s \in [t_{j-1},t_j]$ and $(s - t_{j-1/2}) = \frac{1}{2}\omega'(s)$, so we obtain

$$\big(K\hat{U}\big)(\cdot,s) = \vartheta(\cdot,s) + \tfrac{1}{2}\omega'(s)\delta_t \psi^j, \quad s \in (t_{j-1},t_j).$$

We employ (3) with $w := \hat{U}$ to express the error in (x,t_m), $x \in \Omega$, $m \le M$. Let again $\Gamma := G(x,t_m;\cdot,\cdot)$ and use integration by parts. Then

$$|U^m - u(x,t_m)| \le \left|\int_0^{t_m} \langle \Gamma(\cdot,s), \vartheta(\cdot,s)\rangle \,\mathrm{d}s\right| + \frac{1}{2}\left|\sum_{j=1}^{m}\int_{t_{j-1}}^{t_j} \big\langle \Gamma_s(\cdot,s), \omega(s)\delta_t\psi^j\big\rangle \,\mathrm{d}s\right|. \tag{17}$$

Note that $\frac{1}{6}\tau_j^2$ is the average of ω on (t_{j-1},t_j), and set $\widetilde{\omega}(s) := \omega(s) - \frac{1}{6}\tau_j^2$ for $s \in (t_{j-1},t_j)$. Then, with the notation $W^j := \tau_j^2\delta_t\psi^j - \tau_m^2\delta_t\psi^m$, we get the representation

$$\omega(s)\delta_t\psi^j = \tfrac{1}{6}\tau_m^2\delta_t\psi^m + \widetilde{\omega}(s)\delta_t\psi^j + \tfrac{1}{6}W^j \ \text{ for } \ s \in (t_{j-1},t_j).$$

Next, using the identity

$$\int_{t_{j-1}}^{s} \widetilde{\omega}(\sigma)\,\mathrm{d}\sigma = \tfrac{1}{3}(t_j - s)(s - t_{j-1})(s - t_{j-1/2}) =: \pi_j(s), \ \ s \in [t_{j-1},t_j]$$

and integration by parts, we obtain

$$\begin{aligned}
|U^m - u(x,t_m)| \le{}& \left|\int_0^{t_m} \langle \Gamma(\cdot,s), \vartheta(\cdot,s)\rangle \,\mathrm{d}s\right| + \frac{1}{2}\left|\int_{t_{m-1}}^{t_m} \langle \Gamma_s(\cdot,s), \omega(s)\delta_t\psi^m\rangle \,\mathrm{d}s\right| \\
&+ \frac{1}{2}\left|\left\langle \int_{t_0}^{t_{m-1}} \Gamma_s(\cdot,s)\,\mathrm{d}s, \tau_m^2\delta_t\psi^m \right\rangle\right| \\
&+ \frac{1}{12}\sum_{j=1}^{m-1}\left|\int_{t_{j-1}}^{t_j} \big\langle \Gamma_s(\cdot,s), W^j\big\rangle \,\mathrm{d}s\right| \\
&+ \frac{1}{2}\sum_{j=1}^{m-1}\left|\int_{t_{j-1}}^{t_j} \big\langle \Gamma_{ss}(\cdot,s), \pi_j(s)\delta_t\psi^j\big\rangle \,\mathrm{d}s\right|.
\end{aligned}$$

Now, an application of Hölder's inequality yields

$$\begin{aligned}\|U^m - u(\cdot,t_m)\|_{\infty,\Omega} \le{}& \frac{1}{2}\,\|\delta_t\psi^m\|_{\infty,\Omega}\int_{t_{m-1}}^{t_m}\|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,\omega(s)\,\mathrm{d}s\\ &+\frac{\tau_m^2}{12}\,\|\delta_t\psi^m\|_{\infty,\Omega}\underbrace{\Big(\|\Gamma(\cdot,0)\|_{1,\Omega}+\|\Gamma(\cdot,t_{m-1})\|_{1,\Omega}\Big)}_{\le\beta_{m,0}+\beta_{m,m-1}}\\ &+\frac{1}{2}\sum_{j=1}^{m-1}\left\|\delta_t\psi^j\right\|_{\infty,\Omega}\int_{t_{j-1}}^{t_j}\|\partial_{ss}\Gamma(\cdot,s)\|_{1,\Omega}\left|\pi_j(s)\right|\,\mathrm{d}s\\ &+\frac{1}{12}\sum_{j=1}^{m-1}\left\|W^j\right\|_{\infty,\Omega}\underbrace{\int_{t_{j-1}}^{t_j}\|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,\mathrm{d}s}_{\le\nu_{m,j}}\\ &+\sum_{j=1}^{m}\|\vartheta\|_{\infty,\Omega\times(t_{j-1},t_j)}\underbrace{\int_{t_{j-1}}^{t_j}\|\Gamma(\cdot,s)\|_{1,\Omega}\,\mathrm{d}s}_{\le\kappa_0\tau_j\beta_{m,j}}.\end{aligned}$$

Using Ass. 1, we evaluate the constants not obtained in §3.1:

$$\frac{1}{2}\int_{t_{m-1}}^{t_m}\|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,\omega(s)\,\mathrm{d}s \le \kappa_1\frac{\tau_m^2}{4}+\kappa_1'\frac{\tau_m^3}{12}$$

and

$$\frac{1}{2}\int_{t_{j-1}}^{t_j}\|\partial_{ss}\Gamma(\cdot,s)\|_{1,\Omega}\left|\pi_j(s)\right|\,\mathrm{d}s \le \frac{\beta_{m,j}}{2}\int_{t_{j-1}}^{t_j}\left\{\frac{\kappa_2}{(t_m-s)^2}+\kappa_2'\right\}\left|\pi_j(s)\right|\,\mathrm{d}s =: \zeta_{m,j}^{\mathrm{CN}}.$$

We summarize our results.

