Thesis for the Degree of Licentiate of Philosophy

Smoothing Properties and Approximations of Time Derivatives in Time Stepping Methods for Homogeneous Parabolic Equations

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Abstract

We study smoothing properties and approximations of time derivatives of time discretization schemes with constant and variable time steps for an abstract homogeneous linear parabolic problem. The time stepping schemes are based on using rational fuctions $r(z)$ 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. We first consider the problem in a Hilbert space setting with a selfadjoint, positive definite, unbounded elliptic operator occuring in the parabolic equation in which case $\theta = 0$, and then extend the results to a general Banach space with a more general elliptic operator. Both smooth and nonsmooth data error estimates of optimal order for the approximation of time derivatives are proved. In case of variable time steps only first and second order approximations are discussed, and under certain restrictions on the time steps. We also apply the results in the constant time step case in both L_2 and L_∞ norms to fully discrete methods for the homogeneous heat equation using linear finite elements in space.

Keywords: parabolic, smoothing, time derivatives, single step time stepping schemes, fully discrete schemes, error estimates, finite element methods

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Contents

1. Introduction

We consider smoothing properties of time stepping methods and error estimates of the approximations of time derivatives in the parabolic problem

$$u_t + Au = 0 \quad \text{for } t > 0, \quad \text{with } u(0) = v, \tag{1.1}$$

in a general Banach space $\mathcal{B}$, and we also apply the results obtained to error estimates for fully discrete methods based on finite elements for the homogeneous heat equation in a spatial doman Ω in both L_2 and L_∞ norms.

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, with $\delta \in (0, \pi/2)$,

$$\rho(A) \supset \Sigma_\delta = \{z \in \mathbf{C}; \delta \le |\arg z| \le \pi, z \ne 0\} \cup \{0\}, \tag{1.2}$$

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

$$\|R(z; A)\| \le M|z|^{-1}, \quad \text{for } z \in \Sigma_\delta, \quad \text{with } M \ge 1, \tag{1.3}$$

where $\|\cdot\|$ is the norm in $\mathcal{B}$.

Under these assumptions $-A$ is the infinitesimal generator of a uniformly bounded analytic semigroup $E(t) = e^{-tA}$, $t \ge 0$, which is the solution operator of (1.1). It may be represented as

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

where $\Gamma = \{\, z : |\arg z| = \psi \in (\,\delta, \pi/2\,)$, with $\operatorname{Im} z$ increasing$\}$. In particular the smoothing properties of analytic semigroups are valid for positive time. More precisely, cf., e.g., Pazy [15], if $v \in \mathcal{B}$, we have, with $D_t = \partial/\partial t$,

$$\|D_t^j E(t)v\| = \|A^j E(t)v\| \le Ct^{-j}\|v\|, \quad \text{for } t > 0, \ j \ge 0. \tag{1.4}$$

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

Let k be a time step and $t_n = nk$, with $n \ge 1$. We define a single step discrete method to approximate $u(t_n) = E(t_n)v$ by U^n, using a rational function $r(z)$ approximating e^{-z}, so that U^n is defined recursively by

$$U^n = E_k U^{n-1} \quad \text{for } n \ge 1, \quad \text{with } U^0 = v, \tag{1.5}$$

where $E_k = r(kA)$, with the rational function $r(z)$ defined 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 $p \ge 1$, if

$$r(z) - e^{-z} = O(z^{p+1}), \quad \text{as } z \to 0. \tag{1.6}$$

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 polynomials of degree 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., Thomée [19] and references therein. For instance, if A satisfies (1.2) and (1.3), and $r(z)$ is $A(\theta)$-stable, with $\theta \in (\delta, \pi/2]$, i.e., $|r(z)| \le 1$ for

$|\arg z| \leq \theta$, and (1.6) holds, then, we have, see, e.g., Larsson, Thomée and Wahlbin [11] and Crouzeix, Larsson, Piskarev, and Thomée [7],

$$\|U^n - u(t_n)\| = \|E_k^n v - E(t_n)v\| \leq Ck^p \|A^p v\|, \quad \text{for } v \in \mathcal{D}(A^p). \tag{1.7}$$

To obtain optimal order error estimates for nonsmooth initial data, the 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, see, e.g., [11] and [7],

$$\|U^n - u(t_n)\| = \|E_k^n v - E(t_n)v\| \leq Ck^p t_n^{-p} \|v\|, \quad \text{for } t_n > 0. \tag{1.8}$$

The condition $|r(\infty)| < 1$ ensures that oscillating components of the error are efficiently damped.

If $|r(\infty)| = 1$, the discrete method (1.5) is not smoothing. However, Luskin and Rannacher [12] and Rannacher [16] analyzed modified methods in Hilbert space which combine a stable method of order p and a few steps of method of order $p-1$ with good smoothing properties, and showed nonsmooth data error estimates of order p. For instance, if one uses the Crank-Nicolson method combined with the backward Euler method at two time steps, then a second order nonsmooth data error estimates holds. The results in [12] and [16] are generalized by Hansbo [10] to the Banach space case.

Let us now recall some results about smoothing properties of time discretization schemes and error estimates for the approximations of time derivatives of the solution of (1.1). When $\mathcal{B}$ is a Hilbert space $\mathcal{H}$ and A a linear, selfadjoint, positive definite, unbounded operator, a smoothing property is shown in Thomée [19] for stable time discretization scheme with $r(\infty) = 0$, namely

$$\|A^j U^n\| = \|A^j E_k^n v\| \leq C t_n^{-j} \|v\|, \quad \text{for } t_n \geq t_j, \quad v \in \mathcal{H}. \tag{1.9}$$

Hansbo [10] extends this result to general Banach space, and shows that, if A satisfies (1.2) and (1.3), and $r(z)$ is $A(\theta)$-stable, with $\theta \in (\delta, \frac{1}{2}\pi]$ and $r(\infty) = 0$, then (1.9) holds. Hansbo [10] also shows an optimal order error estimate in the nonsmooth data case for the approximation of the first order time derivative of the solution of (1.1). More precisely, if $r(z)$ is $A(\theta)$-stable with $r(\infty) = 0$, then

$$\|AU^n - u_t(t_n)\| \leq Ck^p t_n^{-p-1} \|v\|, \quad \text{for } n \geq 1, \quad v \in \mathcal{B}. \tag{1.10}$$

However, we show in Section 3 that (1.9) is not valid when $r(\infty) \neq 0$. In the present paper we shall discuss smoothness properties for $A(\theta)$-stable discretizations under the assumption $|r(\infty)| < 1$. These will be based on using difference quotients in time rather than the elliptic operator A in the discrete analogue of (1.4).

Baker, Bramble and Thomée [4] study finite difference approximations for time derivatives $D_t^j u(t_n)$ of the solution of (1.1) of the form

$$Q_k^j U^n = \frac{1}{k^j} \sum_{\nu=-m_1}^{m_2} c_\nu U^{n+\nu}, \quad \text{for } n \geq m_1, \tag{1.11}$$

where m_1, m_2 are nonnegative integers. When the operator Q_k^j is an approximation of order $p \geq 1$ to D_t^j, that is, when for any smooth real-valued functions u,

$$D_t^j u(t_n) = Q_k^j u^n + O(k^p), \quad \text{as } k \to 0, \quad \text{with } u^n = u(t_n), \tag{1.12}$$

then the following nonsmooth data error estimate for the approximation Q_k^j of D_t^j in Hilbert space $\mathcal{H}$ is obtained in [4]: If $|r(\lambda)| < 1$ for $\lambda > 0$, and $|r(\infty)| < 1$, then

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C k^p t_n^{-(p+j)} \|v\|, \quad \text{for } n \ge m_1,\ v \in \mathcal{H}. \tag{1.13}$$

In our paper, we will again consider the approximation of time derivatives of the form (1.11). In Theorem 2.1, we show the following smooth data error estimate for an $A(\theta)$-stable discretization scheme,

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C k^p \|A^{p+j} v\|, \quad \text{for } n \ge m_1,\ v \in \mathcal{D}(A^{p+j}). \tag{1.14}$$

For $A(\theta)$-stable discretization schemes with $|r(\infty)| < 1$, we find that the discrete smoothing property (1.9) holds when we replace A with $\bar\partial$, where $\bar\partial$ is the first order backward difference operator, i.e, $\bar\partial U^n = (U^n - U^{n-1})/k$. It is easy to check that $\bar\partial^j$ is an approximation of order $p = 1$ to D_t^j. More generally, we show, in Theorem 2.5, that if A satisfies (1.2) and (1.3), and $r(z)$ is $A(\theta)$-stable, with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$, then

$$\|Q_k^j U^n\| \le C t_n^{-j} \|v\|, \quad \text{for } n \ge j,\ v \in \mathcal{B}. \tag{1.15}$$

Under the assumptions of Theorem 2.5, we also obtain a nonsmooth data error estimate similar to (1.13) in a general Banach space.

Let us now discuss some properties of the cofficients c_ν in (1.11). With $u(t) = e^t$ in (1.12) we have at $t_n = 0$

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

Using Taylor expansion of $e^{\nu k}$ at $k = 0$, we therefore easily find that (1.12) is equivalent to

$$P(e^z) - z^j = O(z^{p+j}), \quad \text{as } z \to 0, \tag{1.16}$$

where z is allowed to be complex valued.

We also note that (1.11) has the form

$$Q_k^j U^n = k^{-j} P(E_k) E_k^n v, \tag{1.17}$$

which will be useful in later sections of this paper.

We now present some examples of finite difference approximation $Q_k^j u^n$ of $D_t^j u(t_n)$ for different orders of accuracy. It is easy to check that $Q_k^1 u^n = \bar\partial u^n = (u^n - u^{n-1})/k$ and $Q_k^1 u^n = (\frac{3}{2}u^n - 2u^{n-1} + \frac{1}{2}u^{n-2})/k$ are two examples of approximations of $D_t u(t_n)$, and (1.16) then reads

$$P(e^z) - z = 1 - e^z - z = O(z^2), \quad \text{as } z \to 0,$$

and

$$P(e^z) - z = \frac{3}{2} - 2e^z + \frac{1}{2}e^{2z} - z = O(z^3), \quad \text{as } z \to 0,$$

respectively. Their orders of accuracy are $p = 1$ and $p = 2$, respectively.

An example of an approximation of $D_t^2 u(t_n)$ with $p = 2$ is

$$Q_k^2 u^n = (u^{n+1} - 2u^n + u^{n-1})/k^2,$$

and (1.16) now reads

$$P(e^z) - z^2 = e^z - 2 + e^{-z} - z^2 = O(z^4), \quad \text{as } z \to 0.$$

A difference quotient approximating $D_t^3 u(t_n)$ is given by

$$Q_k^3 u^n = \frac{1}{2k^3}(-u^{n+3} + 6u^{n+2} - 12u^{n+1} + 10u^n - 3u^{n-1}),$$

which is accurate of order $p = 2$. The corresponding relation is

$$P(e^z) - z^3 = \frac{1}{2}(-e^{3z} + 6e^{2z} - 12e^z + 10 - 3e^{-z}) = O(z^5), \quad \text{as } z \to 0.$$

In Section 4, we apply the results obtained in Section 3 for the abstract time stepping method to error estimates for fully discrete methods. We then consider the following initial boundary value problem for the homogeneous heat equation

$$u_t = \Delta u \quad \text{in } \Omega, \quad \text{for } t > 0, \tag{1.18}$$

$$u = 0 \quad \text{on } \partial\Omega, \quad \text{for } t > 0, \quad \text{with } u(\cdot, 0) = v \quad \text{in } \Omega,$$

where Ω is a bounded domain in R^d with smooth boundary $\partial\Omega$. We define $H^s = H^s(\Omega)$, for s a nonnegative integer, by the norm

$$\|v\|_s = \|v\|_{H^s} = \Big(\sum_{|\alpha| \le s} \|D^\alpha v\|^2\Big)^{1/2}, \quad \text{where } \|\cdot\| = \|\cdot\|_{L_2}.$$

We assume that we are given a family of finite dimensional subspaces S_h of $L_2 = L_2(\Omega)$ and a corresponding family of operators $T_h : L_2 \to S_h$, approximating $T = (-\Delta)^{-1}$, with the properties for some $r \ge 2$,

(i) T_h is selfadjoint, positive semidefinite on L_2 and positive definite on S_h,

(ii) $\|(T_h - T)f\| \le Ch^{s+2}\|f\|_s$, for $f \in H^s = H^s(\Omega)$, $0 \le s \le r - 2$;

the number r is referred to as the order of accuracy of the family $\{S_h\}$.

We now introduce a discrete Laplacian $\Delta_h : S_h \to S_h$ by $\Delta_h = -T_h^{-1}$. When $S_h \subset H_0^1(\Omega)$, i.e., when the elements of S_h vanish on $\partial\Omega$ and S_h satisfies

$$\inf_{\chi \in S_h} \{\|v - \chi\| + h\|\nabla(v - \chi)\|\} \le Ch^s\|v\|_s, \quad \text{for } 1 \le s \le r,$$

then the discrete Laplacian may be defined by

$$(\Delta_h \psi, \chi) = -(\nabla\psi, \nabla\chi), \quad \forall \psi, \chi \in S_h, \tag{1.19}$$

and $\Delta_h = -T_h^{-1}$ satisfies (i) and (ii).

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

$$u_{h,t} = \Delta_h u_h, \qquad \text{for } t > 0, \qquad \text{with } u_h(0) = v_h. \tag{1.20}$$

We now apply our above time stepping procedure (1.5) to the semidiscrete equation (1.20). This defines the fully discrete approximation $U^n \in S_h$ of $u(t_n)$ recursively by

$$U^n = E_{kh}U^{n-1} \qquad \text{for } n \ge 1, \qquad \text{where } E_{kh} = r(-k\Delta_h), \quad \text{with } U^0 = v_h. \tag{1.21}$$

In Theorem 3.7, we show an L_2 error estimate for the approximation $Q_k^j U^n$ of $D_t^j u(t_n)$ in the nonsmooth data case: if $|r(\lambda)| < 1$ for $\lambda > 0$, and $|r(\infty)| < 1$, and if $v_h = P_h v$, then

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C(h^r t_n^{-r/2-j} + k^p t_n^{-p-j})\|v\|, \quad \text{for } t_n > 0, \quad v \in L_2.$$

Theorem 3.8 contains a smooth data error estimate: for any stable discrete scheme and any initial data $v_h \in S_h$, we have

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C(h^r |v|_{r+2j} + k^p |v|_{2p+2j}) + \|\Delta_h^j v_h - \Delta^j v\|, \quad \text{for } t_n \ge 0,$$

where the norm $|\cdot|$ is defined by $|v|_s = \|(-\Delta)^{s/2} v\| = ((-\Delta)^s v, v)^{1/2}$ for $s \ge 0$.

As for the Banach space case, we restrict our discussion to the problem (1.18) in two space dimensions, using approximation in space by piecewise linear finite elements on quasiuniform triangulations of Ω. Under the assumption that $r(z)$ is A-stable and $|r(\infty)| < 1$, and $v_h = P_h v$, we get the following L_∞ error estimate in the nonsmooth data case, with $\ell_h = \ln(1/h)$,

$$\|Q_k^j U^n - D_t^j u(t_n)\|_{L_\infty} \le C(h^2 \ell_h^{j+3} t_n^{-j-1} \|v\|_{L_\infty} + k^p t_n^{-p-j} \|v\|_{L_\infty}), \quad \text{for } t_n > 0,$$

For any A-stable discretization scheme we also show the smooth data error estimate

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

In Section 5, we return to consider the abstract parabolic problem (1.1) in a general Banach space with variable time steps. Let $0 = t_0 < t_1 < \cdots < t_n < \cdots$ be a partition of the time axis and $k_n = t_n - t_{n-1}$ the variable time steps. Then the discrete approximation U^n of the exact solution $u(t_n)$ of the parabolic problem at t_n will be defined in terms of a rational approximation $r(z)$ of e^{-z}, by the recursion formula

$$U^n = E_{k_n} U^{n-1} \quad \text{for } n \ge 1, \quad E_{k_n} = r(k_n A), \quad \text{with } U^0 = v, \tag{1.22}$$

where the rational function $r(z)$ is defined on $\sigma(k_j A)$ for $j \le n$ and (1.6) holds.

