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

YUBIN YAN

Abstract. We study smoothing properties and approximation of time derivatives for time discretization schemes with variable time steps for a homogeneous parabolic problem formulated as an abstract initial value problem in a Banach space. The time stepping methods are based on using rational functions $r(z) \approx e^{-z}$ which are $A(\theta)$-stable for suitable $\theta \in (0, \pi/2]$ and satisfy $|r(\infty)| < 1$. First and second order approximations of time derivatives based on using difference quotients are considered. Smoothing properties are derived and error estimates are established under the so called *increasing quasi-quasiuniform* assumption on the time steps.

1. Introduction

Let us consider the following homogeneous linear parabolic problem

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

where A is a closed, linear operator, with dense domain $\mathcal{D}(A) \subset \mathcal{B}$, where $\mathcal{B}$ is a Banach space with norm $\|\cdot\|$ and $v \in \mathcal{B}$. We shall study time discretization schemes with variable time steps and show error estimates for the approximations of $u(t)$ and u_t.

We assume that $-A$ is the infinitesimal generator of a bounded analytic semigroup $E(t) = e^{-tA}$ and that $0 \in \rho(A)$, where $\rho(A)$ denotes the resolvent set of A. This is equivalent to saying that there is an angle $\delta \in (0, \pi/2)$ such that

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

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

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

where $\|\cdot\|$ denotes the standard norm of bounded linear operators on $\mathcal{B}$.

Under these assumptions $E(t)$ may be represented as

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

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where $\Gamma = \{ z : |\arg z| = \psi\}$ with $\psi \in (\delta, \pi/2)$ and Imz is decreasing along Γ. Furthermore, the smoothing properties of analytic semigroups are valid. More precisely, see Pazy [11], we have

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

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

Let $0 = t_0 < t_1 < \cdots < t_n < \cdots$ be a partition of the time axis and let $k_n = t_n - t_{n-1},\ n \ge 1$, be the variable time steps. An approximate solution $U^n \approx u(t_n) = E(t_n)v$ of (1.1.1) may be defined by

$$U^n = E_{k_n} U^{n-1}, \quad \text{for } n \ge 1, \quad \text{with } U^0 = v, \tag{1.1.5}$$

where $E_{k_n} = r(k_n A)$ and r is a rational function that satisfies certain conditions. For example, $r(z) = 1/(1-z)$ and $r(z) = (1+z/2)/(1-z/2)$ correspond to the backward Euler and Crank-Nicolson methods, respectively.

We say that r is $A(\theta)$-stable with $\theta \in [0, \pi/2]$ if

$$|r(z)| \le 1, \quad \text{for } |\arg z| \le \theta, \tag{1.1.6}$$

and accurate of order $p \ge 1$, if

$$r(z) - e^{-z} = O(z^{p+1}), \quad \text{as } z \to 0. \tag{1.1.7}$$

Let us recall some results for the time stepping method (1.1.5) with constant time step k. If A satisfies (1.1.2) and (1.1.3), and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, then we have the stability estimate, with $E_k = r(kA)$,

$$\|U^n\| = \|E_k^n v\| \le C\|v\|, \quad \text{for } t_n \ge 0,\ v \in \mathcal{B}, \tag{1.1.8}$$

see, e.g., Crouzeix, Larsson, Piskarev, and Thomée [3] and Palencia [9], [10]. If A satisfies (1.1.2) and (1.1.3), and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$ and accurate of order $p \ge 1$, then the following smooth data error estimate holds:

$$\|U^n - u(t_n)\| \le Ck^p \|A^p v\|, \quad \text{for } t_n \ge 0,\ v \in \mathcal{D}(A^p). \tag{1.1.9}$$

Moreover, if $|r(\infty)| < 1$, then the following nonsmooth data error estimate holds:

$$\|U^n - u(t_n)\| \le Ck^p t_n^{-p} \|v\|, \quad \text{for } t_n > 0,\ v \in \mathcal{B}. \tag{1.1.10}$$

The condition $|r(\infty)| < 1$ ensures that oscillating components of the error are efficiently damped, see, e.g., Le Roux [8], Larsson, Thomée, and Wahlbin [7], Fujita and Suzuki [5].

Smoothing properties and approximation of time derivatives for (1.1.5) with constant time step have also been studied by some authors. Let $j \ge 1$ be fixed. If A satisfies (1.1.2) and (1.1.3), and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and with $r(\infty) = 0$, then the following smoothing property holds:

$$\|A^j U^n\| = \|A^j E_k^n v\| \le Ct_n^{-j}\|v\|, \quad \text{for } t_n \ge t_j,\ v \in \mathcal{B}, \tag{1.1.11}$$

see, e.g., Thomée [12] for the Hilbert space case and Hansbo [6] for the Banach space case. However (1.1.11) is not true in general when $r(\infty) \ne 0$.

Let us introduce the finite difference quotients,

$$Q_k^j U^n = \frac{1}{k^j} \sum_{\nu=-m_1}^{m_2} c_\nu U^{n+\nu}, \quad \text{for } n \geq m_1, \tag{1.1.12}$$

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

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

We then have the following smoothing property and nonsmooth data error estimates: If A satisfies (1.1.2) and (1.1.3), and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$, then we have

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

and, if further $r(z)$ is accurate of order $p \geq 1$,

$$\|Q_k^j U^n - D_t^j u(t_n)\| \leq C k^p t_n^{-(p+j)} \|v\|, \quad \text{for } n \geq m_1,\ t_n > 0,\ v \in \mathcal{B}, \tag{1.1.14}$$

see Yan [13]

For the smooth data error estimate, the condition $|r(\infty)| < 1$ is not necessary. In fact, we have, for any $A(\theta)$-stable discretization scheme with $\theta \in (\delta, \pi/2]$,

$$\|Q_k^j U^n - D_t^j u(t_n)\| \leq C k^p \|A^{p+j} v\|, \quad \text{for } n \geq m_1,\ v \in \mathcal{D}(A^{p+j}), \tag{1.1.15}$$

see, e.g., Baker, Bramble, and Thomée [2] for the Hilbert space case and Yan [13] for the Banach space case.

Now let us mention some results for the variable time steps which are related to the present paper. Stability results have been considered by some authors. For example, Palencia [9] shows that, if A satisfies (1.1.2) and (1.1.3), and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, if the time steps $\{k_j\}_{j=1}^{\infty}$ satisfy, with some constant μ,

$$0 < \mu^{-1} \leq \frac{k_i}{k_j} \leq \mu < \infty, \quad \text{for } i, j \geq 1, \tag{1.1.16}$$

then there exists a constant $C(\mu)$ such that the following stability result holds

$$\Big\| \prod_{j=1}^{n} E_{k_j} \Big\| \leq C(\mu), \quad \text{where } E_{kj} = r(k_j A). \tag{1.1.17}$$

We observe that the stability bound will depend on the maximum ratio μ between the steps, but not on the steps themselves. In this way, the stability bound does not blow up when the maximum time step goes to zero, as long as μ remains bounded. In particular, a family of quasi-uniform grids with $k_{max} \leq \mu k_{min}$ satisfies the assumption (1.1.16), where $k_{max} = \max_{1 \leq j \leq n} k_j$, $k_{min} = \min_{1 \leq j \leq n} k_j$. More precisely, Bakaev [1] shows that if A satisfies (1.1.2) and (1.1.3), and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, then

$$\Big\| \prod_{j=1}^{n} E_{k_j} \Big\| \leq C \ln(1+\mu), \quad \text{where } \mu = \frac{k_{max}}{k_{min}}. \tag{1.1.18}$$

Palencia [10] further finds that if $|r(\infty)| < 1$, then the stability bound holds without any restriction on the time steps.