Theorem 2 *Let U^m be the approximation of $u(\cdot,t_m)$ obtained by the semidiscrete Crank-Nicolson method* (16) *on the mesh ω_t. Then, under Assumption 1, one has*

$$\|U^m - u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^{\mathrm{CN}} := \eta_{\mathrm{osc}}^{\mathrm{CN}}+\eta_{\mathrm{t}}^{\mathrm{CN}}+\eta_{\mathrm{t},\dagger}^{\mathrm{CN}}+\eta_{\mathrm{t,W}}^{\mathrm{CN}}$$

where

$$\eta_{\mathrm{osc}}^{\mathrm{CN}} := \kappa_0\sum_{j=1}^{m}\beta_{m,j}\tau_j\,\|\psi-\hat\psi\|_{\infty,\Omega\times(t_{j-1},t_j]}\,,\quad \eta_{\mathrm{t}}^{\mathrm{CN}} := \sum_{j=1}^{m}\zeta_{m,j}^{\mathrm{CN}}\left\|\delta_t\psi^j\right\|_{\infty,\Omega},$$

$$\eta_{\mathrm{t},\dagger}^{\mathrm{CN}} := \tau_m^2\mu_m^{\mathrm{CN}}\,\|\delta_t\psi^m\|_{\infty,\Omega}\,,\quad \eta_{\mathrm{t,W}}^{\mathrm{CN}} := \frac{1}{12}\sum_{j=1}^{m}\nu_{m,j}\left\|W^j\right\|_{\infty,\Omega}$$

with $\psi = L\hat U + f(\cdot,\cdot,\hat U)$, its piecewise linear interpolant $\hat\psi$, and the quantities $\beta_{m,j}$, $\nu_{m,j}$ and $\zeta_{m,j}^{\mathrm{CN}}$ defined above, $\mu_m^{\mathrm{CN}} := \frac{1}{12}\left\{3\kappa_1+\kappa_1'\tau_m+\kappa_0\left(\beta_{m,0}+\beta_{m,m-1}\right)\right\}$ and $W^j := \tau_j^2\delta_t\psi^j-\tau_m^2\delta_t\psi^m$.

			Theorem 2		[12]		
M	$\|u-U\|_{\infty,\Omega}$	rate	η^{CN}	C_{eff}	$\eta^{\mathrm{CN}}_{[12]}$	C_{eff}	$\frac{C_{\mathrm{eff}}}{\ln(T/\tau_M)+12}$
2^6	1.519e-05	2.00	2.078e-04	13.68	3.770e-04	24.81	1.54
2^7	3.798e-06	2.00	5.222e-05	13.75	9.812e-05	25.84	1.53
2^8	9.494e-07	2.00	1.310e-05	13.79	2.551e-05	26.87	1.53
2^9	2.373e-07	2.00	3.280e-06	13.82	6.624e-06	27.91	1.53
2^{10}	5.934e-08	2.00	8.210e-07	13.84	1.718e-06	28.96	1.53
2^{11}	1.483e-08	2.00	2.054e-07	13.85	4.451e-07	30.00	1.53
2^{12}	3.709e-09	—	5.148e-08	13.88	1.152e-07	31.05	1.53

Table 2 Maximum-norm error at final time $t_M = T = 1/2$ for problem (5), $\varepsilon = 10^{-6}$. Semidiscrete Crank-Nicolson scheme, uniform mesh in time. Comparison of the error estimators from Theorem 2 and [12] (in the form of (18)).

Remark 3 Under Assumption 1, a version of [12, Theorem 5.1] gives the a posteriori error bound

$$\begin{aligned}
&\|U^m - u(\cdot,t_m)\|_{\infty,\Omega} \\
&\le \eta^{\mathrm{CN}}_{[12]} := \kappa_0 \sum_{j=1}^{m} \beta_{m,j}\tau_j \|\psi-\hat{\psi}\|_{\infty,\Omega\times(t_{j-1},t_j]} + \frac{\kappa_0}{2}\tau_m^2 \|\delta_t \psi^m\|_{\infty,\Omega} \\
&\qquad + \frac{\kappa_1}{8}\ln\left(\frac{t_m}{\tau_m}\right) \max_{j=1,\dots,m-1} \beta_{m,j}\tau_j^2 \left\|\delta_t \psi^j\right\|_{\infty,\Omega} + \frac{\kappa_1'}{12}\sum_{j=1}^{m-1} \beta_{m,j}\,\tau_j^3 \left\|\delta_t \psi^j\right\|_{\infty,\Omega},
\end{aligned} \tag{18}$$

which involves the logarithmic factor $\ln(t_m/\tau_m)$.

Numerical test. Again we consider the test problem (5) and compare the a posteriori error estimator η^{CN} of Theorem 2 on one side and $\eta^{\mathrm{CN}}_{[12]}$ from (18) on the other. Because the operator L is independent of time we have

$$\|\psi-\hat{\psi}\|_{\infty,\Omega\times(t_{j-1},t_j]} = \left\|\varphi-\hat{\varphi}\right\|_{\infty,\Omega\times(t_{j-1},t_j]}, \quad j=1,\dots,M.$$

This time we have to sample the nodal interpolation error for a piecewise linear interpolation of f on the mesh ω_t.

Table 2 displays the errors and error estimators for the semidiscrete Crank-Nicolson method. Similarly to the backward Euler discretisation, the new error estimator (of Theorem 2) clearly gives sharper error bounds than the one from [12]. Again, most importantly, no logarithmic dependence of the new error estimator on the time-step size is observed.

3.3 Semidiscrete methods for the semilinear model problem

Consider the semilinear reaction-diffusion equation (2) in $\Omega \subset \mathbb{R}^n$, with $\rho \ge 0$. It should be noted that the second bound in Assumption 1 is not readily available for this problem unless f is linear as described in parts (i)–(iii) of §2.1. So, strictly speaking, the results of Theorems 1 and 2 do not apply to this problem in the general semilinear

M	$\|u-U\|_{\infty,\Omega}$	rate	$\widetilde{\eta}^{\mathrm{E}}$	C_{eff}
2^6	8.011e-03	1.00	1.133e-01	14.14
2^7	4.013e-03	1.00	5.694e-02	14.19
2^8	2.008e-03	1.00	2.856e-02	14.22
2^9	1.005e-03	1.00	1.431e-02	14.24
2^{10}	5.024e-04	1.00	7.160e-03	14.25
2^{11}	2.512e-04	1.00	3.582e-03	14.26
2^{12}	1.256e-04	1.00	1.791e-03	14.26

Table 3 Maximum-norm error at final time $t_M = T = 1/2$ for problem (6), $\varepsilon = 10^{-6}$. Semidiscrete backward Euler scheme, uniform mesh in time. The error estimator (19).

case. Nevertheless, for the problem classes described in parts (iv), (v) of §2.1, one enjoys Assumption 1*. Using this somewhat weaker version of Assumption 1, one can still obtain a posteriori error estimates, similar to those in Theorems 1 and 2, as we now describe.