Variable time steps are particularly useful when the solution changes rapidly in certain regions of time. Stability results have been considered by, e.g., Bakaev [2], [3], and Palencia [13], [14]. In the present paper we will consider smoothing properties of the time discretization scheme (4.1) and the approximation of the time derivative $u_t(t_n)$ of the solution of (1.1). Before doing this, we show some estimates for the approximation U^n of the solution of $u(t_n)$ of (1.1). Our first result is the error estimate in the smooth data case: If the scheme is $A(\theta)$-stable, with $\theta \in (\delta, \pi/2]$, then

$$\|U^n - u(t_n)\| \le C k_{max}^p \|A^p v\| \quad \text{for } t_n \ge 0, \quad \text{where } k_{max} = \max_{j \le n} k_j.$$

To obtain error estimates in the nonsmooth data case, we introduce the notion of *increasing quasi-quasiuniform grids* $\mathcal{T}$ in time. Let $\{\mathcal{T}\}$ be a family of partitions of the time axis, $\mathcal{T} = \{t_n,\ 0 = t_0 < t_1 < \cdots < t_n < \cdots\}$. $\mathcal{T}$ is called a family of *quasi-quasiuniform grids* if there exist positive constants c, C, such that

$$c k_{n+1} \le k_n \le C t_n / n. \tag{1.23}$$

Further, if $k_1 \le k_2 \le \cdots \le k_n \le \cdots$, we call $\{\mathcal{T}\}$ is a family of *increasing quasi-quasiuniform grids.*

For example, if we choose the variable time steps $k_n = n^s k$ for some fixed $s \ge 1$, with $k > 0$, then $t_n = k\Big(\sum_{j=1}^n j^s\Big)$, and the corresponding family of partitions $\{\mathcal{T}\}$ is a family of *increasing quasi-quasiuniform grids.* In fact, it is obvious that $k_n / k_{n+1} = n^s/(n+1)^s \ge 1/2^s$. Further, since $t_n/k = \sum_{j=1}^n j^s \ge c n^{s+1}$ for some positive constant c, we have $k_n \le C t_n / n$ for some positive constant C.

In Theorem 4.4, we show a nonsmooth data error estimate: if $\{\mathcal{T}\}$ is a family of *increasing quasi-quasiuniform grids*, and $r(z)$ is $A(\theta)$-stable and $|r(\infty)| < 1$, then

$$\|U^n - u(t_n)\| \le Ck_n^p t_n^{-p}\|v\|, \quad \text{for } t_n > 0, \quad v \in \mathcal{B}.$$

In order to approximate the time derivative $u_t(t_n)$ we use the variable step first order approximation

$$\bar{\partial}U^n = \frac{U^n - U^{n-1}}{k_n}. \tag{1.24}$$

Assume that $r(z)$ is $A(\theta)$-stable, and that k_j, $1 \le j \le n$ is increasing, then we have the following error estimate in the smooth data case

$$\|\bar{\partial}U^n - D_t u(t_n)\| \le Ck_n\|A^2 v\|, \quad \text{for } t_n \ge 0, \ v \in \mathcal{D}(A^2).$$

Under the assumptions of Theorem 4.4, we have the following smoothing property

$$\|\bar{\partial}U^n\| \le Ct_n^{-1}\|v\|, \quad \text{for } t_n > 0, \quad v \in \mathcal{B}$$

and the nonsmooth data error estimate

$$\|\bar{\partial}U^n - D_t u(t_n)\| \le Ck_n t_n^{-2}\|v\|, \quad \text{for } t_n > 0, \quad v \in \mathcal{B}.$$

We also consider an approximation of the time derivative $u_t(t_n)$ by means of the second order backward difference quotient

$$\bar{\partial}^2 U^n = a_n\bar{\partial}U^n + b_n\bar{\partial}U^{n-1} = a_n\frac{U^n - U^{n-1}}{k_n} + b_n\frac{U^{n-1} - U^{n-2}}{k_{n-1}}, \tag{1.25}$$

$$a_n = (2k_n + k_{n-1})/(k_n + k_{n-1}), \quad b_n = -k_n/(k_n + k_{n-1}).$$

This is a second order approximation of $u_t(t_n)$ in the sense that it is exact for polynomials of degree 2 and it is easy to check that for smooth u we have

$$\bar{\partial}^2 u(t_n) = u_t(t_n) + O(k_n^2 + k_{n-1}^2), \quad \text{as } k_n, k_{n-1} \to 0.$$

For this approximation of $u_t(t_n)$ we show smoothing properties and error estimates in both smooth and nonsmooth data cases.

In Section 6, we give some numerical examples to illustrate our theoretical results.

By C and c we denote large and small 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 Banach Space

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 in 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 (1.5) and $u(t_n)$ is the exact solution of (1.1).

We first show that (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,

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

For example, if

$$r(\lambda) = \frac{1-(1-\theta)\lambda}{1+\theta\lambda}, \quad \text{with } \frac{1}{2} < \theta < 1, \tag{2.1}$$

we have $|r(\lambda)| < 1$ for $\lambda > 0$, and $r(\infty) = (1-\theta)/\theta \neq 0$. It is easy to check that $r(\lambda)$ is accurate of order $p = 1$. Another example is the so called Calahan scheme defined by

$$r(\lambda) = 1 - \frac{\lambda}{1+b\lambda} - \frac{\sqrt{3}}{6}(\frac{\lambda}{1+b\lambda})^2, \text{ with } b = \frac{1}{2}(1+\frac{\sqrt{3}}{3}). \tag{2.2}$$

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 $p = 3$.

This above argument uses that A is unbounded. When A is bounded with maximal eigenvalue $\lambda_{\max}$ and $|r(\infty)| < 1$, we obtain instead

$$t_n\|AE_k^n\| \leq C\max(1,\ k\lambda_{\max}e^{-cn}). \tag{2.3}$$

In fact, it suffices to show

$$n|\lambda r(\lambda)^n| \leq C\max(1,\ k\lambda_{\max}e^{-cn}), \quad \text{for } \lambda \in \sigma(-k\Delta_h),$$

which we will prove now.

Since $r(\lambda) = e^{-\lambda} + O(\lambda^2)$ as $\lambda \to 0$, we have that, for λ_0 small enough,

$$|r(\lambda)| \leq e^{-c\lambda}, \quad \text{for } 0 \leq \lambda \leq \lambda_0, \quad \text{with } 0 < c < 1. \tag{2.4}$$

Thus

$$n|\lambda r(\lambda)|^n \leq n\lambda e^{-cn\lambda} \leq C, \quad \text{for } 0 \leq \lambda \leq \lambda_0.$$

For large λ, we have, since $|r(\infty)| < 1$, that

$$|r(\lambda)| \leq e^{-c}, \quad \text{for } \lambda \geq \lambda_0. \tag{2.5}$$

Therefore,

$$n|\lambda r(\lambda)|^n \leq n(k\lambda_{max})e^{-cn} \leq Ck\lambda_{max}e^{-c_1 n} \quad \text{for } \lambda_0 < \lambda \leq k\lambda_{\max}.$$

Together these estimates complete the proof of (2.3).

In the application to the fully discrete case using quasiuniform triangulations, if we take $A = -\Delta_h$ and $E_k^n = r(-k\Delta_h)$ in (1.9), where Δ_h is the discrete Laplacian defined by (1.19), we get, noting that $\lambda_{\max} = O(h^{-2})$, where h is the spatial mesh size, see, e.g., Luskin and Rannacher [12],

$$t_n\|AE_k^n\| \le C\max(1,\ kh^{-2}e^{-cn}). \tag{2.6}$$

This shows that the estimate (1.10) is not valid for $A = -\Delta_h$ since in this case the bound of $\|\Delta_h U^n\|$ will turn to ∞ when $h \to 0$ for fixed k and n. Note, however, that $kh^{-2}e^{-cn}$ decreases exponentially as n grows, so that $\max(1, kh^{-2}e^{-cn}) = 1$ after some steps. Our numerical example will illustrate this.

Before we study the smoothing properties of the discrete method (1.5), we will show an error estimate for the approximation (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), are smooth. Recall the error estimate (1.7) in approximating the exact solution $u(t_n)$ by U^n, which shows that for $v \in \mathcal{D}(A^p)$, the error estimate 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) *and* (1.5)*. Assume that A satisfies* (1.2) *and* (1.3)*, and that $r(z)$ is accurate of order $p \ge 1$ and $A(\theta)$-stable, with $\theta \in (\delta, \pi/2]$. Let $j \ge 1$ and assume that Q_k^j be an approximation of D_t^j, which is accurate of order p. Then, there is a constant C such that, if $v \in \mathcal{D}(A^{p+j})$, we have*

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le Ck^p\|A^{p+j}v\|, \quad \textit{for } n \ge m_1.$$

For the proof we write, by (1.17),

$$Q_k^j U^n - D_t^j u(t_n) = \frac{1}{k^j}(P(E_k)E_k^n v - (-kA)^j E(t_n)v).$$

With

$$G_n(x) = P(r(x))r(x)^n - (-x)^j e^{-nx}, \tag{2.7}$$

our result will follow from

$$\|G_n(kA)A^{-(p+j)}\| \le Ck^{p+j}, \quad \text{for } n \ge m_1. \tag{2.8}$$

Before we prove Theorem 2.1 in a general Banach space, we consider the Hilbert space case and assume that A is a linear, selfadjoint, positive definite operator. By spectral representation, (2.8) may be written as

$$\Big|G_n(\lambda)\Big| \le C\lambda^{p+j}, \quad \text{for } \lambda \in \sigma(kA). \tag{2.9}$$

Since $\sigma(kA) \subset [0, \infty)$, it suffices to show (2.9) for $\lambda \ge 0$, which we will now do.

First we consider small λ. By (2.4), we have

$$\begin{aligned} \Big|r(\lambda)^n - e^{-n\lambda}\Big| &= \Big|(r(\lambda) - e^{\lambda})\sum_{j=0}^{n-1} r(\lambda)^{n-1-j}e^{-j\lambda}\Big| \\ &\le Cn\lambda^{p+1}e^{-c(n-1)\lambda} \le C\lambda^p, \quad \text{for } 0 \le \lambda \le \lambda_0. \end{aligned} \tag{2.10}$$

Further, with λ_0 possibly further restricted,

$$|P(r(\lambda)) - (-\lambda)^j| \le C\lambda^{p+j}, \quad \text{for } 0 \le \lambda \le \lambda_0. \tag{2.11}$$

In fact, with $1 + x = e^{\lambda}$, or $\lambda = \ln(1 + x)$, we have, by (1.16),

$$P(1 + x) = P(e^{\lambda}) = O(\lambda^j) = O((\ln(1 + x))^j) = O(x^j), \quad \text{as } x \to 0, \tag{2.12}$$

which implies that $P(x) = O((x-1)^j)$ as $x \to 1$, and hence $P'(x) = O((x-1)^{j-1})$ as $x \to 1$. Thus, Taylor's formula shows that, for $0 \le \lambda \le \lambda_0$,

$$|P(r(\lambda)) - P(e^{-\lambda})| = |P'(\xi_\lambda)(r(\lambda) - e^{-\lambda})| \le C|\xi_\lambda - 1|^{j-1}\lambda^{p+1} \le C\lambda^{p+j},$$

where ξ_λ lines between $r(\lambda)$ and $e^{-\lambda}$, and where we have used above the obvious estimate $|\xi_\lambda - 1| \le |r(\lambda) - e^{-\lambda}| + |e^{-\lambda} - 1| \le C\lambda$ for $0 \le \lambda \le \lambda_0$. Together with (1.16) this shows (2.11).

Thus, by (2.10) and (2.11),

$$\begin{aligned} |G_n(\lambda)| &= \Big|(P(r(\lambda)) - (-\lambda)^j)r(\lambda)^n + (-\lambda)^j(r(\lambda)^n - e^{-n\lambda})\Big| \\ &\le C\lambda^{p+j}, \quad \text{for } 0 \le \lambda \le \lambda_0. \end{aligned}$$

For $\lambda \ge \lambda_0$, we have, noting that $P(r(\lambda))r(\lambda)^n = \sum_{\nu=-m_1}^{m_2} c_\nu r(\lambda)^{n+\nu}$ with $n \ge m_1$,

$$|G_n(\lambda)| = |P(r(\lambda))r(\lambda)^n - (-\lambda)^j e^{-n\lambda}| \le C + \lambda^j \le C\lambda^{p+j},$$

which shows (2.9)

We remark that estimates similar to (2.4), (2.10), and (2.11) also hold in the Banach space case treated below, with λ replaced with z and $|z| \le R$, $|\arg z| \le \psi$ for arbitrary R and $\psi \in (0, \theta)$.

We now turn to the proof of Theorem 2.1 in a general Banach space. We need the following lemmas, cf., e.g., Thomée [19].

Lemma 2.2. *Assume that* (1.2) *and* (1.3) *hold and let* $r(z)$ *be a rational function which is bounded for* $|\arg z| \le \psi$, $|z| \ge \epsilon > 0$, *where* $\psi \in (0, \pi/2)$, *and for* $|z| \ge R$. *Then, if* $\epsilon > 0$ *is so small that* $\{z; |z| \le \epsilon\} \subset \rho(A)$, *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 sense.*

Lemma 2.3. *Assume that* (1.2) *and* (1.3) *hold, let* $\psi \in (0, \pi/2)$, *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* $\operatorname{Im} z$ *is decreasing along* $\gamma_\epsilon \cup \Gamma_\epsilon$. *When* $j \ge 0$, *we may take* $\epsilon = 0$.

Proof of Theorem 2.1. With $G_n(z)$ given in (2.7), it suffices to show that, for A satisfying (1.2) and (1.3),

$$\|G_n(A)A^{-(p+j)}\| \le C. \tag{2.13}$$

In fact, with A also kA satisfies (1.2) and (1.3) since, for $z \in \Sigma_\delta$,

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

Hence (2.13) applied to kA yields the desired bound.

By Lemma 2.2 we have, with $\psi \in (0, \theta)$,

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

and here, since the integrand is of order $O(|z|^{-p-j-1})$ for large z, we may let R tend to ∞. Using also Lemma 2.3 we have

$$G_n(A)A^{-(p+j)} = \frac{1}{2\pi i}\int_{\gamma_\epsilon\cup\Gamma_\epsilon} G_n(z)z^{-(p+j)}R(z;A)\,dz. \tag{2.14}$$

Following the proof of (2.9), we find

$$G_n(z) = O(z^{p+j}), \quad \text{as } z\to 0, \quad |\arg z|\le\psi. \tag{2.15}$$

Combining this with the fact that $0\in\rho(A)$, we have that the integrand in (2.14) is continuous at $z=0$, so that we may let $\epsilon\to 0$. It follows that

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

We now estimate the above integral. Again using (2.15) and the fact that $0\in\rho(A)$, we find, for η small enough,

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

Further, using (1.3) and (2.7) as well as the boundedness of $r(z)$ and e^{-tz} on Γ,

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

Thus

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

Together these estimates complete the proof. □

We now turn to a smoothing property of an $A(\theta)$-stable discretization scheme with $|r(\infty)|<1$. Before doing this, we show that $Q_k^jU^n$ defined by (1.11) can be expressed as a linear combination of $\bar\partial^jU^{n+\nu}$ for some integers ν. We have the following lemma:

Lemma 2.4. *Let $j\ge 1$ and $Q_k^jU^n$ be defined by* (1.11). *Then there exist constants α_μ, $-m_1+j\le\mu\le m_2$, such that*

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

Proof. We introduce the translation operator J: $U^{n+1}=JU^n$. Noting that, with $P(x)=\sum_{\nu=-m_1}^{m_2}c_\nu x^\nu$,

$$k^jQ_k^jU^n = \sum_{\nu=-m_1}^{m_2}c_\nu J^\nu U^n = P(J)U^n,$$

we associate with this difference operator with the rational function $P(x)$. We observe that the operator $\bar\partial^jU^{n+\mu}$ corresponds to the rational function $\tilde P(x) = x^\mu(1-x^{-1})^j$, since

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

Thus we only need to show that there exist α_μ such that

$$P(x) = (1 - x^{-1})^j \sum_{\mu=-m_1+j}^{m_2} \alpha_\mu x^\mu. \tag{2.16}$$

But by (1.16) we find $P^{(l)}(1) = 0$ for $0 \le l \le j - 1$, which implies that $P(x)$, and hence $x^{m_1}P(x)$ has the factor $(1 - x)^j$, that is, there exist a polynomial $\bar{P}(x)$ of degree $m_1 + m_2 - j$ such that $x^{m_1}P(x) = (1 - x)^j \bar{P}(x)$. Denoting $\bar{P}(x) = \sum_{k=0}^{m_1+m_2-j} \beta_k x^k$ for some constants β_k, we get that there exist some constants α_μ such that

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

which shows (2.16). □

Theorem 2.5. *Let U^n be the solutions of* (1.5). *Assume that* (1.2) *and* (1.3) *hold, and $r(z)$ is accurate of order $p = 1$ and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$. Let $j \ge 1$ and assume that Q_k^j is an approximation of D_t^j, which is accurate of order p. Then, there is a constant C such that,*

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

Proof. By Lemma 2.4, it suffices to show

$$\|\bar{\partial}^j U^n\| \le C t_n^{-j} \|v\|, \quad \text{for } n \ge j, \tag{2.17}$$

which we shall now do. In this case $\bar{\partial}^j U^n = k^{-j} P(E_k) E_k^n v$ for $P(x) = x^{-j}(x - 1)^j$.