In the present paper, we first consider error estimates for (1.1.5) in both smooth and nonsmooth data cases. We show, in Theorem 2.1, that if A satisfies (1.1.2) and (1.1.3) and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$ and accurate of order $p \geq 1$, then the following smooth data error estimate holds:

$$\|U^n - u(t_n)\| \leq C k_{max}^p \|A^p v\|, \quad \text{for } t_n \geq 0, \ v \in \mathcal{D}(A^p).$$

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

$$ck_{n+1} \leq k_n \leq Ct_n/n, \quad \text{for } n \geq 1. \tag{1.1.19}$$

Further, if $k_1 \leq k_2 \leq \cdots \leq k_n \leq \cdots$, then we call $\{\mathcal{T}\}$ a family of *increasing quasi-quasiuniform grids.* We note that *increasing quasi-quasiuniform* implies that $k_n \sim k_{n+1}$ and $nk_n \sim t_n$, where $a_n \sim b_n$ means that a_n/b_n is bounded above and below.

For example, if we choose the variable time steps $k_n = n^s k$ for some fixed $s \geq 1$, 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 $k_n/k_{n+1} = n^s/(n+1)^s \geq 1/2^s$. Further, since $t_n/k = \sum_{j=1}^n j^s \geq Cn^{s+1}$ for some positive constant C, we have $k_n \leq Ct_n/n$.

Under these assumptions we have the following nonsmooth data error estimate: If A satisfies (1.1.2) and (1.1.3), and r is $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$ and accurate of order $p \geq 1$, if further $|r(\infty)| < 1$ and $\{\mathcal{T}\}$ is a family of *increasing quasi-quasiuniform grids*, then we have

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

We note that these two error estimates correspond to (1.1.9) and (1.1.10) for constant time step, respectively.

As for the smoothing property, we show that, if $r(\infty) = 0$, and $\{\mathcal{T}\}$ satisfies (1.1.16), then

$$\Big\| A \prod_{j=1}^{n} E_{k_j} v \Big\| \leq C t_n^{-1} \|v\|, \quad \text{for } t_n > 0, \ v \in \mathcal{B}.$$

As in the constant time step case, see Yan [13], the above smoothing property is not true in the case of $r(\infty) \neq 0$. However, if $|r(\infty)| < 1$, then we introduce similar difference quotients as (1.1.12) with variable time steps. For simplicity we only consider the following first and second order approximations of time derivative $u_t(t_n)$ defined by

$$\bar{\partial} U^n = \frac{U^n - U^{n-1}}{k_n}, \quad \text{for } n \geq 1, \tag{1.1.20}$$

and

$$\bar{\partial}^2 U^n = a_n \bar{\partial} U^n + b_n \bar{\partial} U^{n-1} = a_n \frac{U^n - U^{n-1}}{k_n} + b_n \frac{U^{n-1} - U^{n-2}}{k_{n-1}}, \quad \text{for } n \geq 2, \tag{1.1.21}$$

where

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

In both cases, under the assumption of *increasing quasi-quasiuniform grids*, we obtain a smoothing property and error estimates for time derivative in the nonsmooth data case which are similar to (1.1.13) and (1.1.14), respectively. We also show a smooth data error estimate without any restrictions on the time steps.

The paper is organized as follows. In Section 2 we show error estimates for the approximation U^n of u^n in both smooth and nonsmooth data cases. In Section 3 we consider the first order approximation (1.1.20) of $u_t(t_n)$ and show a smoothing property and error estimates for time derivative. In Section 4 we consider the second order approximation (1.1.21) and obtain similar results as in Section 3.

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. Error Estimates

In this section we will consider error estimates for the approximation U^n defined by (1.1.5) of the solution $u(t_n)$ of (1.1.1). 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 2.1. *Let U^n and $u(t_n)$ be the solutions of* (1.1.5) *and* (1.1.1)*. Assume that A satisfies* (1.1.2) *and* (1.1.3)*, and that $r(z)$ is accurate of order $p \geq 1$, and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$. Let $k_j, 1 \leq j \leq n$, be time steps. Then we have*

$$\|U^n - u(t_n)\| \leq C k_{max}^p \|A^p v\|, \quad \text{for } t_n \geq 0,\ v \in \mathcal{D}(A^p),$$

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

In order to prove Theorem 2.1, we need the following lemmas which are simple consequences of (1.1.6) and (1.1.7). The first lemma is quoted from Thomée [12, Lemma 8.2].

Lemma 2.2. *Assume that $r(z)$ is $A(\theta)$-stable with $\theta \in (0, \pi/2]$, and accurate of order $p \geq 1$. Then for arbitrary $R > 0$ and $\psi \in (0, \theta)$ there is $c > 0$ such that*

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

Lemma 2.3. *Assume that $r(z)$ is $A(\theta)$-stable with $\theta \in (0, \pi/2]$, 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, with $F_n(z) = \prod_{j=1}^n r(k_j z) - e^{-t_n z}$,*

$$|F_n(z)| \leq Cn|k_{max} z|^{p+1} e^{-ct_n|z|}, \quad \text{for } |k_{max} z| \leq R,\ |\arg z| \leq \psi, \tag{2.2.1}$$

and

$$|F_n(z)| \le C|k_{max}z|^p t_n |z| e^{-ct_n|z|}, \quad \text{for } |k_{max}z| \le R, \ |\arg z| \le \psi, \tag{2.2.2}$$

where $k_{max} = \max_{1\le j\le n} k_j$.

Proof. Since $r(z)$ is accurate of order $p \ge 1$, there exists a small $\eta > 0$ such that

$$|r(z) - e^{-z}| \le C|z|^{p+1}, \quad \text{for } |z| \le \eta.$$

Further, by (1.1.6), we have, for arbitrary $R > 0$ and $\psi \in (0, \theta)$,

$$|r(z) - e^{-z}| \le C|z|^{p+1}, \quad \text{for } |z| \le R, \ |\arg z| \le \psi. \tag{2.2.3}$$

We next observe that, if $c \le \cos\psi$,

$$|e^{-z}| = e^{-\mathrm{Re} z} \le e^{-c|z|}, \quad \text{for } |\arg z| \le \psi. \tag{2.2.4}$$

It is easy to show that

$$|F_n(z)| \le C \sum_{j=1}^{n} (k_j|z|)^{p+1} e^{-c(t_n-k_j)|z|}, \quad \text{for } |k_{max}z| \le R, \ |\arg z| \le \psi. \tag{2.2.5}$$

In fact, using Lemma 2.2, (2.2.3) and (2.2.4), we have, for $|k_{max}z| \le R, \ |\arg z| \le \psi$,

$$|F_1(z)| = |r(k_1 z) - e^{-k_1 z}| \le C(k_1|z|)^{p+1} e^{-c(t_1-k_1)|z|},$$

and

$$\begin{aligned} |F_2(z)| &= |(r(k_1 z) - e^{-k_1 z}) r(k_2 z) + e^{-k_1 z}(r(k_2 z) - e^{-k_2 z})| \\ &\le C|k_1 z|^{p+1} e^{-c(t_2-k_1)|z|} + Ce^{-c(t_2-k_2)|z|}|k_2 z|^{p+1} \\ &= C \sum_{j=1}^{2} (k_j|z|)^{p+1} e^{-c(t_n-k_j)|z|}. \end{aligned}$$