First, let U^m be the approximation of $u(\cdot,t_m)$ obtained by the semidiscrete *backward Euler* method (7) on the mesh ω_t. Now, following the proof of Theorem 1, one again gets (11). As the first bound in (4) holds true, the estimation of the second sum in (11) remains unchanged. For the first sum, however, we use the splitting $\partial_s\Gamma = \partial_s(\Gamma - g) + \partial_s g$, where, by Assumption 1*, $\partial_s(\Gamma - g)$ satisfies the second bound of (4), while $\int_0^T \|\partial_s g(x,t;\cdot,s)\|_{1,\Omega}\,\mathrm{d}s \le \kappa_3$. So for the first sum in (13), with $\partial_s\Gamma$ replaced by $\partial_s(\Gamma - g)$, we also proceed as in the proof of Theorem 1, while for the remaining sum, also employing (12), we get

$$\sum_{j=1}^{m} \left\|\delta_t U^j\right\|_{\infty,\Omega} \int_{t_{j-1}}^{t_j} \|\partial_s g(\cdot,s)\|_{1,\Omega}\,(t_j - s)\,\mathrm{d}s \le \kappa_3 \max_{j=1,\dots,m} \tau_j \left\|\delta_t U^j\right\|_{\infty,\Omega}.$$

Combining these observations, one arrives at

$$\|U^m - u(\cdot,t_m)\|_{\infty,\Omega} \le \widetilde{\eta}^{\mathrm{E}} := \eta^{\mathrm{E}} + \kappa_3 \max_{j=1,\dots,m} \tau_j \left\|\delta_t U^j\right\|_{\infty,\Omega}, \tag{19}$$

where η^{E} is the estimator from Theorem 1.

Comparing the a posteriori error estimate (19) with the one of Theorem 1, we note that the additional term in (19) is of the same order 1 as the method, and does not exhibit any logarithmic dependence on the time-step size.

Next, let U^m be the approximation of $u(\cdot,t_m)$ obtained by the semidiscrete *Crank-Nicolson* method (16) on the mesh ω_t. We modify the proof of Theorem 2 in a similar manner starting from (17) and then employing $\partial_s\Gamma = \partial_s(\Gamma - g) + \partial_s g$ for the first sum in (17). So one gets

$$\|U^m - u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^{\mathrm{CN}} + \frac{\kappa_3}{8} \max_{j=1,\dots,m} \tau_j^2 \left\|\delta_t \psi^j\right\|_{\infty,\Omega}, \tag{20}$$

where η^{CN} and ψ^j are from Theorem 2. Again we note that, in comparison with the estimator of Theorem 2, the additional term in (20) is of the expected order 2, and does not involve any logarithmic terms.

Numerical test. We consider the semilinear test problem (6) and test the a posteriori error estimator (19); see Table 3. As κ_3 remains unknown, we set $\kappa_3 := 1$. As expected, no logarithmic dependence of the new error estimator on the time-step size is observed.

4 Full discretisations

In order to obtain a method that can be implemented on a computer any of the semidiscretisations discussed in §3 must be followed by a discretisation in space. For this we shall consider finite element methods (FEM) in a general framework. To simplify the presentation, mesh coarsening will not be addressed.

4.1 Elliptic problems and elliptic reconstructions

Consider the semilinear elliptic problem of finding $v \in H_0^1(\Omega)$ such that

$$Lv + g(\cdot, v) = 0 \quad \text{in } \Omega. \tag{21}$$

Denoting by $a : H_0^1(\Omega)^2 \to \mathbb{R}$ the bilinear form associated with L, we rewrite (21) in variational form as

$$a(v,w) + \langle g(\cdot, v), w\rangle = 0 \quad \forall w \in H_0^1(\Omega).$$

Given a finite element space $V_h \subset H_0^1(\Omega) \cap C(\bar{\Omega})$, we seek an approximate solution $v_h \in V_h$ that satisfies

$$a_h\big(v_h, w_h\big) + \langle g(\cdot, v_h), w_h\rangle_h = 0 \quad \forall w_h \in V_h, \tag{22}$$

where $a_h(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle_h$ discretisations of $a(\cdot,\cdot)$ and $\langle\cdot,\cdot\rangle$ which for example involve quadrature.

Assumption 2 *There exists an a posteriori error estimator* η *for the FEM* (22) *applied to the elliptic problem* (21) *with*

$$\big\|v_h - v\big\|_{\infty,\Omega} \le \eta\big(V_h, v_h, g(\cdot, v_h)\big).$$

Remark 4 A few error estimators of this type are available in the literature. We mention some of them.

- Nochetto et al. [18] study the semilinear problem $-\Delta u + g(\cdot, u) = 0$ in up to three space dimensions. They give a posteriori error bounds for arbitrary order FEM on quasiuniform triangulations.
- Demlow & Kopteva [4] too consider arbitrary order FEM on quasiuniform triangulations, but for the singularly perturbed equation $-\varepsilon^2\Delta u + g(\cdot, u) = 0$. A posteriory error estimates are established that are robust in the perturbation parameter. Furthermore, in [10] for the same problem P_1-FEM on *anisotropic* meshes are investigated.
- In [15,16] arbitrary order FEM for the linear problem $-\varepsilon^2 u'' + ru = g$ in $(0,1)$, $u(0) = u(1) = 0$ are considered. In contrast to the afore mentioned contributions all constants appearing in the error estimator are given explicitely.

In our numerical experiments, we shall use the estimator from [15].