As in the proof of Theorem 2.1, we first consider the case of a Hilbert space $\mathcal{H}$. We then need to show that, for $n \ge j$,

$$|P(r(\lambda)) r(\lambda)^n| = |r(\lambda)^{n-j}(r(\lambda) - 1)^j| \le C n^{-j}, \quad \text{for } \lambda \ge 0,\ n \ge j. \tag{2.18}$$

For small λ, using (2.4) and $r(\lambda) = 1 + O(\lambda)$ as $\lambda \to 0$, we have

$$|r(\lambda)^{n-j}(r(\lambda) - 1)^j| \le C\lambda^j e^{-cn\lambda} \le C n^{-j}, \quad \text{for } 0 \le \lambda \le \lambda_0,\ n \ge j. \tag{2.19}$$

For large λ, we have, by (2.5) and the stability of $r(\lambda)$,

$$|r(\lambda)^{n-j}(r(\lambda) - 1)^j| \le C e^{-c(n-j)} \le C e^{-cn} \le C n^{-j}, \quad \text{for } \lambda \ge \lambda_0, \quad \text{with } n \ge j.$$

Together these estimates show (2.18).

We now turn to the proof in a general Banach space. We show that

$$\|P(r(A)) r(A)^n\| = \|r(A)^{n-j}(r(A) - 1)^j\| \le C n^{-j} \quad \text{for } n \ge j.$$

As in the proof of Theorem 2.1 this then also holds with A replaced by kA, and thus shows the result stated.

Since $r(z)$ is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$, we have by Lemma 2.2

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

Clearly $|r(\infty)| \le e^{-c}$, with $c > 0$, so we have, for $n \ge j$,

$$|r(\infty)^{n-j}(r(\infty) - 1)^j| \le C e^{-cn} \le C n^{-j}.$$

To bound the integrals over the three components of the path of integration, we first fix $R \geq 1$ large enough that $|r(z)| \leq e^{-c}$ for $|z| = R$ and hence

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

For the other two components of the path of integration, since $0 \in \rho(A)$, we may let ϵ tend to 0, it suffices to bound the integral over Γ_0^R. But by (2.4) and since $r(z) - 1 = O(z)$, as $z \to 0$, we have

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

Together these estimates complete the proof. □

We remark that when $|r(\infty)| = 1$ 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 a compact inverse in Hilbert space $\mathcal{H}$, and A has eigenvalues $\{\lambda_j\}_{j=1}^{\infty}$ and a corresponding basis of orthonormal eigenfunctions $\{\varphi_j\}_{j=1}^{\infty}$. Then, with $v = \varphi_j$, we have, noting that $r(\infty) = -1$,

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

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

$$t_n \|\bar\partial U^n\| \leq C\|v\|, \quad \text{for } n \geq 0, \quad v \in \mathcal{H}.$$

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

$$r(\lambda) = \frac{1 - \frac{1}{2}\lambda + \frac{1}{12}\lambda^2}{1 + \frac{1}{2}\lambda + \frac{1}{12}\lambda^2}, \quad \text{where } r(\infty) = 1. \tag{2.20}$$

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

$$|nr(\lambda)^{n-1}(r(\lambda)-1)| \leq C \quad \text{for } \lambda > 0. \tag{2.21}$$

For small λ this follows directly from (2.19) and it remains to consider large λ. Noting that $|r(\lambda)| \leq e^{-c\lambda^{-1}}$ for $\lambda > \lambda_0$, with constant c, see, e.g., Thomee [19, Lemma 8.2], we have

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

which shows (2.21).

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 on the right. Comparing with the error estimate (1.8), we find that t_n^{-p} has been replaced by t_n^{-p-j} in our theorem. The proof in the Hilbert space case can be found in Baker, Bramble, and Thomée [4]. Here we extend the result to a general Banach space.

Theorem 2.6. *Let $u(t_n)$ and U^n be the solutions of* (1.1) *and* (1.5). *Assume that* (1.2) *and* (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 is an approximation of D_t^j, which is accurate of order p. Then, there is a constant C such that,*

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

To prove this theorem, we need the following lemma, cf., e.g., Thomée [19].

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 (2.7),

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

We set

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

note that $\tilde{G}_n(\infty) = 0$. Since $|\kappa| < 1$ and $\|A(I+A)^{-1}\| \le 2M$, we have

$$\|P(\kappa)\kappa^n A(I+A)^{-1}\| \le 2M|P(\kappa)\kappa^n| \le Cn^{-(p+j)},$$

and 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

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

Note that $\tilde{G}_n(z) = O(1)$ as $z \to 0$ and $0 \in \rho(A)$. Thus the integrand is continuous at $z = 0$, so that we may let ϵ tend to 0. We therefore have, with $\Gamma = \{\, z;\ |arg\, z| = \psi \,\}, \psi \in (0,\theta)$,

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

We write

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

Using the estimates (2.4), (2.10), (2.11) in Banach space case, and $|1/(1+z)| \le 1$ for $Re\, z \ge 0$, we have for $|z| \le 1$,

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

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 and since $|1+z| \ge |z|$ for $|Re z| \ge 0$, we get, for $|z| \ge 1$

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

Thus

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

Together these estimates complete the proof. □

3. Fully Discrete Schemes with Constant Time Steps

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

$$u_t = \Delta u \quad \text{in } \Omega, \quad \text{for } t > 0, \tag{3.1}$$

$$u = 0 \quad \text{on } \partial\Omega, \quad \text{for } t > 0, \; u(\cdot, 0) = v \quad \text{in } \Omega,$$

where Ω is a bounded domain in R^d with smooth boundary $\partial\Omega$.

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

$$u_{h,t}(t) = \Delta_h u_h, \qquad \text{for } t > 0, \qquad \text{with } u_h(0) = v_h, \tag{3.2}$$

where $\Delta_h : S_h \to S_h$ is the discrete Laplacian defined by $\Delta_h = -T_h^{-1}$.

We now apply our above time stepping procedure (1.5) to this semidiscrete equation (3.2). This defines the fully discrete approximation $U^n \in S_h$ of $u(t_n)$ recursively by

$$U^n = E_{kh} U^{n-1} \qquad \text{for } n \geq 1, \qquad \text{where } E_{kh} = r(-k\Delta_h), \quad \text{with } U^0 = v_h. \tag{3.3}$$

We shall first derive L_2 error estimates in the approximations $Q_k^j U^n$ of the time derivatives $D_t^j u(t_n)$ of the solution of (3.1), where U^n is obtained by applying our time stepping methods (1.5) to the spatially semidiscrete equation (3.2). We shall also consider L_∞ error estimates for the same approximations of time derivatives, but here we restrict ourselves to the two-dimensional case and to piecewise linear approximating functions.

3.1. L_2 Error Estimates.

In this subsection, we shall consider L_2 error estimates in the approximation of time derivatives of the solution of (3.1). To do this, we first show some error estimates for time derivatives in the spatially semidiscrete case. For the nonsmooth data case, we quote the following result from Bramble, Schatz, Thomée, and Wahlbin [5].

Theorem 3.1. *Let $u(t)$ and $u_h(t)$ be the solutions of (3.1) and (3.2) and $j \geq 1$. Assume that (i) and (ii) hold, and $v_h = P_h v$. Then we have*

$$\|D_t^j (u_h(t) - u(t))\| \leq C h^r t^{-r/2-j} \|v\| \quad \textit{for } t > 0.$$

The error bound in Theorem 3.1 depends in a singular way on t as t tends to 0, and the singularity is of order $O(t^{-r/2-j})$ when v is only in $L_2 = L_2(\Omega)$. We will show in the following theorems that the order of the sigularity in the error bound depends on the smoothness of v. To express this we shall use the space $\dot{H}^s = \dot{H}^s(\Omega)$ for s a nonnegative integer. Recall that for Ω an appropriately regular domain in R^d, $H^s = H^s(\Omega)$ is defined by the norm

$$\|v\|_s = \|v\|_{H^s} = \Big(\sum_{|\alpha| \leq s} \|D^\alpha v\|^2 \Big)^{1/2}, \quad \text{where } \|\cdot\| = \|\cdot\|_{L_2}.$$

To define $\dot{H}^s$, we consider the eigenvalue problem

$$-\Delta\varphi = \lambda\varphi \quad \text{in } \Omega, \quad \text{with } \varphi = 0 \quad \text{on } \partial\Omega.$$

As is well-known, this eigenvalue problem admits a nondecreasing sequence $\{\lambda_m\}_{m=1}^\infty$ of positive eigenvalues which tend to ∞ with m, and a corresponding sequences

$\{\varphi_m\}_{m=1}^\infty$ of eigenfunctions which form an orthonormal basis for L_2. For $s \ge 0$, let $\dot{H}^s$ be the subspace of L_2 defined by

$$|v|_s = \Big(\sum_{m=1}^{\infty} \lambda_m^s (v, \varphi_m)^2 \Big)^{1/2} < \infty.$$

It is known that, for s a nonnegative integer, see, e.g., Thomée [19],

$$\dot{H}^s = \{ v \in H^s ; \Delta^j v = 0 \quad \text{on } \partial\Omega, \quad \text{for } j < s/2 \},$$

where the boundary conditions are interpreted in the sense of traces in $L_2(\partial\Omega)$, and that the norms $|\cdot|_s = \|\cdot\|_{\dot{H}^s}$ and $\|\cdot\|_s = \|\cdot\|_{H^s}$ are equivalent in $\dot{H}^s$, with

$$|v|_s = \begin{cases} \|\Delta^p v\|, & \text{if } s = 2p, \\ \| \bigtriangledown \Delta^p v\|, & \text{if } s = 2p+1, \end{cases}$$

where p is a nonnegative integers. Based on the properties of space $\dot{H}^s$, the following regularity result is shown in [19].

Lemma 3.2. *For $v \in L_2$, the solution $u(t) = E(t)v$ of (3.1) belongs to $\dot{H}^s$ for any $s \ge 0$, if $t > 0$. If $0 \le s \le q$ and $l \ge 0$, and if $v \in \dot{H}^s$, we have*

$$|D_t^l u(t)|_q = |D_t^l E(t) v|_q \le C t^{-(q-s)/2-l} |v|_s, \quad \textit{for } t > 0.$$

To clarify how the order of t of the singularity in the error bound depends on the smoothness of v, let us first consider the case $v \in \dot{H}^r$. We find in the following theorem in this case that the order will be $O(t^{-j})$, instead of the $O(t^{-r/2-j})$ in the case of $v \in L_2$, i.e., the singularity is weaker for these more regular initial data.

Theorem 3.3. *Let $u(t)$ and $u_h(t)$ be the solutions of (3.1) and (3.2) and $j \ge 1$. Assume that (i) and (ii) hold, and $v_h = P_h v$. Then, if $v \in \dot{H}^r$, we have*

$$\|D_t^j (u_h(t) - u(t))\| \le C h^r t^{-j} |v|_r \quad \textit{for } t > 0.$$

The proof of the result depends on the following lemma, see, e.g., Thomée [19],

Lemma 3.4. *Assume that T_h is positive semidefinite on L_2 and that*

$$T_h e_t + e = \rho, \quad \textit{for } t \ge 0, \quad \textit{with } T_h e(0) = 0.$$

Then, for $\epsilon > 0$ arbitrary,

$$\|e(t)\| \le \epsilon \sup_{s \le t} (s \|\rho_t(s)\|) + C_\epsilon \sup_{s \le t} \|\rho(s)\|, \quad \textit{for } t \ge 0.$$

Proof of Theorem 3.3. The proof will be by induction over j. The case $j = 0$ can be found in Thomée [19, Theorem 3.1]. Assume thus that the result is already shown for $j-1$ with $j \ge 1$. We note that this semidiscrete analogue of (3.1) may also be written

$$T_h u_{h,t} + u_h = 0, \quad \text{for } t > 0, \quad \text{with } u_h(0) = v_h. \tag{3.4}$$

Similarly, for the continuous problem, we have

$$T u_t + u = 0, \quad \text{for } t > 0, \quad \text{with } u(0) = v. \tag{3.5}$$

Setting $e = u_h - u$, we have by (3.4) and (3.5)

$$T_h e_t + e = \rho, \quad \text{where } \rho = -(T_h - T)\Delta u. \tag{3.6}$$

Denoting $e^{(j)} = D_t^j e$, we have, by differentiation of (3.6),

$$T_h e_t^{(j)} + e^{(j)} = \rho^{(j)}, \quad \text{where } \rho^{(j)} = D_t^j \rho = -(T_h - T) D_t^{j+1} \rho. \tag{3.7}$$

We further set $w = w(j,t) = t^j e^{(j)}$, and write

$$\begin{aligned} T_h w_t + w &= T_h (t^j e^{(j)})_t + t^j e^{(j)} \\ &= t^j \rho^{(j)} + j t^{j-1} T_h e^{(j)} = t^j \rho^{(j)} + j t^{j-1} (\rho^{(j-1)} - e^{(j-1)}) = \eta. \end{aligned}$$

By Lemma 3.4 we find

$$\|w(t)\| \le \epsilon \sup_{s\le t} (s \|\eta_t(s)\|) + C_\epsilon \sup_{s \le t} \|\eta(s)\|.$$

Here

$$\|\eta(s)\| \le s^j \|\rho^{(j)}(s)\| + j s^{j-1} \|\rho^{(j-1)}(s)\| + j \|w(j-1,s)\|$$

and

$$\begin{aligned} s\|\eta_t(s)\| \le\ & 2 j s^j \|\rho^{(j)}(s)\| + s^{j+1} \|\rho^{(j+1)}(s)\| + j(j-1) s^{j-1} \|\rho^{(j-1)}(s)\| \\ & + j(j-1) s^{j-1} \|e^{(j-1)}(s)\| + j \|w(j,s)\|. \end{aligned}$$

With $\epsilon = 1/(4j)$, say, we conclude, for all $t \ge 0$,

$$\|w(j,t)\| \le \frac{1}{2} \sup_{s \le t} \|w(j,s)\| + C \sup_{s\le t} \Big(\sum_{l=-1}^{1} s^{j+l} \|\rho^{(j+l)}(s)\| + \|w(j-1,s)\| \Big).$$

Choose $\tau = \tau(t)$ such that $\sup_{s\le t} \|w(j,s)\| = \|w(j,\tau)\|$, we have,

$$\|w(j,t)\| \le \|w(j,\tau)\| \le C \sup_{s\le t} \Big(\sum_{l=-1}^{1} s^{j+l} \|\rho^{(j+l)}(s)\| + \|w(j-1,s)\| \Big).$$

Now since $\rho^{(q)} = -(T_h - T) u^{(q+1)}$, we have by (ii) and Lemma 3.2, for any $q \ge 0$,

$$s^q \|\rho^{(q)}(s)\| \le C h^r s^q |u^{(q+1)}(s)|_{r-2} \le C h^r |v|_r,$$

and, using our induction assumption, $\|w(j-1,s)\| = \|s^{j-1} e^{(j-1)}(s)\| \le C h^r |v|_r$, which completes the proof of Theorem 3.3. □

Theorems 3.1 and 3.3 show error estimates for $v \in L_2$ and $v \in \dot{H}^r$, separately. Using interpolation theory, we obtain the following theorem which shows how the singularity in an optimal order error bound depends on the smoothness of v.

Theorem 3.5. *Let $u(t)$ and $u_h(t)$ be the solutions of* (3.1) *and* (3.2) *and $j \ge 1$. Assume that (i) and (ii) hold, and $v_h = P_h v$. Then, if $v \in \dot{H}^s$ and $0 \le s \le r$, we have*

$$\|D_t^j u_h(t) - D_t^j u(t)\| \le C h^r t^{-(r-s)/2-j} |v|_s, \quad \textit{for } t > 0.$$

We now consider error estimates for time derivatives for the semidiscrete problem which hold uniformly down to $t = 0$. In this case, in order to obtain optimal order results, a special choice of initial data has to be made and more smoothness than before has to be required from the initial data.

Theorem 3.6. *Let $u(t)$ and $u_h(t)$ be the solutions of* (3.1) *and* (3.2) *and $j \ge 1$. Assume that (i) and (ii) hold, and $v_h = P_h v$. Then, if $v \in \dot{H}^{r+2j}$, we have*

$$\|D_t^j u_h(t) - D_t^j u(t)\| \le C h^r |v|_{r+2j} + C \|\Delta_h^j v_h - \Delta^j v\| \quad \textit{for } t \ge 0. \tag{3.8}$$

Proof. We assume first $v_h = T_h^j(-\Delta)^j v$. In this case $\Delta_h^j v_h = \Delta^j v$, so that the second term on the right in (3.8) vanishes. Recall that $e^{(j)}$ satisfies

$$T_h e_t^{(j)} + e^{(j)} = \rho^{(j)}.$$

With $v_h = T_h^j(-\Delta)^j v$, we have

$$T_h e^{(j)}(0) = T_h(\Delta_h^j v_h - \Delta^j v) = 0.$$

Hence by Lemma 3.2 and (ii), for $s \geq 0$,

$$\begin{aligned}\|\rho^{(j)}(s)\| &= \|(T_h - T)D_t^{j+1}u(s)\| \leq Ch^r\|D_t^{j+1}u(s)\|_{r-2}\\ &= Ch^r|\Delta^{j+1}u(s)|_{r-2} \leq Ch^r|v|_{r+2j},\end{aligned}$$

and

$$\begin{aligned}s\|\rho_t^{(j)}(s)\| &= s\|(T_h - T)D_t^{j+2}u(s)\| \leq Ch^r s|D_t^{j+2}u(s)|_{r-2}\\ &\leq Ch^r s|\Delta^{j+2}u(s)|_{r-2} \leq Ch^r s|u(s)|_{2j+r+2} \leq Ch^r|v|_{r+2j},\end{aligned}$$

Together with Lemma 3.4 these estimates show

$$\|D_t^j u_h(t) - D_t^j u(t)\| \leq Ch^r|v|_{r+2j}, \quad \text{for } t \geq 0, \tag{3.9}$$

which completes the proof of (3.8) for the present choice of v_h.