In general, for $n \ge 3$,

$$\begin{aligned} |F_n(z)| &= \Big| \Big(r(k_1 z) - e^{-k_1 z}\Big) \prod_{j=2}^{n} r(k_j z) + e^{-k_1 z}\Big(r(k_2 z) - e^{-k_2 z}\Big) \prod_{j=3}^{n} r(k_j z) \\ &\quad + \cdots + \Big(\prod_{j=1}^{n-1} e^{-k_j z}\Big)\Big(r(k_n z) - e^{-k_n z}\Big) \Big| \\ &\le C \sum_{j=1}^{n} \Big(e^{-ct_{j-1}|z|} (k_j|z|)^{p+1} e^{-c(t_n-t_j)|z|} \Big) \\ &= C \sum_{j=1}^{n} (k_j|z|)^{p+1} e^{-c(t_n-k_j)|z|}. \end{aligned}$$

Thus, by (2.2.5), we get, using $k_j|z| \le |k_{\max}z| \le R, \ 1 \le j \le n$,

$$|F_n(z)| \le Cn|k_{max}z|^{p+1} e^{-ct_n|z|}, \quad \text{for } |k_{max}z| \le R, \ |\arg z| \le \psi,$$

and

$$\begin{aligned}|F_n(z)| &\le Ce^{-ct_n|z|}\sum_{j=1}^{n}(k_j|z|)^{p+1}\\ &\le C|k_{max}z|^p t_n|z|e^{-ct_n|z|}, \quad \text{for } |k_{max}z|\le R,\ |\arg z|\le\psi.\end{aligned}$$

Together these estimates complete the proof. □

The following lemma gives the Dunford-Taylor spectral representation of a rational function of the operator A when the rational function is bounded in a sector in the right halfplane, see Thomée [12, Lemma 8.1].

Lemma 2.4. *Assume that* (1.1.2) *and* (1.1.3) *hold and let* $r(z)$ *be a rational function which is bounded for* $|\arg z|\le\psi$, $|z|\ge\epsilon>0$, *where* $\psi\in(\delta,\pi/2)$, *and for* $|z|\ge R$. *If* $\epsilon>0$ *is so small that* $\{z:|z|\le\epsilon\}\subset\rho(A)$, *then we have*

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

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

For our error estimates we shall apply the following spectral representation of the semigroup, see Thomée [12, Lemma 8.3].

Lemma 2.5. *Assume that* (1.1.2) *and* (1.1.3) *hold, let* $\psi\in(\delta,\pi/2)$, *and* j *be any integer. Then we have for* $\epsilon>0$ *sufficiently small*

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

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

Proof of Theorem 2.1. Since $U^n-u(t_n)=\prod_{j=1}^n r(k_jA)v-e^{-t_nA}v=F_n(A)v$, we need to show $\|F_n(A)v\|\le Ck_{max}^p\|A^pv\|$, or in operator norm,

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

which we will do now. Let $\bar r(z)=\prod_{j=1}^n r(k_jz)(k_{max}z)^{-p}$. Since $r(z)$ is $A(\theta)$-stable with $\theta\in(\delta,\pi/2]$, we find that $\bar r(z)$ is bounded for $|\arg z|\le\psi$, $|z|\ge\epsilon$ with some $\psi\in(\delta,\theta)$ and any $\epsilon>0$. Further $\bar r(z)$ is also bounded for $|z|\ge R$ with R sufficiently large, since $\bar r(\infty)=0$. Thus, applying Lemma 2.4 to the rational function $\bar r(z)$, we have

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

By (1.1.3) and (1.1.6), we know that the integrand is of order $O(z^{-p-1})$ for large z which implies that the integrand has no poles when $|z| \geq R$, so that we may let R tend to ∞. Using also Lemma 2.5 we conclude

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

Now by (2.2.1) we see that $F_n(z) = O(z^{p+1})$ as $z \to 0$. Combining this with (1.1.3) we have that the integrand is bounded on the small domain with boundary $\gamma_\epsilon \cup \Gamma_0^\epsilon$, so that we may let $\epsilon \to 0$. It follows that, using also (1.1.3),

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

By (2.2.2), we have, for arbitrary $R > 0$,

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

Since $r(z)$ and e^{-tz} are bounded on Γ, where $\Gamma = \{z : |\arg z| = \psi\}$, we find

$$\int_{R/k_{max}}^\infty |F_n(\rho e^{\pm i\psi})|(k_{max}\rho)^{-p}\,\frac{d\rho}{\rho} \leq C\int_{R/k_{max}}^\infty (k_{max}\rho)^{-p}\,\frac{d\rho}{\rho} \leq C.$$

Together these estimates complete the proof. □

We now show a nonsmooth data error estimate.

Theorem 2.6. *Let U^n and $u(t_n)$be the solutions of* (1.1.5) *and* (1.1.1). *Assume that A satisfies* (1.1.2) *and* (1.1.3), *and that $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$ 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*

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

To prove Theorem 2.6 we need the following lemma.

Lemma 2.7. *If the rational function $r(z)$ is $A(\theta)$-stable with $\theta \in (0, \pi/2]$ and $|r(\infty)| < 1$, then for any $\psi \in (0,\theta)$ and $R > 0$ there are positive c and C such that, for any sequences $k_1 \leq k_2 \leq \cdots \leq k_n$, with $\kappa = r(\infty)$,*

$$\Big|\prod_{j=1}^n r(k_j z) - \kappa^n\Big| \leq C|k_1 z|^{-1}e^{-cn}, \quad \text{for } |k_1 z| \geq R,\ |\arg z| \leq \psi. \tag{2.2.6}$$

Proof. Since $r(z) - \kappa$ vanishes at infinity and $r(z)$ is $A(\theta)$-stable with $\theta \in (0, \pi/2]$, we have, see Thomée [12, Lemma 8.5],

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

Further,

$$|r(z)| \leq e^{-c}, \quad \text{for } |z| \geq R,\ |\arg z| \leq \psi. \tag{2.2.7}$$

In fact, $|\kappa| < 1$ implies that (2.2.7) holds for $|z| \le \tilde{R}$ with $\tilde{R}$ sufficiently large. By (1.1.6) and the maximum-principle we have $|r(z)| < 1$ for $|\arg z| < \theta$, $z \ne 0$. In particular, $|r(z)| < 1$ on the compact set $\{z : R \le |z| \le \tilde{R},\ |\arg z| \le \psi\}$, which shows (2.2.7).