Elliptic reconstructions. Let $a^j(\cdot,\cdot)$ be the bilinear form associated with L^j and $a_h^j(\cdot,\cdot)$ its finite-element approximation on V_h. Given an approximation $u_h^j \in V_h$ of $u(\cdot,t_j)$, let $\psi_h^j \in V_h$ satisfy

$$a_h^j\big(u_h^j, w_h\big) = \big\langle \psi_h^j - f\big(\cdot,t_j,u_h^j\big), w_h\big\rangle_h, \quad j=0,\dots,M. \tag{23}$$

We may consider u_h^j to be the FE-approximation of $R^j \in H_0^1(\Omega)$, the solution of the elliptic problem

$$a^j\big(R^j, w\big) = \big\langle \psi_h^j - f\big(\cdot,t_j,u_h^j\big), w\big\rangle \quad \forall w \in H_0^1(\Omega) \tag{24}$$

or

$$L^j R^j = \psi_h^j - f(\cdot,t_j,u_h^j) \quad \text{in } \ \Omega, \tag{25}$$

for short. Therefore, supposing Assumption 2 we have the bound

$$\big\|u_h^j - R^j\big\|_{\infty,\Omega} \le \eta^j := \eta\big(V_h, u_h^j, \psi_h^j - f(\cdot,t_j,u_h^j)\big). \tag{26}$$

The function R^j is referred to as *elliptic reconstruction* of u_h^j, [17].

4.2 Fully discrete backward Euler method

We consider an arbitrary nonuniform mesh ω_t in the time direction and associate an approximate FEM solution $u_h^j \in V_h$ with the time level t_j and require it to satisfy

$$\big\langle \delta_t u_h^j, w_h\big\rangle_h + a_h^j\big(u_h^j, w_h\big) + \big\langle f\big(\cdot,t_j,u_h^j\big), w_h\big\rangle_h = 0 \quad \forall w_h \in V_h, \quad j=1,\dots,M \tag{27}$$

with an approximation $u_h^0 \in V_h$ of the initial condition u_0.

Note that for this method, (23) and (27) yield the simple representation

$$\psi_h^j = -\delta_t u_h^j, \ \ j=1,\dots,M. \tag{28}$$

We like to estimate the maximum-norm error at time t_m, $m \le M$. First, the triangle inequality gives

$$\begin{aligned}\|u_h^m - u(\cdot,t_m)\|_{\infty,\Omega} &\le \|u_h^m - R^m\|_{\infty,\Omega} + \|R^m - u(\cdot,t_m)\|_{\infty,\Omega} \\ &\le \eta^m + \|R^m - u(\cdot,t_m)\|_{\infty,\Omega}\,,\end{aligned}$$

by (26). The second term on the right-hand side will be bounded using (3).

For $t \in (t_{j-1},t_j]$, let

$$\psi_R(\cdot,t) := L(t)R^j + f(\cdot,t,R^j), \qquad \vartheta(\cdot,t) := f(\cdot,t_j,R^j) - f(\cdot,t_j,u_h^j). \tag{29}$$

Then, by (28) and (25)

$$\partial_t \hat{u}_h = \delta_t u_h^j = -\psi_h^j = -L^j R^j - f(\cdot,t_j,u_h^j) = -\bar{\psi}_R + \vartheta \quad \text{in } \ (t_{j-1},t_j],$$

and

$$K\bar{R} = \partial_t \left(\bar{R} - \bar{u}_h\right) + \partial_t \left(\bar{u}_h - \hat{u}_h\right) + \psi_R - \bar{\psi}_R + \vartheta$$

Set $\chi^j := R^j - u_h^j - \left(R^m - u_h^m\right)$, $j = 0, \ldots, m$. Note that $\chi^m = 0$ and $\partial_t \bar{\chi} = \partial_t \left(\bar{R} - \bar{u}_h\right)$. Therefore,

$$K\bar{R} = \partial_t \bar{\chi} + \partial_t \left(\bar{u}_h - \hat{u}_h\right) + \psi_R - \bar{\psi}_R + \vartheta.$$

Fix $x \in \Omega$ and let $\Gamma := G(x, t_m; \cdot, \cdot)$. Then, using (3) with $w := \bar{R}$, we obtain

$$\begin{aligned} R^m(x) - u(x, t_m) &= \left(\bar{R} - u\right)(x, t_m) \\ &= \left\langle \Gamma(\cdot, 0), R^0 - u_0 \right\rangle + \int_0^{t_m} \left\langle \Gamma(\cdot, s), \partial_s \bar{\chi}(\cdot, s) \right\rangle \mathrm{d}s \\ &\quad + \int_0^{t_m} \left\langle \Gamma(\cdot, s), \partial_s (\bar{u}_h - \hat{u}_h)(\cdot, s) \right\rangle \mathrm{d}s + \int_0^{t_m} \left\langle \Gamma(\cdot, s), (\psi_R - \bar{\psi}_R + \vartheta)(\cdot, s) \right\rangle \mathrm{d}s. \end{aligned}$$

Apply integration by parts to the second and third integral on the right-hand side.

$$\begin{aligned} &R^m(x) - u(x, t_m) \\ &\quad = \left\langle \Gamma(\cdot, 0), u_h^0 - u_0 \right\rangle + \left\langle \Gamma(\cdot, 0), R^m - u_h^m \right\rangle - \int_0^{t_m} \left\langle \partial_s \Gamma(\cdot, s), \bar{\chi}(\cdot, s) \right\rangle \mathrm{d}s \\ &\qquad - \int_0^{t_m} \left\langle \partial_s \Gamma(\cdot, s), (\bar{u}_h - \hat{u}_h)(\cdot, s) \right\rangle \mathrm{d}s + \int_0^{t_m} \left\langle \Gamma(\cdot, s), (\psi_R - \bar{\psi}_R + \vartheta)(\cdot, s) \right\rangle \mathrm{d}s. \end{aligned} \tag{30}$$

The fourth term on the right-hand side can be bounded using the technique from §3.1. To this end we introduce $w_h^j := \frac{1}{2}\left[(u_h^j - u_h^{j-1}) - (u_h^m - u_h^{m-1})\right]$ and obtain

$$\begin{aligned} &\left| \int_0^{t_m} \left\langle \partial_s \Gamma(\cdot, s), (\bar{u}_h - \hat{u}_h)(\cdot, s) \right\rangle \mathrm{d}s \right| \\ &\qquad \le \sum_{j=1}^{m-1} \zeta_{m,j}^{\mathrm{E}} \left\| \delta_t u_h^j \right\|_{\infty,\Omega} + \sum_{j=1}^{m-1} \nu_{m,j} \left\| w_h^j \right\|_{\infty,\Omega} + \tau_m \mu_m^{\mathrm{E}} \left\| \delta_t u_h^m \right\|_{\infty,\Omega}. \end{aligned}$$