It remains to consider the contribution to the semidiscrete solution of the initial data $v_h - T_h^j(-\Delta)^j v$. If $E_h(t) = e^{\Delta_h t}$ is the solution operator of the semidiscrete problem (3.2), then we have by (3.9)

$$\|D_t^j E_h(t)(T_h^j(-\Delta)^j v) - D_t^j u(t)\| \leq Ch^r|v|_{r+2j}.$$

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

$$\|D_t^j E_h(t)(v_h - T_h^j(-\Delta)^j v)\| = \|E_h(t)(\Delta_h^j v_h - \Delta^j v)\| \leq C\|\Delta_h^j v_h - \Delta^j v\|.$$

Together these estimates complete the proof of (3.8). □

We remark that if $v \in \dot{H}^{\max(r+2l-2,2p+2j)}$, with $l > j$, we also obtain the optimal order convergence for the choice of initial data $v_h = T_h^l(-\Delta)^l v$, which follows from Theorem 3.6 and the following fact, for present choice of v_h,

$$\begin{aligned}\|\Delta_h^j v_h - \Delta^j v\| &= \|(-T_h)^{l-j}\Delta^l v - \Delta^j v\| = \sum_{m=1}^{l-j} T_h^{m-1}(T_h - T)\Delta^{j+m}v\|\\ &\leq Ch^r\|(T_h - T)\Delta^l v\| \leq Ch^r|v|_{r+2l-2}.\end{aligned}$$

With (j,l) replaced by (m,j) this means that the error bound of Theorem 3.6 holds also for $\|D_t^m(u_h - u)\|$ when $m < j$. A similar remark applies to Theorems 3.8 and 3.17 below.

We are now ready to consider the fully discrete schemes defined by application of our time stepping procedure to the semidiscrete equation (3.2). We begin with a nonsmooth data error estimate.

Theorem 3.7. *Let $u(t_n)$ and U^n be the solutions of* (3.1) *and* (3.3). *Assume that (i) and (ii) hold, and that the time stepping method defined by* (3.3) *is accurate of order p, with $p \geq 1$, and $|r(\lambda)| < 1$ for $\lambda > 0$ and $|r(\infty)| < 1$. Let $j \geq 1$ and assume that Q_k^j is an approximation of D_t^j, which is also accurate of order p. Then, if $v_h = P_h v$, we have*

$$\|Q_k^j U^n - D_t^j u(t_n)\| \leq C(h^r t_n^{-r/2-j} + k^p t_n^{-p-j})\|v\|, \quad \textit{for } t_n > 0.$$

Proof. By Theorem 2.6, applied to the semidiscrete equation (3.2), we have

$$\|Q_k^j U^n - D_t^j u_h(t_n)\| \le Ck^p t_n^{-p-j}\|P_h v\| \le Ck^p t_n^{-p-j}\|v\|.$$

Together with Theorem 3.1 this completes the proof. □

We shall now turn to error estimates in the smooth data case. In this case, in order to obtain optimal order results uniformly down to $t = 0$, as in the semidscrete approximation considered above, a special choice of discrete initial data v_h and smoothness of the initial data v for the continous problem have to be required.

Theorem 3.8. *Let $u(t_n)$ and U^n be the solutions of (3.1) and (3.3). Assume that (i) and (ii) hold, and that the time stepping method defined by (3.3) is accurate of order p, with $p \ge 1$, and $|r(\lambda)| < 1$ for $\lambda > 0$. Let $j \ge 1$ and ssume that Q_k^j is an approximation of D_t^j, which is also accurate of order p. Then, if $v \in \dot{H}^{max(r+2j,2p+2j)}$, we have*

(3.10)
$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C(h^r|v|_{r+2j} + k^p|v|_{2p+2j}) + C\|\Delta_h^j v_h - \Delta^j v\|, \quad \textit{for } t_n \ge 0.$$

In order to show the estimate stated, we need the following lemma.

Lemma 3.9. *Assume that the discretization scheme is accurate of order p, with $p \ge 1$, and that $|r(\lambda)| < 1$ for $\lambda > 0$. Let $\tilde{G}_{n,s} = G_n(-k\Delta_h)T_h^s$, where $G_n(\lambda)$ is given by (2.7). Then, we have*

$$\|\tilde{G}_{n,l+j}\| \le Ck^{l+j}, \quad \textit{for } 0 \le l \le p,\ n \ge 0, \tag{3.11}$$

and

$$\|\tilde{G}_{n,l}\| \le Ck^l n^{-j}, \quad \textit{for } 0 \le l \le p,\ n > 0. \tag{3.12}$$

Proof. Since

$$\|\tilde{G}_{n,l+j}\| \le k^{l+j} \sup_{\lambda\in\sigma(-k\Delta_h)} |\lambda^{-(l+j)}G_n(\lambda)|,$$

it suffices for the proof of (3.11) to show that $|G_n(\lambda)| \le C\lambda^{l+j}$ for $\lambda > 0$, $0 \le l \le p$. But, by (2.9), we have, with $\lambda_0 \in (0,1)$,

$$|G_n(\lambda)| \le C\lambda^{l+j}, \quad \text{for } 0 \le l \le p, \quad 0 \le \lambda \le \lambda_0,$$

and, using the stability of $r(\lambda)$,

$$|G_n(\lambda)| \le C + C\lambda^j \le C\lambda^{l+j}, \quad \text{for } 0 \le l \le p, \quad \lambda > \lambda_0,$$

which shows (3.11).

To prove (3.12), we need to show

$$|G_n(\lambda)| \le C\lambda^l n^{-j}, \quad \text{for } 0 \le l \le p, \quad \lambda > 0. \tag{3.13}$$

We have, by (1.16) and (2.4), with $\lambda_0 \in (0,1)$,

$$|(P(r(\lambda)) - (-\lambda)^{-j})r(\lambda)^n| \le (C\lambda^{l+j})e^{-cn\lambda} \le C\lambda^l n^{-j}, \quad \text{for } 0 \le \lambda \le \lambda_0, \tag{3.14}$$

and, by (2.10),

$$|(-\lambda)^j(r(\lambda)^n - e^{-n\lambda})| \le C\lambda^j(C\lambda^{l+1}ne^{-c(n-1)\lambda}) \le C\lambda^l n^{-j}, \quad \text{for } 0 \le \lambda \le \lambda_0,$$

which shows that (3.13) holds for $0 \le \lambda \le \lambda_0$. Further, using (2.11),

$$\lambda^{-l}n^j|P(r(\lambda))r(\lambda)^n| \le C\lambda_0^{-l}n^j e^{-c(n-m_1)} \le C, \quad \text{for } \lambda > \lambda_0,\ 0 \le l \le p,$$

and

$$\lambda^{-l} n^j |(-\lambda)^j e^{-n\lambda}| \le \lambda_0^{-l} |(n\lambda)^j e^{-n\lambda}| \le C, \quad \text{for } \lambda > \lambda_0,\ 0 \le l \le p.$$

Hence, (3.13) holds also for $\lambda > \lambda_0$. Together these estimates complete the proof. □

Proof of Theorem 3.8. Assuming first that $v_h = T_h^j(-\Delta)^j v$ we may write

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

We now note that if we set

$$v_k = \sum_{k\lambda_l \le 1} (v, \varphi_l)\varphi_l,$$

where φ_l and λ_l are the eigenfunctions and eigenvalues of the differential operator $-\Delta$, with vanishing boundary values, then $v_k \in \dot{H}^s$ for each $s \ge 0$. Further, by the definition of the norm in $\dot{H}^s$, we find easily

$$\|(-\Delta)^j (v - v_k)\| \le C k^p |v|_{2p+2j}, \tag{3.15}$$

$$\|(-\Delta)^{p+j} v_k\| \le C \|(-\Delta)^{p+j} v\| = C|v|_{2p+2j}, \tag{3.16}$$

and

$$|v_k|_{r+2l+2j} \le k^{-l} |v|_{r+2j}, \quad \text{for } 0 \le l \le p-1. \tag{3.17}$$

Applying now the identity

$$v = \sum_{l=0}^{p-1} T_h^l (T - T_h)(-\Delta)^{l+1} v + T_h^p (-\Delta)^p v, \quad \text{for } v \in \dot{H}^{2p+2j},$$

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

$$\begin{aligned} \tilde{G}_{n,j}(-\Delta)^j v_k &= G_n(-k\Delta_h) T_h^j (-\Delta)^j v_k \\ &= \sum_{l=0}^{p-1} \tilde{G}_{n,l+j} (T - T_h)(-\Delta)^{l+j+1} v_k + \tilde{G}_{n,p+j} (-\Delta)^{p+j} v_k. \end{aligned} \tag{3.18}$$

Here, by (3.11) and (3.16),

$$\|\tilde{G}_{n,p+j}(-\Delta)^{p+j} v_k\| \le C k^{p+j} \|(-\Delta)^{p+j} v_k\| \le C k^{p+j} |v_k|_{2p+2j} \le C k^{p+j} |v|_{2p+2j}.$$

Further, using also property (ii) of T_h and (3.17), we obtain

$$\begin{aligned} \|\tilde{G}_{n,l+j}(T - T_h)(-\Delta)^{l+j+1} v_k\| &\le C k^{l+j} \|(T - T_h)(-\Delta)^{l+j+1} v_k\| \\ &\le C k^{l+j} h^r \|(-\Delta)^{l+j+1} v_k\|_{r-2} = C k^{l+j} h^r |v_k|_{r+2l+2j} \\ &\le C k^j h^r |v|_{r+2j}, \quad \text{for } 0 \le l \le p-1. \end{aligned}$$

Together these estimates imply

$$\|\tilde{G}_{n,j}(-\Delta)^j v_k\| \le C k^j (h^r |v|_{r+2j} + k^p |v|_{2p+2j}).$$

Since obviously, by (3.11) and (3.15),

$$\begin{aligned} \|\tilde{G}_{n,j}(-\Delta)^j (v - v_k)\| &= \|G_n(-k\Delta_h) T_h^j (-\Delta)^j (v - v_k)\| \\ &\le C k^j \|(-\Delta)^j (v - v_k)\| \le C k^{p+j} |v|_{2p+2j}, \end{aligned}$$

we conclude that

$$\|Q_k^j U^n - D_t^j u_h(t_n)\| = \|k^{-j} \tilde{G}_{n,j}(-\Delta)^j v\| \le C(h^r |v|_{r+2j} + k^p |v|_{2p+2j}), \tag{3.19}$$

which completes the proof of (3.10) for the present choice of v_h.

It remains to consider the contribution to the fully discrete solution of $v_h - T_h^j(-\Delta)^j v$. By (3.19), we have

$$\|Q_k^j E_{kh}^n T_h^j(-\Delta)^j v - D_t^j u_h(t_n)\| \le C(h^r|v|_{r+2j} + k^p|v|_{2p+2j}).$$

Further, using (2.11) and the stability of $r(\lambda)$,

$$\begin{aligned}\|Q_k^j E_{kh}^n (v_h - T_h^j(-\Delta)^j)v\| &\le \sup_{\lambda\in\sigma(-k\Delta_h)} \left|P(r(\lambda))r(\lambda)^n\lambda^{-j}\right| \|\Delta_h^j v_h - \Delta^j v\| \\ &\le C\|\Delta_h^j v_h - \Delta^j v\|.\end{aligned}$$

Together with the estimate (3.8) for the semidiscrete problem this completes the proof of Theorem 3.8. □

Theorem 3.8 shows that the optimal order convergence uniformly down to $t = 0$ depends upon the smoothness of v and the choice of initial data v_h. One may want to choose $v_h = P_h v$, where v is smooth enough. In this case, we are able to obtain optimal order convergence, but not uniformly down to $t = 0$. We close this section by stating an estimate for $v \in \dot{H}^{\max(r,2p)}$ and $v_h = P_h v$. We omit the proof which is similar to the proof of Theorem 3.8.

Theorem 3.10. *Let $u(t_n)$ and U^n be the solutions of* (3.1) *and* (3.3). *Assume that (i) and (ii) hold, and that the time stepping method defined by* (3.3) *is accurate of order p, with $p \ge 1$, and $|r(\lambda)| < 1$ for $\lambda > 0$. Let $j \ge 1$ and assume that Q_k^j is an approximation of D_t^j, which is also accurate of order p. Then, if $v \in \dot{H}^{max(r,2p)}$ and $v_h = P_h v$, we have*

$$\|Q_k^j U^n - D_t^j u(t_n)\| \le C t_n^{-j}(h^r|v|_r + k^p|v|_{2p}), \quad \textit{for } t_n > 0.$$

3.2. L_∞ **Error Estimates.** In this subsection, we will derive L_∞ error estimates for approximations of time derivatives of the solution of (3.1) in two spatial variables, using piecewise linear approximating functions in space on quasiuniform triangulations of the spatial domain.

We first show some L_∞ error estimates in the spatially semidiscrete case. We begin with an error estimate in the nonsmooth data case.

Theorem 3.11. *Let $u(t)$ and $u_h(t)$ be the solutions of* (3.1) *and* (3.2) *and $j \ge 1$. Then, if $v \in L_\infty$ and $v_h = P_h v$, we have*

$$\|D_t^j u_h(t) - D_t^j u(t)\|_{L_\infty} \le C h^2 \ell_h^{3+j} t^{-j-1}\|v\|_{L_\infty}, \quad \textit{where } \ell_h = \ln(1/h).$$

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 3.12. *Let $u(t)$ be the solution of* (3.1) *and $j \ge 1$. Then, we have, for $\rho = (R_h - I)u$ and $\eta = (P_h - I)u$,*

$$t^{j+1}\left(\|\rho^{(j)}(t)\|_{L_\infty} + \ell_h\|\eta^{(j)}(t)\|_{L_\infty}\right) \le C h^2 \ell_h^2 \|v\|_{L_\infty}. \tag{3.20}$$

Proof. With I_h the standard interpolation operator into S_h, we have, cf., e.g., Brenner and Scott [6],

$$\|I_h u - u\|_{L_\infty} \le C h^{2-2/s}\|u\|_{W_s^2}, \quad \text{for } 2 \le s \le \infty,\ u \in \dot{W}_s^2 = W_s^2 \cap H_0^1.$$

Noting that by the logarithmic maximum-norm stability of R_h in L_∞, i.e., (cf., Schatz and Wahlbin [18]), $\|R_h u\|_{L_\infty} \le C\ell_h \|u\|_{L_\infty}$, we have, since $\rho^{(j)} = (R_h - I)D_t^j u = (R_h - I)(D_t^j u - I_h D_t^j u)$,

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

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

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

we hence obtain, using also the smoothing property (1.4),

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

With $s = \ell_h$ this shows the bound in (3.20) for $\rho^{(j)}(t)$. The proof of the bound for $\eta^{(j)}(t)$ is analogous, with one less factor ℓ_h because P_h is bounded in L_∞. □

We also need the following lemma which shows that the discrete solution operator $E_h(t)$ is stable in L_∞ norm and has a smoothing property.

