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Runge-Kutta Convolution Quadrature for Operators Arising in Wave Propagation

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Runge-Kutta convolution quadrature for operators arising in wave propagation

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Abstract

An error analysis of Runge-Kutta convolution quadrature is presented for a class of non-sectorial operators whose Laplace transform satisfies, besides the standard assumptions of analyticity in a half-plane $\operatorname{Re} s > \sigma_0$ and a polynomial bound $\mathrm{O}(s^{\mu_1})$ there, the stronger polynomial bound $\mathrm{O}(s^{\mu_2})$ in convex sectors of the form $|\arg s| \le \pi/2 - \theta < \pi/2$ for $\theta > 0$. The order of convergence of the Runge-Kutta convolution quadrature is determined by μ_2 and the underlying Runge-Kutta method, but is independent of μ_1.

Time domain boundary integral operators for wave propagation problems have Laplace transforms that satisfy bounds of the above type. Numerical examples from acoustic scattering show that the theory describes accurately the convergence behaviour of Runge-Kutta convolution quadrature for this class of applications. Our results show in particular that the full classical order of the Runge-Kutta method is attained away from the scattering boundary.

1 Introduction

Convolution quadrature is a numerical scheme to evaluate expressions of the form

$$u(t) = \int_0^t k(t-\tau) g(\tau) d\tau, \qquad 0 \le t \le T, \tag{1.1}$$

for given g and k. We refer to [11] for a recent review of convolution quadrature and its applications, to [12] and [3] for Runge-Kutta convolution quadratures, and to [10] for the type of analysis that will be used in the present paper. The basis of the numerical realization as well as the analysis of convolution quadrature is not the function k but its Laplace transform $K = \mathscr{L}k$, which is important since in many applications it is the transfer function K, and not the kernel k, that is known explicitly and more easily analysed and computed with. This fact and the excellent stability properties of convolution quadrature have resulted in numerous recent papers investigating its use in applications and its fast numerical implementation [2, 4, 5, 6, 8, 13, 14, 15].

In the present paper, we focus on the convergence analysis of Runge-Kutta convolution quadrature for non-sectorial transfer functions K, or, more generally, operators K, that are analytic in a half-plane $\operatorname{Re} s > \sigma_0$ and polynomially bounded there. Such operators appear naturally in the context of time-domain wave propagation problems, [1, 9]. For multistep-based convolution quadrature, it has been observed already in [10] that the achievable convergence order is limited by $p = 2$ due to the requirement of A-stability of the underlying ODE-solver for this class of problems. On the other hand, A-stable Runge-Kutta methods of arbitrary order are available and convolution quadratures based on them often outperform those based on linear multistep methods; see [2, 13] for numerical comparisons of convolution quadratures based on Radau IIA Runge-Kutta methods

and on BDF multistep methods. An analysis of Runge-Kutta-based convolution quadrature for non-sectorial operators has recently been presented in [3]. The analysis of [3] is sharp for the class of kernels with Laplace transforms K that are polynomially bounded in a half-plane, i.e., that satisfy (2.1) below. Several kernel transforms K arising in practice, however, have more structure in that they satisfy a more stringent growth condition on convex sectors of the form $|\arg s| \leq \pi/2 - \theta$ ($\theta > 0$ arbitrary) than on the half-plane $\operatorname{Re} s > \sigma_0$. Assumption 2.1 below formalizes this behaviour. Indeed, as is seen for example from the results of [1] and [9], Assumption 2.1 is the appropriate setting for various kernel transforms K arising in wave propagation problems. As an application of our convergence result Theorem 3.2, we will also study in Section 5 a Runge-Kutta convolution quadrature for a boundary integral equation formulation of a wave scattering problem. The numerical results for this scattering problem show that the theory of the present paper accurately describes the behaviour of Runge-Kutta convolution quadrature for this problem class. This was not possible with previously available theories.

The present paper, therefore, concentrates on kernels with Laplace transforms K that conform to Assumption 2.1. In this setting, we prove that the order of convergence attainable by Runge-Kutta convolution quadrature is controlled by the growth properties of K on sectors of the form $|\arg s| < \pi/2 - \theta$ rather than growth conditions on the half-plane $\operatorname{Re} > \sigma_0$. Our numerical examples indicate that our theoretical error estimates are sharp.

