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by

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Abstract

An error analysis is given for convolution quadratures based on strongly A-stable Runge-Kutta methods, for the non-sectorial case of a convolution kernel with a Laplace transform that is polynomially bounded in a half-plane. The order of approximation depends on the classical order and stage order of the Runge-Kutta method and on the growth exponent of the Laplace transform. Numerical experiments with convolution quadratures based on the Radau IIA methods are given on an example of a time-domain boundary integral operator.

1 Introduction

The numerical approximation of convolutions

$$\int_0^t k(t-\tau)\, g(\tau)\, d\tau, \qquad t>0, \tag{1}$$

and of integral equations containing convolutions of this type is of interest in a variety of application areas, and in particular in boundary integral equations of time-domain wave scattering problems. Convolution quadrature methods based on numerical methods for ordinary differential equations, such as multistep or Runge-Kutta methods, have proved very effective: they offer built-in stability, they require only knowledge of the Laplace transform $K(s)$ of the convolution kernel $k(t)$ rather than the kernel itself, and they yield accurate approximations also for singular or non-smooth kernels; see the review [15], numerous references therein, and, e.g., the recent papers [2, 3, 8, 11, 18].

Numerical experiments show that Runge-Kutta based convolution quadrature methods often outperform those based on multistep methods; see [2, 17], where numerical comparisons of convolution quadratures based on Radau IIA Runge-Kutta methods and on BDF multistep methods are presented. In particular, when the Laplace transform is analytic and polynomially bounded only in a half-space $\operatorname{Re} s \geq \sigma$, then one must resort to A-stable methods, which can have arbitrary order in the case of Runge-Kutta methods, but which have at most order 2 in the case of multistep methods by Dahlquist's order barrier [6].

Most of the existing error analysis for convolution quadratures refers to methods based on multistep methods [7, 12, 13, 14, 15]. For Runge-Kutta based convolution quadrature methods, there is an error bound in [16] for the case of Laplace transforms that are analytic and bounded by a negative power of $|s|$ in a sector $|\arg s| \leq \pi-\varphi$ with $\varphi<\pi/2$. No such sectorial assumption is made in [5], where error bounds for the application of Runge-Kutta convolution quadrature methods for Volterra convolution equations $u(t)=u_0+\int_0^t a(t-\tau)\, u(\tau)\, d\tau$ with a constant u_0 are obtained. This corresponds to a convolution (1) with a kernel whose Laplace transform is $K(s)=(I-A(s))^{-1}$ and with the particular case $g(\tau)\equiv u_0$.

In this paper we give an error analysis of Runge-Kutta based convolution quadrature in the general, non-sectorial case when the Laplace transform is analytic and polynomially bounded only in a half-space $\operatorname{Re} s \geq \sigma$. This is the situation encountered in boundary integral equations for acoustic, elastic or electro-magnetic wave problems.

In Section 2 we recall some properties of Runge-Kutta methods and turn to Runge-Kutta based convolution quadrature in Section 3. The following Sections 4 and 5 develop the error analysis, first for decaying Laplace transforms, then for polynomially bounded Laplace transforms. The order of approximation depends on the classical order p of the Runge-Kutta method, on the stage order q, and on the growth exponent μ of the Laplace transform $K(s)$. The paper concludes with numerical experiments.

2 Runge-Kutta methods

An m-stage Runge-Kutta discretization of $y' = f(t, y)$, $y(0) = y_0$, is given by

$$\begin{aligned} Y_{ni} &= y_n + h \sum_{j=1}^{m} a_{ij} f(t_n + c_j h, Y_{nj}), \qquad i = 1, \dots, m, \\ y_{n+1} &= y_n + h \sum_{j=1}^{m} b_j f(t_n + c_j h, Y_{nj}), \end{aligned}$$

where h is the time-step, $t_n = nh$, and the internal stages Y_{ni} and grid values y_n are approximations to $y(t_n + c_i h)$ and $y(t_n)$, respectively. In the following we will use the notation

$$A = (a_{ij})_{i,j=1}^{m}, \quad b = (b_1, b_2, \dots, b_m)^T, \quad \mathbb{1} = (1, 1, \dots, 1)^T.$$