For the third term in (30) note that, $\bar{\chi} = 0$ on $(t_{m-1}, t_m]$. Applying Hölder's inequality and the bound (14) for $\partial_s \Gamma$, we get

$$\left| \int_0^{t_m} \left\langle \partial_s \Gamma(\cdot, s), \bar{\chi}(\cdot, s) \right\rangle \mathrm{d}s \right| \le \sum_{j=1}^{m-1} \nu_{m,j} \left\| \chi^j \right\|_{\infty,\Omega}.$$

Theorem 3 *Let u_h^m be the approximation of $u(\cdot, t_m)$ obtained by (27) on the mesh ω_t. Then, under Assumption 1, one has*

$$\left\| u_h^m - u(\cdot, t_m) \right\|_{\infty,\Omega} \le \eta^{\mathrm{E}} := \eta_{\mathrm{init}} + \eta_{\mathrm{ell}}^{\mathrm{E}} + \eta_{\mathrm{osc}}^{\mathrm{E}} + \eta_{\mathrm{t}}^{\mathrm{E}} + \eta_{\mathrm{t},\dagger}^{\mathrm{E}} + \eta_{\mathrm{t,W}}^{\mathrm{E}}$$

with

$$\eta_{\text{init}} := \kappa_0 \beta_{m,0} \left\|u_h^0 - u_0\right\|_{\infty,\Omega}, \quad \eta_{\text{ell}}^{\text{E}} := \kappa_0 \left(1+\beta_{m,0}\right) \eta^m + \sum_{j=1}^{m-1} \nu_{m,j} \left\|\chi^j\right\|_{\infty,\Omega},$$

$$\eta_{\text{osc}}^{\text{E}} := \kappa_0 \sum_{j=1}^{m} \beta_{m,j} \tau_j \left\|\psi_R - \bar{\psi}_R + \vartheta\right\|_{\infty,\Omega\times(t_{j-1},t_j]}, \quad \eta_{\text{t}}^{\text{E}} := \sum_{j=1}^{m-1} \zeta_{m,j}^{\text{E}} \left\|\delta_t U^j\right\|_{\infty,\Omega},$$

$$\eta_{\text{t},\dagger}^{\text{E}} := \tau_m \mu_m^{\text{E}} \left\|\delta_t U^m\right\|_{\infty,\Omega}, \quad \eta_{\text{t,W}}^{\text{E}} := \sum_{j=1}^{m-1} \nu_{m,j} \left\|W^j\right\|_{\infty,\Omega},$$

and the constants $\beta_{m,j}$, $\nu_{m,j}$, μ_m^{E} *and* $\zeta_{m,j}^{\text{E}}$ *as in Theorem 1,* η^m *from* (26), (28), ψ_R *and* ϑ *from* (29), *and* $\chi^j = \left(R^j - u_h^j\right) - \left(R^m - u_h^m\right)$ *defined using* (25).

Remark 5 [12, §9] gives a version of the estimator (15) for the fully discrete method (27), which also involves the log factor $\ln(t_m/\tau_m)$ in the term $\eta_{\text{ell}}^{\text{E}}$, capturing the errors of the spatial discretisation. The estimator of Theorem 3 appears superior as it does not involve any such factor.

Remark 6 Let $L(t) = L$ be independent of time. Consequently, the bilinear forms $a(t)(\cdot,\cdot)$ and $a_h^j(\cdot,\cdot)$ are also independent of time, so we write $a(\cdot,\cdot)$ and $a_h(\cdot,\cdot)$. From (23) and (24) we have

$$a_h\left(u_h^m - u_h^j, w_h\right) = \left\langle \psi_h^m - \psi_h^j - f\left(\cdot,t_m,u_h^m\right) + f\left(\cdot,t_j,u_h^j\right), w_h \right\rangle_h \quad \forall w_h \in V_h$$

and

$$a\left(R^m - R^j, w\right) = \left\langle \psi_h^m - \psi_h^j - f\left(\cdot,t_m,u_h^m\right) + f\left(\cdot,t_j,u_h^j, w\right\rangle \quad \forall w \in H_0^1(\Omega).$$

Therefore, we may regard $u_h^m - u_h^j$ as a FE-approximation of $R^m - R^j$ and apply the a posteriori error estimator of §4.1. We get

$$\left\|\chi^j\right\|_{\infty,\Omega} \le \eta_*^j := \eta\left(V_h, u_h^m - u_h^j, \psi_h^m - \psi_h^j - f\left(\cdot,t_m,u_h^m\right) + f\left(\cdot,t_j,u_h^j\right)\right). \tag{31}$$

Hence

$$\eta_{\text{ell}}^{\text{E}} \le \kappa_0 \left(1+\beta_{m,0}\right) \eta^m + \sum_{j=1}^{m-1} \nu_{m,j} \eta_*^j. \tag{32}$$

Numerical test. We like to apply Theorem 3 to our test problem (5), which we associate with $L = \varepsilon^2 \frac{d^2}{dx^2} + r$ and $f(x,t,u) = -\varphi(x,t)$. As L is independent of time, we compute $\eta_{\text{ell}}^{\text{E}}$ using (32), (26) and (31) combined with $\psi_h^j = -\delta_t u_h^j$ (by (28)) and $f(\cdot,t_j,u_h^j) = -\varphi(\cdot,t_j)$. So η_{init}, η_{ell} and η_{t} are computable. Furthermore, for this problem (29) yields $\vartheta \equiv 0$ and $\psi_R - \bar{\psi}_R + \vartheta = -(\varphi - \bar{\varphi})$. So

$$\eta_{\text{osc}}^{\text{E}} = \kappa_0 \sum_{j=1}^{m} \beta_{m,j} \tau_j \left\|\varphi - \bar{\varphi}\right\|_{\infty,\Omega\times(t_{j-1},t_j]}.$$

This term captures the oscillations of the right-hand side φ and – like η_{init} – requires sampling.

For the spatial discretisation we use P_1-FEM on a Bakhvalov mesh with N mesh intervals and the error estimator derived in [15]. In that paper the integrals in (22) are approximated as follows

$$\langle v, w_h \rangle \approx \langle v, w_h \rangle_h := \left\langle v^I, w_h \right\rangle, \quad v \in C(\bar{\Omega}),\ w_h \in V_h,$$

where v^I is the piecewise linear nodal interpolant on the given spatial mesh. We balance the spatial and temporal accuracy by letting $N \sim \sqrt{M}$, because the method is first order in time, but second order in space.