(2.2.6) is obvious for $n = 1$. When $n \ge 2$, we have, for $|k_1 z| \ge R$, noting that $\kappa \le e^{-c}$ and $k_1 \le k_2 \le \cdots \le k_n$,

$$\Big|\prod_{j=1}^{n} r(k_j z) - \kappa^n\Big| = \Big|(r(k_1 z) - \kappa)\prod_{j=2}^{n} r(k_j z) + \cdots + \kappa^{n-1}(r(k_n z) - \kappa)\Big|$$

$$\le Ce^{-cn}\sum_{j=1}^{n} |k_j z|^{-1} \le C|k_1 z|^{-1} n e^{-cn} \le C|k_1 z|^{-1} e^{-cn},$$

which completes the proof of Lemma 2.7. □

Proof of Theorem 2.6. The case $n = 1$ follows from the constant time step case, see Thomée [12]. We now consider $n \ge 2$. With $F_n(z)$ as in Lemma 2.3, we need to show $\|F_n(A)\| \le Ck_n^p t_n^{-p}$. Since $t_n \le nk_n$, it suffices to show

$$\|F_n(A)\| \le Cn^{-p}.$$

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

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

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 $z = \infty$, we may use Lemmas 2.4 and 2.5 to see that

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

where $\Gamma = \{z : |\arg z| = \psi\}$ for some $\psi \in (\delta, \theta)$. By (1.1.3), we get

$$\|\tilde{F}_n(A)\| \le C\int_0^{\infty} |\tilde{F}_n(\rho e^{\pm i\psi})|\, \frac{d\rho}{\rho}.$$

Let R be arbitrary. We will bound the above integral over the intervals $[0, R/k_n] \cup [R/k_n, R/k_1] \cup [R/k_1, \infty)$. We rewrite $\tilde{F}_n(z) = (\prod_{j=1}^{n} r(k_j z) - \kappa^n) + \kappa^n/(1 + k_n z) - e^{-t_n z}$. Using (2.2.4) and Lemma 2.7 and $|1 + k_n z| \ge |k_n z|$ for $\mathrm{Re}\, z \ge 0$, we get

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

Obviously,

$$\int_{R/k_1}^{\infty} e^{-cn}(k_1\rho)^{-1}\, \frac{d\rho}{\rho} \le \int_{R}^{\infty} e^{-cn} x^{-2}\, dx \le Cn^{-p},$$

and, using $k_1 \le k_n$,

$$\int_{R/k_1}^{\infty} |\kappa|^n (k_n\rho)^{-1}\, \frac{d\rho}{\rho} \le \int_{R}^{\infty} |\kappa|^n (k_n k_1^{-1})^{-1} x^{-2}\, dx \le Cn^{-p},$$

and, using $nk_1 \le t_n$,

$$\int_{R/k_1}^{\infty} e^{-ct_n\rho}\,\frac{d\rho}{\rho} \le C\int_{R/k_1}^{\infty} (t_n\rho)^{-p}\,\frac{d\rho}{\rho} \le C\int_{R}^{\infty} (t_n k_1^{-1})^{-p} x^{-p-1}\,dx \le Cn^{-p}.$$

Thus

$$\int_{R/k_1}^{\infty} |\tilde{F}_n(\rho e^{\pm i\psi})|\,\frac{d\rho}{\rho} \le Cn^{-p}, \quad \text{for } n \ge 2. \tag{2.2.8}$$

Using (2.2.1) and $|1/(1+k_n z)| \le 1$ for $\mathrm{Re}\, z \ge 0$, we have, since $nk_n \sim t_n$,

$$\begin{aligned}\int_0^{R/k_n} |\tilde{F}_n(\rho e^{\pm i\psi})|\,\frac{d\rho}{\rho} &\le \int_0^{R/k_n} |F_n(\rho e^{\pm i\psi})|\,\frac{d\rho}{\rho} + \int_0^{R/k_n} |\kappa|^n k_n\,d\rho \\ &\le C\int_0^{R/k_n} (k_n\rho)^{p+1} e^{-ct_n\rho} n\,\frac{d\rho}{\rho} + C|\kappa|^n \\ &\le C\int_0^{R} x^p e^{-c(t_n/k_n)x} n\,dx + C|\kappa|^n \le Cn^{-p}, \quad \text{for } n \ge 2.\end{aligned}$$

It remains to consider the integral over the interval $[R/k_n, R/k_1]$ for $n \ge 2$. By Lemma 2.2 and (2.2.7) there exist 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 $|z| \ge R$, $|\arg z| \le \psi$, where c_2 can be chosen arbitrarily small. Therefore, assuming that $z \in \Gamma_{R/k_{m+1}}^{R/k_m}$ with some $m : 1 \le m \le n-1$ so that $k_j|z| \le R$ for $j \le m$, we have

$$\Big|\prod_{j=1}^{n} r(k_j z)\Big| \le e^{-c_1 t_m |z|} e^{-c_2(n-m)} \le e^{-c_2 n}\Big(e^{c_2 m} e^{-c_1 t_m |z|}\Big), \quad \text{for } n \ge 2.$$

Further, by (1.1.19),

$$c_1 t_m |z| = c_1 (t_m/k_m)(k_m/k_{m+1})(k_{m+1}|z|) \ge c_1 c_0 C_0^{-1} R m = c_3 m. \tag{2.2.9}$$

Thus if we choose $c_2 \le c_3$ and let $c_4 = c_3 - c_2$, we get

$$\Big|\prod_{j=1}^{n} r(k_j z)\Big| \le e^{-c_2 n} e^{-c_4 m}, \quad \text{if } z \in \Gamma_{R/k_{m+1}}^{R/k_m},\ 1 \le m \le n-1. \tag{2.2.10}$$

We rewrite $\tilde{F}_n(z) = \prod_{j=1}^n r(k_j z) - e^{-t_n z} - \kappa^n k_n z/(1+k_n z)$. Using (2.2.10) and noting that $\ln(k_{m+1}/k_m) \le \ln C \le C$, we get

$$\begin{aligned}\int_{R/k_n}^{R/k_1} \Big| \prod_{j=1}^n r(k_j \rho e^{\pm i\psi}) \Big| \frac{d\rho}{\rho} &\le \sum_{m=1}^{n-1} \int_{R/k_{m+1}}^{R/k_m} \Big| \prod_{j=1}^n r(k_j \rho e^{\pm i\psi}) \Big| \frac{d\rho}{\rho} \\ &\le \sum_{m=1}^{n-1} \int_{R/k_{m+1}}^{R/k_m} e^{-c_2 n} e^{-c_4 m} \frac{d\rho}{\rho} \le e^{-c_2 n} \sum_{m=1}^{n-1} \Big(e^{-c_4 m} \ln(k_{m+1}/k_m) \Big) \\ &\le C e^{-c_2 n} \Big(\sum_{m=1}^{n-1} e^{-c_4 m} \Big) \le C e^{-c_2 n} \le C n^{-p}, \quad \text{for } n \ge 2.\end{aligned} \tag{2.2.11}$$

Further, using (2.2.4) and noting that (1.1.19) implies $t_n \rho \ge c(nk_n)\rho \ge cn$ for $\rho \in [R/k_n, R/k_1]$, we have, since $\ln(k_n/k_1) = \sum_{m=1}^{n-1} \ln(k_{m+1}/k_m) \le Cn$,

$$\begin{aligned}\int_{R/k_n}^{R/k_1} \Big(|e^{-t_n \rho e^{\pm i\psi}}| + \frac{k_n \rho}{1+k_n\rho} \kappa^n \Big) \frac{d\rho}{\rho} &\le \int_{R/k_n}^{R/k_1} (e^{-cn} + \kappa^n) \frac{d\rho}{\rho} \\ &\le (e^{-cn} + \kappa^n) \ln(k_n/k_1) \le Cn(e^{-cn} + \kappa^n) \le Cn^{-p}, \quad \text{for } n \ge 2.\end{aligned} \tag{2.2.12}$$

Hence

$$\int_{R/k_n}^{R/k_1} \Big| \tilde{F}_n(\rho e^{\pm i\psi}) \Big| \frac{d\rho}{\rho} \le Cn^{-p}, \quad \text{for } n \ge 2.$$

Together these estimates complete the proof. □

3. Approximation of time derivative — first order

In this section, we shall consider a smoothing property of the time discretization scheme (1.1.5) and error estimates for the first order approximation of time derivative $u_t(t_n)$ defined by

$$\bar{\partial} U^n = \frac{U^n - U^{n-1}}{k_n}, \quad \text{for } n \ge 1. \tag{3.3.1}$$

We begin with a smooth data error estimate for the approximation (3.3.1).