The Runge-Kutta method is said to be of (classical) order p and stage order $q+1$ if for sufficiently smooth right-hand sides f

$$Y_{0i} - y(c_i h) = \mathrm{O}(h^{q+1}), \text{ for } i = 1, \dots, m, \quad \text{and} \quad y_1 - y(t_1) = \mathrm{O}(h^{p+1}),$$

as $h \to 0$. The order and stage order are characterized in terms of the Runge-Kutta coefficients by well-known order conditions (see [4, 9]), which in particular imply the following relation that will be used later: for $k = 1, \dots, p$,

$$b^T (I - zA)^{-1} (kAc^{k-1} - c^k) = \mathrm{O}(z^{p-k}) \quad \text{as } z \to 0, \tag{2}$$

where $c^k = (c_1^k, \dots, c_m^k)^T$. When the Runge-Kutta method is applied to $y' = \lambda y$, the numerical solution is $y_n = R(h\lambda)^n y_0$ with the stability function

$$R(z) = 1 + z b^T (I - zA)^{-1} \mathbb{1},$$

which satisfies, for $z \to 0$,

$$R(z) - e^z = \mathrm{O}(z^{p+1}). \tag{3}$$

We consider Runge-Kutta methods that are A-stable, that is, the stability function is bounded as

$$|R(z)| \le 1 \quad \text{for } \operatorname{Re} z \le 0, \text{ and } I - zA \text{ is non-singular for } \operatorname{Re} z \le 0. \tag{4}$$

We further require that the matrix A is non-singular and

$$|R(\mathrm{i}\omega)| < 1 \quad \text{for all real } \omega \ne 0 \quad \text{and} \quad R(\infty) = 0. \tag{5}$$

All the above conditions are satisfied by Radau IIA methods (with order $p = 2m-1$ and stage order $q = m$) and Lobatto IIIC methods (with $p = 2m-2$ and $q = m-1$). For these methods we have in addition that $(b_1, \dots, b_m)$ equals the last row of A, so that $y_{n+1} = Y_{nm}$ and $b^T A^{-1} = (0, \dots, 0, 1)$.

We end this preparatory section with recalling an explicit formula of the error of the Runge-Kutta method when applied to $y' = \lambda y + g$ with a polynomial function g.

Lemma 2.1. *[16] The error at time t_n of the Runge-Kutta method applied to $y' = \lambda y + t^l/l!$, $y(0) = 0$ is given by*

$$e_n = \lambda^{-l-1}(R(h\lambda)^n - e^{nh\lambda}) - \sum_{k=q+1}^{p} h^k \sum_{\nu=1}^{n-1} r_{n-1-\nu}^{(k)}(h\lambda) \lambda^{k-l-1} \sum_{\kappa=0}^{l-k} \frac{(\lambda t_\nu)^\kappa}{\kappa!}, \tag{6}$$

with

$$r_n^{(k)}(z) := R(z)^n z b^T (I - zA)^{-1} \delta^{(k)} \quad \text{and} \quad \delta^{(k)} = Ac^{k-1} - c^k/k.$$

3 Runge-Kutta based convolution quadrature

Let $K(s)$ be analytic in the half-plane $\mathrm{Re}\, s \geq \sigma$ and for some real exponent μ and constant M be bounded by

$$|K(s)| \leq M\,|s|^{-\mu} \qquad \text{for } \; \mathrm{Re}\, s \geq \sigma. \tag{7}$$

Let us for the moment assume that $\mu > 1$. Then, the inverse Laplace transform

$$k(t) = \frac{1}{2\pi \mathrm{i}} \int_{\sigma + \mathrm{i}\mathbb{R}} e^{\lambda t} K(\lambda)\, d\lambda, \qquad t \geq 0, \tag{8}$$

defines a continuous, exponentially bounded function. We are interested in computing the convolution of the kernel k with a continuous function g,

$$u(t) = \big(K(\partial_t) g\big)(t) := \int_0^t k(t-\tau)\, g(\tau)\, d\tau, \qquad t \geq 0. \tag{9}$$

The motivation for the notation $K(\partial_t)g$ comes from identities of the type $(\partial_t^{-1} g)(t) = \int_0^t g(\tau) d\tau$ and $K_2(\partial_t)K_1(\partial_t)g = (K_2K_1)(\partial_t)g$. Substituting (8) into the convolution (9) and interchanging integrals we obtain

$$u(t) = \frac{1}{2\pi \mathrm{i}} \int_{\sigma + \mathrm{i}\mathbb{R}} K(\lambda)\, y_\lambda(t)\, d\lambda, \tag{10}$$

where $y_\lambda(t) = \int_0^t e^{\lambda(t-\tau)} g(\tau) d\tau$ is the solution of the initial value problem

$$y' = \lambda y + g, \qquad y(0) = 0. \tag{11}$$

For $\mu \leq 1$, we instead consider $K_r(s) := K(s)/s^r$ with $r + \mu > 1$ and define, for sufficiently differentiable functions g,

$$u(t) = \big(K(\partial_t) g\big)(t) := \left(\frac{d}{dt}\right)^r \big(K_r(\partial_t) g\big)(t) = \left(\frac{d}{dt}\right)^r \int_0^t k_r(\tau)\, g(t-\tau)\, d\tau, \qquad t > 0,$$

with $k_r(t) = \frac{1}{2\pi \mathrm{i}} \int_{\sigma+\mathrm{i}\mathbb{R}} e^{\lambda t} K_r(\lambda)\, d\lambda$. An easy calculation using partial integration shows that for $\mu \in (0, 1]$ formula (10) still remains valid.