Table 4 contains the results of our test computations for $\varepsilon = 10^{-6}$. It displays the actual errors (estimated by the double mesh principle), the rate of convergence, the value of the error estimator and the efficiency index (estimator divided by error). Additionally, it contains the various terms of the error estimator. The errors are overestimated by a factor of 6, but, most importantly, in contrast to the estimator from [12], no logarithmic dependence on the time-step size is observed.

4.3 The Crank-Nicolson method

We consider an arbitrary nonuniform mesh ω_t in the time direction and associate an approximate FEM solution $u_h^j \in V_h$ with the time level t_j and require it to satisfy

$$\begin{aligned}\left\langle \delta_t u_h^j, w_h \right\rangle_{V_h} &+ \tfrac{1}{2}\left\{ a_h^j\left(u_h^j, w_h\right) + a_h^{j-1}\left(u_h^{j-1}, w_h\right)\right\} \\ &+ \tfrac{1}{2}\left\langle f\left(\cdot, t_j, u_h^j\right) + f\left(\cdot, t_{j-1}, u_h^{j-1}\right), w_h \right\rangle_h = 0 \\ &\qquad \forall w_h \in V_h, \quad j = 1, \dots, M\end{aligned} \tag{33}$$

with an approximation $u_h^0 \in V_h$ of the initial condition u_0.

M	N	error rate	η^{E} C_{eff}	$\eta^{\mathrm{E}}_{\mathrm{init}}$ $\eta^{\mathrm{E}}_{\mathrm{t}}$	$\eta^{\mathrm{E}}_{\mathrm{osc}}$ $\eta^{\mathrm{E}}_{\mathrm{t},\dagger}$	$\eta^{\mathrm{E}}_{\mathrm{ell}}$ $\eta^{\mathrm{E}}_{\mathrm{t,W}}$
2^{10}	256	1.066e-03	6.773e-03	4.566e-05	1.965e-04	5.156e-03
		0.94	6.35	3.892e-05	8.854e-04	4.508e-04
2^{11}	360	5.543e-04	3.407e-03	2.309e-05	9.820e-05	2.597e-03
		0.99	6.15	1.949e-05	4.428e-04	2.258e-04
2^{12}	512	2.796e-04	1.685e-03	1.142e-05	4.909e-05	1.280e-03
		1.00	6.03	9.753e-06	2.214e-04	1.130e-04
2^{13}	728	1.402e-04	8.343e-04	5.646e-06	2.454e-05	6.320e-04
		0.97	5.95	4.879e-06	1.107e-04	5.652e-05
2^{14}	1024	7.157e-05	4.201e-04	2.854e-06	1.227e-05	3.190e-04
		0.99	5.87	2.440e-06	5.535e-05	2.827e-05
2^{15}	1448	3.604e-05	2.099e-04	1.427e-06	6.135e-06	1.593e-04
		0.99	5.82	1.220e-06	2.767e-05	1.414e-05
2^{16}	2048	1.811e-05	1.049e-04	7.135e-07	3.068e-06	7.960e-05
		—	5.79	6.101e-07	1.384e-05	7.069e-06

Table 4 Maximum-norm error at final time $t_M = T = 1/2$ for problem (5), $\varepsilon = 10^{-6}$. Fully discrete backward Euler.

Again, we estimate the maximum-norm error at time t_m, $m \le M$. Similar to the backward Euler discretisation we have

$$\|u_h^m - u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^m + \|R^m - u(\cdot,t_m)\|_{\infty,\Omega}\,.$$

For the second term on the right-hand side we will use (3) with $w = \hat{R}$. To this end we have to determine $K\hat{R}$.

From (24) and (33) we have

$$\partial_t \hat{u}_h(\cdot,t) = \delta_t u_h^j = -\tfrac{1}{2}\left(\psi_h^j + \psi_h^{j-1}\right), \ \ t \in (t_{j-1},t_j].$$

Introducing $\psi_R := L\hat{R} + f(\cdot,\cdot,\hat{R})$, we have

$$K\hat{R} = \partial_t \hat{R} + \psi_R = \partial_t\left(\hat{R} - \hat{u}_h\right) + \hat{\psi}_h - \tfrac{1}{2}\left(\psi_h^j + \psi_h^{j-1}\right) + \psi_R - \hat{\psi}_h \ \text{ in } (t_{j-1},t_j].$$

Let $\chi^j := R^j - u_h^j - \left(R^m - u_h^m\right)$, $j = 0,\dots,m$. Clearly, $\chi^m = 0$ and $\partial_t \hat{\chi} = \partial_t\left(\hat{R} - \hat{u}_h\right)$. Furthermore, cf. §3.2,

$$\hat{\psi}_h(\cdot,s) - \tfrac{1}{2}\left(\psi_h^j + \psi_h^{j-1}\right) = \left(s - t_{j-1/2}\right)\delta_t \psi_h^j, \quad s \in (t_{j-1},t_j].$$

Hence,

$$\left(K\hat{R}\right)(\cdot,s) = \partial_t \hat{\chi}(\cdot,s) + \left(s - t_{j-1/2}\right)\delta_t \psi_h^j + \left(\psi_R - \hat{\psi}_h\right)(\cdot,s), \quad s \in (t_{j-1},t_j].$$

Now fix $x \in \Omega$ and let again $\Gamma := G(x,t_m;\cdot,\cdot)$. Then, by (3) with $w := \hat{R}$, we have

$$\begin{aligned}
&R^m(x) - u(x,t_m) = \left(\hat{R} - u\right)(x,t_m)\\
&\quad = \left\langle \Gamma(\cdot,0), R^0 - u_0 \right\rangle + \int_0^{t_m} \langle \Gamma(\cdot,s), \partial_s \hat{\chi}(\cdot,s)\rangle \,\mathrm{d}s\\
&\qquad + \int_0^{t_m} \left\langle \Gamma(\cdot,s), \left(s - t_{j-1/2}\right)\delta_t \psi_h^j(\cdot,s) \right\rangle \mathrm{d}s + \int_0^{t_m} \langle \Gamma(\cdot,s), (\psi_R - \hat{\psi}_h)(\cdot,s)\rangle \,\mathrm{d}s.
\end{aligned}$$

