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*PREPRINT 2002–01*

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NO 2002–01
ISSN 1404–4382

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Printed in Sweden
Chalmers University of Technology
Göteborg, Sweden 2002

# APPROXIMATION OF TIME DERIVATIVES FOR PARABOLIC EQUATIONS IN BANACH SPACE: CONSTANT TIME STEPS

YUBIN YAN

Abstract. We study smoothing properties and approximation of time derivatives for time discretization schemes with constant time steps for a homogeneous parabolic problem formulated as an abstract initial value problem in a Banach space. The time stepping schemes are based on using rational functions $r(z) \approx e^{-z}$ which are $A(\theta)$-stable for suitable $\theta \in [0, \pi/2]$ and satisfy $|r(\infty)| < 1$, and the approximations of time derivatives are based on using difference quotients in time. Both smooth and nonsmooth data error estimates of optimal order for the approximation of time derivatives are proved. Further, we apply the results to obtain error estimates of time derivatives in the supremum norm for fully discrete methods based on discretizing the spatial variable by a finite element method.

## 1. Introduction

In this paper, we consider single step time stepping methods for the following homogeneous linear parabolic problem

$$u_t + Au = 0 \quad \text{for } t > 0, \quad \text{with } u(0) = v, \tag{1.1.1}$$

in a Banach space $\mathcal{B}$. We first study the smoothing properties of the time stepping methods, then we consider approximations of time derivatives based on difference quotients of the approximate solutions of (1.1.1). Both smooth and nonsmooth data error estimates of the approximations of time derivatives are obtained. As an application we show error estimates in the supremum norm for fully discrete methods based on finite element methods in a spatial domain $\Omega \subset \mathbf{R}^2$.

We assume that $A$ is a closed, densely defined, linear operator defined in $\mathcal{D}(A) \subset \mathcal{B}$, that the resolvent set $\rho(A)$ of $A$ is such that, for some $\delta \in (0, \pi/2)$,

$$\rho(A) \supset \Sigma_\delta = \{z \in \mathbf{C} : \delta \le |\arg z| \le \pi, z \ne 0\} \cup \{0\}, \tag{1.1.2}$$

and that the resolvent, $R(z; A) = (zI - A)^{-1}$, satisfies

$$\|R(z; A)\| \le M|z|^{-1}, \quad \text{for } z \in \Sigma_\delta,\ z \ne 0, \quad \text{with } M \ge 1. \tag{1.1.3}$$

Throughout this paper $\|\cdot\|$ denotes both the norm in $\mathcal{B}$ and the norm of bounded linear operators on $\mathcal{B}$.

*Date*: February 21, 2002.

*Key words and phrases.* Banach space, parabolic, smoothing, time derivative, single step time stepping methods, fully discrete schemes, error estimates, finite element methods.

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We assume that $0 \in \rho(A)$ for simplicity, but this is not essential. In the case of $0 \notin \rho(A)$ we can add a multiple $\delta' u$ of $u$ to (1.1.1), thus replacing the operator $A$ by $A + \delta' I$ for some positive number $\delta' > 0$.

Under these assumptions $-A$ is the infinitesimal generator of a uniformly bounded analytic semigroup $E(t) = e^{-tA}$, $t \geq 0$, which is the solution operator of (1.1.1), so that $u(t) = E(t)v$. It may be represented as

$$E(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{-zt} R(z; A)\, dz,$$

where $\Gamma = \{\, z : |\arg z| = \psi \}$ with $\psi \in (\,\delta, \pi/2\,)$ and $\mathrm{Im} z$ decreasing along $\Gamma$. In particular the smoothing properties of analytic semigroups are valid, see, e.g., Pazy [13]. More precisely, we have

$$\|D_t^j E(t)v\| = \|A^j E(t)v\| \leq C_j t^{-j} \|v\|, \quad \text{for } t > 0,\ v \in \mathcal{B}, \tag{1.1.4}$$

which shows that the solution is regular for positive time even if the initial data are not.

Let $U^n$ be an approximation of the solution $u(t_n) = E(t_n)v$ of (1.1.1) at time $t_n = nk$, where $k$ is the time step, defined by a single step method,

$$U^n = E_k U^{n-1} \quad \text{for } n \geq 1, \quad \text{with } U^0 = v, \tag{1.1.5}$$

where $E_k = r(kA)$, and where the rational function $r(z)$ has no poles on $\sigma(kA)$. We may thus write $U^n = E_k^n v$.

We say that the time discretization scheme is accurate of order $p$, with $p \geq 1$, if

$$r(z) - e^{-z} = O(z^{p+1}), \quad \text{as } z \to 0. \tag{1.1.6}$$

For example, the backward Euler method, given by $r(z) = 1/(1+z)$, is first order accurate and the Crank-Nicolson method, defined by $r(z) = (1 - \frac{1}{2}z)/(1 + \frac{1}{2}z)$, is second order. As another example, the method defined by the $(q, q+1)$ subdiagonal Padé approximation $r(z) = p_1(z)/p_2(z)$, where $p_1$ and $p_2$ are certain polynomials of degrees $q$ and $q+1$, respectively, is accurate of order $2q+1$.

Stability and error estimates for single step methods have been studied by many authors, see, e.g., Bakaev [2], [3], Palencia [11], [12], Thomée [16] and references therein. For instance, if $A$ satisfies (1.1.2) and (1.1.3), and $r(z)$ is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, i.e., $|r(z)| \leq 1$ for $|\arg z| \leq \theta$, and (1.1.6) holds, then we have

$$\|U^n - u(t_n)\| = \|E_k^n v - E(t_n)v\| \leq C k^p \|A^p v\|, \quad \text{for } v \in \mathcal{D}(A^p), \tag{1.1.7}$$

see, e.g., Larsson, Thomée, and Wahlbin [9] and Crouzeix, Larsson, Piskarev, and Thomée [7]. Due to the assumption $v \in \mathcal{D}(A^p)$, we refer to this as a smooth data error estimate.

To obtain optimal order error estimates for nonsmooth initial data, the $A(\theta)$-stability of the scheme is not sufficient. However, if we require in addition that $|r(\infty)| < 1$, then the following nonsmooth data result is valid:

$$\|U^n - u(t_n)\| = \|E_k^n v - E(t_n)v\| \leq C k^p t_n^{-p} \|v\|, \quad \text{for } t_n > 0,\ v \in \mathcal{B}, \tag{1.1.8}$$

see, e.g., Larsson, Thomée, and Wahlbin [9] and Crouzeix, Larsson, Piskarev, and Thomée [7]. The condition $|r(\infty)| < 1$ ensures that oscillating components of the error are efficiently damped.

Let us recall some results about the smoothing properties of the time discretization schemes (1.1.5). When $\mathcal{B}$ is a Hilbert space $\mathcal{H}$ and $A$ a linear, selfadjoint, positive definite, unbounded operator, the following smoothing property holds for $A(0)$-stable time discretization schemes with $r(\infty) = 0$:

$$\|A^j U^n\| = \|A^j E_k^n v\| \le C_j t_n^{-j} \|v\|, \quad \text{for } t_n \ge t_j,\ v \in \mathcal{H}, \tag{1.1.9}$$

see, e.g., Thomée [16, Lemma 7.3]. Hansbo [8] extends this result to Banach space, and shows that, if $A$ satisfies (1.1.2) and (1.1.3), and $r(z)$ is $A(\theta)$-stable with $\theta \in (\delta, \frac{1}{2}\pi]$ and $r(\infty) = 0$, then (1.1.9) holds. Hansbo [8] also shows an optimal order error estimate in the nonsmooth data case for the approximation $(-A)U^n \approx (-A)u(t_n) = u_t(t_n)$ of the first order time derivative of the solution of (1.1.1). More precisely, if $r(z)$ is $A(\theta)$-stable with $\theta \in (\delta, \frac{1}{2}\pi]$ and $r(\infty) = 0$, then

$$\|(-A)U^n - u_t(t_n)\| \le C k^p t_n^{-p-1} \|v\|, \quad \text{for } t_n > 0,\ v \in \mathcal{B}. \tag{1.1.10}$$

However, we observe in Section 2 below that the smoothing property (1.1.9) is not valid when $r(\infty) \ne 0$. Therefore it is natural to investigate the smoothing properties of (1.1.5) when $r(\infty) \ne 0$. If $|r(\infty)| = 1$, the discrete method (1.1.5) is not smoothing. However, if such a method of order $p \ge 2$ is combined with a few steps of a smoothing method of order $p-1$, then we have nonsmooth data error estimate of order $p$. For instance, if one uses the Crank-Nicolson method combined with two steps of the backward Euler method, then a second order nonsmooth data error estimate holds. This analysis is carried out in Hilbert space by Luskin and Rannacher [10] and Rannacher [14]. Hansbo [8] extends the results to Banach space.