Theorem 3.1. *Let U^n and $u(t_n)$be the solutions of* (1.1.5) *and* (1.1.1). *Assume that A satisfies* (1.1.2) *and* (1.1.3), *and that $r(z)$ is accurate of order $p \ge 1$, and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$. Let $k_j, 1 \le j \le n$, be increasing. Then we have*

$$\|\bar{\partial} U^n - u_t(t_n)\| \le Ck_n \|A^2 v\|, \quad \textit{for } t_n > 0. \tag{3.3.2}$$

Proof. The case $n = 1$ follows from the result in constant time step case, see Yan [13]. Now we consider the case when $n \ge 2$. 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

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

Let $\bar{r}(z) = \Big(\prod_{j=1}^{n-1} r(k_jz)(r(k_nz)-1)\Big)(k_nz)^{-2}$. As in the proof of Theorem 2.1, applying Lemma 2.4 to the rational function $\bar{r}(z)$ and using also Lemma 2.5 we conclude

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

Since $0 \in \rho(A)$, we have, by (1.1.3),

$$\|R(z;A)\| \le C, \quad \text{for } \delta \le |\arg z| \le \pi. \tag{3.3.3}$$

We will show that

$$G_n(z) = O(z^2) \quad \text{as } z \to 0. \tag{3.3.4}$$

Combining this with (3.3.3) shows that the integrand is bounded on the small domain with boundary $\gamma_\epsilon \cup \Gamma_0^\epsilon$, so that we may let $\epsilon \to 0$. It follows that, with $\Gamma = \{z : |\arg z| = \psi\}$ for some $\psi \in (\delta, \theta)$,

$$G_n(A)(k_nA)^{-2} = \frac{1}{2\pi i}\int_{\Gamma} G_n(z)(k_nz)^{-2}R(z;A)\,dz. \tag{3.3.5}$$

In order to show (3.3.4), we write

$$G_n(z) = G_n^1(z) + G_n^2(z) + G_n^3(z), \quad \text{for } n \ge 2,$$

where

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

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

$$G_n^2(z) = -k_nz\prod_{j=1}^{n-1} r(k_jz)(1 - r(k_nz)), \quad G_n^3(z) = -k_nzF_n(z).$$

By (1.1.7), there exists a small $\eta > 0$ such that

$$|r(z)| \le C,\ |r(z)-1| \le C|z|,\ |r(z)-1-z| \le C|z|^2, \quad \text{for } |z| \le \eta. \tag{3.3.6}$$

Combining this with (2.2.2) shows $|G_n(z)| \le C|k_nz|^2$ for $|k_nz| \le \eta$, which is (3.3.4).

It remains to consider (3.3.5). Let us first consider the integral over Γ_0^{η/k_n}. By (1.1.2) and (1.1.3), $R(z;A)$ is analytic in the domain $\{z : \delta \le |\arg z| \le \pi\}$, and hence $G_n(z)(k_nz)^{-2}R(z;A)$ is analytic in the domain bounded by $\Gamma_0^{\eta/k_n} \cup \gamma^{\eta/k_n}$ (see Lemmas 2.4 and 2.5 for the definition of the curves). We then can replace the path of integration in (3.3.5) by $\tilde{\Gamma} = \gamma^{\eta/k_n} \cup \Gamma_{\eta/k_n}$. We find, using $|G_n(z)| \le C|k_nz|^2$ for $|k_nz| \le \eta$,

$$\Big\|\int_{\gamma^{\eta/k_n}} G_n(z)(k_nz)^{-2}R(z;A)\,dz\Big\| \le \int_{\gamma^{\eta/k_n}} \frac{|dz|}{|z|} = C, \tag{3.3.7}$$

and, by the boundedness of $r(z)$ and $e^{-t_n z}$ over Γ,

$$\Big\| \int_{\Gamma_{\eta/k_n}} G_n(z)(k_n z)^{-2} R(z;A)\, dz \Big\| \le C \int_{\eta/k_n}^{\infty} (C + C(k_n\rho))(k_n\rho)^{-2} \frac{d\rho}{\rho} \le C. \tag{3.3.8}$$

Together these estimates complete the proof. □

We now turn to smoothing properties of (1.1.5). Recall from the introduction that the smoothing property (1.1.11) is not valid if $r(\infty) \neq 0$. However, if $r(\infty) = 0$, the analogue of (1.1.11) holds also for some special schemes $r(z)$ with no restriction on the time steps, see Eriksson, Johnson, and Larsson [4]. For a general scheme $r(z)$ we have the following smoothing property:

Theorem 3.2. *Assume that* (1.1.2) *and* (1.1.3) *hold, and r(z) is accurate of order* $p \ge 1$ *and* $A(\theta)$*-stable with* $\theta \in (\delta, \pi/2]$*, and that* $r(\infty) = 0$*. Let* $\{k_j\}$ *satisfy* $ck_j \le k_{j+1} \le Ck_j$*. Then there is a constant C such that*

$$\Big\| A \prod_{j=1}^{n} r(k_j A) v \Big\| \le C t_n^{-1} \|v\|, \quad \textit{for } t_n > 0. \tag{3.3.9}$$

Proof. The case $n = 1$ follows the result in the constant time step case, see Hansbo [6]. Here we consider the case when $n \ge 2$. 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 $r(\infty) = 0$, we have, see Thomée [12, Lemma 7.3],

$$|r(z)| \le \frac{1}{1 + c|z|}, \quad \text{for } |\arg z| \le \psi, \tag{3.3.10}$$

which implies that $g_n(z)$ is bounded for $|\arg z| \le \psi$ and $g_n(\infty) = 0$. Thus there exists $R > 0$ such that $g_n(z)$ is bounded for $|z| \ge R$. Lemma 2.4 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 $z \to 0$, $|\arg z| \le \psi$, we may let $R \to \infty$ and $\epsilon \to 0$, so that

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

where $\Gamma = \{z : |\arg z| = \psi\}$ for some $\psi \in (\delta, \theta)$. We split the path of integration as $\Gamma = \Gamma_0^{R/t_n} \cup \Gamma_{R/t_n}$. By (2.2.7), we have

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

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

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

so that $\sum_{l\neq j} k_l k_j \geq t_n^2/2$ and hence

$$\prod_{j=1}^{n}(1+ck_j\rho) = 1 + c\Big(\sum_{j=1}^{n} k_j\Big)\rho + c\rho^2\Big(\sum_{l\neq j} k_l k_j\Big) + \cdots \geq ct_n^2\rho^2,$$

which implies that, by (3.3.10),

$$\Big\| \int_{\Gamma_{R/t_n}} g_n(z)R(z;A)\,dz \Big\| \leq C\int_{R/t_n}^{\infty} \frac{t_n\rho}{\prod_{j=1}^{n}(1+ck_j\rho)}\,\frac{d\rho}{\rho}$$
$$\leq C\int_{R/t_n}^{\infty} \frac{t_n}{c\rho^2 t_n^2}\,d\rho \leq C.$$

If $k_{max} \geq t_n/2$, then, assuming that $k_{max} = k_m$ for some m with $1 \leq m \leq n$, and since $n \geq 2$, we have