The third term on the right-hand side is bounded using the argument from §3.2. We introduce $w_h^j := \tau_j^2 \delta_t \psi_h^j - \tau_m^2 \delta_t \psi_h^m$, $j = 1,\dots,m$, and bound

$$\begin{aligned}
&\frac{1}{2}\left| \int_0^{t_m} \left\langle \Gamma(\cdot,s), \left(s - t_{j-1/2}\right)\delta_t \psi_h^j(\cdot,s) \right\rangle \mathrm{d}s \right|\\
&\qquad \le \tau_m^2 \mu_m^{\mathrm{CN}} \|\delta_t \psi_h^m\|_{\infty,\Omega} + \sum_{j=1}^{m-1} \zeta_{m,j}^{\mathrm{CN}} \left\|\delta_t \psi_h^j\right\|_{\infty,\Omega} + \frac{1}{12}\sum_{j=1}^{m-1} \nu_{m,j} \left\|w_h^j\right\|_{\infty,\Omega}.
\end{aligned}$$

Applying integration by parts to the second integral on the right-hand side, we get

$$\begin{aligned}
&\left\langle \Gamma(\cdot,0), R^0 - u_0 \right\rangle + \int_0^{t_m} \langle \Gamma(\cdot,s), \partial_s \hat{\chi}(\cdot,s)\rangle \,\mathrm{d}s\\
&\qquad = \left\langle \Gamma(\cdot,0), u_h^0 - u_0 \right\rangle + \langle \Gamma(\cdot,0), R^m - u_h^m\rangle - \int_0^{t_m} \langle \partial_s \Gamma(\cdot,s), \hat{\chi}(\cdot,s)\rangle \,\mathrm{d}s.
\end{aligned}$$

This can be bounded as in §4.2. Also note, that

$$\|\hat{\chi}^j\|_{\infty,\Omega\times[t_{j-1},t_j]} = \max\left\{\left\|\chi^{j-1}\right\|_{\infty,\Omega}, \left\|\chi^j\right\|_{\infty,\Omega}\right\},$$

because $\hat{\chi}$ is linear on $[t_{j-1},t_j]$. Gathering these results, we obtain our a posteriori error estimator for the Crank-Nicolson scheme.

Theorem 4 *Let u_h^m be the approximation of $u(\cdot,t_m)$ obtained by* (33) *on the mesh ω_t. Then, under Assumption 1, one has*

$$\|u_h^m - u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^{\mathrm{CN}} := \eta_{\mathrm{init}} + \eta_{\mathrm{ell}}^{\mathrm{CN}} + \eta_{\mathrm{osc}}^{\mathrm{CN}} + \eta_{\mathrm{t}}^{\mathrm{CN}} + \eta_{\mathrm{t},\dagger}^{\mathrm{CN}} + \eta_{\mathrm{t,W}}^{\mathrm{CN}}$$

with η_{init} as in Theorem 3,

$$\eta_{\mathrm{ell}}^{\mathrm{CN}} := \kappa_0\,(1+\beta_{m,0})\,\eta^m + \sum_{j=1}^{m-1} \nu_{m,j} \max\left\{ \|\chi^{j-1}\|_{\infty,\Omega}\,, \|\chi^j\|_{\infty,\Omega} \right\},$$

$$\eta_{\mathrm{t}}^{\mathrm{CN}} := \sum_{j=1}^{m-1} \zeta_{m,j}^{\mathrm{CN}} \left\|\delta_t \psi_h^j\right\|_{\infty,\Omega}, \quad \eta_{\mathrm{t},\dagger}^{\mathrm{CN}} := \tau_m^2 \mu_m^{\mathrm{CN}} \|\delta_t \psi_h^m\|_{\infty,\Omega}\,,$$

$$\eta_{\mathrm{t,W}}^{\mathrm{CN}} := \frac{1}{12}\sum_{j=1}^{m-1} \nu_{m,j} \left\|w_h^j\right\|_{\infty,\Omega}, \quad \eta_{\mathrm{osc}}^{\mathrm{CN}} := \kappa_0 \sum_{j=1}^{m} \beta_{m,j}\tau_j\,\|\psi_R - \hat{\psi}_h\|_{\infty,\Omega\times(t_{j-1},t_j]}\,,$$

with ψ_h^j from (23)*, η^j from* (26) *and $w_h^j := \tau_j^2 \delta_t \psi_h^j - \tau_m^2 \delta_t \psi_h^m$, while $\psi_R = L\hat{R} + f(\cdot,\cdot,\hat{R})$ and $\chi^j = \left(R^j - u_h^j\right) - \left(R^m - u_h^m\right)$ are defined using* (25).

Numerical test. Once more, we consider (5). As L is independent of time, similarly to the backward Euler scheme, for χ^j we have (31), while $L\hat{R} = \hat{\psi}_h - \hat{f}(\cdot,\cdot,\hat{u}_h)$, so the oscillation term simplifies to

$$\eta_{\mathrm{osc}}^{\mathrm{CN}} = \kappa_0 \sum_{j=1}^{m} \beta_{m,j}\tau_j\,\|\varphi - \hat{\varphi}\|_{\infty,\Omega\times(t_{j-1},t_j]}\,.$$

Again this term requires sampling.

In space we use P_1-FEM (as in §4.3) on a Bakhvalov mesh with N mesh intervals and the error estimator from [15]. Because the method is second order both in time and in space, we let $N = 16M$,

Table 5 contains the results of our test computations for $\varepsilon = 10^{-6}$. It displays the actual errors, the rate of convergence, the value of the error estimator and the efficiency constant. It contains the various terms of the error estimator also. The errors are overestimated by a factor of ≈ 5.5. Similar to the backward Euler discretisation, there is no logarithmic dependence on the time-step size.

4.4 Fully discrete methods for the semilinear model problem

Consider the semilinear reaction-diffusion equation (2) in $\Omega \subset \mathbb{R}^n$, with $\rho \ge 0$. As discussed in §3.3, strictly speaking, the results of Theorems 3 and 4 do not apply to this problem in the general semilinear case. Nevertheless, using Assumption 1*, one can obtain a posteriori error estimates, similar to those in Theorems 3 and 4.