Discretizing (11) with the Runge-Kutta method and substituting the result into (10), we obtain the Runge-Kutta based convolution quadrature approximation of (9), as introduced in [16]. There it is shown that for a Runge-Kutta method with $R(\infty) = 0$, the approximation at time $t = (n+1)h$ obtained in this way is given by

$$u_{n+1} = b^T A^{-1} h \sum_{\nu=0}^{n} W_{n-\nu}(K) G_\nu, \tag{12}$$

where $G_n = (g(t_n + c_i h))_{i=1}^m$ and the $m \times m$ matrix $W_n(K)$ is given as the nth coefficient of the generating function

$$h \sum_{n=0}^{\infty} W_n(K) \zeta^n = K\left(\frac{\Delta(\zeta)}{h}\right), \tag{13}$$

with

$$\Delta(\zeta) = \left(A + \frac{\zeta}{1-\zeta} \mathbb{1} b^T\right)^{-1}.$$

The stage approximation $U_{ni} \approx u(t_n + c_i h)$ is given by the vector $U_n = (U_{ni})_{i=1}^m$ via

$$U_n = \big(K(\underline{\partial_t}^h) g\big)_n := h \sum_{\nu=0}^{n} W_{n-\nu}(K) G_\nu. \tag{14}$$

Note that the composition rule $(K_2K_1)(\partial_t)g = K_2(\partial_t)K_1(\partial_t)g$ still holds for the stage approximation:

$$(K_2K_1)(\underline{\partial_t}^h)g = K_2(\underline{\partial_t}^h)K_1(\underline{\partial_t}^h)g.$$

With this notation, (12) simplifies to

$$u_{n+1} = b^T A^{-1}\big(K(\underline{\partial_t}^h)g\big)_n.$$

We have derived the above discrete convolutions via formula (10) which does not hold for $\mu \le 0$ even if we assume that higher-order derivatives of g are zero at $t = 0$. Nevertheless, the discrete convolutions (12) and (14) still make sense for $\mu \le 0$ and we will prove that they give a convergent approximation to the continuous convolution. We first derive uniform error estimates for the case $\mu > 0$ and afterwards give ℓ^2 estimates of the error that hold for the whole range $\mu \in \mathbb{R}$.

4 ℓ^∞ error bound for $\mu > 0$

In [16] an error bound of Runge-Kutta based convolution quadrature methods was given for the case of *sectorial* Laplace transforms, for which a bound (7) holds not only in a half-plane, but in a larger sector $|\arg s| \le \pi - \varphi$ with $\varphi < \pi/2$. The following result extends the error bound to the *non-sectorial* case (7). Surprisingly, there is no order reduction compared to the sectorial case: the order is $\min(p, q + 1 + \mu)$ when the convolution quadrature is applied to smooth functions g that have sufficiently many vanishing derivatives at 0.

Theorem 4.1. *Let $K(s)$ be analytic for $\mathrm{Re}\, s \ge \sigma$ and bounded as in (7), with $\mu > 0$. Let $g \in C^p[0, T]$. Consider a Runge-Kutta method of order p and stage order q that is A-stable and satisfies the additional condition (5). Then, there exist $h_0 > 0$ such that, for $0 < h \le h_0$ and $nh \le T$, the error of the convolution quadrature (12) is bounded as*

$$|u_n - u(t_n)| \le C \sum_{l=0}^{q} h^{\min(p,l+\mu)} |g^{(l)}(0)| + C h^{\min(p,q+1+\mu)} \left(\sum_{l=q+1}^{p-1} |g^{(l)}(0)| + \max_{0\le\tau\le t_n} |g^{(p)}(\tau)| \right).$$

The constants C and h_0 depend only on the Runge-Kutta method, on the constants M and σ in (7), and on T. In case that $p = l + \mu$ for some $l = 0, \ldots, q+1$, then the corresponding factor $h^{\min(p,l+\mu)}$ must be replaced by $h^p |\log h|$. An analogous error bound holds for the internal stages with p replaced by $\min(q + 1, p)$.

Proof. As in [16] we first prove the result for the case $g(t)$ is a polynomial of degree at most $p-1$; cf. [16, Lemma 5.1]. The general case then follows by applying this result to the Peano kernel representation of the remainder in the Taylor expansion of g at 0; for details of this step in the proof see [16, Lemma 5.2].