In the present paper we consider the case $|r(\infty)| < 1$. For fixed $j \ge 1$ we introduce the finite difference quotient,

$$Q_k^j U^n = \frac{1}{k^j} \sum_{\nu=-m_1}^{m_2} c_\nu U^{n+\nu}, \quad \text{for } n \ge m_1, \tag{1.1.11}$$

where $m_1, m_2$ are nonnegative integers, and $c_\nu$ are real numbers, such that the operator $Q_k^j$ is an approximation of order $p \ge 1$ to $D_t^j$, that is, for any smooth real-valued function $u$,

$$D_t^j u(t_n) = Q_k^j u^n + O(k^p), \quad \text{as } k \to 0, \quad \text{with } u^n = u(t_n). \tag{1.1.12}$$

As an example with $j = 1,\ m_1 = 1,\ m_2 = 0,\ p = 1$, we have

$$D_t u(t_n) = \frac{1}{k}(-u^{n-1} + u^n) + O(k), \quad \text{as } k \to 0.$$

As an example with $j = 2,\ m_1 = 1,\ m_2 = 1,\ p = 2$, we have

$$D_t^2 u(t_n) = \frac{1}{k^2}(u^{n-1} - 2u^n + u^{n+1}) + O(k^2), \quad \text{as } k \to 0.$$

In Theorem 2.5, we show that, if $A$ satisfies (1.1.2) and (1.1.3), and $r(z)$ is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$, then the following smoothing property holds:

$$\|Q_k^j U^n\| \le C t_n^{-j} \|v\|, \quad \text{for } n \ge m_1,\ t_n > 0,\ v \in \mathcal{B}. \tag{1.1.13}$$

Now let us turn to error estimates for approximations of time derivatives of the form (1.1.11). We show, in Theorem 2.1, the following smooth data error estimate for an $A(\theta)$-stable discretization scheme:

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C k^p \|A^{p+j} v\|, \quad \text{for } n \ge m_1,\ v \in \mathcal{D}(A^{p+j}). \tag{1.1.14}$$

To obtain an optimal order error estimate for nonsmooth data, the $A(\theta)$-stability is not suffient. Baker, Bramble, and Thomée [5] shows the following nonsmooth data error estimate in Hilbert space $\mathcal{H}$ by using a spectral argument: if $|r(\lambda)| \le 1$ for $\lambda \ge 0$, and $|r(\infty)| < 1$, then

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C k^p t_n^{-(p+j)} \|v\|, \quad \text{for } n \ge m_1,\ t_n > 0,\ v \in \mathcal{H}. \tag{1.1.15}$$

We extend in Theorem 2.6 this result to Banach space, that is, (1.1.15) also holds under the assumptions of Theorem 2.5.

The above results are proved under the assumption that the time step is constant. Some results for variable steps are presented in Yan [18].

Let us now discuss some properties of the coefficients $c_\nu$ in (1.1.11). With $u(t) = e^t$ in (1.1.12) we have at $t_n = 0$

$$k^j = P(e^k) + O(k^{p+j}), \quad \text{as } k \to 0, \quad \text{where } P(x) = \sum_{\nu=-m_1}^{m_2} c_\nu x^\nu. \tag{1.1.16}$$

Using Taylor expansion of $e^{\nu k}$ at $k = 0$, we therefore easily find that (1.1.12) is equivalent to

$$P(e^z) - z^j = O(z^{p+j}), \quad \text{as } z \to 0, \tag{1.1.17}$$

where $z$ is allowed to be complex-valued. For later use we note that (1.1.11) has the form

$$Q_k^j U^n = k^{-j} P(E_k) E_k^n v. \tag{1.1.18}$$

The paper is organized as follows. In Section 2, we show the smoothing properties of the abstract time stepping method, and give the optimal order error estimates of the approximation of the time derivatives for both smooth and nonsmooth data. In Section 3, we apply the results obtained in Section 2 to a fully discrete scheme. In Section 4, we give some numerical examples to illustrate our theoretical results.

By $C$ and $c$ we denote positive constants independent of the functions and parameters concerned, but not necessarily the same at different occurrences. When necessary for clarity we distinguish constants by subscripts.

## 2. Smoothing Properties and Error Estimates

In this section, we discuss smoothing properties of time stepping methods in the general Banach space situation and show smooth and nonsmooth data error estimates for the approximation $Q_k^j U^n$ of $D_t^j u(t_n)$ in the case of constant time steps, where $U^n$ is defined by (1.1.5), $u(t_n)$ is the solution of (1.1.1), and $Q_k^j$ is defined by (1.1.11).

We first show that (1.1.9) is not valid for a scheme with $r(\infty) \neq 0$. In fact, if $\mathcal{B}$ is a separable Hilbert space $\mathcal{H}$ and $A$ is a linear, selfadjoint, positive definite, unbounded operator, we have, by spectral representation,

$$t_n \|AE_k^n\| = t_n \|Ar(kA)^n\| = \sup_{\lambda \in \sigma(kA)} |n\lambda r(\lambda)^n| = \infty, \quad \text{for fixed } n \geq 1,$$

which implies that (1.1.9) does not hold for $j = 1$. Similar arguments work for any $j > 1$.

As an example of a scheme with $r(\infty) \neq 0$, we consider the $\theta$-method:

$$r(\lambda) = \frac{1 - (1-\theta)\lambda}{1 + \theta\lambda}, \quad \text{with } \frac{1}{2} < \theta < 1. \tag{2.2.1}$$

Here we have $|r(\lambda)| < 1$ for $\lambda > 0$, and $r(\infty) = (\theta - 1)/\theta \neq 0$. It is easy to check that $r(\lambda)$ is accurate of order $p = 1$.

Another example is the so called Calahan scheme defined by

$$r(\lambda) = 1 - \frac{\lambda}{1 + b\lambda} - \frac{\sqrt{3}}{6}\Big(\frac{\lambda}{1 + b\lambda}\Big)^2, \quad \text{with } b = \frac{1}{2}\Big(1 + \frac{\sqrt{3}}{3}\Big). \tag{2.2.2}$$

One can show that $|r(\lambda)| < 1$ for $\lambda > 0$, since $r(\lambda)$ is a decreasing function on $(0, \infty)$ and

$$r(\infty) = 1 - \frac{1}{b} - \frac{\sqrt{3}}{6}\frac{1}{b^2} = 1 - \sqrt{3} > -1.$$

A simple calculation shows that this scheme is accurate of order $p = 3$.

Before we study the smoothing properties of the discrete method (1.1.5), we will show an error estimate for the approximation (1.1.11) of the time derivative $D_t^j u(t_n)$ in the case that the initial data, and hence the solution of (1.1.1), are smooth. Recall the error estimate (1.1.7), which shows that for $v \in \mathcal{D}(A^p)$, the error $U^n - u(t_n)$ has the optimal order of accuracy. Similarly we find in the following theorem that if $v \in \mathcal{D}(A^{p+j})$, then the error estimate for the approximation of $D_t^j u(t_n)$ has the optimal order of accuracy.

**Theorem 2.1.** *Let $u(t_n)$ and $U^n$ be the solutions of* (1.1.1) *and* (1.1.5)*. Assume that $A$ satisfies* (1.1.2) *and* (1.1.3)*, and that $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$. Let $j \geq 1$ and assume that $Q_k^j$, defined in* (1.1.11)*, is an approximation of $D_t^j$, which is accurate of order $p$. Then there is a constant $C$ such that*

$$\|Q_k^j U^n - D_t^j u(t_n)\| \leq Ck^p \|A^{p+j} v\|, \quad \text{for } n \geq m_1,\ v \in \mathcal{D}(A^{p+j}).$$

To prove this theorem we need the following lemmas, which we quote from Thomée [16, Lemmas 8.1, 8.3].

**Lemma 2.2.** *Assume that* (1.1.2) *and* (1.1.3) *hold and let* $r(z)$ *be a rational function which is bounded for* $|\arg z| \le \psi$, $|z| \ge \epsilon > 0$, *where* $\psi \in (\delta, \pi/2)$, *and for* $|z| \ge R$ *with some positive number* $R$. *If* $\epsilon > 0$ *is so small that* $\{z : |z| \le \epsilon\} \subset \rho(A)$, *then we have*

$$r(A) = r(\infty)I + \frac{1}{2\pi i} \int_{\gamma_\epsilon \cup \Gamma_\epsilon^R \cup \gamma^R} r(z) R(z; A)\, dz,$$

*where* $\gamma_\epsilon = \{z : |z| = \epsilon, |\arg z| \le \psi\}$, $\Gamma_\epsilon^R = \{z : |\arg z| = \psi, \epsilon \le |z| \le R\}$, *and* $\gamma^R = \{z : |z| = R, \psi \le |\arg z| \le \pi\}$, *and with the closed path of integration oriented in the negative (clock-wise) sense.*

**Lemma 2.3.** *Assume that* (1.1.2) *and* (1.1.3) *hold, let* $\psi \in (\delta, \pi/2)$, *and* $j$ *be any integer. Then we have for* $\epsilon > 0$ *sufficiently small*

$$A^j E(t) = \frac{1}{2\pi i} \int_{\gamma_\epsilon \cup \Gamma_\epsilon} e^{-zt} z^j R(z; A)\, dz,$$

*where* $\gamma_\epsilon = \{z : |z| = \epsilon, |\arg z| \le \psi\}$ *and* $\Gamma_\epsilon = \{z : |\arg z| = \psi, |z| \ge \epsilon\}$, *and where* $\mathrm{Im} z$ *is decreasing along* $\gamma_\epsilon \cup \Gamma_\epsilon$. *When* $j \ge 0$, *we may take* $\epsilon = 0$.

*Proof of Theorem 2.1.* We have

$$Q_k^j U^n - D_t^j u(t_n) = k^{-j} \Big( P(r(kA)) r(kA)^n - (-kA)^j e^{-nkA} \Big),$$

where $P(x)$ is defined by (1.1.16). With

$$G_n(z) = P(r(z)) r(z)^n - (-z)^j e^{-nz}, \tag{2.2.3}$$

our result will follow from

$$\|G_n(kA)(kA)^{-(p+j)}\| \le C.$$

Note that with $A$ also $kA$ satisfies (1.1.2) and (1.1.3) since, for $z \in \Sigma_\delta$,

$$\|R(z; kA)\| = \|k^{-1}(zk^{-1}I - A)^{-1}\| \le k^{-1} M |zk^{-1}|^{-1} = M|z|^{-1}.$$

Therefore it suffices to show

$$\|G_n(A) A^{-(p+j)}\| \le C, \tag{2.2.4}$$

which we will prove now. Let $\bar{r}(z) = P(r(z)) r(z)^n z^{-(p+j)}$. Since $n \ge m_1$ and $r(z)$ is $A(\theta)$-stable, we find that $\bar{r}(z)$ is bounded for $|\arg z| \le \psi$, $|z| \ge \epsilon > 0$, with some $\psi \in (\delta, \theta)$. Further $\bar{r}(z)$ is also bounded for $|z| \ge R$ with $R$ sufficiently large since $\bar{r}(\infty) = 0$. Thus, applying Lemma 2.2 to the rational function $\bar{r}(z) = P(r(z)) r(z)^n z^{-(p+j)}$, we have

$$P(r(A)) r(A)^n A^{-(p+j)} = \frac{1}{2\pi i} \int_{\gamma_\epsilon \cup \Gamma_\epsilon^R \cup \gamma^R} P(r(z)) r(z)^n z^{-(p+j)} R(z; A)\, dz.$$