2 Preparation

2.1 Problem class

We are interested in computing convolutions of the form (1.1). Throughout this paper, we will assume that the Laplace transform $K(s) = \mathscr{L}k\,(s)$of the (possibly distributional) kernel $k(t)$ has the following property:

Assumption 2.1. *K is analytic in the half-plane $\operatorname{Re} s > \sigma_0$ and satisfies, for some real exponent μ_1 and bounding factor $M_1(\sigma_0) > 0$,*

$$|K(s)| \leq M_1(\sigma_0)|s|^{\mu_1} \quad \text{for } \operatorname{Re} s > \sigma_0. \tag{2.1}$$

Furthermore, there is an exponent $\mu_2 \leq \mu_1$ such that for every $r > 0$ there exists $M_2(\sigma_0, r) > 0$ such that

$$|K(s)| \leq M_2(\sigma_0, r)|s|^{\mu_2} \quad \text{for } |s| > \sigma_0 \text{ and } 0 \leq \frac{|\operatorname{Im} s|}{\operatorname{Re} s} \leq r. \tag{2.2}$$

An important class of transfer functions K satisfies bounds of the form (2.3) below. These are covered by Assumption 2.1 as a direct calculation shows:

Lemma 2.2. *Let K be analytic in the half-plane $\operatorname{Re} s > \sigma_0 > 0$ and satisfy for some real exponent μ and $\nu \geq 0$*

$$|K(s)| \leq M(\sigma_0)\frac{|s|^{\mu}}{(\operatorname{Re} s)^{\nu}} \text{ for all } \operatorname{Re} s > \sigma_0. \tag{2.3}$$

Then K satisfies Assumption 2.1 with $\mu_1 = \mu$, $\mu_2 = \mu - \nu$, $M_1(\sigma_0) = \frac{M(\sigma_0)}{\sigma_0^{\nu}}$, and $M_2(\sigma_0, r) = M(\sigma_0)(\sqrt{1+r^2})^{\nu}$.

If we write $K(s) = s^{\ell}K_{\ell}(s)$ with an integer $\ell > \mu_1 + 1$, then the Laplace inversion formula

$$k_{\ell}(t) = \frac{1}{2\pi\,\mathrm{i}}\int_{\sigma+i\mathbb{R}} e^{st}\,K_{\ell}(s)\,ds, \quad t \geq 0 \quad (\sigma > \sigma_0)$$

defines a continuous and exponentially bounded function k_ℓ, which has k as its ℓth distributional derivative. We write the convolution with k as

$$u(t) = K(\partial_t)g\,(t) = (k * g)(t) = \Big(\frac{d}{dt}\Big)^\ell \int_0^t k_\ell(t-\tau)\,g(\tau)\,d\tau, \qquad t > 0,$$

for functions g on $[0,T]$ whose extension to $t < 0$ by 0 is ℓ times continuously differentiable.

2.2 Runge-Kutta methods

We employ standard notation for m-stage Runge-Kutta discretizations based on the Butcher tableau described by the matrix $A = (a_{ij})_{i,j=1}^m \in \mathbb{R}^{m\times m}$ and the vectors $b = (b_1,\dots,b_m)^T \in \mathbb{R}^m$ and $c = (c_1,\dots,c_m)^T \in [0,1]^m$. In terms of A, b, c, an m-stage Runge-Kutta discretization of the initial value problem $y' = f(t,y)$, $y(0) = y_0$, is given by the recurrence

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

here, h is the time-step and $t_j = jh$. The values Y_{ni} and y_n are approximations to $y(t_n + c_i h)$ and $y(t_n)$, respectively. This Runge-Kutta method is said to be of (classical) order $p \geq 1$ and stage order q if for sufficiently smooth right-hand side 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 $h \to 0$. Furthermore, we recall that the weights b_i and nodes c_i define a quadrature formula of order p:

$$\sum_{i=1}^m b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1,2,\dots,p. \tag{2.4}$$

Using the notation

$$\mathbb{1} = (1,1,\dots,1)^T,$$

the Runge-Kutta method is said to be A-stable if $\mathrm{I} - zA$ is non-singular for $\mathrm{Re}\, z \leq 0$ and the stability function

$$R(z) = 1 + zb^T(I - zA)^{-1}\mathbb{1} \tag{2.5}$$

satisfies $|R(z)| \leq 1$ for $\mathrm{Re}\, z \leq 0$. Note that if A^{-1} exists, then $R(\infty) = 1 - b^T A^{-1}\mathbb{1}$.

For the analysis in the remainder of the paper we will make some extra assumptions on the Runge-Kutta method. We list these next.

Assumption 2.3. *(a) The Runge-Kutta method is A-stable with (classical) order $p \geq 1$ and stage order $q \leq p$.*

(b) The stability function satisfies $|R(\mathrm{i}\,y)| < 1$ for all real $y \neq 0$.

(c) $R(\infty) = 0$.

(d) The Runge-Kutta coefficient matrix A is invertible.