The convolution quadrature error is

$$u_n - u(t_n) = \int_{\sigma + i\mathbb{R}} K(\lambda)\, e_n(h, \lambda)\, d\lambda$$

where $e_n(h, \lambda)$ is the error at time t_n of the Runge-Kutta method when applied to $y' = \lambda y + g(t)$, $y(0) = 0$. For $g(t) = t^l/l!$, this error is given explicitly by Lemma 2.1. We investigate the two terms in this error separately.

Let us write $\lambda = \sigma + i\omega$ with fixed $\sigma > 0$ and note that $|e^{nh\lambda}| = e^{\sigma nh}$, and under our assumptions on the stability function, $|R(h\lambda)^n| \le e^{c\sigma nh}$ for an arbitrary constant $c > 1$, provided that h is sufficiently small. For the remainder of the proof C will denote a generic constant that is allowed to depend on T via a factor $e^{c\sigma T}$ or a power of T.

(a) We show that

$$\left| \int_{\sigma+\mathrm{i}\mathbb{R}} K(\lambda)\lambda^{-l-1}(R(h\lambda)^n - e^{nh\lambda})\, d\lambda \right| = \begin{cases} \mathrm{O}(h^p), & l+\mu > p \\ \mathrm{O}(h^p|\log h|), & l+\mu = p \\ \mathrm{O}(h^{l+\mu}), & l+\mu < p. \end{cases} \tag{15}$$

(i) $|\lambda h| \le 1$: From the approximation property (3) we have that for $nh \le T$,

$$|R(h\lambda)^n - e^{nh\lambda}| \le C(\lambda h)^p$$

and hence

$$\left| \int_{\sigma+\mathrm{i}[-1/h,1/h]} K(\lambda)\lambda^{-l-1}(R(h\lambda)^n - e^{nh\lambda}) d\lambda \right| \le Ch^p \int_{\sigma+\mathrm{i}[-1/h,1/h]} |\lambda|^{p-\mu-l-1}|d\lambda|,$$

which is bounded by the right-hand side of (15).

(ii) $|\lambda h| \ge 1$: We now use the uniform boundedness of $|R(h\lambda)^n|$ and $|e^{nh\lambda}|$ for $nh \le T$ on the integration contour to show that

$$\left| \int_{\sigma+\mathrm{i}\mathbb{R}\setminus[-1/h,1/h]} K(\lambda)\lambda^{-l-1}(R(h\lambda)^n - e^{nh\lambda}) d\lambda \right| \le C \int_{\sigma+\mathrm{i}\mathbb{R}\setminus[-1/h,1/h]} |\lambda|^{-\mu-l-1}|d\lambda| \le Ch^{\mu+l}.$$

(b) Next, we prove

$$\left| \sum_{k=q+1}^{p} h^k \int_{\mathrm{Re}\,\lambda=\sigma} K(\lambda) \sum_{\nu=0}^{n-1} r_{n-1-\nu}^{(k)}(h\lambda)\lambda^{k-l-1} \sum_{\kappa=0}^{l-k} \frac{(\lambda t_\nu)^\kappa}{\kappa!} d\lambda \right| = \begin{cases} \mathrm{O}(h^p), & q+1+\mu > p \\ \mathrm{O}(h^p|\log h|), & q+1+\mu = p \\ \mathrm{O}(h^{q+1+\mu}), & q+1+\mu < p. \end{cases} \tag{16}$$

(i) We first consider the part of the integral with $|\lambda h| \le 1$. We write again $z = h\lambda$. Below we will repeatedly require the following consequence of (3) and (5):

$$\frac{|z|}{|1-R(z)|} \le Const., \quad \text{for } |z| \le 1,\ \mathrm{Re}\, z = h\sigma. \tag{17}$$

We define

$$f_n^{(k)}(z) := \sum_{\nu=0}^{n} R(z)^{-\nu}\nu^k$$

and prove that

$$|zR(z)^n f_n^{(k)}(z)| \le C_k\,(n + |z|^{-1})^k\, e^{ch\sigma n} \qquad \text{for } |z| \le 1,\ \mathrm{Re}\, z = h\sigma. \tag{18}$$

First, notice that

$$\frac{df_n^{(k)}}{dz}(z) = -R'(z) \sum_{\nu=0}^{n} R(z)^{-\nu-1}\nu^{k+1} = -\frac{R'(z)}{R(z)} f_n^{(k+1)}(z),$$

therefore

$$f_n^{(k+1)}(z) = -\frac{R(z)}{R'(z)} \frac{df_n^{(k)}}{dz}(z).$$

Next, note that

$$f_n^{(0)}(z) = \frac{1-R(z)^{-n-1}}{1-R(z)^{-1}} = \frac{R(z)-R(z)^{-n}}{R(z)-1}$$

and hence

$$|zR(z)^n f_n^{(0)}(z)| \le |R(z)^{n+1} - 1| \frac{|z|}{|1-R(z)|} \le C_0\, e^{ch\sigma n}.$$