Lemma 3.13. *With S_h the piecewise linear finite element spaces and $E_h(t)$ the solution operator of* (3.2), *we have*

$$\|E_h(t)v_h\|_{L_\infty} + (t+h^2)\|E_h'(t)v_h\|_{L_\infty} \le C\|v_h\|_{L_\infty}, \quad \textit{for } t > 0. \tag{3.21}$$

Proof. We know from Thomée and Wahlbin [20] that

$$\|E_h(t)v_h\|_{L_\infty} + t\|E_h'(t)v_h\|_{L_\infty} \le C\|v_h\|_{L_\infty}, \quad \text{for } t > 0.$$

By the inverse property $\|\Delta_h \chi\|_{L_\infty} \le Ch^{-2}\|\chi\|_{L_\infty}$ for $\chi \in S_h$, we get

$$\|E_h'(t)v_h\|_{L_\infty} = \|\Delta_h E_h(t)v_h\|_{L_\infty} \le C\|\Delta_h v_h\|_{L_\infty} \le Ch^{-2}\|v_h\|_{L_\infty}.$$

Together these estimates complete the proof. □

Proof of Theorem 3.11. The proof will be by induction over j. The case $j = 0$ can be found in Thomée [19, Theorem 5.4]. Assuming now that the result is already shown for $j-1$, with $j \ge 1$, we write $u_h(t) - u(t) = (u_h(t) - P_h u(t)) + (P_h u(t) - u(t)) = \zeta + \eta$. Here $\eta^{(j)}$ is bounded as desired by Lemma 3.12 and it remains to bound $\zeta^{(j)} = D_t^j \zeta = D_t^j(u_h(t) - P_h u(t))$. Since

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

we find

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

Thus, we obtain by integration, noting that $E_h(t-s)\Delta_h = E_h'(t-s)$,

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

By the induction assumption, $s^j\|\zeta^{(j-1)}(s)\|_{L_\infty} \le Ch^2\ell_h^{2+j}\|v\|_{L_\infty}$. Thus, combining this with Lemma 3.13, we have, for $h \le h_0$ and t bounded,

$$\|I\|_{L_\infty} \le C\int_0^t \frac{1}{t-s+h^2} s^j\|\zeta^{(j-1)}(s)\|_{L_\infty} ds$$
$$\le Ch^2\ell_h^{2+j}\ln((h^2+t)/h^2)\|v\|_{L_\infty} \le Ch^2\ell_h^{3+j}\|v\|_{L_\infty}.$$

Similarly, by Lemma 3.12 and 3.13, we have

$$\|II\|_{L_\infty} + \|III\|_{L_\infty} \le Ch^2\ell_h^2\int_0^t \frac{1}{t-s+h^2} ds\|v\|_{L_\infty} \le Ch^2\ell_h^3\|v\|_{L_\infty}.$$

Together these estimates complete the proof. □

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

Theorem 3.14. *Let $u(t)$ and $u_h(t)$ be the solutions of* (3.1) *and* (3.2) *and $j \ge 1$. Then, if $v \in \dot W_\infty^{2j+2}$, we have*

$$(3.22)\qquad \|D_t^j u_h(t) - D_t^j u(t)\|_{L_\infty} \le Ch^2\ell_h^2\|v\|_{W_\infty^{2j+2}} + C\|\Delta_h^j v_h - R_h\Delta^j v\|_{L_\infty}.$$

The proof will depend on the following:

Lemma 3.15. *Let $u(t)$ be the solution of* (3.1) *and $j \ge 1$. Then we have, for $\rho = R_h u - u$,*

$$\|\rho^{(j)}(t)\|_{L_\infty} + t\|\rho^{(j+1)}(t)\|_{L_\infty} \le Ch^2\ell_h^2\|v\|_{W_\infty^{2j+2}}, \quad \textit{for } j \ge 0, \quad v \in \dot W_\infty^{2j+2}$$

Proof. The case $j = 0$ can be found in Thomée [19, Lemma 5.6]. Hence

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

which completes the proof. □

Proof of Theorem 3.14. We assume first $v_h = T_h^{j+1}(-\Delta)^{j+1}v$. In this case $\Delta_h^j v_h = R_h\Delta^j v$, so that the second term on the right in (3.22) vanishes. We write, with $\tilde\theta = D_t^j(u_h - R_h u)$ and $\tilde\rho = D_t^j(R_h u - u)$,

$$\tilde e(t) = D_t^j u_h(t) - D_t^j u(t) = \tilde\theta(t) + \tilde\rho(t).$$

Here $\tilde\rho(t)$ is bounded as desired by Lemma 3.15. To estimate $\tilde\theta(t)$ we write, noting that $\tilde\theta(0) = 0$,

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

Here by Lemmas 3.13 and 3.15,

$$\|II\|_{L_\infty} \le C\int_{t/2}^t \|\tilde\rho_t(s)\|_{L_\infty} ds \le Ch^2\ell_h^2\|v\|_{W_\infty^{2j+2}}.$$

For I we integrate by parts to obtain

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

Again using Lemmas 3.13 and 3.15 we have

$$\|E_h(t-s)P_h\tilde\rho(s)\|_{L_\infty} \le C\|\tilde\rho(s)\|_{L_\infty} \le Ch^2\ell_h^2\|v\|_{W_\infty^{2j+2}}, \quad \text{for } s = 0, t/2.$$

and, using $\|E_h'(t)\| \leq Ct^{-1}\|v_h\|_{L_\infty}$,

$$\Big\| \int_0^{t/2} E_h'(t-s)P_h\tilde{\rho}(s)ds \Big\|_{L_\infty} \leq C\int_0^{t/2}(t-s)^{-1}\|\tilde{\rho}(s)\|_{L_\infty}ds \leq Ch^2\ell_h^2\|v\|_{W_\infty^{2j+2}},$$

which shows (3.22) for present choice of v_h.

The argument of the proof of Theorem 3.6 completes the proof for a general choice of v_h. □

Now we consider error estimates for the fully discrete scheme (3.3). Combining Theorem 3.11, for the error estimate in semidiscrete case, and Theorem 2.6, applied to the semidiscrete equation (3.2), we obtain the following error estimate in the nonsmooth data case.

Theorem 3.16. *Let $u(t_n)$ and U^n be the solutions of (3.1) and (3.3). Assume that the time stepping method defined by (3.3) is accurate of order p, with $p \geq 1$, and that $r(z)$ is A-stable and accurate of order p and $|r(\infty)| < 1$. Let $j \geq 1$ and assume that Q_k^j is an approximation of D_t^j, which is also accurate of order p. Then, if $v \in L_\infty$ and $v_h = P_h v$, we have*

$$\|Q_k^j U^n - D_t^j u(t_n)\|_{L_\infty} \leq C(h^2\ell_h^{j+3}t_n^{-j-1} + k^p t_n^{-p-j})\|v\|_{L_\infty}, \quad \text{for } t_n > 0.$$

We now show an error estimate in the smooth data case.

Theorem 3.17. *Let $u(t_n)$ and U^n be the solutions of (3.1) and (3.3). Assume that the time stepping method defined by (3.3) is accurate of order p, with $p \geq 1$, and that $r(z)$ is A-stable and accurate of order p. Let $j \geq 1$ and assume that Q_k^j is an approximation of D_t^j, which is also accurate of order p. Then, if $v \in \mathcal{D}(\Delta^{p+j})$, we have*

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

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

Lemma 3.18. *Assume that $r(z)$ is A-stable and accurate of order p and that $j \geq 1$. With $\tilde{G}_{n,s}$ given in Lemma 3.9, we have*

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

Proof. By Pazy [15, Theorem 2.5.2], we see that (3.21) implies that $E_h(t)$ is an analytic semigroup, uniformly in h, and lead to a resolvent estimate on an appropriate sector in the complex plane

$$\|R(z, -\Delta_h)\|_{L_\infty} \leq C|z|^{-1}, \quad \psi \leq |arg\ z| \leq \pi,\ \psi \in [0, \pi/2).$$

Applying Theorem 2.1, we obtain

$$\|\tilde{G}_{n,l+j}w\|_{L_\infty} = \|G_n(-k\Delta_h)T_h^{l+j}w\| \leq Ck^{l+j}\|w\|_{L_\infty}, \quad \text{for } 0 \leq l \leq p. \tag{3.23}$$

Note that if $r(z)$ is accurate of p it is also accurate of order l with $1 \leq l \leq p$, which shows (3.23) for $1 \leq l \leq p$. The case $l = 0$ follows by the direct proof as in the case $l = p$. □

Proof of Theorem 3.17. By Theorem 3.14, Lemma 3.15 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

(3.24)

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

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

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

From Thomée [19, Theorem 8.6], we choose $\tilde{v}_k$, such that, with C independent of s,

$$\|(-\Delta)^j(v - \tilde{v}_k)\|_{L_\infty} \le Ck^p\|\Delta^{p+j}v\|_{L_\infty} \le Ck^p\|v\|_{W_\infty^{2(p+j)}} \tag{3.25}$$

$$\|(-\Delta)^{p+j}\tilde{v}_k\|_{L_\infty} \le C\|\Delta^{p+j}v\|_{L_\infty} \le \|v\|_{W_\infty^{2(p+j)}} \tag{3.26}$$

$$k^l\|(-\Delta)^{l+j}\tilde{v}_k\|_{W_s^2} \le Cs\|\Delta^j v\|_{W_s^2} \quad \text{for } 0 \le l \le p-1,\ 2 \le s < \infty. \tag{3.27}$$

Following the proof of Theorem 3.8, we will use the equality, cf., (3.18),

$$\begin{aligned}\tilde{G}_{n,j}(-\Delta)^j\tilde{v}_k &= G_n(-k\Delta_h)T_h^j(-\Delta)^j\tilde{v}_k \\ &= \sum_{l=0}^{p-1}\tilde{G}_{n,l+j}(T - T_h)(-\Delta)^{l+j+1}\tilde{v}_k + \tilde{G}_{n,p+j}(-\Delta)^{p+j}\tilde{v}_k.\end{aligned}$$

By Lemma 3.18, we have, since $(T - T_h)\Delta = R_h - I$,

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

Using the following bound for the Ritz projection in maximum-norm, see, e.g., Thomée [19, 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 choosing $s = \ell_h$ we therefore obtain

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

For the case $l = p$ we have by (3.26),

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

Together these estimates imply

$$\|\tilde{G}_{n,j}(-\Delta)^j\tilde{v}_k\|_{L_\infty} \le Ck^j(h^2\ell_h^2\|\Delta^j v\|_{W_\infty^{2j+2}} + k^p\|v\|_{W_\infty^{2(p+j)}}), \quad \text{for } t_n \ge 0.$$

Since obviously, by Lemma 3.18 and (3.25), we have

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

We conclude that

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

which shows (3.24) for present choice of v_h. Following the proof Theorem 3.8, we also need to show

$$\|P(r(-k\Delta_h))r(-k\Delta_h)^n(-k\Delta_h)^{-j}\|_{L_\infty} \le C. \tag{3.28}$$

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 Γ,

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

which shows (3.28). The proof is now complete. □

4. Variable Time Steps

In this section we will consider time stepping methods with variable time steps. Let $0 = t_0 < t_1 < \cdots < t_n < \cdots$ be a partition of the time axis and $k_n = t_n - t_{n-1}$ the variable time steps. Recall from introduction we have defined the following single step discrete method for (1.1),

$$(4.1) \qquad U^n = E_{k_n} U^{n-1} \quad \text{for } n \geq 1, \quad E_{k_n} = r(k_n A), \quad \text{with } U^0 = v,$$

where the rational function $r(z)$ is defined on $\sigma(k_j A)$ for $j \leq n$ and (1.6) holds.

We will study the smoothing properties of the time discretization scheme (4.1) and show error estimates for the first and second order approximations of the time derivative $D_t u(t_n) = u_t(t_n)$ of the solution of (1.1).

4.1. Some Basic Stability and Error Estimates.

We first quote the following stability result, see, e.g., Palencia [13].

Theorem 4.1. *Assume that A satisfies (1.2) and (1.3), and that $r(z)$ is accurate of order $p = 1$ and $A(\theta)$-stable, with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$. Let $k_j, 1 \leq j \leq n$, be time steps. Then there is a constant C such that*

$$(4.2) \qquad \Big\| \prod_{j=1}^{n} r(k_j A) v \Big\| \leq C \|v\|, \quad \text{for } t_n \geq 0.$$

If we remove the restriction $|r(\infty)| < 1$, the bound on the right side of (4.2) will depends on the variable time stepsizes. More precisely, if $|r(\infty)| \leq 1$, we have, see, e.g., Bakaev [2],

$$\Big\| \prod_{j=1}^{n} r(k_j A) v \Big\| \leq C \ln(1 + k_{max}/k_{min}) \|v\|, \quad \text{for } t_n \geq 0,$$

where $k_{max} = \max_{1 \leq j \leq n} k_j$, $k_{min} = \min_{1 \leq j \leq n} k_j$.

We begin with some error estimates for the approximation U^n defined by (4.1) of the solution $u(t_n)$ of (1.1). Our first result is an error estimate in the smooth data case in which there is no restriction on the time steps k_n.

Theorem 4.2. *Let $u(t_n)$ and U^n be the solutions of (1.1) and (4.1). Assume that A satisfies (1.2) and (1.3), and that $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable, with $\theta \in (\delta, \pi/2]$. Let $k_j, 1 \leq j \leq n$, be time steps. Then, there is a C such that*

$$\|U^n - u(t_n)\| \leq C k_{max}^p \|A^p v\|, \quad \text{for } n \geq 1.$$

In order to prove Theorem 4.2, we need the following lemma.

Lemma 4.3. *Assume that $r(z)$ is $A(\theta)$-stable and accurate of order $p \geq 1$. Let k_j, $1 \leq j \leq n$, be any positive numbers. Then for arbitrary $R > 0$ and $\psi \in (0, \theta)$ there are $c, C > 0$ such that, for $|k_{max} z| \leq R$, $|arg\ z| \leq \psi$,*

$$\Big| \prod_{j=1}^{n} r(k_j z) - e^{-t_n z} \Big| \leq C |k_{max} z|^p t_n |z| e^{-c t_n |z|} \leq C n |k_{max} z|^{p+1} e^{-c t_n |z|}.$$

Proof. Since $r(z)$ is $A(\theta)$-stable and accurate of order $p \geq 1$, we have

$$(4.3) \qquad |r(z) - e^{-z}| \leq C |z|^{p+1} \quad \text{for } |z| \leq R, \ |arg\ z| \leq \psi.$$

We also have, with $c = \cos\psi$,

(4.4) $$|e^{-z}| = e^{-Re z} \le e^{-c|z|} \quad \text{for } |arg\ z| \le \psi.$$

Thus we have, for $|k_{max} z| \le R$,

$$\begin{aligned}
&\Big|\prod_{j=1}^{n} r(k_j z) - e^{-t_n z}\Big| \\
&= \Big|\Big(r(k_1 z) - e^{-k_1 z}\Big)\prod_{j=2}^{n} r(k_j z) + \cdots + \Big(\prod_{j=1}^{n-1} e^{-k_j z}\Big)\Big(r(k_n z) - e^{-k_n z}\Big)\Big| \\
&\le \sum_{j=1}^{n}\Big|\prod_{s=1}^{j-1} e^{-k_s z}\Big(r(k_j z) - e^{-k_j z}\Big)\prod_{l=j+1}^{n} r(k_l z)\Big| \\
&\le C\sum_{j=1}^{n}\Big(e^{-ct_{j-1}|z|}(k_j|z|)^{p+1}e^{-c(t_n - t_j)|z|}\Big) \\
&\le Ce^{-ct_n|z|}\sum_{j=1}^{n}(k_j|z|)^{p+1} \le C(k_{max}|z|)^p t_n |z| e^{-ct_n|z|} \\
&\le Cn|k_{max} z|^{p+1}e^{-ct_n|z|},
\end{aligned}$$

which completes the proof of Lemma 4.3. □

Proof of Theorem 4.2. With $F_n(z) = \prod_{j=1}^{n} r(k_j z) - e^{-t_n z}$, it suffices to show

$$\|F_n(A)(k_{max}A)^{-p}\| \le C.$$

Since $\prod_{j=1}^{n} r(k_j z)(k_{max} z)^{-p}R(z;A)$ is bounded for $|z| \ge \tilde{R}$, with some positive $\tilde{R} > 0$, thus, we have, by Lemma 2.2,

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

We may further let $\tilde{R}$ tend to ∞ since the integrand has no poles when $|z| \ge \tilde{R}$. Using also Lemma 2.3 we therefore have

$$F_n(A)(k_{max}A)^{-p} = \frac{1}{2\pi i}\int_{\gamma_\epsilon \cup \Gamma_\epsilon} F_n(z)(k_{max} z)^{-p}R(z;A)\, dz.$$

By Lemma 4.3 we see that $F_n(z) = O(z^{p+1})$ as $z \to 0$ and thus the integrand is bounded, so that we may let $\epsilon \to 0$. It follows that

$$\|F_n(A)(k_{max}A)^{-p}\| \le C\int_0^\infty (|F_n(\rho e^{\pm i\psi})| + |F_n(\rho e^{\pm i\psi})|)(k_{max}\rho)^{-p}\frac{d\rho}{\rho}.$$

Noting that $r(z)^n$ and e^{-tz} are bounded on Γ we find

$$\int_{R/k_{max}}^{\infty} |F_n(\rho e^{\pm i\psi})|(k_{max}\rho)^{-p}\frac{d\rho}{\rho} \le C\int_R^\infty \frac{dx}{x^{p+1}} \le C.$$

Further, we have, by Lemma 4.3,

$$\int_0^{R/k_{max}} |F_n(\rho e^{\pm i\psi})|(k_{max}\rho)^{-p}\frac{d\rho}{\rho} \le C\int_0^{R/k_{max}} e^{-ct_n\rho}t_n d\rho \le C.$$

Together these estimates complete the proof. □

We now show a nonsmooth data error estimate. To do this, we need the notion of *increasing quasi-quasiuniform grids* introduced in the introduction. Let $\{\mathcal{T}\}$ be a family of partitions of the time axis, $\mathcal{T} = \{t_n,\ 0 = t_0 < t_1 < \cdots < t_n < \cdots\}$. $\{\mathcal{T}\}$ is called a family of *quasi-quasiuniform grids* if there exist positive constants c_0, C_0, such that

$$c_0 k_{n+1} \le k_n \le C_0 t_n/n. \tag{4.5}$$

Further if $k_1 \le k_2 \le \cdots \le k_n \le \cdots$, we call $\{\mathcal{T}\}$ is a family of *increasing quasi-quasiuniform grids.* We have the following

Theorem 4.4. *Let $u(t_n)$ and U^n be the solutions of (1.1) and (4.1). Assume that A satisfies (1.2) and (1.3), and that $r(z)$ is accurate of order $p \ge 1$ and $A(\theta)$-stable, with $\theta \in (\delta, \pi/2]$ and $|r(\infty)| < 1$. Assume further that $\{\mathcal{T}\}$ is a family of increasing quasi-quasiuniform grids. Then, there is a constant C such that*

$$\|U^n - u(t_n)\| \le C k_n^p t_n^{-p} \|v\|, \quad \textit{for } n \ge 1.$$

To prove Theorem 4.4, we need the following lemma.