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

Together these estimates complete the proof. □

As in Yan [13] for the constant time step case, if $|r(\infty)| < 1$, using difference quotients in time rather than the elliptic operator A in (3.3.9), we have a following smoothing property:

Theorem 3.3. *Let U^n be the solution of* (1.1.5). *Assume that* (1.1.2) *and* (1.1.3) *hold and that the discretization scheme is accurate of order $p \geq 1$, and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$. Assume that $\{\mathcal{T}\}$ is a family of increasing quasi-quasiuniform grids. Then there is a constant C such that*

$$\|\bar{\partial}U^n\| \leq Ct_n^{-1}\|v\|, \quad \textit{for } t_n > 0. \tag{3.3.11}$$

Proof. The case $n = 1$ follows from the constant time step case, see Yan [13]. We now consider the case when $n \geq 2$. We want to show that, with $\tilde{g}_n(z) = \prod_{j=1}^{n-1} r(k_j z)(r(k_n z)-1)$,

$$\|\tilde{g}_n(A)\| \leq Cn^{-1}, \quad \text{for } n \geq 2.$$

Since $t_n \leq nk$ this implies $\|\tilde{g}_n(A)\| \leq Ck_n t_n^{-1}$.

Since $|r(\infty)| < 1$ we find that $\tilde{g}_n(\infty)$ exists, which implies that there is $\tilde{R} > 0$, such that for fixed n, $\tilde{g}_n(z)$ is bounded for $|z| \geq \tilde{R}$. Further, by (1.1.6), $\tilde{g}_n(z)$ is bounded for $|z| \geq \epsilon$, $|\arg z| \leq \psi$ with $\psi \in (\delta, \theta)$. Applying Lemma 2.4, we get

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

Since the integrand is bounded for $|z| \geq \tilde{R}$, we may let $\tilde{R}$ tend to ∞. Moreover, by (3.3.6), we have $\tilde{g}_n(z) = O(z)$ as $z \to 0$, so that we may let $\epsilon \to 0$. Thus

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

where $\Gamma = \{z : |\arg z| = \psi\}$ for some $\psi \in (\delta, \theta)$.

Clearly,

$$\|\tilde{g}_n(\infty)I\| \le |r(\infty)^{n-1}(r(\infty)-1)| \le Ce^{-cn} \le Cn^{-1}.$$

Since $|r(\infty)| < 1$, there exist $R > 0$ and $c > 0$ such that

$$|r(z)| \le e^{-c}, \quad \text{for } |z| \ge R, \tag{3.3.12}$$

which shows that the integrand has no poles when $|z| \ge R/k_1,\ \delta \le |\arg z| \le \pi$. In fact, using also (3.3.3), we have

(3.3.13)

$$\|\tilde{g}_n(z)R(z;A)\| \le Ce^{-c(n-1)}(e^{-c}+1) \le Ce^{-cn}, \quad \text{for } |z| \ge R/k_1,\ \delta \le |\arg z| \le \pi.$$

Thus we can replace the path of the integration by $\tilde{\Gamma} = \Gamma_0^{R/k_n} \cup \Gamma_{R/k_n}^{R/k_1} \cup \gamma^{R/k_1}$. We have, since $|\tilde{g}_n(z)| \le Ce^{-cn}$ for $|z| \ge R/k_1$,

$$\Big\| \int_{\gamma^{R/k_1}} \tilde{g}_n(z)R(z;A)\,dz \Big\| \le C \int_{\gamma^{R/k_1}} e^{-cn} \frac{|dz|}{|z|} \le Cn^{-1}.$$

By (1.1.6) and (3.3.6), we know that, for arbitrary R,

$$|r(z)-1| \le C|z|,\ |r(z)-1-z| \le C|z|^2, \quad \text{for } |z| \le R,\ |\arg z| \le \psi. \tag{3.3.14}$$

Using this, Lemma 2.2 and $t_{n-1}/k_n = (t_{n-1}/k_{n-1})(k_{n-1}/k_n) \ge C(t_{n-1}/k_{n-1}) \ge C(n-1)$, we have

$$\Big\| \int_{\Gamma_0^{R/k_n}} \tilde{g}_n(z)R(z;A)\,dz \Big\| \le C \int_0^{R/k_n} e^{-ct_{n-1}\rho}(k_n\rho)\,\frac{d\rho}{\rho}$$
$$\le C\int_0^R e^{-c(t_{n-1}/k_n)x}\,dx \le C\int_0^R e^{-cnx}\,dx \le Cn^{-1}.$$

Finally, we write

$$\int_{\Gamma_{R/k_n}^{R/k_1}} \tilde{g}_n(z)R(z;A)\,dz = \Big(\int_{\Gamma_{R/k_n}^{R/k_{n-1}}} + \int_{\Gamma_{R/k_{n-1}}^{R/k_1}} \Big) \tilde{g}_n(z)R(z;A)\,dz = I + II.$$

If $n = 2$, we have, by Lemma 2.2 and $\ln(k_2/k_1) \le C$,

$$\Big\| \int_{\Gamma_{R/k_2}^{R/k_1}} \tilde{g}_n(z)R(z;A)\,dz \Big\| \le \int_{R/k_2}^{R/k_1} e^{-ck_1\rho}\,\frac{d\rho}{\rho} \le C \le Cn^{-1}.$$

If $n \ge 3$, using Lemma 2.2 and (1.1.6) and (2.2.9) with $m = n-1$, we obtain, for $z \in \Gamma_{R/k_{m+1}}^{R/k_m}$, $1 \le m \le n-2$,

$$|\tilde{g}_n(z)| \le C\Big|\prod_{j=1}^{n-1} r(k_j z)\Big| \le Ce^{-ct_{n-1}|z|} \le Ce^{-c_3(n-1)},$$

which implies that, since $k_{n-1} \sim k_n$,

$$\|I\| \le C\int_{R/k_n}^{R/k_{n-1}} e^{-c_3(n-1)}\,\frac{d\rho}{\rho} \le Ce^{-cn}\ln(k_n/k_{n-1}) \le Ce^{-cn}.$$

Further, by (1.1.6) and (2.2.10),

$$|\tilde{g}_n(z)| \leq \Big|\prod_{j=1}^{n-1} r(k_j z)\Big| \leq Ce^{-c_2(n-1)}e^{-c_4 m}, \quad \text{for } z \in \Gamma_{R/k_{m+1}}^{R/k_m},\ 1 \leq m \leq n-2,$$

which shows that, following the proof of (2.2.11),

$$\|II\| \leq C \sum_{m=1}^{n-2} \int_{R/k_{m+1}}^{R/k_m} e^{-c_2(n-1)}e^{-c_4 m}\,\frac{d\rho}{\rho} \leq Ce^{-cn}.$$

We therefore obtain

$$\Big\|\int_{\Gamma_{R/k_n}^{R/k_1}} \tilde{g}_n(z)R(z;A)\,dz\Big\| \leq Ce^{-cn} \leq Cn^{-1}, \quad \text{for } n \geq 3. \tag{3.3.15}$$

Together these estimates complete the proof. □

Our next result is a nonsmooth data error estimate.

Theorem 3.4. *Let U^n and $u(t_n)$be the solutions of* (1.1.5) *and* (1.1.1). *Assume that A satisfies* (1.1.2) *and* (1.1.3), *and that $r(z)$ is accurate of order $p \geq 1$ and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$ 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*

$$\|\bar{\partial}U^n - D_t u(t_n)\| \leq Ck_n t_n^{-2}\|v\|, \quad \textit{for } t_n > 0.$$

Proof. The case $n = 1$ follows from the constant time step case, see Yan [13]. Here we consider the case when $n \geq 2$.