Hence the bound (18) holds for $f_n^{(0)}$. Next,

$$f_n^{(1)}(z) = -\frac{R(z)}{R'(z)}\frac{df_n^{(0)}}{dz}(z) = -\frac{R(z)+nR(z)^{-n}}{R(z)-1} + \frac{R(z)^2 - R(z)^{-n+1}}{(R(z)-1)^2}.$$

Hence,

$$|zR(z)^n f_n^{(1)}(z)| \le C_1\,(n+|z|^{-1})e^{ch\sigma n},$$

where in the last step we have again used (17). Continuing, it is seen that $|zR(z)^{n-1} f_n^{(1)}(z)|$ is bounded by a sum of terms of the form $n^i|z|^{-j}$ with $i+j=k$, from which the required result follows.

With the above notation, the second expression in the error formula (6) can be rewritten, with $z = h\lambda$,

$$\widetilde{e}_n = h^{l+1}\sum_{k=q+1}^{p} b^T(I-zA)^{-1}\delta^{(k)}z^{k-l-1}\sum_{\kappa=0}^{l-k}\frac{z^\kappa}{\kappa!}\cdot zR(z)^{n-1}f_{n-1}^{(\kappa)}(z).$$

With the bounds (2) and (18) we thus obtain, for $l \ge q+1$ and $|z| \le 1$ with $\operatorname{Re} z = h\sigma$ and $nh \le T$,

$$\begin{aligned}|\widetilde{e}_n| &\le C\,h^{l+1}\sum_{k=q+1}^{p}|z|^{p-k}|z|^{k-l-1}\sum_{\kappa=0}^{l-k}|z|^\kappa(n+|z|^{-1})^\kappa \\ &\le C\,h^p|\lambda|^{p-l-1}\,(1+nh|\lambda|)^{l-q-1} \le C\,h^p|\lambda^{p-q-2}|.\end{aligned}$$

With this estimate, it follows that the integral of $\widetilde{e}_n(h,\lambda)$ over the segment $\operatorname{Re}\lambda = \sigma$, $|\operatorname{Im}\lambda| \le 1/h$ is bounded by

$$Ch^p\int_{\operatorname{Re}\lambda=\sigma,|\lambda|\le 1/h}|\lambda|^{-\mu}\cdot|\lambda|^{p-q-2}\,|d\lambda| = \begin{cases}\mathrm{O}(h^p), & q+1+\mu > p\\ \mathrm{O}(h^p|\log h|), & q+1+\mu = p\\ \mathrm{O}(h^{q+1+\mu}), & q+1+\mu < p.\end{cases}$$

(ii) For the part of the integral with $|h\lambda| = |z| \ge 1$, we use $|R(z)| \le \rho < 1$ to estimate

$$|R(z)^n f_n^{(k)}(z)| \le C_k\,n^k \qquad \text{for } |z|\ge 1,\ \operatorname{Re} z = h\sigma. \tag{19}$$

We then obtain the bound, for $nh \le T$,

$$|\widetilde{e}_n| \le Ch^{l+1}\sum_{k=q+1}^{p}|z|^{k-l-1}\sum_{\kappa=0}^{l-1}|z|^\kappa\,n^\kappa \le Ch^{q+1}|\lambda|^{-1}.$$

The corresponding part of the integral is thus bounded by

$$Ch^{q+1}\int_{\operatorname{Re}\lambda=\sigma,|\lambda|\ge 1/h}|\lambda|^{-\mu}\cdot|\lambda|^{-1}\,|d\lambda| = \mathrm{O}(h^{q+1+\mu}).$$

This completes the proof of (16) and thus of the desired bound of $|u_n - u(t_n)|$ for $g(t) = t^l/l!$. As mentioned in the beginning of the proof, the error bound for general smooth functions g then follows with the Peano kernel argument of [16]. We omit the proof of the error bound for the internal stages, which is similar. □

5 ℓ^2 error bound for $\mu \le 0$

To obtain ℓ^2 error bounds, we will need to bound

$$K\left(\frac{\Delta(\zeta)}{h}\right) = \frac{1}{2\pi\mathrm{i}}\oint_\Gamma K(z/h)\,(zI-\Delta(\zeta))^{-1}\,dz \qquad \text{for } |\zeta| \le e^{-h\widetilde{\sigma}},$$

where the contour Γ encloses the eigenvalues of $\Delta(\zeta)$. This task is facilitated by the following result proved in [16].