Since the integrand is of order $O(|z|^{-p-j-1})$ for large $z$, we may let $R$ tend to $\infty$. Using also Lemma 2.3 we conclude

$$G_n(A) A^{-(p+j)} = \frac{1}{2\pi i} \int_{\gamma_\epsilon \cup \Gamma_\epsilon} G_n(z) z^{-(p+j)} R(z; A)\, dz. \tag{2.2.5}$$

We shall show that

$$G_n(z) = O(z^{p+j}), \quad \text{as } z \to 0, \quad \text{with } |\arg z| \le \psi. \tag{2.2.6}$$

Assuming this and combining this with the fact that $0 \in \rho(A)$, we have that the integrand in (2.2.5) is bounded on the small domain with boundary $\gamma_\epsilon \cup \Gamma_0^\epsilon$, so that we may let $\epsilon \to 0$. It follows that

$$G_n(A)A^{-(p+j)} = \frac{1}{2\pi i}\int_\Gamma G_n(z)z^{-(p+j)}R(z;A)\,dz,$$

where $\Gamma = \{z : |\arg z| = \psi\}$. We now estimate the above integral. Again using (2.2.6) and the fact that $0 \in \rho(A)$, we find, for $\eta$ small enough,

$$\|G_n(z)R(z;A)\| \le C|z|^{p+j}, \quad \text{for } |z| \le \eta, \quad |\arg z| = \psi.$$

Further, noting that $P(r(z))r(z)^n$ is bounded on $\Gamma$, since $n \ge m_1$ and $r(z)$ is $A(\theta)$-stable, we have, using (1.1.3) and (2.2.3) as well as the boundedness of $e^{-nz}$ on $\Gamma$,

$$\|G_n(z)R(z;A)\| \le M(C + |z|^j)|z|^{-1}, \quad \text{for } |z| \ge \eta, \ |\arg z| = \psi.$$

Thus

$$\|G_n(A)A^{-(p+j)}\| \le C\int_0^\eta \rho^{p+j}\rho^{-(p+j)}\,d\rho + M\int_\eta^\infty (C+\rho^j)\rho^{-(p+j+1)}\,d\rho \le C.$$

It remains to prove (2.2.6). Since $r(z) = e^{-z} + O(z^2)$ as $z \to 0$, we have that, for $\tilde\eta > 0$ small enough,

$$|r(z)| \le e^{-c|z|}, \quad \text{for } |z| \le \tilde\eta, \quad |\arg z| \le \psi, \quad \text{with } 0 < c < 1. \tag{2.2.7}$$

Thus, using also (1.1.6),

$$\begin{aligned} |r(z)^n - e^{-nz}| &= \Big|(r(z) - e^{-z})\sum_{j=0}^{n-1} r(z)^{n-1-j}e^{-jz}\Big| \\ &\le Cn|z|^{p+1}e^{-c(n-1)|z|} \le C|z|^p, \quad \text{for } |z| \le \tilde\eta, \ |\arg z| \le \psi. \end{aligned} \tag{2.2.8}$$

Further, with $\tilde\eta$ possibly further restricted,

$$|P(r(z)) - (-z)^j| \le C|z|^{p+j}, \quad \text{for } |z| \le \tilde\eta. \tag{2.2.9}$$

In fact, by Taylor's formula, we have

$$\begin{aligned} P(r(z)) - P(e^{-z}) &= \sum_{l=1}^{j-1}\frac{P^{(l)}(e^{-z})}{l!}(r(z)-e^{-z})^l \\ &\quad + (r(z)-e^{-z})^j\int_0^1 \frac{(1-s)^{j-1}}{(j-1)!}P^{(j)}(r(z)+s(r(z)-e^{-z}))\,ds. \end{aligned}$$

Since $P(e^{-z})$ is an analytic function of $z$ and $P(e^{-z}) = O(z^j)$ as $z \to 0$ by (1.1.17), we have $P^{(l)}(e^{-z}) = O(z^{j-l})$, $0 \le l \le j$ as $z \to 0$. Moreover, since $r(z) \to 1$, $e^{-z} \to 1$ as $z \to 0$, it is easy to see that there exist constants $c_1 > 0$, $c_2 > 0$ and small $\tilde\eta$ such that $c_1 \le |r(z) + s(r(z) - e^{-z})| \le c_2$ for $|z| \le \tilde\eta$, $0 \le s \le 1$, which implies that $|P^{(j)}(r(z) +$

$s(r(z)-e^{-z}))| \le C$ for $|z| \le \tilde{\eta}$, $0 \le s \le 1$, since $P(x)$ has the form $P(x) = \sum_{\nu=-m_1}^{m_2} c_\nu x^\nu$. Thus, using also (1.1.6) we get

$$|P(r(z)) - P(e^{-z})| = \sum_{l=1}^{j-1} O(z^{j-l})O(z^{l(p+1)}) + O(z^{j(p+1)}) = O(z^{p+j}), \quad \text{as } z \to 0.$$

Combining this with (1.1.17) shows (2.2.9).

Thus, by (2.2.8) and (2.2.9),

$$\begin{aligned} |G_n(z)| &= \left|(P(r(z)) - (-z)^j)r(z)^n + (-z)^j(r(z)^n - e^{-nz})\right| \\ &\le C|z|^{p+j}, \quad \text{for } |z| \le \tilde{\eta}, \quad |\arg z| \le \psi, \end{aligned}$$

which is (2.2.6). □

We next prove a smoothing property for $A(\theta)$-stable discretization schemes with $|r(\infty)| < 1$. Before doing this, we show that $Q_k^j U^n$ defined by (1.1.11) can be expressed as a linear combination of the backward difference quotients $\bar{\partial}^j U^{n+\mu}$ for some integers $\mu$.

**Lemma 2.4.** *Let $j \ge 1$ and $Q_k^j U^n$ be defined by* (1.1.11)*. Then there exist constants $\alpha_\mu$, $-m_1 + j \le \mu \le m_2$, such that*

$$Q_k^j U^n = \sum_{\mu=-m_1+j}^{m_2} \alpha_\mu \bar{\partial}^j U^{n+\mu}, \quad \textit{where} \quad \bar{\partial} U^n = (U^n - U^{n-1})/k.$$

*Proof.* With $P(x) = \sum_{\nu=-m_1}^{m_2} c_\nu x^\nu$, we have

$$k^j Q_k^j U^n = \sum_{\nu=-m_1}^{m_2} c_\nu E_k^\nu U^n = P(E_k)U^n, \quad \text{where } E_k = r(kA),$$

i.e., the difference operator is associated with the rational function $P(x)$. Similarly the operator $k^j \bar{\partial}^j U^{n+\mu}$ corresponds to the rational function $\tilde{P}(x) = x^\mu(1-x^{-1})^j$, since

$$k^j \bar{\partial}^j U^{n+\mu} = (1 - E_k^{-1})^j E_k^{n+\mu} v = (I - E_k^{-1})^j E_k^\mu U^n = \tilde{P}(E_k)U^n.$$

Thus we only need to show that there exist $\alpha_\mu$ such that

$$P(x) = \sum_{\mu=-m_1+j}^{m_2} \alpha_\mu \tilde{P}(x) = (1-x^{-1})^j \sum_{\mu=-m_1+j}^{m_2} \alpha_\mu x^\mu. \tag{2.2.10}$$

But by (1.1.17) we find $P^{(l)}(1) = 0$ for $0 \le l \le j-1$, which implies that $P(x)$, and hence $x^{m_1}P(x)$ contains the factor $(x-1)^j$, that is, there exists a polynomial $\bar{P}(x)$ of degree $m_1 + m_2 - j$ such that $x^{m_1}P(x) = (x-1)^j \bar{P}(x)$. Denoting $\bar{P}(x) = \sum_{k=0}^{m_1+m_2-j} \beta_k x^k$ for some constants $\beta_k$, we get that there exist constants $\alpha_\mu$ such that

$$x^{m_1}P(x) = (x-1)^j \sum_{k=0}^{m_1+m_2-j} \beta_k x^k = (x-1)^j \sum_{\mu=-m_1+j}^{m_2} \alpha_\mu x^{\mu+m_1-j},$$

which shows (2.2.10). □

**Theorem 2.5.** *Let $U^n$ be the solution of* (1.1.5). *Assume that* (1.1.2) *and* (1.1.3) *hold, and $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$. Let $j \geq 1$ and assume that $Q_k^j$, defined in* (1.1.11), *is an approximation of $D_t^j$, which is accurate of order $p$. Then there is a constant $C$ such that*

$$\|Q_k^j U^n\| \leq C t_n^{-j} \|v\|, \quad \text{for } n \geq m_1,\ t_n > 0,\ v \in \mathcal{B}.$$

*Proof.* By Lemma 2.4, it suffices to show

$$\|\bar{\partial}^j U^n\| \leq C t_n^{-j} \|v\|, \quad \text{for } n \geq j. \tag{2.2.11}$$

In fact, this implies, for $n \geq m_1,\ t_n > 0$,

$$\begin{aligned}\|Q_k^j U^n\| = \Big\| \sum_{\mu=-m_1+j}^{m_2} \alpha_\mu \bar{\partial}^j U^{n+\mu} \Big\| &\leq C \sum_{\mu=-m_1+j}^{m_2} t_{n+\mu}^{-j} \|v\| \\ &\leq C t_{n-m_1+j}^{-j} \|v\| \leq C t_n^{-j} \|v\|.\end{aligned}$$

We know show (2.2.11). Noting that $\bar{\partial}^j U^n = k^{-j} \tilde{P}(E_k) E_k^n v$ for $\tilde{P}(x) = (1 - x^{-1})^j = x^{-j}(x-1)^j$, we need to show

$$\|\tilde{P}(r(A)) r(A)^n\| = \|r(A)^{n-j}(r(A) - 1)^j\| \leq C n^{-j}, \quad \text{for } n \geq j.$$

As in the proof of Theorem 2.1 this then also holds with $A$ replaced by $kA$, and thus shows (2.2.11).