Lemma 4.5. *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 $\kappa = r(\infty)$, for any sequences $k_1 \le k_2 \le \cdots \le k_n$*

$$\Big|\prod_{j=1}^{n} r(k_j z) - \kappa^n\Big| \le C|k_1 z|^{-1} e^{-cn}, \quad \textit{for } |k_1 z| \ge R,\ |arg\, z| \le \psi.$$

Proof. Since $r(z) - \kappa$ vanishes at infinity and $|r(z)| \le 1$, we have

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

Further, $|\kappa| < 1$ implies that

$$|r(z)| \le e^{-c}, \quad \text{for } |z| \ge R,\ |arg\, z| \le \psi. \tag{4.6}$$

Hence, we have, for $|k_1 z| \ge R$, noting that $\kappa \le e^{-c}$ for some c,

$$\begin{aligned}\Big|\prod_{j=1}^{n} r(k_j z) - \kappa^n\Big| &= \Big|(r(k_1 z) - \kappa)\prod_{j=2}^{n} r(k_j z) + \cdots + \kappa^{n-1}(r(k_n z) - \kappa)\Big| \\ &\le C e^{-cn} \sum_{j=1}^{n} |k_j z|^{-1} \le C|k_1 z|^{-1} n e^{-cn} \le C|k_1 z|^{-1} e^{-cn},\end{aligned}$$

which completes the proof of Lemma 4.5. □

Proof of Theorem 4.4. With $F_n(z)$ as in the proof of Theorem 4.2, we need to show

$$\|F_n(A)\| \le C k_n^p t_n^{-p}.$$

Set $\tilde{F}_n(z) = F_n(z) - \kappa^n k_n z/(1 + k_n z)$. Since $|\kappa| < 1$, and by the obvious fact that $\|k_n A(I + k_n A)^{-1}\| \le C$, we have, noting that $t_n/k_n \le n$,

$$\|\kappa^n k_n A(I + k_n A)^{-1}\| \le C|\kappa|^n \le C n^{-p} \le C k_n^p t_n^{-p},$$

and it remains to show the same bound for the operator norm of $\tilde{F}_n(A)$. Since $\prod_{j=1}^{n} r(k_j z) - \kappa^n k_n z/(1 + k_n z)$ vanishes at $z = \infty$, and $0 \in \rho(A)$, we may use Lemmas 2.2 and 2.3 to see that with $\Gamma = \{z : |arg\, z| = \psi,\ \psi \in (\delta, \theta)\}$,

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

Since $\tilde{F}_n(z) = (\prod_{j=1}^n r(k_j z) - \kappa^n) + \kappa^n/(1+k_n z) - e^{-t_n z}$, Lemma 4.5 shows

$$\int_{R/k_1}^{\infty} |\tilde{F}_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} \le C \int_{R/k_1}^{\infty} \left(e^{-cn}(k_1\rho)^{-1} + |\kappa|^n (k_n\rho)^{-1} + e^{-ct_n\rho} \right) \frac{d\rho}{\rho} \le C k_n^p t_n^{-p}.$$

Using also Lemma 4.3 and $|1/(1+k_n z)| \le 1$ for $Re\, z \ge 0$, we have

$$\begin{aligned}
\int_0^{R/k_n} |\tilde{F}_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} &\le \int_0^{R/k_n} |F_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} + \int_0^{R/k_n} |\kappa|^n k_n d\rho \\
&\le C \int_0^{R/k_n} (k_n\rho)^{p+1} e^{-ct_n\rho} n \frac{d\rho}{\rho} + C|\kappa|^n \\
&= C k_n^p t_n^{-p} \int_0^{R/k_n} (t_n\rho)^p e^{-ct_n\rho} (nk_n) d\rho + C|\kappa|^n \qquad (4.7) \\
&\le C k_n^p t_n^{-p} \int_0^{R/k_n} e^{-ct_n\rho} t_n d\rho + C|\kappa|^n \le C k_n^p t_n^{-p}.
\end{aligned}$$

It remains to consider the integral over the interval $[R/k_n, R/k_1]$. To explain our estimates in a precise way we introduce constants c_1 and c_2 such that $|r(z)| \le e^{-c_1|z|}$ for $|z| \le R, |arg\, z| \le \psi$, and $|r(z)| \le e^{-c_2}$ for $|z| \ge R, |arg\, z| \le \psi$. We remark that c_2 can be chosen arbitrary small. Assuming that $|k_m z| \le R, |k_{m+1} z| > R$, with some $m < n$, we have, for c_2 small enough,

$$\left| \prod_{j=1}^n r(k_j z) \right| \le e^{-c_1 t_m |z|} e^{-c_2(n-m)} \le e^{-c_2 n} \left(e^{c_2 m} e^{-c_1 t_m |z|} \right) \le e^{-c_2 n} e^{-c_3 m}, \qquad (4.8)$$

because it follows from (4.5) that $c_1 t_m |z| = c_1 (t_m/k_m)(k_m/k_{m+1})(k_{m+1}|z|) \ge c_1 c_0 C_0^{-1} R m = c_3 m$, so that (4.8) holds if $c_2 \le c_3$.

We write $\tilde{F}_n(z) = \prod_{j=1}^n r(k_j z) - e^{-t_n z} - k_n z (1+k_n z)^{-1} \kappa^n$. We have, using (4.8) and noting that $\ln(k_{m+1}/k_m) \le \ln C \le C$,

$$\begin{aligned}
\int_{R/k_n}^{R/k_1} \left| \prod_{j=1}^n r(k_j \rho e^{\pm i\psi}) \right| \frac{d\rho}{\rho} &\le \sum_{m=1}^{n-1} \int_{R/k_{m+1}}^{R/k_m} \left| \prod_{j=1}^n r(k_j \rho e^{\pm i\psi}) \right| \frac{d\rho}{\rho} \\
&\le \sum_{m=1}^{n-1} \int_{R/k_{m+1}}^{R/k_m} e^{-c_2 n} e^{-cm} \frac{d\rho}{\rho} \le e^{-c_2 n} \sum_{m=1}^{n-1} e^{-cm} \ln(k_{m+1}/k_m) \qquad (4.9) \\
&\le C e^{-c_2 n} \sum_{m=1}^{n-1} e^{-cm} \le C e^{-c_2 n} \le C n^{-p} \le C k_n^p t_n^{-p}.
\end{aligned}$$

Further, we have, using (4.4) and noting that (4.5) implies $t_n \rho \ge cn$ for $\rho \in [R/k_n R/k_1]$, and $\ln(k_n/k_1) = \sum_{m=1}^{n-1} \ln(k_{m+1}/k_m) \le Cn$,

$$\begin{aligned}
\int_{R/k_n}^{R/k_1} \left(\left| e^{-t_n \rho e^{\pm i\psi}} \right| + \frac{k_n \rho}{1 + k_n \rho} \kappa^n \right) \frac{d\rho}{\rho} &\le \int_{R/k_n}^{R/k_1} e^{-cn} \frac{d\rho}{\rho} \qquad (4.10) \\
&\le e^{-cn} \ln(k_n/k_1) \le C n e^{-cn} \le C k_n^p t_n^{-p}.
\end{aligned}$$

Hence we get

$$\int_{R/k_n}^{R/k_1} \left| \tilde{F}_n(\rho e^{\pm i\psi}) \right| \frac{d\rho}{\rho} \le C k_n^p t_n^{-p}.$$

Together these estimates complete the proof. □

4.2. **A First Order Approximation of the Time Derivative.** In this section, we shall consider smoothing properties of the time discretization scheme (4.1) and error estimates for the first order approximation of the time derivative $u_t(t_n)$ of the solution of (1.1) defined by

$$\bar{\partial} U^n = \frac{U^n - U^{n-1}}{k_n}, \quad \text{for } n \geq 1. \tag{4.11}$$

We begin with a smooth data error estimate for the approximation (4.11).

Theorem 4.6. *In addition to the assumptions of Theorem 4.2, let $k_j, 1 \leq j \leq n$, be increasing. Then, there is a constant C such that*

$$\|\bar{\partial} U^n - u_t(t_n)\| \leq C k_n \|A^2 v\|, \quad \textit{for } n \geq 1. \tag{4.12}$$

Proof. Setting $G_n(z) = \prod_{j=1}^{n-1} r(k_j z)(r(k_n z) - 1) - (-k_n z) e^{-t_n z}$, our result will follow from

$$\|G_n(A)(k_n A)^{-2}\| \leq C, \quad \text{for } n \geq 1.$$

For the same reason as in the proof of Theorem 4.2, we have

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

From the proof below we see that the integrand is bounded, so that we may let $\epsilon \to 0$. It follows that

$$G_n(A)(k_n A)^{-2} = \frac{1}{2\pi i} \int_\Gamma G_n(z)(k_n z)^{-2} R(z, A) dz.$$

We now estimate the integral. Since $0 \in \rho(A)$ and $r(z) - 1 + z = O(z^2)$ for $z \to 0$, there exists a constant $R > 0$, such that $|R(z, A)| \leq C$, $|r(z) - 1 + z| \leq C|z|^2$, and $|r(z) - 1| \leq C|z|$ for $|z| \leq R$. We write

$$G_n(z) = G_n^1(z) + G_n^2(z) + G_n^3(z),$$

where

$$G_n^1(z) = \prod_{j=1}^{n-1} r(k_j z)(r(k_n z) - 1 + k_n z),$$

and, with $F_n(z) = \prod_{j=1}^{n} r(k_j z) - e^{-t_n z}$,

$$G_n^2(z) = k_n z \prod_{j=1}^{n-1} r(k_j z)(1 - r(k_n z)), \quad G_n^3(z) = k_n z F_n(z).$$

We have, using Lemma 4.3,

$$\left\| \int_{\Gamma_0^{R/k_n}} G_n(z)(k_n z)^{-2} R(z, A) dz \right\| \leq \sum_{l=1}^{3} \left\| \int_{\Gamma_0^{R/k_n}} G_n^l(z)(k_n z)^{-2} R(z, A) dz \right\| \tag{4.13}$$
$$\leq C \int_0^{R/k_n} e^{-ct_{n-1}\rho} d\rho + C \int_0^{R/k_n} (k_n \rho)\Big((k_n \rho) e^{-ct_n \rho} t_n \rho\Big)(k_n \rho)^{-2} \frac{d\rho}{\rho} \leq C.$$

Further, by the boundedness of $G_n(z)$,

$$\left\| \int_{\Gamma_{R/k_n}^\infty} G_n(z)(k_n z)^{-2} R(z, A) dz \right\| \leq C \int_{R/k_n}^\infty (k_n \rho)^{-2} \frac{d\rho}{\rho} \leq C.$$

Together these estimates complete the proof. □

We now turn to smoothing properties of (4.1). Recall from the introduction that the smoothing property (1.9) is not valid even with constant time steps if $r(\infty) \neq 0$. However, if $r(\infty) = 0$, the analogue of (1.9) holds also for some special schemes $r(z)$ with no restriction on the time steps, cf., Eriksson, Johnson, and Larsson [8]. We have the following smoothing property for general $r(z)$.

Theorem 4.7. *Assume that* (1.2) *and* (1.3) *hold, and r(z) is accurate of order* $p = 1$ *and* $A(\theta)$*-stable with* $\theta \in (\delta, \pi/2]$, *and that* $\kappa = r(\infty) = 0$. *Let* $\{k_j\}$ *satisfy* $ck_j \le k_{j+1} \le Ck_j$. *Then there is a constant C such that*

$$\Big\| A \prod_{j=1}^{n} r(k_j A) v \Big\| \le C t_n^{-1} \|v\|, \quad \textit{for } n \ge 2. \tag{4.14}$$

Proof. We show that, with $g_n(z) = t_n z \prod_{j=1}^{n} r(k_j z)$,

$$\|g_n(A)\| \le C, \quad \text{for } n \ge 2.$$

Since $\kappa = 0$, we have, see, e.g., Thomée [19, Lemma 7.3],

$$|r(z)| \le \frac{1}{1 + c|z|}, \quad \text{for } |arg\, z| \le \psi, \tag{4.15}$$

which implies that $g_n(z)$ is bounded for $|arg\, z| \le \psi$ and $g_n(\infty) = 0$. Thus there exists a positive R such that $g_n(z)$ is bounded for $|z| \ge R$. Lemma 2.2 shows that

$$g_n(A) = \frac{1}{2\pi i} \int_{\gamma_\epsilon \cup \Gamma_\epsilon^R \cup \gamma^R} g_n(z) R(z, A) dz.$$

Noting that $g_n(z)$ is analytic for $|z| \ge R$, $\psi \le |arg\, z| \le \pi$, and $g_n(z) = O(|z|)$ as $z \to 0$, we may let $R \to \infty$ and $\epsilon \to 0$, so that

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

We split the path of integration as $\Gamma = \Gamma_0^{R/t_n} \cup \Gamma_{R/t_n}^\infty$. Noting that $|r(z)| \le e^{-c_1|z|}$ for $|z| \le R$, $|arg\, z| \le \psi$, we have

$$\Big\| \int_{\Gamma_0^{R/t_n}} g_n(z) R(z, A) dz \Big\| \le C \int_0^{R/t_n} t_n \rho e^{-c_1 t_n \rho} \frac{d\rho}{\rho} \le C.$$

We now consider the integral over Γ_{R/t_n}^∞. If $k_{max} \le t_n/2$, we have

$$t_n^2 = \sum_{l=1}^{n} k_l^2 + \sum_{l \neq j} k_l k_j \le k_{max} t_n + \sum_{l \neq j} k_l k_j \le t_n^2/2 + \sum_{l \neq j} k_l k_j,$$

and hence by (4.15)

$$\Big\| \int_{R/t_n}^\infty g_n(z) R(z, A) dz \Big\| \le C \int_{R/t_n}^\infty \frac{t_n \rho}{\prod_{j=1}^{n} (1 + ck_j \rho)} \frac{d\rho}{\rho}$$
$$\le C \int_{R/t_n}^\infty \frac{t_n}{1 + ct_n\rho + c\rho^2 \sum_{l \neq j} k_l k_j} d\rho \le C \int_{R/t_n}^\infty \frac{t_n}{1 + c\rho^2 t_n^2} d\rho \le C.$$

If $k_{max} \ge t_n/2$, we have $k_m = k_{max}$ for some m with $1 \le m \le n$. Hence, using that k_{m-1}/k_m is bounded above and below, we have, since $n \ge 2$,

$$\Big\| \int_{R/t_n}^{\infty} g_n(z)R(z,A)dz \Big\| \le C \int_{R/t_n}^{\infty} \frac{t_n}{(1+ck_m\rho)^2} d\rho$$
$$\le C \int_{R/t_n}^{\infty} \frac{t_n}{(1+ct_n\rho)^2} d\rho \le C.$$

Together these estimates complete the proof. □

As for the constant time step case, using difference quotients in time rather than the elliptic operator A in (4.14), we have a smoothing property as follows.