Lemma 5.1. *We have*

$$(zI - \Delta(\zeta))^{-1} = A(zA - I)^{-1} - \frac{\zeta}{1 - R(z)\zeta}(I - zA)^{-1}\mathbb{1}b^T(I - zA)^{-1}.$$

Lemma 5.2. *Assuming (7) with $\mu \le 0$ and under the assumptions of Theorem 4.1 on the Runge-Kutta method, we have that for every $\widetilde{\sigma} > \sigma$, there exists $h_0 > 0$ such that for $0 < h \le h_0$, the eigenvalues of $\Delta(\zeta)$ lie in the half-plane $\mathrm{Re}\, z \ge h\sigma$ for $|\zeta| \le e^{-h\widetilde{\sigma}}$ and*

$$\sup_{|\zeta| \le e^{-h\widetilde{\sigma}}} \left\| K\left(\frac{\Delta(\zeta)}{h}\right)\right\| \le CM\, h^{\mu}.$$

The constant C depends only on the Runge-Kutta method.

Proof. We fix ζ with $|\zeta| \le e^{-h\widetilde{\sigma}}$. Using the Cauchy representation formula and Lemma 5.1, we have that

$$\begin{aligned} K\left(\frac{\Delta(\zeta)}{h}\right) &= \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma} K(z/h) A(zA - I)^{-1} dz \\ &\quad - \frac{1}{2\pi\mathrm{i}} \oint_{\Gamma} K(z/h) \frac{\zeta}{1 - R(z)\zeta}(I - zA)^{-1}\mathbb{1}b^T(I - zA)^{-1} dz. \end{aligned} \tag{20}$$

The contour Γ is chosen to enclose all the singularities of both integrands. We will see in a moment that the singularities all have real part greater than $h\sigma$, so that $K(z/h)$ is defined on the contour and satisfies the bound (7). For the first integral we can deform the contour to a contour Γ_1 that encloses the eigenvalues of A^{-1}, all of which have positive real part by the assumption (4) of A-stability. We then bound, using (7),

$$\left|\frac{1}{2\pi\mathrm{i}} \oint_{\Gamma_1} K(z/h) A(zA - I)^{-1} dz\right| \le \frac{1}{2\pi} \oint_{\Gamma_1} M|z/h|^{-\mu}\, \|(zI - A^{-1})^{-1}\|\, |dz| \le CM\, h^{\mu}.$$

The second integrand in (20) has singularities at the eigenvalues of A^{-1} and in addition at points where $R(z) = \zeta^{-1}$. We consider a contour $\Gamma(r)$ that is composed of a circular arc $|z| = r$, $\mathrm{Re}\, z \ge h\sigma$ and a vertical line segment $\mathrm{Re}\, z = h\sigma$, $|z| \le r$. We arbitrarily fix small $\rho > 0$ and $\delta > 0$ and note that by condition (5), there exists $r > 0$ such that $\Gamma(r)$ encloses all points z with $|1 - R(z)\zeta| \le \delta$ for $|\zeta - 1| > \rho$. For such ζ, we can estimate the second contour integral in (20) over $\Gamma(r)$ as before to obtain that it is bounded by CMh^{μ}.

It remains to consider ζ near 1. Since $R(0) = 1$ and $R'(0) = 1$, the implicit function theorem yields that for ζ near 1, there is a unique solution $w(\zeta)$ to

$$R(w(\zeta)) = \zeta^{-1}, \quad w(1) = 0.$$

We also note $w'(1) = -1$, so that for sufficiently small h we have $\mathrm{Re}\, w(\zeta) \ge h\sigma$ if $|\zeta| \le e^{-h\widetilde{\sigma}}$ and $|\zeta - 1| \le \rho$. We can then split the second integral in (20) into the contribution from the pole at $w(\zeta)$ and the remaining integral over the contour Γ_1 in the right half-plane that encloses the eigenvalues of A^{-1} and is bounded away from the origin. The latter integral is bounded by CMh^{μ} by the same argument as before. The contribution from the pole at $w(\zeta)$ is

$$-\frac{1}{R'(z)} K(z/h)(I - zA)^{-1}\mathbb{1}b^T(I - zA)^{-1}\Big|_{z = w(\zeta)},$$

which is again bounded by CMh^{μ}. □

We now give estimates for the ℓ^2 error that are valid for $\mu \le 0$.