Since $n \geq j$ and $r(z)$ is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$ and $|r(\infty)| < 1$, which implies that $r(z)^{n-j}(r(z)-1)^j$ is bounded for $|\arg z| \leq \psi,\ |z| \geq \epsilon$ with some $\psi \in (\delta, \theta)$ and arbitrary $\epsilon > 0$, and also bounded for $|z| \geq R$ with $R$ sufficiently large, we therefore have, by Lemma 2.2,

$$\begin{aligned} r(A)^{n-j}(r(A)-1)^j = & r(\infty)^{n-j}(r(\infty)-1)^j I \\ & + \frac{1}{2\pi i} \int_{\gamma_\epsilon \cup \Gamma_\epsilon^R \cup \gamma^R} r(z)^{n-j}(r(z)-1)^j R(z; A)\, dz. \end{aligned}$$

By $|r(\infty)| < 1$, we have, for fixed $R \geq 1$ large enough,

$$|r(z)| \leq e^{-c}, \quad \text{for } |z| \geq R. \tag{2.2.12}$$

Clearly then $|r(\infty)| \leq e^{-c}$, so that

$$|r(\infty)^{n-j}(r(\infty)-1)^j| \leq C e^{-cn} \leq C n^{-j}, \quad \text{for } n \geq 1.$$

To bound the integrals over the three components of the path of integration, we have, by (2.2.12),

$$\Big\| \frac{1}{2\pi i} \int_{\gamma^R} r(z)^{n-j}(r(z)-1)^j R(z; A)\, dz \Big\| \leq C e^{-cn} \int_{\gamma^R} \frac{|dz|}{|z|} \leq C n^{-j}, \quad \text{for } n \geq 1.$$

For the other two components of the path of integration, since $r(z)$ is $A(\theta)$-stable and $0 \in \rho(A)$ and accurate of order $p \geq 1$, which imply that the integrand is bounded on the small domain with boundary $\gamma_\epsilon \cup \Gamma_0^\epsilon$, we may let $\epsilon$ tend to 0. Thus it suffices to bound the integral over $\Gamma_0^R$. But by $A(\theta)$-stability and the maximum-principle we have $|r(z)| < 1$ for

$|\arg z| < \theta,\ z \neq 0$. In particular, $|r(z)| < 1$ on the compact set $\{z : \tilde{\eta} \leq |z| \leq R,\ |\arg z| \leq \psi\}$, which means that the inequality (2.2.7) also holds for $|z| \leq R,\ |\arg z| \leq \psi$ with $c$ sufficiently small. Thus, we have, noting that $r(z) - 1 = O(z)$ as $z \to 0$,

$$\Big\| \frac{1}{2\pi i} \int_{\Gamma_0^R} r(z)^{n-j} (r(z)-1)^j R(z;A)\, dz \Big\| \leq C \int_0^R e^{-cn\rho} \rho^{j-1}\, d\rho \leq C n^{-j}.$$

Together these estimates complete the proof. □

We remark that if $|r(\infty)| = 1$ with $r(\infty) \neq 1$, then the conclusion of Theorem 2.5 is not valid. For example, let us consider the Crank-Nicolson scheme, with $r(\infty) = -1$. Assume that $A$ is a linear selfadjoint, positive definite, unbounded operator with compact inverse in Hilbert space $\mathcal{H}$, and $A$ has eigenvalues $\{\lambda_j\}_{j=1}^{\infty}$ and a corresponding basis of orthonormal eigenvectors $\{\varphi_j\}_{j=1}^{\infty}$. Then, with $v = \varphi_j$, we have, noting that $r(\infty) = -1$,

$$\begin{aligned} t_n \|\bar{\partial} U^n\| &= n \|r(kA)^{n-1}(r(kA) - 1)v\| \\ &= n |r(k\lambda_j)^{n-1}(r(k\lambda_j) - 1)| \to 2n, \quad \text{as } j \to \infty, \end{aligned}$$

which implies that there does not exist a constant $C$ such that

$$t_n \|\bar{\partial} U^n\| \leq C \|v\|, \quad \text{for } n \geq 1, \quad v \in \mathcal{H}.$$

However, if $r(\infty) = 1$, then the conclusion of Theorem 2.5 holds in special cases: Let us consider the $(2, 2)$ Padé scheme,

$$r(\lambda) = \frac{1 - \frac{1}{2}\lambda + \frac{1}{12}\lambda^2}{1 + \frac{1}{2}\lambda + \frac{1}{12}\lambda^2}, \quad \text{where } r(\infty) = 1. \tag{2.2.13}$$

We show that in this case $t_n \|\bar{\partial} U^n\| \leq C \|v\|$. In fact, for this it suffices to show

$$|n r(\lambda)^{n-1}(r(\lambda) - 1)| \leq C, \quad \text{for } \lambda > 0. \tag{2.2.14}$$

For small $\lambda$ this follows directly from the fact that $|r(\lambda)| \leq e^{-c\lambda},\ |r(\lambda) - 1| \leq C\lambda$ for $0 \leq \lambda \leq \lambda_0$ and it remains to consider large $\lambda$. Noting that $|r(\lambda)| \leq e^{-c\lambda^{-1}}$ with some constant $c$ and $|r(\lambda) - 1| \leq C\lambda^{-1}$ for $\lambda > \lambda_0$, see, e.g., Thomée [16, Lemma 8.2], we have

$$|n r(\lambda)^{n-1}(r(\lambda) - 1)| \leq C(n\lambda^{-1}) e^{-c(n-1)\lambda^{-1}} \leq C,$$

which shows (2.2.14).

Our next result is an error estimate in the nonsmooth data case. The estimate has optimal order of accuracy for $t_n$ bounded away from zero, but contains a negative power of $t_n$. Comparing with the error estimate (1.1.8), we find that $t_n^{-p}$ is replaced by $t_n^{-p-j}$ in our theorem. The proof in the Hilbert space case can be found in Baker, Bramble, and Thomée [5]. Here we extend the result to Banach space.

**Theorem 2.6.** *Let $u(t_n)$ and $U^n$ be the solutions of* (1.1.1) *and* (1.1.5)*. Assume that* (1.1.2) *and* (1.1.3) *hold, and $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$. Let $j \geq 1$ and assume that $Q_k^j$, defined in* (1.1.11)*, is an approximation of $D_t^j$, which is accurate of order $p$. Then there is a constant $C$ such that*

$$\|Q_k^j U^n - D_t^j u(t_n)\| \leq C k^p t_n^{-(p+j)} \|v\|, \quad \textit{for } n \geq m_1,\ t_n > 0,\ v \in \mathcal{B}.$$

To prove this theorem, we need the following lemma, which we quote from Thomée [16, Lemma 8.5].

**Lemma 2.7.** *Assume that the rational function $r(z)$ is $A(\theta)$-stable with $\theta \le \pi/2$, and that $|r(\infty)| < 1$. Then for any $\psi \in (0, \theta)$ and $R > 0$ there are positive $C$ and $c$ such that, with $\kappa = r(\infty)$,*

$$|r(z)^n - \kappa^n| \le C|z|^{-1}e^{-cn}, \quad \text{for } |z| \ge R,\ |\arg z| \le \psi,\ n \ge 1.$$

*Proof of Theorem 2.6.* As above we now need to show, with $G_n(z)$ given by (2.2.3),

$$\|G_n(A)\| \le Cn^{-(p+j)}.$$

We set $\kappa = r(\infty)$ and

$$\tilde{G}_n(z) = G_n(z) - P(\kappa)\kappa^n z/(1+z).$$

Obviously $\tilde{G}_n(\infty) = 0$. Since $|\kappa| < 1$, we have $|\kappa| \le e^{-c}$ for some $c > 0$. Noting that $\|A(I+A)^{-1}\| \le 2M$, we have, since $n \ge m_1,\ n \ge 1$,

$$\begin{aligned}\|P(\kappa)\kappa^n A(I+A)^{-1}\| \le 2M|P(\kappa)\kappa^n| &\le 2M\Big|\sum_{\nu=-m_1}^{m_2} c_\nu e^{-c(n+\nu)}\Big| \\ &\le Ce^{-cn} \le Cn^{-(p+j)}.\end{aligned}$$

It remains to show the same bound for the operator norm of $\tilde{G}_n(A)$. We may now use Lemmas 2.2 and 2.3 to see that, with $\psi \in (\delta, \theta)$,

$$\tilde{G}_n(A) = \frac{1}{2\pi i}\int_{\gamma_\epsilon \cup \Gamma_\epsilon} \tilde{G}_n(z)R(z;A)\,dz.$$

Since $n \ge m_1$ and $r(z)$ is $A(\theta)$-stable and $0 \in \rho(A)$, the integrand is bounded on the small domain with boundary $\gamma_\epsilon \cup \Gamma_0^\epsilon$, so that we may let $\epsilon$ tend to 0. We therefore have, with $\Gamma = \{\, z : \ |\arg z| = \psi \,\}$,

$$\tilde{G}_n(A) = \frac{1}{2\pi i}\int_{\Gamma} \tilde{G}_n(z)R(z;A)\,dz.$$

We write

$$\tilde{G}_n(z) = \Big(P(r(z)) - (-z)^{-j}\Big)r(z)^n + (-z)^j\Big(r(z)^n - e^{-nz}\Big) - P(\kappa)\kappa^n z/(1+z).$$

Using the estimates (2.2.7), (2.2.8), (2.2.9) and $|1/(1+z)| \le 1$ for $\mathrm{Re}\, z \ge 0$ and the boundedness of $R(z;A)$, we have, for $z \in \Gamma,\ |z| \le 1,\ n \ge 1$,

$$\|\tilde{G}_n(z)R(z;A)\| \le \Big(C|z|^{p+j}e^{-cn|z|} + |z|^j(Cn|z|^{p+1}e^{-cn|z|})\Big) + C\kappa^n \le Cn^{-p-j}.$$