First, let u_h^m be the approximation of $u(\cdot,t_m)$ obtained by (27) on the mesh ω_t. We proceed as in §3.3, i.e. follow the proof of Theorem 3, arrive at (30), and then use

M	error	$\eta^{\rm CN}$	$\eta^{\rm CN}_{\rm init}$	$\eta^{\rm CN}_{\rm osc}$	$\eta^{\rm CN}_{\rm ell}$
	rate	$C_{\rm eff}$	$\eta^{\rm CN}_{t}$	$\eta^{\rm CN}_{\rm t,\dagger}$	$\eta^{\rm CN}_{\rm t,W}$
2^6	7.193e-05	3.855e-04	2.854e-06	7.424e-05	1.749e-04
	1.99	5.36	1.879e-06	9.750e-05	3.413e-05
2^7	1.815e-05	9.716e-05	7.135e-07	1.852e-05	4.424e-05
	1.99	5.35	4.632e-07	2.429e-05	8.929e-06
2^8	4.559e-06	2.440e-05	1.784e-07	4.627e-06	1.113e-05
	2.00	5.35	1.145e-07	6.062e-06	2.291e-06
2^9	1.142e-06	6.114e-06	4.459e-08	1.156e-06	2.790e-06
	2.00	5.35	2.841e-08	1.514e-06	5.811e-07
2^{10}	2.859e-07	1.530e-06	1.115e-08	2.890e-07	6.984e-07
	2.00	5.35	7.067e-09	3.783e-07	1.465e-07
2^{11}	7.153e-08	3.829e-07	2.787e-09	7.223e-08	1.747e-07
	2.00	5.35	1.762e-09	9.456e-08	3.678e-08
2^{12}	1.789e-08	9.575e-08	6.967e-10	1.806e-08	4.370e-08
	—	5.35	4.396e-10	2.364e-08	9.217e-09

Table 5 Maximum-norm error at final time $t_M = T = 1/2$ for problem (5), $\varepsilon = 10^{-6}$. Fully discrete Crank-Nicolson method, $N = 16M$.

the splitting $\partial_s\Gamma = \partial_s(\Gamma - g) + \partial_s g$, where, by Assumption 1*, $\partial_s(\Gamma - g)$ satisfies the second bound of (4), while $\int_0^T \|\partial_s g(x,t;\cdot,s)\|_{1,\Omega}\, ds \le \kappa_3$. Hence one gets

$$\|u_h^m - u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^{\rm E} + \kappa_3 \max_{j=1,\ldots,m}\Big(\tau_j \big\|\delta_t u_h^j\big\|_{\infty,\Omega} + \big\|\chi^j\big\|_{\infty,\Omega}\Big),$$

where $\eta^{\rm E}$ is the estimator from Theorem 3 (note that $\chi^m = 0$).

Let us discuss the computation of the components $\eta^{\rm E}_{\rm ell}$ and $\eta^{\rm E}_{\rm osc}$ of $\eta^{\rm E}$ in the semilinear case. It is convenient to associate the bilinear forms $a^j(\cdot,\cdot)$ and $a_h^j(\cdot,\cdot)$ in (23) and (24), as well as the elliptic estimator $\eta(\cdot,\cdot,\cdot)$ in (26), with the operator $L = -\varepsilon^2\Delta + \rho^2$. So we rewrite the equation $\partial_t u - \varepsilon^2\Delta u + f(\cdot,\cdot,u) = 0$ from (2) as $\partial_t u + Lu + \widetilde{f}(\cdot,\cdot,u) = 0$. So $\widetilde{f}(\cdot,\cdot,u) := f(\cdot,\cdot,u) - \rho^2 u$ will replace f in (23)–(26). Now, as L is independent of time, we compute $\eta^{\rm E}_{\rm ell}$ using (32), (26) and (31) combined with $\psi_h^j = -\delta_t u_h^j$ (by (28)) and $f(\cdot,t_j,u_h^j)$ replaced by $\widetilde{f}(\cdot,t_j,u_h^j)$. Next, consider $\eta^{\rm E}_{\rm osc}$, for which (29) yields $\psi_R - \bar\psi_R = f(\cdot,t,R^j) - f(\cdot,t_j,R^j)$ and $\|\vartheta(\cdot,t)\|_{\infty,\Omega\times(t_{j-1},t_j]} = \|\widetilde{f}(\cdot,t_j,R^j) - \widetilde{f}(\cdot,t_j,u_h^j)\|_{\infty,\Omega} \le (\bar\rho^2 - \rho^2)\eta^j$, Finally, $\psi_R - \bar\psi_R = f(\cdot,t,u_h^j) - f(\cdot,t_j,u_h^j) + O\big(\tau_j\eta^j\big)$ (see [12, Remark 8.4]).

Next, let u_h^m be the approximation of $u(\cdot,t_m)$ obtained by (33) on the mesh ω_t. By modifying the proof of Theorem 4 in a similar manner, one gets

$$\|U^m - u(\cdot,t_m)\|_{\infty,\Omega} \le \eta^{\rm CN} + \kappa_3 \max_{j=1,\ldots,m}\left(\frac{1}{8}\tau_j^2 \left\|\delta_t\psi_h^j\right\|_{\infty,\Omega} + \|\chi^j\|_{\infty,\Omega}\right), \qquad (34)$$

where $\eta^{\rm CN}$ and ψ_h^j are from Theorem 4.

Note also that the components $\eta^{\rm CN}$ in the semilinear case are computed similarly to the components of $\eta^{\rm E}$, with the exception of $\eta^{\rm CN}_{\rm osc}$, which now involves $\psi_R - \hat\psi_h$. As $L = -\varepsilon^2\Delta + \rho^2$ is independent of time, one has $L\hat R = \hat\psi_h - \hat f(\cdot,\cdot,\hat u_h)$. Consequently, $\psi_R - \hat\psi_h = f(\cdot,\cdot,\hat R) - \hat f(\cdot,\cdot,\hat u_h)$ can be bounded as described in [12, Remark 8.5].

Finally, we note that, in comparison with the estimators of Theorems 3 and 4, the additional terms in the above two estimators are of the expected order in time (1 and 2 respectively), and do not involve any logarithmic terms.

5 Conclusion

For linear and semilinear second-order parabolic equations, we have given a posteriori error estimates in the maximum norm that improve upon recent results in the literature. In particular, our estimators do not exhibit logarithmic dependence on the time step size. Numerical experiments support our theoretical findings.

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