Theorem 5.3. *Assume (7), with $\mu \le 0$, and let $g(0) = g'(0) = \cdots = g^{(r)}(0) = 0$ for r such that $r + \mu > 0$. Then, under the conditions of Theorem 4.1 on the Runge-Kutta method and assuming $p \ge q+1$, there exists $h_0 > 0$ such that for all $0 < h < h_0$ and $Nh \le T$,*

$$\left(h \sum_{n=0}^{N} |u_n - u(t_n)|^2 \right)^{1/2} \le C \sum_{l=0}^{q} h^{\min(q+1+\mu, l+r+\mu)} |g^{(l+r)}(0)| + Ch^{q+1+\mu} \max_{0 \le \tau \le T} |g^{(q+1+r)}(\tau)|.$$

The constants C and h_0 depend only on the Runge-Kutta method, on the constants M and σ in (7), and on T.

Proof. We first write the error e as a sum of two terms each of which we will estimate separately:

$$e := K(\partial_t)g - b^T A^{-1} K(\underline{\partial_t}^h)g = e_1 + e_2$$

with

$$e_1 := K_r(\partial_t)g^{(r)} - b^T A^{-1} K_r(\underline{\partial_t}^h)g^{(r)}, \qquad e_2 := b^T A^{-1} K_r(\underline{\partial_t}^h)g^{(r)} - b^T A^{-1} K(\underline{\partial_t}^h)g,$$

where again $K_r(s) = K(s)/s^r$.

Theorem 4.1 can be applied to bound the error e_1 since $|K_r(s)| \le C|s|^{-\mu-r}$ and r was chosen such that $r + \mu > 0$.

To estimate e_2 we will first need to rewrite $K_r(\underline{\partial_t}^h)g^{(r)}$. By the composition rule,

$$K_r(\underline{\partial_t}^h)g^{(r)} = K(\underline{\partial_t}^h)(\underline{\partial_t}^h)^{-r} g^{(r)}.$$

Therefore

$$e_2(t_{n+1}) = b^T A^{-1} h \sum_{\nu=0}^{n} W_{n-\nu}(K) \left(h \sum_{l=0}^{\nu} W_{\nu-l}(s^{-r}) G_l^{(r)} - G_\nu \right).$$

The term in brackets is just the stage error of the Runge-Kutta method applied to the rth-order differential equation $y^{(r)} = g^{(r)}$ with zero initial values. It is bounded by

$$E_\nu = \sum_{l=0}^{\nu} W_{\nu-l}(s^{-r}) G_l^{(r)} - G_\nu = \mathrm{O}(h^{q+1}).$$

Using Parseval's formula recalling (13) and applying the estimate of Lemma 5.2, we obtain

$$\left(h \sum_{n=0}^{N} |e_2(t_{n+1})|^2 \right)^{1/2} \le e^{\widetilde{\sigma} T} \sup_{|\zeta| \le e^{-h\widetilde{\sigma}}} \left\| K\left(\frac{\Delta(\zeta)}{h} \right) \right\| \left(h \sum_{n=0}^{N} |E_n|^2 \right)^{1/2} = \mathrm{O}(h^{q+1+\mu})$$

and the proof is complete. □

6 Numerical examples

6.1 A scalar example

Let us consider the case

$$K_\mu(s) = \frac{s^{-\mu}}{1 - e^{-s}}.$$

Clearly, $K(s)$ is analytic in the right half-plane and bounded as $|K(s)| \le C|s|^{-\mu}$ for $\operatorname{Re} s \ge \sigma > 0$. The exact solution is

$$K_\mu(\partial_t)g = \sum_{j=0}^{\infty} (\partial_t^{-\mu} g)(t - j),$$

where $(\partial_t^{-\mu} g)(t) = \int_0^t (t-\tau)^{\mu-1}/\Gamma(\mu)\, g(\tau)\, d\tau$ for $\mu > 0$, and $\partial_t^{-\mu} g = \partial_t^r (\partial_t^{-\mu-r} g)$ with $r + \mu > 0$ for $\mu \le 0$.

We approximate this convolution by the convolution quadrature based on the 3-stage Radau IIA method (stage order $q = 3$) with

$$g(t) = e^{-0.4t} \sin^6 t, \qquad t \ge 0.$$

In the following table we show the relative ℓ^2 error up to $T = 2$ divided by $h^{4+\mu}$. Since for fractional μ we cannot easily obtain the analytical solution, instead of the exact solution we have used the numerical solution with $N = 2^{10}$.

N	$\mu = 1$	$\mu = 1/2$	$\mu = -1/2$	$\mu = -1$
2	0.00	0.02	0.27	0.76
4	0.04	0.04	0.18	0.68
8	0.05	0.06	0.15	0.75
16	0.05	0.04	0.19	0.80
32	0.04	0.03	0.20	0.81
64	0.04	0.02	0.20	0.81
128	0.04	0.03	0.20	0.81

These results confirm that the convergence rates we have proved are also optimal.