Further, we rewrite

$$\tilde{G}_n(z) = \Big(P(r(z))r(z)^n - P(\kappa)\kappa^n\Big) + P(\kappa)\kappa^n/(1+z) - (-z)^j e^{-nz}.$$

By Lemma 2.7 we have, for $z \in \Gamma,\ |z| \geq 1$ and $n \geq m_1$,

$$\begin{aligned}|P(r(z))r(z)^n - P(\kappa)\kappa^n| &= \Big| \sum_{\nu=-m_1}^{m_2} c_\nu \Big( r(z)^{n+\nu} - \kappa^{n+\nu} \Big) \Big| \\ &\leq C|z|^{-1} \sum_{\nu=-m_1}^{m_2} |c_\nu| e^{-c(n+\nu)} \\ &\leq C|z|^{-1} e^{-c(n-m_1)} \leq C|z|^{-1} e^{-cn}.\end{aligned}$$

Thus, since $|1+z| \geq |z|$ for $\mathrm{Re} z \geq 0$, we get, for $z \in \Gamma,\ |z| \geq 1,\ n \geq m_1$ and $n \geq 1$,

$$\begin{aligned}\|\tilde{G}_n(z) R(z;A)\| &\leq \Big( C|z|^{-1} e^{-cn} + \kappa^n |z|^{-1} \Big) |z|^{-1} + C|z|^{-p-1} |z|^{p+j} e^{-cn|z|} \\ &\leq Cn^{-p-j} (|z|^{-2} + |z|^{-p-1}) \leq Cn^{-p-j} |z|^{-2}.\end{aligned}$$

We therefore obtain

$$\|\tilde{G}_n(A)\| \leq \int_0^1 Cn^{-p-j}\, d\rho + \int_1^\infty Cn^{-p-j} \rho^{-2}\, d\rho \leq Cn^{-p-j}.$$

Together these estimates complete the proof. □

## 3. Fully Discrete Schemes

In this section we study fully discrete schemes of the initial boundary value problem

$$\left\{ \begin{array}{l} u_t = \Delta u \quad \text{in } \Omega, \quad \text{for } t > 0, \\ u = 0 \quad \text{on } \partial\Omega, \quad \text{for } t > 0, \quad u(\cdot, 0) = v \quad \text{in } \Omega, \end{array} \right. \tag{3.3.1}$$

where $\Omega$ is a bounded domain in $\mathbf{R}^2$ with smooth boundary $\partial\Omega$.

Let $L_p = L_p(\Omega)$ denote the usual real Lebesgue spaces with norms

$$\|v\|_{L_p} = \left\{ \begin{array}{l} \Big( \int_\Omega |v(x)|^p\, dx \Big)^{\frac{1}{p}},\ 1 \leq p < \infty, \\ \operatorname{ess\,sup}\{|v(x)| : x \in \Omega\},\ p = \infty, \end{array} \right. \tag{3.3.2}$$

and let $k$ be a nonnegative integer and let $W_p^k = W_p^k(\Omega)$ be the standard real Sobolev spaces with norms $\|\cdot\|_{W_p^k}$ defined by

$$\|v\|_{W_p^k} = \Big( \sum_{|\alpha| \leq k} \|D^\alpha v\|_{L_p}^p \Big)^{\frac{1}{p}},$$

for $1 \leq p \leq \infty$ with the usual modification in the case $p = \infty$. In the case $p = 2$, we set $H^k = W_2^k$, which is a Hilbert space with the inner product

$$(v, w)_{H^k} = \sum_{|\alpha| \leq k} \int_\Omega D^\alpha v D^\alpha w\, dx.$$

Moreover we denote $H_0^1 = \{v \in H^k :\ v = 0 \text{ on } \partial\Omega\}$, and $\dot{W}_p^k = \{v \in W_p^k :\ (-\Delta)^l v = 0 \text{ on } \partial\Omega,\ \text{for } l < k/2\}$.

In (3.3.1), we consider $A = -\Delta$ with $\mathcal{D}(A^j) = \dot{W}_p^{2j}$ for $j \geq 1$. It is known that $\Delta$ generates a strongly continuous and analytic semigroup $E(t) = e^{t\Delta}$ in $L_p$ for $1 < p < \infty$, but for $p = \infty$ the strong continuity at $t = 0$ is lost. Nevertheless, the corresponding stability and smoothing estimates are valid:

$$\|E(t)v\|_{L_p} + \|E'(t)\|_{L_p} \leq Ct^{-1}\|v\|_{L_p}, \quad \text{for } v \in L_p,\ 2 \leq p \leq \infty, \tag{3.3.3}$$

see, e.g., Thomée [16, Chapter 5] for more details.

We assume that $\Omega$ is approximated by a quasi-uniform family of triangular finite element meshes $\tau_h$ such that the union of the elements determines a polygonal domain $\Omega_h$ with boundary nodes on $\partial\Omega$. For simplicity we assume that $\Omega$ is convex and let $S_h$ be the space of continuous functions that are linear on each element and vanish outside $\Omega_h$, so that $S_h \subset H_0^1$. We define the discrete Laplacian $\Delta_h$ by

$$(\Delta_h \psi, \chi) = -(\nabla\psi, \nabla\chi), \quad \forall \psi, \chi \in S_h. \tag{3.3.4}$$

The spatially semidiscrete problem is then to find $u_h : [0, \infty) \to S_h$, such that

$$u_{h,t} = \Delta_h u_h, \quad \text{for } t > 0, \quad \text{with } u_h(0) = v_h, \tag{3.3.5}$$

where $v_h \in S_h$ is some approximation of $v$. Let $P_h$ denote the orthogonal projection of $v$ onto $S_h$ with respect to the inner product to the $L_2$ norm, i.e.,

$$(P_h v, \chi) = (v, \chi), \quad \forall \chi \in S_h, \quad \text{for } v \in L_2. \tag{3.3.6}$$

We also need the so called elliptic or Ritz projection $R_h$ onto $S_h$ defined as the orthogonal projection with respect to the inner product $(\nabla v, \nabla w)$, so that

$$(\nabla R_h v, \nabla\chi) = (\nabla v, \nabla\chi), \quad \forall \chi \in S_h, \quad \text{for } v \in H_0^1. \tag{3.3.7}$$

Note that

$$\Delta_h R_h = P_h \Delta, \tag{3.3.8}$$

which we need in the proof of our theorems.

We now apply our above time stepping procedure (1.1.5) to this semidiscrete equation (3.3.5). This defines the fully discrete approximation $U^n \in S_h$ of $u(t_n)$ recursively by

$$U^n = E_{kh}U^{n-1}, \quad \text{for } n \geq 1, \quad \text{where } E_{kh} = r(-k\Delta_h), \quad \text{with } U^0 = v_h. \tag{3.3.9}$$

We shall derive $L_\infty$ error estimates for the approximations $Q_k^j U^n$ of the time derivatives $D_t^j u(t_n)$ of the solution of (3.3.1), where $U^n$ is defined by (3.3.9). We first show some $L_\infty$ error estimates in the spatially semidiscrete case. We begin with an error estimate in the nonsmooth data case.

**Theorem 3.1.** *Let $u(t)$ and $u_h(t)$ be the solutions of* (3.3.1) *and* (3.3.5) *and $j \geq 0$. If $v \in L_\infty$ and $v_h = P_h v$, then we have*

$$\|D_t^j u_h(t) - D_t^j u(t)\|_{L_\infty} \leq Ch^2 \ell_h^2 t^{-j-1}\|v\|_{L_\infty}, \quad \text{where } \ell_h = \ln(1/h).$$

The proof of the result depends on the following lemmas. The first lemma concerns error bounds for the $L_2$ and Ritz projections in maximum-norm.

**Lemma 3.2.** *Let $u(t)$ be the solution of* (3.3.1) *and* $j \geq 0$. *Then, we have, for* $\rho = (R_h - I)u$ *and* $\eta = (P_h - I)u$ ,

$$t^{j+1}\Big(\|D_t^j\rho(t)\|_{L_\infty} + \ell_h\|D_t^j\eta(t)\|_{L_\infty}\Big) \leq Ch^2\ell_h^2\|v\|_{L_\infty}. \tag{3.3.10}$$

*Proof.* With $I_h : C(\bar{\Omega}) \to S_h$ the standard Lagrange interpolation operator, we have, see, e.g., Brenner and Scott [6],

$$\|I_h u - u\|_{L_\infty} \leq Ch^{2-2/s}\|u\|_{W_s^2}, \quad \text{for } 2 \leq s \leq \infty,\ u \in \dot{W}_s^2.$$

Since $D_t^j\rho = (R_h - I)D_t^j u = (R_h - I)(I - I_h)D_t^j u$, using the logarithmic maximum-norm stability of $R_h$, i.e., $\|R_h u\|_{L_\infty} \leq C\ell_h\|u\|_{L_\infty}$, see, e.g., Schatz and Wahlbin [15], we have,

$$\|D_t^j\rho\|_{L_\infty} \leq C\ell_h\|(I - I_h)D_t^j u\|_{L_\infty} \leq C\ell_h h^{2-2/s}\|D_t^j u\|_{W_s^2}.$$

By the Agmon-Douglis-Nirenberg [1] regularity estimate

$$\|u\|_{W_s^2} \leq Cs\|\Delta u\|_{L_s}, \quad \text{for } 2 \leq s < \infty,\ u \in \dot{W}_s^2,$$

we hence obtain, using also the smoothing property (3.3.3),

$$\begin{aligned}\|D_t^j\rho(t)\|_{L_\infty} &\leq Ch^{2-2/s}\ell_h s\|\Delta D_t^j u(t)\|_{L_s}\\ &\leq Ch^{2-2/s}\ell_h s t^{-j-1}\|v\|_{L_s} \leq Ch^{2-2/s}\ell_h s t^{-j-1}\|v\|_{L_\infty}.\end{aligned}$$

With $s = \ell_h$ this shows the bound in (3.3.10) for $D_t^j\rho(t)$. The proof of the bound for $D_t^j\eta(t)$ is analogous, with one less factor $\ell_h$ because $P_h$ is bounded in $L_\infty$, see Thomée [16, Lemma 5.7]. □

We also need the following lemma which shows that the discrete solution operator $E_h(t) = e^{t\Delta_h}$ is stable in the $L_\infty$ norm and has a smoothing property, uniformly in $h$, see Thomée and Wahlbin [17], and Bakaev, Thomée, and Wahlbin [4].