With the notation of Theorem 3.1 and since $t_n \leq nk_n$ we need to show

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

We set, with $\kappa = r(\infty)$,

$$\tilde{G}_n(z) = G_n(z) - \kappa^{n-1}(\kappa - 1)k_n z/(1 + k_n z). \tag{3.3.16}$$

For the same reason as in the proof of Theorem 2.6, we have

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

and

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

where $\Gamma = \{z : |\arg z| = \psi\}$ for some $\psi \in (\delta, \theta)$.

We write

$$\tilde{G}_n(z) = \Big(\prod_{j=1}^{n-1} r(k_j z)(r(k_n z) - 1) - \kappa^{n-1}(\kappa - 1)\Big) + \kappa^{n-1}(\kappa - 1)/(1 + k_n z) - (-k_n z)e^{-t_n z}. \tag{3.3.17}$$

By Lemma 2.7 and $|1+k_n z| \geq |k_n z|$ for $\mathrm{Re}\, z \geq 0$, we have

$$\int_{R/k_1}^{\infty} |\tilde{G}_n(\rho e^{\pm i\psi})| \, \frac{d\rho}{\rho} \leq C \int_{R/k_1}^{\infty} \Big(e^{-cn}(k_1\rho)^{-1} + |\kappa|^n (k_n\rho)^{-1} + (k_n\rho) e^{-ct_n\rho} \Big) \, \frac{d\rho}{\rho}$$
$$\leq Cn^{-2}.$$

Using $|1/(1+k_n z)| \leq 1$ for $\mathrm{Re}\, z \geq 0$, we have, by (3.3.16), with $G_n^l(z), l = 1, 2, 3$, as in the proof of Theorem 3.1,

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

Obviously, we have, by Lemma 2.2 and (3.3.14) and $t_{n-1}/k_n \geq C(n-1)$,

$$\int_0^{R/k_n} (|G_n^1| + |G_n^2|) \, \frac{d\rho}{\rho} \leq C \int_0^{R/k_n} e^{-ct_{n-1}\rho} (k_n\rho)^2 \, \frac{d\rho}{\rho} \tag{3.3.18}$$
$$\leq \int_0^{R} e^{-c(t_{n-1}/k_n)x} x \, dx \leq \int_0^{R} e^{-c(n-1)x} x \, dx \leq Cn^{-2},$$

and, by (2.2.1) with $p = 1$ and $nk_n \sim t_n$,

$$\int_0^{R/k_n} |G_n^3| \, \frac{d\rho}{\rho} \leq C \int_0^{R/k_n} (k_n\rho)(k_n\rho)^2 e^{-ct_n\rho} n \, \frac{d\rho}{\rho} = \int_0^{R} x^2 e^{-c(t_n/k_n)x} n \, dx$$
$$\leq C \int_0^{R} x^2 e^{-cnx} n \, dx \leq Cn^{-2}.$$

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

$$\int_0^{R/k_n} |\tilde{G}_n(\rho e^{\pm i\psi})| \, \frac{d\rho}{\rho} \leq Cn^{-2}, \quad \text{for } n \geq 2.$$

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, since $t_n\rho = (t_n/k_n)k_n\rho \geq Cn$ for $\rho \in [R/k_n, R/k_1]$,

$$\int_{R/k_n}^{R/k_1} e^{-t_n\rho e^{\pm i\psi}} (k_n\rho) \, \frac{d\rho}{\rho} \leq \int_{R/k_n}^{R/k_1} e^{-ct_n\rho} k_n d\rho \leq e^{-cn} \int_{R/k_n}^{R/k_1} e^{-\frac{c}{2}t_n\rho} t_n d\rho \tag{3.3.19}$$
$$\leq e^{-cn} \int_0^{\infty} e^{-\frac{c}{2}x} \, dx \leq Ce^{-cn} \leq Cn^{-2},$$

and, since $\ln(k_n/k_1) \le Cn$,

$$\int_{R/k_n}^{R/k_1} \frac{k_n\rho}{1+k_n\rho}(\kappa^n - \kappa^{n-1})\,\frac{d\rho}{\rho} \le C\kappa^n \ln(k_n/k_1) \le Cn^{-2}. \tag{3.3.20}$$

Combining this with (3.3.15) shows

$$\int_{R/k_n}^{R/k_1} |\tilde{G}_n(\rho e^{\pm i\psi})|\,\frac{d\rho}{\rho} \le Cn^{-2}, \quad \text{for } n \ge 2.$$

The proof is complete. □

4. Approximation of time derivative — second order

In this section we shall consider the following second order approximation of $u_t(t_n)$ of the solution of (1.1.1),

$$\bar{\partial}_2 U^n = a_n\bar{\partial}U^n + b_n\bar{\partial}U^{n-1} = a_n\frac{U^n - U^{n-1}}{k_n} + b_n\frac{U^{n-1}-U^{n-2}}{k_{n-1}}, \tag{4.4.1}$$

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

where U^n is the discrete solution of (1.1.1) defined by (1.1.5). Combining (4.4.1) and Theorem 3.3, we obtain the following smoothing property of discrete scheme (1.1.5).

Theorem 4.1. *Let U^n be the solution of* (1.1.5)*. Assume that* (1.1.2) *and* (1.1.3) *hold and that the discretization scheme is accurate of order $p \ge 1$, and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$, and $|r(\infty)| < 1$. Assume that $\{\mathcal{T}\}$ is a family of increasing quasi-quasiuniform grids. Then there is a constant C such that*

$$\|\bar{\partial}_2 U^n\| \le Ct_n^{-1}\|v\|, \quad \textit{for } n \ge 2.$$

Note that (4.4.1) can also be written in the form

$$\bar{\partial}_2 U^n = \frac{1}{k_n}\Big(c_0U^n + c_1U^{n-1} + c_2U^{n-2}\Big), \quad \text{for } n \ge 2, \tag{4.4.2}$$

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 error estimates for the approximation (4.4.1). We begin with a smooth data error estimate.

Theorem 4.2. *Let U^n and $u(t_n)$be the solutions of* (1.1.5) *and* (1.1.1)*. Assume that A satisfies* (1.1.2) *and* (1.1.3)*, and that $r(z)$ is accurate of order $p \ge 2$, and $A(\theta)$-stable with $\theta \in (\delta, \pi/2]$. Let $k_j, 1 \le j \le n$, be increasing. Then we have*

$$\|\bar{\partial}_2 U^n - D_t u(t_n)\| \le Ck_n^2\|A^3 v\|, \quad \textit{for } n \ge 2. \tag{4.4.3}$$

Proof. With $P(x,y) = c_0 + c_1y^{-1} + c_2x^{-1}y^{-1}$ and

$$G_n(z) = \prod_{j=1}^{n} r(k_j z)P(r(k_{n-1}z), r(k_n z)) - (-k_n z)e^{-t_n z}, \quad \text{for } n \ge 2,$$

we want to prove

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

Let $\bar{r}(z) = \Big(\prod_{j=1}^n r(k_jz)P(r(k_{n-1}z), r(k_nz))\Big)(k_nz)^{-3}$. As in the proof of Theorem 2.1, applying Lemma 2.4 to the rational function $\bar{r}(z)$ and using also Lemma 2.5 we conclude

$$G_n(A)(k_nA)^{-3} = \frac{1}{2\pi i}\int_{\gamma_\epsilon\cup\Gamma_\epsilon} G_n(z)(k_nz)^{-3}R(z;A)\,dz.$$