6.2 An operator example

Let Ω be a bounded subdomain of $\mathbb{R}^3$ with boundary Γ. The single layer boundary integral potential for the equation $-\Delta \widehat{u} + s^2 \widehat{u} = 0$ is given by

$$S(s)\varphi(x) := \int_\Gamma \frac{e^{-s|x-y|}}{4\pi|x-y|} \varphi(y) d\Gamma_y, \quad x \in \Omega.$$

Its restriction to the boundary we denote by

$$V(s)\varphi(x) := \int_\Gamma \frac{e^{-s|x-y|}}{4\pi|x-y|} \varphi(y) d\Gamma_y, \quad x \in \Gamma.$$

In [1] it is shown that the operator $V(s)$ is invertible for $\operatorname{Re} s > 0$ and that its inverse is bounded as

$$\|V^{-1}(s)\|_{H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)}\, C(\sigma) \frac{|s|^2}{\operatorname{Re} s} \qquad \text{for } \operatorname{Re} s \ge \sigma > 0. \tag{21}$$

Given $g(\cdot, t) \in H^{1/2}(\Gamma)$, let

$$\psi = V^{-1}(\partial_t) g. \tag{22}$$

Then $u = S(\partial_t)\psi$ satisfies the wave equation

$$\begin{aligned} \partial_t^2 u(x,t) &= \Delta u(x,t), && (x,t) \in \Omega^\pm \times [0,T], \\ u(x,0) &= \partial_t u(x,0) = 0, && x \in \Omega^\pm, \\ u(x,t) &= g(x,t), && (x,t) \in \Gamma \times [0,T] \end{aligned}$$

both in the interior $\Omega^- = \Omega$ and the exterior $\Omega^+ = \mathbb{R}^3 \setminus \overline{\Omega}$ domain.

For the special case $g(x,t) = g(t)$ and $\Gamma = \mathbb{S}^2$ the unit sphere, it turns out that $\psi = K(\partial_t) g$ with $K(s) = 2s/(1 - e^{-2s})$, and hence a convergence rate $\mathrm{O}(h^q)$ of a Runge-Kutta convolution quadrature of (22) is obtained; this example was the motivation behind the set of experiments in Section 6.1.

N	5	10	15	20	30
e_N	8.7×10^{-2}	1.6×10^{-2}	4.5×10^{-3}	1.9×10^{-3}	5.7×10^{-4}
order	–	2.5	3.1	3.0	3.0

Table 1: Convergence of the 3-stage Radau IIA convolution quadrature of a time-domain boundary integral operator.

In the general case, however, the bound in (21) suggests a convergence rate $\mathrm{O}(h^{q-1})$. We have performed numerical experiments with the right-hand side

$$g(x,t) = \cos\left(\frac{1}{2}\pi(t-\alpha\cdot x)\right) e^{-\left(\frac{t-\alpha\cdot x-4}{\sqrt{2}}\right)^2}, \quad \alpha = (1,0,0)^T,$$

a non-convex domain Ω defined in [2], and a time interval of length $T = 6$. We have used a piecewise-constant Galerkin discretization in space, with 1.4×10^4 triangular panels discretizing Γ. All the computations have been done with the techniques described in [2]. Since no analytic solution is known we have estimated the error by

$$e_N = \left(h \sum_{j=0}^{N} \|\psi_N(t_j) - \psi_{2N}(t_j)\|^2_{H^{-1/2}(\Gamma)} \right)^{1/2},$$

where ψ_N is the discrete solution obtained by convolution quadrature with time-step $h = T/N$, i.e., we have compared the numerical solution with the numerical solution obtained with the time-step halved. In order to make sure that the space discretization is not significantly affecting the results, we have computed e_N for $N = 20$ with a finer space discretization of 2.3×10^4 panels; this computation gave the same result up to two digits accuracy.

The results of these numerical experiments, as documented in Table 1, suggest a convergence order $\mathrm{O}(h^3)$ when computing (22) using the 3-stage Radau IIA method. The 3-stage Radau IIA method being of stage order $q = 3$, this is one order better than our present theory is able to predict.

This final experiment suggests that it is also of interest to consider a class of operators bounded as

$$|K(s)| \le M \frac{|s|^{-\mu}}{(\operatorname{Re} s)^{\nu}}, \qquad \operatorname{Re} s > \sigma. \tag{23}$$

All standard boundary integral operators and operators related to transmission problems, BEM-FEM coupling, etc., see [11], satisfy bounds of this more general form. Our present analysis does not give more favourable estimates for this class of operators when $\nu > 0$.

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