**Lemma 3.3.** *Let $E_h(t)$ be the solution operator of* (3.3.5). *Then*

$$\|E_h(t)v_h\|_{L_\infty} + t\|E_h'(t)v_h\|_{L_\infty} \leq C\|v_h\|_{L_\infty}, \quad \textit{for}\ t > 0. \tag{3.3.11}$$

*Proof of Theorem 3.1.* We write $u_h - u = (u_h - P_h u) + (P_h u - u) = \zeta + \eta$. Here $D_t^j\eta$ is bounded as desired by Lemma 3.2 and it remains to bound $\zeta^{(j)} = D_t^j\zeta = D_t^j(u_h - P_h u)$. We will show, by induction, that for each $j \geq 0$ there is $C$, such that

$$\sup_{0\leq s\leq t}\,(s^{j+1}\|\zeta^{(j)}(s)\|_{L_\infty}) \leq Ch^2\ell_h^2\|v\|_{L_\infty}. \tag{3.3.12}$$

The case $j = 0$ can be found in Thomée [16, Theorem 5.4]. Assuming now that the result is already shown with $j$ replaced by $j - 1$. Since

$$\zeta_t - \Delta_h\zeta = -\Delta_h P_h\rho,$$

we find

$$\begin{aligned}(t^{j+1}\zeta^{(j)})_t - \Delta_h(t^{j+1}\zeta^{(j)}) &= (j+1)t^j\zeta^{(j)} + t^{j+1}(\zeta_t^{(j)} - \Delta_h\zeta^{(j)})\\ &= (j+1)t^j(\Delta_h\zeta^{(j-1)} - \Delta_h P_h\rho^{(j-1)}) - t^{j+1}\Delta_h P_h\rho^{(j)}.\end{aligned} \tag{3.3.13}$$

Thus, by Duhamel's principle, we have, noting that $E_h(t-s)\Delta_h = E_h'(t-s)$,

$$\begin{aligned} t^{j+1}\zeta^{(j)}(t) = \int_0^t E_h'(t-s)\Big((j+1)s^j\zeta^{(j-1)}(s) \\ - (j+1)s^j P_h\rho^{(j-1)}(s) - s^{j+1}P_h\rho^{(j)}(s)\Big)ds = I + II + III. \end{aligned}$$

For $II$, we write

$$II = -\Big(\int_0^{t/2} + \int_{t/2}^t\Big)E_h'(t-s)(j+1)s^jP_h\rho^{(j-1)}(s)\,ds = II_1 + II_2.$$

Here, using Lemmas 3.2 and 3.3,

$$\|II_1\|_{L_\infty} \le C\int_0^{t/2}(t-s)^{-1}s^j\|\rho^{(j-1)}(s)\|_{L_\infty}\,ds \le Ch^2\ell_h^2\|v\|_{L_\infty}.$$

Further, after integration by parts,

$$\begin{aligned} II_2 =& \Big[E_h(t-s)(j+1)s^jP_h\rho^{(j-1)}(s)\Big]_{t/2}^t \\ &- \int_{t/2}^t E_h(t-s)(j+1)P_h\Big(js^{j-1}\rho^{(j-1)}(s) + s^j\rho^{(j)}(s)\Big)\,ds, \end{aligned}$$

and thus by Lemmas 3.2 and 3.3, we get

$$\|II_2\|_{L_\infty} \le Ch^2\ell_h^2\|v\|_{L_\infty}.$$

Therefore $\|II\|_{L_\infty} \le Ch^2\ell_h^2\|v\|_{L_\infty}$. Following the estimate of $II$, we can also show $\|III\|_{L_\infty} \le Ch^2\ell_h^2\|v\|_{L_\infty}$.

Now we turn to $I$, and write, with $a > 1$,

$$I = \Big(\int_0^{t/a} + \int_{t/a}^t\Big)E_h'(t-s)(j+1)s^j\zeta^{(j-1)}(s)\,ds = I_1 + I_2.$$

Here, using Lemma 3.3 and the induction assumption, we have

$$\|I_1\|_{L_\infty} \le C\int_0^{t/a}(t-s)^{-1}s^j\|\zeta^{(j-1)}(s)\|_{L_\infty}\,ds \le C\ln(\frac{a}{a-1})h^2\ell_h^2\|v\|_{L_\infty}.$$

Further, after integration by parts,

$$\begin{aligned} I_2 =& -\Big[E_h(t-s)(j+1)s^j\zeta^{(j-1)}(s)\Big]_{t/a}^t \\ &+ \int_{t/a}^t E_h(t-s)(j+1)s^{-1}(js^j\zeta^{(j-1)}(s) + s^{j+1}\zeta^{(j)}(s))\,ds. \end{aligned}$$

By Lemma 3.3 and the induction assumption, we have

$$\|E_h(t-s)(j+1)s^j\zeta^{(j-1)}(s)\|_{L_\infty} \le Ch^2\ell_h^2\|v\|_{L_\infty},$$

and

$$\Big\| \int_{t/a}^{t} E_h(t-s)(j+1)s^{-1}(js^j \zeta^{(j-1)}(s))\, ds \Big\|_{L_\infty} \leq C \ln(a) h^2 \ell_h^2 \|v\|_{L_\infty}.$$

Thus

$$\|I_2\|_{L_\infty} \leq (C + C\ln(a)) h^2 \ell_h^2 \|v\|_{L_\infty} + C\ln(a) \sup_{0\leq s\leq t} \|s^{j+1}\zeta^{(j)}\|_{L_\infty}.$$

Therefore, with $C_a = C + C\ln(a) + C\ln(\frac{a}{a-1})$,

$$\|I\|_{L_\infty} \leq C_a h^2 \ell_h^2 \|v\|_{L_\infty} + C\ln(a) \sup_{0\leq s\leq t} \|s^{j+1}\zeta^{(j)}(s)\|_{L_\infty}.$$

By (3.3.13), we get

$$\sup_{0\leq s\leq t} \|s^{j+1}\zeta^{(j)}(s)\|_{L_\infty} \leq C_a h^2 \ell_h^2 \|v\|_{L_\infty} + C\ln(a) \sup_{0\leq s\leq t} \|s^{j+1}\zeta^{(j)}(s)\|_{L_\infty}.$$

Choosing $a$ such that $C\ln(a) \leq 1/2$, we obtain (3.3.12). The proof is complete. □

We now turn to an error estimate in the smooth data case.

**Theorem 3.4.** *Let $u(t)$ and $u_h(t)$ be the solutions of* (3.3.1) *and* (3.3.5) *and $j \geq 0$. If $v \in \dot{W}_\infty^{2j+2}$, then we have*

$$\|D_t^j u_h(t) - D_t^j u(t)\|_{L_\infty} \leq Ch^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}} + C\|\Delta_h^j v_h - R_h \Delta^j v\|_{L_\infty}. \tag{3.3.14}$$

The proof will depend on the following:

**Lemma 3.5.** *Let $u(t)$ be the solution of* (3.3.1) *and $j \geq 0$. Then we have, for $\rho = R_h u - u$, $\rho^{(j)} = D_t^j \rho$,*

$$\|\rho^{(j)}(t)\|_{L_\infty} + t\|\rho^{(j+1)}(t)\|_{L_\infty} \leq Ch^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}}, \quad \textit{for } v \in \dot{W}_\infty^{2j+2}.$$

*Proof.* The case $j = 0$ can be found in Thomée [16, Lemma 5.6]. Hence

$$\|\rho^{(j)}(t)\|_{L_\infty} + t\|\rho^{(j+1)}(t)\|_{L_\infty} \leq Ch^2 \ell_h^2 \|D_t^j u(0)\|_{W_\infty^2} \leq Ch^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}},$$

which completes the proof. □

*Proof of Theorem 3.4.* First we assume $v_h = T_h^{j+1}(-\Delta)^{j+1} v$, where $T_h = (-\Delta_h)^{-1}$, which implies that $\Delta_h^j v_h = R_h \Delta^j v$. In this case, we want to show

$$\|D_t^j u_h(t) - D_t^j u(t)\|_{L_\infty} \leq Ch^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}},$$

which we will do now.

We write, with $\rho^{(j)} = D_t^j \rho$ and $\theta^{(j)} = D_t^j \theta$, where $\theta = u_h - R_h u$ and $\rho = R_h u - u$,

$$D_t^j u_h - D_t^j u = \theta^{(j)} + \rho^{(j)}.$$

Here $\rho^{(j)}$ is bounded as desired by Lemma 3.5. To estimate $\theta^{(j)}$ we note that

$$D_t \theta^{(j)} - \Delta_h \theta^{(j)} = -P_h \rho^{(j+1)},$$

so that, by Duhamel's principle and $\theta^{(j)}(0) = \Delta_h^j v_h - R_h \Delta^j v = 0$,

$$\theta^{(j)}(t) = -\Big(\int_0^{t/2} + \int_{t/2}^t\Big) E_h(t-s) P_h \rho^{(j+1)}(s)\, ds = I + II.$$

Here by Lemmas 3.3 and 3.5,

$$\|II\|_{L_\infty} \le C \int_{t/2}^t \|\rho^{(j+1)}(s)\|_{L_\infty}\, ds \le C h^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}}.$$

For $I$ we integrate by parts to obtain

$$I = -\Big[E_h(t-s) P_h \rho^{(j)}(s)\Big]_0^{t/2} - \int_0^{t/2} E_h'(t-s) P_h \rho^{(j)}(s)\, ds.$$

Using Lemmas 3.3 and 3.5 we have

$$\|E_h(t-s) P_h \rho^{(j)}(s)\|_{L_\infty} \le C \|\rho^{(j)}(s)\|_{L_\infty} \le C h^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}},$$

and

$$\begin{aligned}\Big\| \int_0^{t/2} E_h'(t-s) P_h \rho^{(j)}(s)\, ds \Big\|_{L_\infty} &\le C \int_0^{t/2} (t-s)^{-1} \|\rho^{(j)}(s)\|_{L_\infty}\, ds \\ &\le C h^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}},\end{aligned}$$

which shows (3.3.14) for present choice of $v_h$.