Theorem 4.8. *Let U^n be the solution of* (4.1). *Assume that* (1.2) *and* (1.3) *hold and that the discretization scheme is accurate of order $p = 1$, and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|\kappa| < 1$. Assume that $\{\mathcal{T}\}$ is a family of increasing quasi-quasiuniform grids. Then, there is a constant C such that*

$$\|\bar{\partial} U^n\| \le C t_n^{-1} \|v\|, \quad \textit{for}\, n \ge 1. \tag{4.16}$$

Proof. We want to show that, with $\tilde{g}_n(z) = t_n/k_n \prod_{j=1}^{n-1} r(k_j z)(r(k_n z) - 1)$

$$\|\tilde{g}_n(A)\| \le C, \quad \text{for } n \ge 1.$$

It is obvious that there exists a positive constant $\tilde{R} > 0$, such that for fixed n, $\tilde{g}_n(z)$ is bounded for $|z| \ge \tilde{R}$. Lemma 2.2 implies that

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

Since the integrand is bounded for $|z| \ge \tilde{R}$, we may let $\tilde{R}$ tend to ∞. Moreover, $\tilde{g}_n(z) = O(|z|)$ as $z \to 0$, so that we may let $\epsilon \to 0$. Thus we have

$$\tilde{g}_n(A) = \tilde{g}_n(\infty)I + \frac{1}{2\pi i} \int_{\Gamma} \tilde{g}_n(z)R(z,A)dz.$$

Clearly, noting that since k_n is increasing we have $t_n/k_n \le n$,

$$\|\tilde{g}_n(\infty)I\| \le |t_n/k_n \kappa^{n-1}(r(\kappa) - 1)| \le Cne^{-cn} \le C.$$

Recall that there exists a positive constant R such that $|r(z)| \le e^{-c_1|z|}$, $|r(z) - 1| \le C|z|$ for $|z| \le R$ and $|r(z)| \le e^{-c_2}$ for $|z| \ge R$. Note that the integrand is bounded when $|z| \ge R/k_1$. In fact, if $|z| \ge R/k_1$, we have $\|\tilde{g}_n(z)R(z,A)\| \le (t_n/k_n)e^{-c_2(n-1)}(e^{-c_2} + 1)$. Therefore the integrand has no poles when $|z| \ge R/k_1$, and hence we can replace the path of the integration by $\tilde{\Gamma} = \Gamma_0^{R/k_{n-1}} \cup \Gamma_{R/k_{n-1}}^{R/k_1} \cup \gamma^{R/k_1}$. We now estimate the integral on the three different parts. We first have, noting that $t_n/t_{n-1} = 1 + k_n/t_{n-1} \le C$,

$$\Big\| \int_{\Gamma_0^{R/k_{n-1}}} \tilde{g}_n(z)R(z,A)dz \Big\| \le C \int_0^{R/k_{n-1}} (t_n/k_n) e^{-c_1 t_{n-1}\rho}(k_n\rho) \frac{d\rho}{\rho}$$
$$\le C \int_0^{R/k_{n-1}} t_{n-1} e^{-c_1 t_{n-1}\rho} d\rho \le C \int_0^{\infty} e^{-c_1 x} dx \le C.$$

Here we have used $|r(k_n z) - 1| \le C k_n |z|$, since $k_n|z| = |(k_n/k_{n-1})k_{n-1}|z| \le CR$, when $|z| \le R/k_{n-1}$, which will be satisfied when we choose CR instead R. The same argument is used in the proofs of Theorems 4.9 and 4.12 below. We also have, using $|r(z)| \le e^{-c_2}$ for $|z| \ge R$, and the stability of $r(z)$ and $t_n/k_n \le n$,

$$\Big\| \int_{\gamma^{R/k_1}} \tilde{g}_n(z) R(z,A)dz \Big\| \le C \int_{\gamma^{R/k_1}} t_n/k_n e^{-c_2(n-1)} \frac{d\rho}{\rho} \le C.$$

Further, recalling (4.9) with $p = 1$, we have, since $k_{n-1}/t_{n-1} \le C k_n/t_n$,

$$\Big\| \int_{R/k_{n-1}}^{R/k_1} \tilde{g}_n(z) R(z,A)dz \Big\| \le \sum_{m=1}^{n-2} \Big\| \int_{R/k_{m+1}}^{R/k_m} \tilde{g}_n(z) R(z,A)dz \Big\|$$
$$\le t_n k_n^{-1} \sum_{m=1}^{n-2} \int_{R/k_{m+1}}^{R/k_m} \Big| \prod_{j=1}^{n-1} r(k_j \rho e^{\pm i\phi}) \Big| \frac{d\rho}{\rho} \le C t_n k_n^{-1} (k_{n-1} t_{n-1}^{-1}) \le C$$

Together these estimates complete the proof. □

Our next result is an error estimate of the approximation (4.11) of time derivative $u_t(t_n)$ of the solution of (1.1) in nonsmooth data case.

Theorem 4.9. *Under the assumptions of Theorem 4.4, there is a constant C, such that*

$$\|\bar{\partial} U^n - D_t u(t_n)\| \le C k_n t_n^{-2} \|v\|, \quad \textit{for } n \ge 1.$$

Proof. With the notation of Theorem 4.6 we need to show

$$\|G_n(A)\| \le C k_n^2 t_n^{-2}, \quad \text{for } n \ge 1.$$

We set $\tilde{G}_n(z) = G_n(z) - \kappa^{n-1}(\kappa - 1) k_n z/(1 + k_n z)$. For the same reason as in the proof of Theorem 4.4, we have

$$\|\kappa^{n-1}(\kappa-1) k_n A (I + k_n A)^{-1}\| \le C|\kappa|^{n-1} \le C n^{-2} \le C k_n^2 t_n^{-2},$$

and we may write

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

Since

$$\tilde{G}_n(z) = \Big(\prod_{j=1}^{n-1} r(k_j z)(r(k_n z) - 1) - \kappa^{n-1}(\kappa - 1) \Big)$$
$$+ \kappa^{n-1}(\kappa-1)/(1 + k_n z) - (-k_n z) e^{-t_n z},$$

we have

$$\int_{R/k_1}^\infty |\tilde{G}_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} \le C \int_{R/k_1}^\infty \Big(e^{-c_2 n}(k_1\rho)^{-1} + |\kappa|^n (k_n \rho)^{-1} + (k_n\rho) e^{-c t_n \rho} \Big) \frac{d\rho}{\rho}$$
$$\le C k_n^2 t_n^{-2}.$$

Using $|1/(1 + k_n z)| \le 1$ for $Re\, z \ge 0$ we have, with $G_n^l(z), l = 1,2,3$ as in the proof of Theorem 4.6,

$$\int_0^{R/k_{n-1}} |\tilde{G}_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} \le \int_0^{R/k_{n-1}} |G_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} + C \int_0^{R/k_{n-1}} |\kappa|^{n-1} k_n d\rho$$
$$\le \sum_{l=1}^3 \int_0^{R/k_{n-1}} |G_n^l| \frac{d\rho}{\rho} + C|\kappa|^n.$$

Obviously

$$\text{(4.17)} \qquad \int_0^{R/k_{n-1}} (|G_n^1| + |G_n^2|)\frac{d\rho}{\rho} \le C\int_0^{R/k_{n-1}} e^{-c_2 t_{n-1}\rho}(k_n\rho)^2 \frac{d\rho}{rho}$$
$$\le Ck_n^2 t_n^{-2}\int_0^{R/k_{n-1}} e^{-c_2 t_{n-1}\rho} t_n^2 \rho d\rho \le Ck_n^2 t_n^{-2}.$$

Here as in the proof of Theorem 4.8, we use $|r(k_n z) - 1 + k_n z| \le Ck_n|z|$ and $|r(k_n z) - 1| \le Ck_n|z|$, since $k_n|z| \le CR$ when $|z| \le R/k_{n-1}$.

Following the proof of (4.7), we have

$$\int_0^{R/k_{n-1}} |G_n^3|\frac{d\rho}{\rho} \le C\int_0^{R/k_{n-1}} (k_n\rho)(k_n\rho)^2 e^{-c_1 t_n\rho} n\frac{d\rho}{\rho}$$
$$\le Ck_n^2 t_n^{-2}\int_0^{R/k_{n-1}} e^{-c_1 t_n \rho}(t_n\rho)^2 nk_n d\rho$$
$$\le Ck_n^2 t_n^{-2}\int_0^{\infty} e^{-c_1 x}x^2 dx \le Ck_n^2 t_n^{-2}.$$

Thus, combining this with $|\kappa|^n \le Cn^{-2} \le Ck_n^2 t_n^{-2}$, we get

$$\int_0^{R/k_{n-1}} |\tilde{G}_n(\rho e^{\pm i\psi})|\frac{d\rho}{\rho} \le Ck_n^2 t_n^{-2}.$$

It remains to consider the integral on interval $[R/k_n, R/k_1]$. We rewrite

$$\tilde{G}_n(z) = \prod_{j=1}^{n-1} r(k_j z)(r(k_n z - 1) - (-k_n z)e^{-t_n z} - \frac{k_n z}{1 + k_n z}(\kappa^n - \kappa^{n-1}).$$

We have, recalling (4.9) with $p = 2$, and noting that $k_{n-1}^2 t_{n-1}^{-2} \le Ck_n^2 t_n^{-2}$,

$$\int_{R/k_{n-1}}^{R/k_1} \Big|\prod_{j=1}^{n} r(k_j\rho e^{\pm i\psi})\Big|\frac{d\rho}{\rho} \le \int_{R/k_{n-1}}^{R/k_1} \Big|\prod_{j=1}^{n-1} r(k_j\rho e^{\pm i\psi})\Big|\frac{d\rho}{\rho}$$
$$\le \sum_{m=1}^{n-2}\int_{R/k_{m+1}}^{R/k_m} \Big|\prod_{j=1}^{n-1} r(k_j\rho e^{\pm i\psi})\Big|\frac{d\rho}{\rho} \le Ck_{n-1}^2 t_{n-1}^{-2} \le Ck_n^2 t_n^{-2}.$$

Further, recalling (4.10), we get, noting that this time $t_n\rho > C(n-1)$ for $\rho \in [R/k_{n-1}, R/k_1]$, since we have $t_n\rho \ge (t_n/k_{n-1})R \ge (t_{n-1}/k_{n-1})R \ge C(n-1)$,

$$\text{(4.18)} \qquad \int_{R/k_{n-1}}^{R/k_1} e^{-t_n\rho e^{\pm i\psi}}(k_n\rho)\frac{d\rho}{\rho} \le \int_{R/k_{n-1}}^{R/k_1} e^{-ct_n\rho}k_n d\rho$$
$$\le e^{-cn}\int_{R/k_{n-1}}^{R/k_1} e^{-\frac{c}{2}t_n\rho}t_n d\rho \le e^{-cn}\int_0^{\infty} e^{-\frac{c}{2}x}dx \le Ck_n^2 t_n^{-2},$$

and

$$\int_{R/k_{n-1}}^{R/k_1} \frac{k_n\rho}{1 + k_n\rho}(\kappa^n - \kappa^{n-1})\frac{d\rho}{\rho} \le Ck_n^2 t_n^{-2}.$$

Thus

$$\int_{R/k_{n-1}}^{R/k_1} |\tilde{G}_n(\rho e^{\pm i\psi})|\frac{d\rho}{\rho} \le Ck_n^2 t_n^{-2}.$$

The proof is now complete. □

4.3. **A Second Order Approximation of the Time Derivative.** In this subsection we shall consider the following second order approximation of $u_t(t_n)$ of the solution of (1.1),

$$\bar{\partial}^2 U^n = a_n \bar{\partial} U^n + b_n \bar{\partial} U^{n-1} = a_n \frac{U^n - U^{n-1}}{k_n} + b_n \frac{U^{n-1} - U^{n-2}}{k_{n-1}}, \tag{4.19}$$

$$a_n = (2k_n + k_{n-1})/(k_n + k_{n-1}), \quad b_n = -k_n/(k_n + k_{n-1}),$$

where U^n is the discrete solution of (1.1) defined by (4.1). Combining (4.19) and Theorem 4.8, we obtain the following smoothing property of discrete scheme (4.1).

Theorem 4.10. *Under the assumptions of Theorem 4.8, there is a constant C, such that*

$$\|\bar{\partial}^2 U^n\| \le C t_n^{-1} \|v\|, \quad \text{for } n \ge 2.$$

Note that (4.19) can also be written in the form

$$\bar{\partial}^2 U^n = \frac{1}{k_n}\Big(c_0 U^n + c_1 U^{n-1} + c_2 U^{n-2}\Big), \tag{4.20}$$

where $c_1 = 1 + \gamma_n, c_2 = \gamma_n^2/(1+\gamma_n)$, $c_0 = c_1 + c_2$ and $\gamma_n = k_n/k_{n-1}$.

We shall now consider the error estimates for the approximation (4.19). We begin with a smooth data estimate.

Theorem 4.11. *Under the assumptions of Theorem 4.6, there is a constant C such that*

$$\|\bar{\partial}^2 U^n - D_t u(t_n)\| \le C k_n^2 \|A^3 v\|, \quad \text{for } n \ge 2. \tag{4.21}$$

Proof. With $P(x, y) = c_0 + c_1 y^{-1} + c_2 x^{-1} y^{-1}$ and

$$G_n(z) = \prod_{j=1}^{n} r(k_j z) P(r(k_{n-1}z), r(k_n z)) - (-k_n z) e^{-t_n z},$$

we want to prove

$$\|G_n(A)(k_n A)^{-3}\| \le C, \quad \text{for } n \ge 2.$$

For the same reason as in the proof of Theorem 4.6, we have

$$G_n(A)(k_n A)^{-3} = \frac{1}{2\pi i} \int_\Gamma G_n(z)(k_n z)^{-3} R(z, A)\, dz.$$

It is easy to check that there exist a constant R, such that, noting that $0 \in \rho(A)$,

$$|R(z, A)| \le C, \quad \text{for } |z| \le R,$$

and

$$|P(e^{-k_{n-1}z}, e^{-k_n z}) - (-k_n z)| \le C |k_n z|^3, \quad \text{for } |k_n z| \le R,$$

and

$$|P(r(k_{n-1}z), r(k_n z)) - P(e^{-k_{n-1}z}, e^{-k_n z})| \le C |k_n z|^3 \quad \text{for } |k_n z| \le R.$$

We write

$$G_n(z) = G_n^1(z) + G_n^2(z) + G_n^3(z), \tag{4.22}$$

where

$$G_n^1(z) = \prod_{j=1}^n r(k_j z)\Big(P(r(k_{n-1}z), r(k_n z)) - P(e^{-k_{n-1}z}, e^{-k_n z})\Big),$$

and, with $F_n(z) = \prod_{j=1}^n r(k_j z) - e^{-t_n z}$,

$$G_n^2(z) = \prod_{j=1}^n r(k_j z) P(e^{-k_{n-1}z}, e^{-k_n z}) - (-k_n z), \quad G_n^3 = k_n z F_n(z).$$

We have, recalling (4.13),

$$\Big\| \int_{\Gamma_0^{R/k_n}} G_n(z)(k_n z)^{-2} R(z,A)dz \Big\| \le \sum_{l=1}^3 \Big\| \int_{\Gamma_0^{R/k_n}} G_n^l(z)(k_n z)^{-3} R(z,A)dz \Big\|$$
$$\le C \int_0^{R/k_n} e^{-ct_{n-1}\rho} d\rho + C \int_0^{R/k_n} (k_n\rho)\Big((k_n\rho)^2 e^{-ct_n\rho}(t_n\rho)\Big)(k_n\rho)^{-3}\frac{d\rho}{\rho} \le C.$$

Further, by the boundedness of $G_n(z)$,

$$\Big\| \int_{\Gamma_{R/k_n}^\infty} G_n(z)(k_n z)^{-3} R(z,A)dz \Big\| \le C \int_{R/k_n}^\infty (k_n\rho)^{-3}\frac{d\rho}{\rho} \le C.$$

Together these estimates complete the proof. □

We close this section with an error estimate of the approximation (4.19) of the time derivative $u_t(t_n)$ of the solution of (1.1) in the nonsmooth data case.