We now show that

$$G_n(z) = O(z^3), \quad \text{as } z \to 0. \tag{4.4.4}$$

In fact, we write

$$G_n(z) = G_n^1(z) + G_n^2(z) + G_n^3(z), \quad \text{for } n \ge 2, \tag{4.4.5}$$

where

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

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

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

It is easy to see that there exists a small $\eta > 0$ such that

$$|r(k_jz)| \le C, \quad \text{for } 1 \le j \le n,\ |k_nz| \le \eta, \tag{4.4.6}$$

and

$$|P(e^{-k_{n-1}z}, e^{-k_nz}) - (-k_nz)| \le C|k_nz|^3, \quad \text{for } |k_nz| \le \eta, \tag{4.4.7}$$

and

$$|P(r(k_{n-1}z), r(k_nz)) - P(e^{-k_{n-1}z}, e^{-k_nz})| \le C|k_nz|^3, \quad \text{for } |k_nz| \le \eta. \tag{4.4.8}$$

Combining this with (2.2.2) shows

$$|G_n(z)| \le C|k_nz|^3, \quad \text{for } |k_nz| \le \eta, \tag{4.4.9}$$

which is (4.4.4). We remark that we can not extend (4.4.7) and (4.4.8) to $|k_nz| \le R$, $|\arg z| \le \psi$ for arbitrary R and $\psi \in (\delta, \theta)$, since $P(x,y)$ is not a polynomial for variables x, y. Combining (3.3.3) with (4.4.9) shows that the integrand is bounded on the small domain with boundary $\gamma_\epsilon \cup \Gamma_0^\epsilon$, so that we may let $\epsilon \to 0$. It follows that, with $\Gamma = \{z : |\arg z| = \psi\}$ for some $\psi \in (\delta, \theta)$,

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

The remainder of the proof is similar to the proof of Theorem 3.1. The proof is complete. □

We close this section with an error estimate in the nonsmooth data case.

Theorem 4.3. *Let U^n and $u(t_n)$be the solutions of* (1.1.5) *and* (1.1.1). *Assume that A satisfies* (1.1.2) *and* (1.1.3), *and that $r(z)$ is accurate of order $p \geq 2$ 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*

$$\|\bar{\partial}_2 U^n - D_t u(t_n)\| \leq C k_n^2 t_n^{-3} \|v\|, \quad \textit{for} \quad n \geq 2. \tag{4.4.10}$$

Proof. With the notation of Theorem 4.2 we need to show

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

Following the argument in the proof of Theorem 3.4, we set, with $\kappa = r(\infty)$,

$$\tilde{G}_n(z) = G_n(z) - \kappa^n P(\kappa, \kappa) k_n z/(1 + k_n z), \tag{4.4.11}$$

and we have

$$\|\kappa^n P(\kappa, \kappa) k_n A (I + k_n A)^{-1}\| \leq C|\kappa|^n \leq C n^{-3},$$

and

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

We write

$$\begin{aligned} \tilde{G}_n(z) = &\Big(\prod_{j=1}^n r(k_j z) P(r(k_{n-1} z), r(k_n z)) - \kappa^n P(\kappa, \kappa) \Big) \\ &+ \kappa^n P(\kappa, \kappa)/(1 + k_n z) - (-k_n z) e^{-t_n z}, \quad \text{for } n \geq 2. \end{aligned} \tag{4.4.12}$$

By Lemma 2.7 and $|1 + k_n z| \geq |k_n z|$ for $\mathrm{Re}\, z \geq 0$, we have, with η as in the proof of Theorem 4.2,

$$\begin{aligned} \int_{\eta/k_1}^\infty |\tilde{G}_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} &\leq C \int_{\eta/k_1}^\infty \Big(e^{-cn} (k_1 \rho)^{-1} + |\kappa|^n (k_n \rho)^{-1} + (k_n \rho) e^{-t_n \rho} \Big) \frac{d\rho}{\rho} \\ &\leq C n^{-3}. \end{aligned}$$

Using $|1/(1+k_n z)| \leq 1$ for $\mathrm{Re}\, z \geq 0$, we have, by (4.4.11), with $G_n^l(z), l = 1, 2, 3$, as in the proof of Theorem 4.2,

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

Obviously, using Lemma 2.2, (4.4.6), (4.4.7) and (4.4.8), we have

$$\int_0^{\eta/k_n} (|G_n^1| + |G_n^2|) \frac{d\rho}{\rho} \leq C n^{-3},$$

and, by (2.2.1) with $p = 2$ and $n k_n \sim t_n$,

$$\int_0^{\eta/k_n} |G_n^3| \frac{d\rho}{\rho} \leq C \int_0^{\eta/k_n} (k_n \rho)(k_n \rho)^3 e^{-c t_n \rho} n \frac{d\rho}{\rho} \leq C n^{-3}.$$

Thus, combining this with $|\kappa|^n \le Cn^{-3}$, we get

$$\int_0^{\eta/k_n} |\tilde G_n(\rho e^{\pm i\psi})| \frac{d\rho}{\rho} \le Cn^{-3}, \quad \text{for } n \ge 2.$$

It remains to consider the integral on the interval $[\eta/k_n, \eta/k_1]$ for $n \ge 2$. If $n = 2$, we write, by (4.4.2),

$$\begin{aligned}\tilde G_2(z) = &\Big(c_0 r(k_1 z) r(k_2 z) + c_1 r(k_1 z) + c_2\Big) - (-k_2 z) e^{-t_2 z}\\ &- \frac{k_2 z}{1 + k_2 z}(c_0 \kappa^2 + c_1 \kappa + c_2) = I + II + III,\end{aligned}$$

where the integrals related to II and III can be bounded by (3.3.19) and (3.3.20), respectively. For I, we have

$$\begin{aligned}&\Big\| \int_{\Gamma_{\eta/k_2}^{\eta/k_1}} \Big(c_0 r(k_1 z) r(k_2 z) + c_1 r(k_1 z) + c_2\Big) R(z; A)\, dz \Big\|\\ &\qquad \le C \int_{\eta/k_2}^{\eta/k_1} \frac{d\rho}{\rho} \le C \ln(k_2/k_1) \le C \le Cn^{-3}.\end{aligned}$$

If $n \ge 3$, we write, by (4.4.2),

$$\begin{aligned}\tilde G_n(z) = &\Big(c_0 \prod_{j=1}^{n} r(k_j z) + c_1 \prod_{j=1}^{n-1} r(k_j z) + c_2 \prod_{j=1}^{n-2} r(k_j z)\Big) - (-k_n z) e^{-t_n z}\\ &- \frac{k_n z}{1 + k_n z}(c_0 \kappa^n + c_1 \kappa^{n-1} + c_2 \kappa^{n-2}) = I + II + III.\end{aligned}$$

We can consider the case for $n = 3$ as for $n = 2$. If $n \ge 4$, the integrals related to II and III can be bounded by (3.3.19) and (3.3.20), respectively. Following the argument in the proof of (3.3.15), we have

$$\int_{\eta/k_n}^{\eta/k_1} \Big| \prod_{j=1}^{n-2} r(k_j \rho e^{\pm i\psi}) \Big| \frac{d\rho}{\rho} \le Ce^{-cn} \le Cn^{-3}.$$

Using this and the boundedness of $r(k_j z)$ on Γ we obtain the desired bound for the integral related to I.

Together these estimates complete the proof. □

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