It remains to consider the contribution to the semidiscrete solution of the initial data $v_h - T_h^{j+1}(-\Delta)^{j+1} v$. We have by the above proof

$$\|D_t^j E_h(t)(T_h^{j+1}(-\Delta)^{j+1} v) - D_t^j u(t)\|_{L_\infty} \le C h^2 \ell_h^2 \|v\|_{W_\infty^{2j+2}}.$$

On the other hand, by the stability of $E_h(t)$,

$$\|D_t^j E_h(t)(v_h - T_h^{j+1}(-\Delta)^{j+1} v)\|_{L_\infty} \le C \|\Delta_h^j v_h - R_h \Delta^j v\|_{L_\infty}.$$

Together these estimates complete the proof of (3.3.14). □

Now we consider the error estimates for the fully discrete scheme (3.3.9). In order to apply the results of Section 2, we have to consider the appropriate bound for the resolvent $R(z; -\Delta_h)$. To do this, we quote the following lemma from Bakaev, Thomée, and Wahlbin [4, Theorem 1.1],

**Lemma 3.6.** *For any $\delta \in (0, \pi/2)$ there exists a constant $C$ such that*

$$\|R(z; -\Delta_h) f\|_{L_\infty} \le C |z|^{-1} \|f\|_{L_\infty}, \quad \textit{for}\; z \in \Sigma_\delta.$$

By using this lemma, we see that $A = -\Delta_h$ satisfies (1.1.2) and (1.1.3), hence we can apply the results in Section 2 with $A = -\Delta_h$, $\mathcal{B} = S_h$ equipped with the $L_\infty$ norm.

We first combine Theorem 3.1, for the error estimate in the semidiscrete case, with Theorem 2.6, applied to the semidiscrete equation (3.3.5), and obtain the following error estimate in the nonsmooth data case.

**Theorem 3.7.** *Let $u(t_n)$ and $U^n$ be the solutions of* (3.3.1) *and* (3.3.9). *Assume that $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable with $\theta \in (0, \pi/2]$ and $|r(\infty)| < 1$. Let $j \geq 1$ and assume that $Q_k^j$, defined in* (1.1.11), *is an approximation of $D_t^j$, which is accurate of order $p$. Then there is a constant $C$ such that, if $v \in L_\infty$ and $v_h = P_h v$, then we have, for $n \geq m_1,\ t_n > 0$,*

$$\|Q_k^j U^n - D_t^j u(t_n)\|_{L_\infty} \leq C(h^2 \ell_h^2 t_n^{-j-1} + k^p t_n^{-p-j}) \|v\|_{L_\infty}.$$

We finish with an error estimate in the smooth data case.

**Theorem 3.8.** *Let $u(t_n)$ and $U^n$ be the solutions of* (3.3.1) *and* (3.3.9). *Assume that $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable with $\theta \in (0, \pi/2]$. Let $j \geq 1$ and assume that $Q_k^j$, defined in* (1.1.11), *is an approximation of $D_t^j$, which is accurate of order $p$. Then there is a constant $C$ such that, if $v \in \dot{W}_\infty^{2p+2j}$ and $v_h = P_h v$, then we have, for $n \geq m_1$,*

$$\|Q_k^j U^n - D_t^j u(t_n)\|_{L_\infty} \leq C(h^2 \ell_h^2 \|v\|_{W_\infty^{2+2j}} + k^p \|v\|_{W_\infty^{2p+2j}}) + C\|\Delta_h^j v_h - \Delta^j v\|_{L_\infty}.$$

In order to prove the theorem, we need the following lemma.

**Lemma 3.9.** *Assume that $r(z)$ is $A(\theta)$-stable with $\theta \in (0, \pi/2]$ and accurate of order $p \geq 1$. Let $j \geq 1$ and let $\tilde{G}_{n,s} = G_n(-k\Delta_h) T_h^s$, where $G_n$ is defined by* (2.2.3) *and $T_h = (-\Delta_h)^{-1}$. Then we have*

$$\|\tilde{G}_{n,l+j} w\|_{L_\infty} \leq C k^{l+j} \|w\|_{L_\infty}, \quad \textit{for } 0 \leq l \leq p,\ n \geq m_1.$$

*Proof.* Using Lemma 3.6, we obtain by Theorem 2.1, for $n \geq m_1$,

$$\|\tilde{G}_{n,l+j} w\|_{L_\infty} = \|G_n(-k\Delta_h) T_h^{l+j} w\|_{L_\infty} \leq C k^{l+j} \|w\|_{L_\infty}, \quad \text{for } 0 \leq l \leq p. \tag{3.3.15}$$

Note that if $r(z)$ is accurate of $p$ it is also accurate of order $l$ with $1 \leq l \leq p$, which shows (3.3.15) for $1 \leq l \leq p$. The case $l = 0$ follows by a direct proof as in the case $l = p$. □

*Proof of Theorem 3.8.* By Theorem 3.4, Lemma 3.5 and the estimate

$$\|\Delta_h^j v_h - R_h \Delta^j v\|_{L_\infty} \leq \|\Delta_h^j v_h - \Delta^j v\|_{L_\infty} + \|(R_h - I)\Delta^j v\|_{L_\infty},$$

we only need to show

$$\|Q_k^j U^n - D_t^j u_h(t_n)\|_{L_\infty} \leq C(h^2 \ell_h^2 \|v\|_{W_\infty^{2+2j}} + k^p \|v\|_{W_\infty^{2p+2j}}) + C\|\Delta_h^j v_h - \Delta^j v\|_{L_\infty}. \tag{3.3.16}$$

Assuming first that $v_h = T_h^j (-\Delta)^j v$, we have

$$Q_k^j U^n - D_t^j u_h(t_n) = k^{-j} \tilde{G}_{n,j} (-\Delta)^j v.$$

Following Thomée [16, Theorem 8.6], we choose $\tilde{v}_k$, such that, with $C$ independent of $s$,

$$\|(-\Delta)^j (v - \tilde{v}_k)\|_{L_\infty} \leq C k^p \|\Delta^{p+j} v\|_{L_\infty} \leq C k^p \|v\|_{W_\infty^{2p+2j}}, \tag{3.3.17}$$

$$\|(-\Delta)^{p+j} \tilde{v}_k\|_{L_\infty} \leq C \|\Delta^{p+j} v\|_{L_\infty} \leq C \|v\|_{W_\infty^{2p+2j}}, \tag{3.3.18}$$

$$k^l \|(-\Delta)^{l+j} \tilde{v}_k\|_{W_s^2} \leq C s \|\Delta^j v\|_{W_s^2}, \quad \text{for } 0 \leq l \leq p-1,\ 2 \leq s < \infty. \tag{3.3.19}$$

Applying now the identity

$$v=\sum_{l=0}^{p-1}T_h^l(T-T_h)(-\Delta)^{l+1}v+T_h^p(-\Delta)^pv,$$

to $(-\Delta)^j\tilde v_k$, we have

$$\begin{aligned}\tilde G_{n,j}(-\Delta)^j\tilde v_k&=G_n(-k\Delta_h)T_h^j(-\Delta)^j\tilde v_k\\&=\sum_{l=0}^{p-1}\tilde G_{n,l+j}(T-T_h)(-\Delta)^{l+j+1}\tilde v_k+\tilde G_{n,p+j}(-\Delta)^{p+j}\tilde v_k.\end{aligned}\tag{3.3.20}$$

By Lemma 3.9, we have, since $(T-T_h)(-\Delta)=I-R_h$,

$$\|\tilde G_{n,l+j}(T-T_h)(-\Delta)^{l+j+1}\tilde v_k\|_{L_\infty}\le Ck^{l+j}\|(I-R_h)(-\Delta)^{l+j}\tilde v_k\|_{L_\infty}.$$

Using the following bound for the Ritz projection in maximum-norm, see, e.g., Thomée [16, Lemma 5.6],

$$\|(R_h-I)v\|_{L_\infty}\le Ch^{2-2/s}\ell_h\|v\|_{W_s^2},\quad \text{for } 2\le s<\infty,$$

and (3.3.19), choosing $s=\ell_h$, we therefore obtain

$$\begin{aligned}\|\tilde G_{n,l+j}(T-T_h)(-\Delta)^{l+j+1}\tilde v_k\|_{L_\infty}&\le Ck^{l+j}h^{2-2/s}\ell_h\|\Delta^{l+j}\tilde v_k\|_{W_s^2}\\&\le Ck^jsh^{2-2/s}\ell_h\|\Delta^jv\|_{W_s^2}\\&\le Ck^jh^2\ell_h^2\|v\|_{W_\infty^{2+2j}},\quad\text{for } 0\le l\le p-1.\end{aligned}$$

For the case $l=p$ we have by (3.3.18),

$$\|\tilde G_{n,p+j}(-\Delta)^{p+j}\tilde v_k\|_{L_\infty}\le Ck^{p+j}\|\Delta^{p+j}\tilde v_k\|_{L_\infty}\le Ck^{p+j}\|v\|_{W_\infty^{2p+2j}}.$$

Together these estimates imply

$$\|\tilde G_{n,j}(-\Delta)^j\tilde v_k\|_{L_\infty}\le Ck^j(h^2\ell_h^2\|v\|_{W_\infty^{2+2j}}+k^p\|v\|_{W_\infty^{2p+2j}}).$$

By Lemma 3.9 and (3.3.17), we have

$$\begin{aligned}\|\tilde G_{n,j}(-\Delta)^j(v-\tilde v_k)\|_{L_\infty}&=\|G_n(-k\Delta_h)T_h^j(-\Delta)^j(v-\tilde v_k)\|_{L_\infty}\\&\le Ck^j\|(-\Delta)^j(v-\tilde v_k)\|_{L_\infty}\le Ck^{p+j}\|v\|_{W_\infty^{2p+2j}}.\end{aligned}$$

We conclude that

$$\begin{aligned}\|Q_k^jU^n-D_t^ju_h(t_n)\|_{L_\infty}&=\|k^{-j}\tilde G_{n,j}(-\Delta)^jv\|_{L_\infty}\\&\le C(h^2\ell_h^2\|v\|_{W_\infty^{2+2j}}+k^p\|v\|_{W_\infty^{2p+2j}}),\end{aligned}$$

which shows (3.3.16) for present choice of $v_h$.