Theorem 4.12. *Under the assumptions of Theorem 4.9, there is a constant C, such that*

$$\|\bar\partial^2 U^n - D_t u(t_n)\| \le C k_n^2 t_n^{-3}\|v\|, \quad \textit{for} \quad n \ge 2. \tag{4.23}$$

Proof. With the notation of Theorem 4.11 we need to show

$$\|G_n(A)\| \le C k_n^3 t_n^{-3}, \quad \text{for } n \ge 2.$$

By the argument in the proof of Theorem 4.9, we may write

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

where $\tilde G(z) = G_n(z) - \kappa^n P(\kappa,\kappa) k_n z/(1 + k_n z)$.
We rewrite

$$\tilde G_n(z) = \Big(\prod_{j=1}^n r(k_j z) P(r(k_{n-1}z), r(k_n z)) - \kappa^n P(\kappa,\kappa)\Big)$$
$$+ \kappa^n P(\kappa,\kappa)/(1 + k_n z) - (-k_n z)e^{-t_n z},$$

we have

$$\int_{R/k_1}^\infty |\tilde G_n(\rho e^{\pm i\psi})|\frac{d\rho}{\rho} \le C \int_{R/k_1}^\infty \Big(e^{-c_2 n}(k_1\rho)^{-1} + |\kappa|^n (k_n\rho)^{-1} + (k_n\rho)e^{-t_n\rho}\Big)\frac{d\rho}{\rho}$$
$$\le C k_n^3 t_n^{-3}.$$

Using $|1/(1+k_nz)| \le 1$ for $Re\, z \ge 0$, we get, with $n > 2$,

$$\int_0^{R/k_{n-2}} |\tilde G_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} + \int_0^{R/k_{n-2}} |\kappa|^n k_n d\rho$$
$$\le \sum_{l=1}^3 \int_0^{R/k_{n-2}} |G_n^l| \frac{d\rho}{\rho} + C \int_0^{R/k_{n-2}} |\kappa|^n k_n d\rho,$$

where $G_n^l(z)$, $l = 1, 2, 3$ are defined by (4.22). Obviously, recalling (4.17),

$$\int_0^{R/k_{n-2}} (|G_n^1| + |G_n^2|) \frac{d\rho}{\rho} \le C k_n^3 t_n^{-3}.$$

Here we use

$$|P(e^{-k_{n-1}z}, e^{-k_n z}) - (-k_n z)| \le C|k_n z|^3,$$

and

$$|P(r(k_{n-1}z), r(k_n z)) - P(e^{-k_{n-1}z}, e^{-k_n z})| \le C|k_n z|^3,$$

which follows from $k_n|z| = (k_n/k_{n-2})(k_{n-2}|z|) \le CR$, when $|z| \le R/k_{n-2}$. Further, recalling (4.7), we have

$$\int_0^{R/k_{n-2}} |G_n^3| \frac{d\rho}{\rho} \le C \int_0^{R/k_{n-2}} (k_n\rho)(k_n\rho)^3 e^{-c_1 t_n \rho} n \frac{d\rho}{\rho} \le C k_n^3 t_n^{-3}.$$

It remains to consider the integral on interval $[R/k_n, R/k_1]$. We rewrite

$$\tilde G_n(z) = c_0 \prod_{j=1}^n r(k_j z) + c_1 \prod_{j=1}^{n-1} r(k_j z) + c_2 \prod_{j=1}^{n-2} r(k_j z) - (-k_n z) e^{-t_n z} - \frac{k_n z}{1 + k_n z}(c_0 \kappa^n + c_1 \kappa^{n-1} + c_2 \kappa^{n-2}). \tag{4.24}$$

Recalling (4.9) with $p = 3$, we have, noting that $k_{n-2}^3 t_{n-2}^{-3} \le C k_n^3 t_n^{-3}$,

$$\int_{R/k_{n-2}}^{R/k_1} \Big| \prod_{j=1}^{n-2} r(k_j \rho e^{\pm i\psi}) \Big| \frac{d\rho}{\rho} \le \sum_{m=1}^{n-3} \int_{R/k_{m+1}}^{R/k_m} \Big| \prod_{j=1}^{n-2} r(k_j \rho e^{\pm i\psi}) \Big| \frac{d\rho}{\rho}$$
$$\le C k_{n-2}^3 t_{n-2}^{-3} \le C k_n^3 t_n^{-3}.$$

Further, recalling (4.18), we have, noting this time that $t_n \rho \ge C(n-2)$ for $\rho \in [R/k_{n-2}, R/k_1]$, since $t_n\rho \ge R(t_n/k_{n-2}) \ge R(t_{n-2}/k_{n-2}) \ge C(n-2)$,

$$\int_{R/k_{n-2}}^{R/k_1} \Big| e^{-t_n \rho e^{\pm i\psi}} \Big| (k_n \rho) \frac{d\rho}{\rho} \le C k_n^3 t_n^{-3},$$

and

$$\int_{R/k_{n-2}}^{R/k_1} \frac{k_n \rho}{1 + k_n \rho} (c_0 \kappa^n + c_1 \kappa^{n-1} + c_2 \kappa^{n-2}) \frac{d\rho}{\rho} \le C k_n^3 t_n^{-3}.$$

Together these estimates complete the proof. □

5. Numerical Illustrations

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

$$u_t - u_{xx} = 0, \quad \text{in } [0,1], \quad \text{with } u(0,t) = u(1,t) = 0, \quad \text{for } t > 0, \tag{5.1}$$

$$u(x,0) = v(x), \quad \text{in } [0,1],$$

where

$$v = \begin{cases} 1, & \text{if } \frac{1}{4} < x < \frac{3}{4}, \\ 0, & \text{otherwise.} \end{cases} \tag{5.2}$$

We have that $v \in \dot{H}^s$, for $0 < s < 1/2$. In fact, we consider the eigenvalue problem

$$-\varphi'' = \lambda\varphi \quad \text{for } 0 < x < 1, \quad \varphi(0) = \varphi(1) = 0.$$

As is well-known, the eigenfuctions $\varphi_n = \sqrt{2}\sin n\pi x$, $n = 1, 2, \cdots$ form an orthonormal basis in $L_2(0,1)$, and the corresponding eigenvalues are $\lambda_n = n^2\pi^2$. Thus, if $0 \le s < 1/2$, we have

$$|v|_s = \sum_{n=1}^{\infty} \lambda_n^s (v, \varphi_n)^2 = \sum_{n=1}^{\infty} 4((2n-1)\pi)^{2s-2} < \infty,$$

which implies that $v \in \dot{H}^s$ for $s < 1/2$. We also note that $v \in L_\infty$, but $v \notin W_\infty^s$ for any $s > 0$.

The exact solution of (5.1) 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 the introduction, the semidiscrete problem may be written

$$u_{h,t} = A_h u_h, \qquad \text{for } t > 0, \qquad \text{with } u_h(0) = P_h v, \tag{5.3}$$

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 (5.1) by applying the constant step time stepping method $U^n = r(kA)U^{n-1}$ to the semidiscrete problem (5.3), 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 (1.10) holds. Recall from (2.3) that this approximation is not so good if $r(\infty) \ne 0$. Therefore we then use Q_kU^n, defined by (1.11) to approximate $u_t(t_n)$, and Theorems 3.7 and 3.16 show error estimates for the fully discrete method with nonsmooth data in L_2 and L_∞ norms. More precisely, if $|r(\infty)| < 1$, we have in L_2 norm, for $0 \le s \le 2$, see, e.g., Thomée [19],

$$\|U^n - u(t_n)\| \le C t_n^{-(1-s/2)}(k + h^2)|v|_s. \tag{5.4}$$

and it follows from Theorem 3.7 that

$$\|\bar\partial U^n - u_t(t_n)\| \le C t_n^{-(2-s/2)}(k + h^2)|v|_s. \tag{5.5}$$

Here, in order to be able to use v in (5.2), for which $v \in \dot{H}^s$, for any $s < 1/2$, we have interpolated between smooth and nonsmooth data error estimates.

For the approximation $-A_h U^n$ of $u_t(t_n)$ when $r(\infty) = 0$, combining (2.3) and Theorem 3.1, we have the same error bound as in (5.5).

In our experiments, we consider different time stepping methods, namely, the backward Euler method, the θ-method defined by (2.1) with $\theta = 2/3$, and the Crank-Nicolson method. Since we are mostly interested in the time stepping, we choose h very small and a moderate and variable k. We will thus use $h = 1/200$ be fixed, and the time step k be chosen as $1/20, 1/40$ and $1/80$.

We begin with the backward Euler method, so that $r(\lambda) = 1/(1 + \lambda)$, with $r(\infty) = 0$. Denote $\varepsilon(k) = \varepsilon(k, t_n) = \|U^n - u(t_n)\|$, and let $\rho(k_1, k_2) = \varepsilon(k_1)/\varepsilon(k_2)$. Table 1 shows the L_2 norm of the error of the approximation U^n of $u(t_n)$ at time t_n. The results show 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 $\varepsilon(k) = \varepsilon(k, t_n) = \|\bar\partial U^n - u_t(t_n)\|$, 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 $t \to 0$. Note that in this case $\bar\partial U^n = -A_h U^n$ so that the approximation using $-A_h U^n$ is the same as $\bar\partial U^n$.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20, 1/40)$	$\rho(1/40, 1/80)$
0.1	4.867E-02	2.629E-02	1.375E-02	1.85	1.91
0.2	3.952E-02	2.062E-02	1.053E-02	1.91	1.95
0.3	2.440E-02	1.217E-02	6.062E-03	2.00	2.00
0.4	1.343E-02	6.398E-03	3.101E-03	2.09	2.06
0.5	6.952E-03	3.154E-03	1.487E-03	2.20	2.11
0.6	3.463E-03	1.494E-03	6.854E-04	2.31	2.17
0.7	1.681E-03	6.886E-04	3.070E-04	2.44	2.24
0.8	8.020E-04	3.112E-04	1.348E-04	2.55	2.30
0.9	3.775E-04	1.385E-04	5.826E-05	2.72	2.37
1.0	1.759E-04	6.099E-05	2.487E-05	2.88	2.45

Table 1: Backward Euler method with the approximation U^n of $u(t_n)$.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20,1/40)$	$\rho(1/40,1/80)$
0.1	8.158E-01	3.113E-01	1.430E-01	2.62	2.17
0.2	3.907E-01	2.036E-01	1.040E-01	1.91	1.95
0.3	2.409E-01	1.202E-01	5.984E-02	2.00	2.00
0.4	1.326E-01	6.315E-02	3.061E-02	2.09	2.06
0.5	6.862E-02	3.113E-02	1.468E-02	2.20	2.11
0.6	3.418E-02	1.474E-02	6.765E-03	2.31	2.17
0.7	1.658E-02	6.797E-03	3.031E-03	2.44	2.24
0.8	7.916E-03	3.071E-03	1.330E-03	2.57	2.30
0.9	3.725E-03	1.367E-03	5.750E-04	2.72	2.37
1.0	1.736E-03	6.020E-04	2.455E-04	2.88	2.45

Table 2: Backward Euler method with the approximation $\bar{\partial}U^n$ of $u_t(t_n)$.

We next consider the θ-method defined by (2.1), with $\theta = 2/3$, i.e., $r(\lambda) = (1-\frac{1}{3}\lambda)/(1+\frac{2}{3}\lambda)$, with $r(\infty) = 1/2$, which is also accurate of order $p = 1$. Table 3 shows the L_2 error estimates of the approximation U^n of $u(t_n)$, and Table 4 shows the L_2 error estimates of the approximation $\bar{\partial}U^n$ of $u_t(t_n)$, Tables 3 and 4 again confirm our theoretical results.

Table 5 shows the L_2 error estimates of the approximation $-A_hU^n$ of $u_t(t_n)$. Since $r(\infty) \neq 0$, the error estimate (5.5) is not valid for $-A_hU^n$. Now $\varepsilon(k) = \varepsilon(k,t_n) = \|A_hU^n - u_t(t_n)\|$. By (2.6), we have $\|A_hU^n\| \le C\max(t_n^{-1},\ h^{-2}e^{-cn})$. When n is small, the term $Ch^{-2}e^{-cn}$ dominates, so that we cannot expect $-A_hU^n$ to be a good approximation of $u_t(t_n)$, but this term becomes exponentially smaller with n. For example, for $t_n = 0.4$ we have $n = 8, 16$, and 32 when k is chosen as $k = 1/20, 1/40$, and $1/80$. We see that $\rho(1/20,1/40)$ is much larger than $\rho(1/40,1/80)$: $Ch^{-2}e^{-cn}$ is much smaller for $n = 16$ than for $n = 8$.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20,1/40)$	$\rho(1/40,1/80)$
0.1	4.453E-02	1.122E-02	4.492E-03	3.96	2.49
0.2	1.420E-02	6.329E-03	3.369E-03	2.24	1.87
0.3	6.661E-03	3.593E-03	1.901E-03	1.85	1.89
0.4	3.284E-03	1.815E-03	9.538E-04	1.80	1.90
0.5	1.565E-03	8.618E-04	4.484E-04	1.81	1.92
0.6	7.206E-04	3.923E-04	2.024E-04	1.83	1.93
0.7	3.231E-04	1.736E-04	8.888E-05	1.86	1.95
0.8	1.420E-04	7.532E-05	3.824E-05	1.88	1.97
0.9	6.146E-05	3.215E-05	1.618E-05	1.91	1.98
1.0	2.628E-05	1.356E-05	6.765E-06	1.93	2.00

Table 3. θ-method, $\theta = 2/3$, with the approximation U^n of $u(t_n)$.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20, 1/40)$	$\rho(1/40, 1/80)$
0.1	2.863E-00	9.914E-01	1.676E-01	2.88	5.91
0.2	6.390E-01	1.540E-01	7.213E-02	4.14	2.13
0.3	1.872E-01	6.786E-02	3.352E-02	2.75	2.02
0.4	6.867E-02	3.048E-02	1.507E-02	2.25	2.02
0.5	2.817E-02	1.331E-02	6.555E-03	2.11	2.03
0.6	1.193E-02	5.729E-03	2.806E-03	2.08	2.04
0.7	5.067E-03	2.430E-03	1.184E-03	2.08	2.05
0.8	2.140E-03	1.019E-03	4.938E-04	2.09	2.06
0.9	8.980E-04	4.240E-04	2.039E-04	2.11	2.07
1.0	3.745E-04	1.749E-04	8.358E-05	2.14	2.09

Table 4. θ-method, $\theta = 2/3$, with the approximation $\bar{\partial}U^n$ of $u_t(t_n)$.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20, 1/40)$	$\rho(1/40, 1/80)$
0.1	2.277E+03	5.674E+02	3.504E+01	4.01	16.1
0.2	5.686E+02	3.532E+01	1.388E-01	16.0	254.5
0.3	1.420E+02	2.198E+00	1.877E-02	64.5	117.4
0.4	3.546E+01	1.380E-01	9.414E-03	256.9	14.6
0.5	8.857E+00	1.204E-02	4.427E-03	735.5	2.71
0.6	2.212E+00	3.909E-03	1.998E-03	565.8	1.95
0.7	5.524E-01	1.714E-03	8.774E-04	322.1	1.95
0.8	1.379E-01	7.435E-04	3.773E-04	185.5	1.97
0.9	3.446E-02	3.174E-04	1.597E-04	108.5	1.98
1.0	8.609E-03	1.338E-04	6.678E-05	64.3	2.00

Table 5. θ-method, $\theta = 2/3$, with the approximation $-A_hU^n$ of $u_t(t_n)$.

In the following Tables 6 and 7 we present maximum-norm error corresponding to Tables 3 and 4.

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 6. θ-method, with the approximation U^n of $u(t_n)$ in L_∞ 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 7. θ-method, with the approximation $\bar{\partial}U^n$ of $u_t(t_n)$ in L_∞ norm.

Finally we consider the Crank-Nicolson method. Tables 8, 9, and 10 show the error in U^n, $\bar{\partial}U^n$ and $-A_hU^n$ in L_2 norm. Note that because this method is not smoothing, the error estimates (5.4) and (5.5) are not valid. Thus, in Table 8 we do not attain the full $O(k^2)$ convergence which holds for smooth data. Further, inTable 9, the error does not decrease with k, because the difference quotient contains a factor k^{-1}. Finally, in Table 10, the error is very large and depends on the multiplication by the ill-conditioned operator A_h of the oscillating components of U^n, which are now not small.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20, 1/40)$	$\rho(1/40, 1/80)$
0.1	1.764E-01	1.249E-01	8.750E-02	1.41	1.42
0.2	1.489E-01	1.047E-01	7.263E-02	1.42	1.44
0.3	1.345E-01	9.437E-02	6.481E-02	1.42	1.45
0.4	1.250E-01	8.752E-02	5.958E-02	1.42	1.46
0.5	1.181E-01	8.249E-02	5.566E-02	1.43	1.48
0.6	1.128E-01	7.856E-02	5.259E-02	1.45	1.49
0.7	1.084E-01	7.534E-02	5.003E-02	1.43	1.50
0.8	1.048E-01	7.263E-02	4.785E-02	1.44	1.51
0.9	1.016E-01	7.030E-02	4.596E-02	1.44	1.52
1.0	9.895E-02	6.825E-02	4.428E-02	1.44	1.54

Table 8. Crank-Nicolson method, with the approximation U^n of $u(t_n)$.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20, 1/40)$	$\rho(1/40, 1/80)$
0.1	0.1369	0.1843	0.2534	0.74	0.72
0.2	0.3691	0.5100	0.70	0.72	0.72
0.3	0.6693	0.9285	1.26	0.72	0.73
0.4	1.0235	1.4207	1.92	0.72	0.73
0.5	1.4242	1.9756	2.65	0.72	0.74
0.6	1.8664	2.5856	3.45	0.72	0.74
0.7	2.3462	3.2450	4.30	0.72	0.75
0.8	2.8607	3.9496	5.19	0.72	0.76
0.9	3.4074	4.6956	6.13	0.72	0.76
1.0	3.9844	5.4802	7.10	0.72	0.77

Table 9. Crank-Nicolson method, with the approximation $\bar{\partial}U^n$ of $u_t(t_n)$.

t	$\varepsilon(1/20)$	$\varepsilon(1/40)$	$\varepsilon(1/80)$	$\rho(1/20, 1/40)$	$\rho(1/40, 1/80)$
0.1	9.109E+03	9.083E+03	8.986E+03	1.00	1.01
0.2	9.100E+03	9.050E+03	8.864E+03	1.00	1.02
0.3	9.091E+03	9.017E+03	8.750E+03	1.01	1.03
0.4	9.083E+03	8.986E+03	8.640E+03	1.01	1.04
0.5	9.074E+03	8.955E+03	8.534E+03	1.01	1.04
0.6	9.066E+03	8.924E+03	8.431E+03	1.02	1.05
0.7	9.056E+03	8.894E+03	8.332E+03	1.02	1.06
0.8	9.050E+03	8.864E+03	8.236E+03	1.02	1.07
0.9	9.042E+03	8.835E+03	8.142E+03	1.02	1.08
1.0	9.033E+03	8.807E+03	8.050E+03	1.03	1.09

Table 10. Crank-Nicolson method, with the approximation $-A_hU^n$ of $u_t(t_n)$.

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