It remains to consider the contribution to the fully discrete solution of $v_h-T_h^j(-\Delta)^jv$. Since

$$Q_k^jE_{kh}^n(v_h-T_h^j(-\Delta)^j)v=P(r(-k\Delta_h))r(-k\Delta_h)^n(-k\Delta_h)^{-j}v,\tag{3.3.21}$$

it suffices to show

$$\|P(r(-k\Delta_h))r(-k\Delta_h)^n(-k\Delta_h)^{-j}\|_{L_\infty} \le C, \tag{3.3.22}$$

where $\|\cdot\|_{L_\infty}$ denotes the operator norm. In fact,

$$P(r(-\Delta_h))r(-\Delta_h)^n(-\Delta_h)^{-j} = \frac{1}{2\pi i}\int_\Gamma P(r(z))r(z)^n z^{-j} R(z;-\Delta_h)\,dz.$$

Since $0 \in \rho(-\Delta_h)$, $P(r(z)) = O(z^j)$ as $z \to 0$, there exists small $\eta > 0$, such that $\|R(z;-\Delta_h)\|_{L_\infty} \le C$ and $|P(r(z))z^{-j}| \le C$ for $|z| \le \eta$. Thus, we have, noting $r(z)$ is bounded on $\Gamma$ and $n \ge m_1$,

$$\Big\| \int_\Gamma P(r(z))r(z)^n z^{-j} R(z;-\Delta_h)\,dz \Big\|_{L_\infty} \le \int_0^\eta d\rho + \int_\eta^\infty \frac{d\rho}{\rho^{j+1}} \le C,$$

which shows (3.3.22). The proof is now complete. □

## 4. Numerical Illustrations

In this section, we show some numerical results illustrating our theoretical analysis. We consider a one-dimensional problem with nonsmooth data,

$$\begin{cases} u_t - u_{xx} = 0, \quad \text{in } [0,1], \quad \text{with } u(0,t) = u(1,t) = 0, \quad \text{for } t > 0, \\ u(x,0) = v(x), \quad \text{in } [0,1], \end{cases} \tag{4.4.1}$$

where

$$v = \begin{cases} 1, & \text{if } \frac{1}{4} < x < \frac{3}{4}, \\ 0, & \text{otherwise.} \end{cases} \tag{4.4.2}$$

We have that $v \in L_\infty$, but $v \notin W_\infty^s$ for any $s > 0$.

The exact solution of (4.4.1) is

$$u(x,t) = \frac{4}{\pi}\sum_{n=1}^{\infty}(-1)^n \sin\frac{(2n-1)\pi}{4}(2n-1)^{-1}e^{-((2n-1)\pi)^2 t}\sin(2n-1)\pi x,$$

and the derivative of $u(x,t)$ is

$$u_t(x,t) = 4\pi\sum_{n=1}^{\infty}(-1)^{n+1}\sin\frac{(2n-1)\pi}{4}(2n-1)e^{-((2n-1)\pi)^2 t}\sin(2n-1)\pi x.$$

We define $S_h$ to be the set of continuous piecewise linear functions on a uniform mesh of size $h$, which vanish at $x = 0$ and $x = 1$. As explained in Section 3, the semidiscrete problem may be written

$$u_{h,t} = A_h u_h, \quad \text{for } t > 0, \quad \text{with } u_h(0) = P_h v, \tag{4.4.3}$$

where $A_h$ is the discrete analogue of $A = -d^2/dx^2$, defined by

$$(A_h\psi, \chi) = \int_0^1 \psi'\chi'\,dx, \quad \forall\, \psi,\, \chi \in S_h.$$

We first compute the approximate solution $U^n$ of (4.4.1) by applying the time stepping method $U^n = r(kA_h)U^{n-1}$ to the semidiscrete problem (4.4.3), where $r(\lambda)$ will be specified in our examples below. As mentioned in the introduction, if $r(\infty) = 0$, then $u_{h,t}(t_n)$ can be approximated by $-A_hU^n$ and the error estimates (1.1.10) holds. In the case of $r(\infty) \neq 0$, we then use $\bar{\partial}U^n = (U^n - U^{n-1})/k$, which is a special case of (1.1.11), to approximate $u_t(t_n)$. Theorem 3.7 shows an error estimate for the fully discrete method with nonsmooth data in the $L_\infty$ norm. More precisely, if $|r(\infty)| < 1$, we have

$$\|\bar{\partial}U^n - u_t(t_n)\| \leq Ct_n^{-2}(k + h^2\ell_h^2)\|v\|_{L_\infty}. \tag{4.4.4}$$

For the approximation $-A_hU^n$ of $u_t(t_n)$ when $r(\infty) = 0$, combining (1.1.10) and Theorem 3.1, we have the same error bound as in (4.4.4).

In our experiment, we consider the $\theta$-method defined by (2.2.1) with $\theta = 2/3$, in this case $|r(\infty)| = 1/2$. Since we are mostly interested in the time stepping, we choose $h$ very small and a sequence of moderate $k$. We thus use $h = 1/200$ fixed, and the time step $k$ is chosen as $1/20, 1/40$ and $1/80$.

Denote $\varepsilon(k) = \varepsilon(k, t_n) = \|U^n - u(t_n)\|_{L_\infty}$, and let $\rho(k_1, k_2) = \varepsilon(k_1)/\varepsilon(k_2)$. Table 1 shows the $L_\infty$ norm of the error of the approximation $U^n$ of $u(t_n)$ at time $t_n$. From Thomée [16], we know that $\|U^n - u(t_n)\| \leq Ct_n^{-1}(k + h^2\ell_h^2)\|v\|_{L_\infty}$. Table 1 shows the expected $O(k)$ order of convergence. We also see that the error becomes large when $t$ tends to 0.

In Table 2, we show the results of the approximation $\bar{\partial}U^n$ of $u_t(t_n)$. Here $\varepsilon(k) = \varepsilon(k, t_n) = \|\bar{\partial}U^n - u_t(t_n)\|_{L_\infty}$, and again $\rho(k_1, k_2) = \varepsilon(k_1)/\varepsilon(k_2)$. The results confirm the expected $O(k)$ order of convergence and the singular behavior of the error as $t \to 0$.

| t | $\varepsilon(1/20)$ | $\varepsilon(1/40)$ | $\varepsilon(1/80)$ | $\rho(1/20, 1/40)$ | $\rho(1/40, 1/80)$ |
|---|---|---|---|---|---|
| 0.1 | 1.669E-01 | 4.343E-02 | 6.465E-03 | 3.84 | 6.71 |
| 0.2 | 4.794E-02 | 8.957E-03 | 4.764E-03 | 5.35 | 1.87 |
| 0.3 | 1.537E-02 | 5.082E-03 | 2.688E-03 | 3.02 | 1.89 |
| 0.4 | 5.498E-03 | 2.570E-03 | 1.348E-03 | 2.13 | 1.90 |
| 0.5 | 2.214E-03 | 1.218E-03 | 6.342E-04 | 1.81 | 1.92 |
| 0.6 | 1.020E-03 | 5.548E-04 | 2.863E-04 | 1.83 | 1.93 |
| 0.7 | 4.572E-04 | 2.456E-04 | 1.257E-04 | 1.86 | 1.95 |
| 0.8 | 2.009E-04 | 1.065E-04 | 5.405E-05 | 1.88 | 1.97 |
| 0.9 | 8.693E-05 | 4.548E-05 | 2.288E-05 | 1.91 | 1.98 |
| 1.0 | 3.717E-05 | 1.918E-05 | 9.568E-06 | 1.93 | 2.00 |

Table 1. $\theta$-method, with the approximation $U^n$ of $u(t_n)$ in $L_\infty$ norm.

| t | $\varepsilon(1/20)$ | $\varepsilon(1/40)$ | $\varepsilon(1/80)$ | $\rho(1/20, 1/40)$ | $\rho(1/40, 1/80)$ |
|---|---|---|---|---|---|
| 0.1 | 9.664E+00 | 4.558E+00 | 6.097E-01 | 2.11 | 7.47 |
| 0.2 | 2.460E+00 | 3.964E-01 | 1.020E-01 | 6.20 | 3.88 |
| 0.3 | 6.737E-01 | 9.585E-02 | 4.741E-02 | 7.02 | 2.02 |
| 0.4 | 1.939E-01 | 4.30E-02 | 2.123E-02 | 4.50 | 2.02 |
| 0.5 | 5.960E-02 | 1.883E-02 | 9.270E-03 | 3.16 | 2.03 |
| 0.6 | 1.970E-02 | 8.102E-03 | 3.969E-03 | 2.43 | 2.04 |
| 0.7 | 7.118E-03 | 3.437E-03 | 1.674E-03 | 2.07 | 2.05 |
| 0.8 | 3.018E-03 | 1.442E-03 | 6.983E-04 | 2.09 | 2.06 |
| 0.9 | 1.268E-03 | 5.996E-04 | 2.884E-04 | 2.11 | 2.07 |
| 1.0 | 5.293E-04 | 2.474E-04 | 1.182E-04 | 2.13 | 2.09 |

Table 2. $\theta$-method, with the approximation $\bar{\partial}U^n$ of $u_t(t_n)$ in $L_\infty$ norm.

**Acknowledgement.** I wish to express my sincere gratitude to my supervisor Prof. Vidar Thomée, who suggested the topic of this paper, for his support and valuable criticism. I am also greatly indebted to my supervisor Dr. Stig Larsson for reading the manuscript carefully and providing many valuable comments on the manuscript.

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