Remark 2.4. Conditions (c), (d) are ensured, for example, for stiffly accurate Runge-Kutta methods, which satisfy $b^T A^{-1} = (0, 0, \ldots, 0, 1)^T$ and therefore $R(\infty) = 0$, [7, Chap. IV, Prop. 3.8]. Important examples of RK-methods satisfying Assumption 2.3 are the stiffly accurate Radau IIA (with order $p = 2m-1$ and stage order $q = m$) and the Lobatto IIIC families (with order $p = 2m-2$ and stage order $q = m-1$), [7]. Conditions (b) and (c) are not satisfied for the Gauss collocation methods (with $p = 2m$ and $q = m$), for which the stability function is of unit modulus along the imaginary axis. ∎

2.3 Miscellaneous order properties of Runge-Kutta methods

Lemma 2.5. *A Runge-Kutta method with invertible coefficient matrix A satisfies*

$$b^T A^{-1}(\mathrm{I} - zA)^{-1}\mathbb{1} = R(z) - R(\infty) \tag{2.6}$$

and, with $e^{cz} := (e^{c_1 z}, e^{c_2 z}, \ldots, e^{c_m z})^T$, the following for small $|z|$:

$$zb^T e^{cz} = e^z - 1 + \mathrm{O}(z^{p+1}), \tag{2.7}$$

$$zAe^{cz} = e^{cz} - \mathbb{1} + \mathrm{O}(z^{q+1}), \tag{2.8}$$

$$b^T(\mathrm{I} - zA)^{-1}e^{cz} = e^z + \mathrm{O}(z^p), \tag{2.9}$$

$$(z - w)b^T(\mathrm{I} - wA)^{-1}e^{cz} = e^z - R(w) + \mathrm{O}(z^{q+1}). \tag{2.10}$$

The implied constant in (2.10) is independent of w bounded away from inverses of eigenvalues of A.

Proof. Identity (2.6) is easily proved:

$$b^T A^{-1}(\mathrm{I} - zA)^{-1}\mathbb{1} = b^T A^{-1}(\mathrm{I} - zA + zA)(\mathrm{I} - zA)^{-1}\mathbb{1} = R(z) - 1 + b^T A^{-1}\mathbb{1} = R(z) - R(\infty).$$

The order condition (2.4) implies (2.7) as follows:

$$zb^T e^{cz} = \sum_{j=0}^{\infty} \frac{1}{j!} z^{j+1} b^T (c_l^j)_{l=1,\ldots,m} = \sum_{j=0}^{p-1} \frac{1}{(j+1)!} z^{j+1} + \mathrm{O}(z^{p+1}) = e^z - 1 + \mathrm{O}(z^{p+1}).$$

Applying one step of the Runge-Kutta method to the initial value problem $y' = y$, $y(0) = 1$, with time step z, gives

$$Y_0 = \mathbb{1} + zAY_0.$$

Substituting the stage order condition $Y_{0i} = e^{c_i z} + \mathrm{O}(z^{q+1})$ implies (2.8).

Similarly, one step of the Runge-Kutta discretization of $y' = e^t + y$, $y(0) = 0$, with time step z, gives

$$y_1 = zb^T(\mathrm{I} - zA)^{-1}e^{cz} = ze^z + \mathrm{O}(z^{p+1}).$$

This proves (2.9).

To prove (2.10) notice that

$$\begin{aligned} zb^T(\mathrm{I} - wA)^{-1}e^{cz} &= zb^T e^{cz} + wb^T(\mathrm{I} - wA)^{-1}zAe^{cz} \\ &\overset{(2.7),(2.8)}{=} e^z - 1 + wb^T(\mathrm{I} - wA)^{-1}(e^{cz} - \mathbb{1} + \mathrm{O}(z^{q+1})) + \mathrm{O}(z^{p+1}) \\ &= e^z - R(w) + wb^T(\mathrm{I} - wA)^{-1}e^{cz} + wb^T(\mathrm{I} - wA)^{-1}\,\mathrm{O}(z^{q+1}) + \mathrm{O}(z^{p+1}). \end{aligned}$$

Rearranging the terms produces the desired result. □

2.4 The spectrum of the Runge-Kutta differentiation symbol

The following matrix-valued function Δ plays a key role in the definition and the analysis of Runge-Kutta convolution quadrature:

$$\Delta(\zeta) := \left(A + \frac{\zeta}{1-\zeta} \mathbb{1} b^T \right)^{-1}. \tag{2.11}$$

In case $R(\infty) = 0$, using the Sherman-Morrison formula and $1 - b^T A^{-1} \mathbb{1} = R(\infty) = 0$ shows that $\Delta(\zeta)$ can be written as a linear polynomial in ζ:

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

Concerning the spectrum $\sigma(\Delta(\zeta))$, we have the following.

Lemma 2.6. *For a Runge-Kutta method with invertible matrix A, the following is true for $|\zeta| < 1$:*

(i) The spectrum of $\Delta(\zeta)$ is given as

$$\sigma(\Delta(\zeta)) = \sigma(A^{-1}) \cup \{ z \in \mathbb{C} \colon R(z)\zeta = 1 \}.$$

Hence, for an A-stable method $\sigma(\Delta(\zeta))$ is contained in the open right half-plane for $|\zeta| < 1$.

(ii) For $z \notin \sigma(\Delta(\zeta))$ we have, if $R(\infty) = 0$,

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

Proof. We start with the following identity of [12, Lemma 2.4]:

$$(z\,\mathrm{I} - \Delta(\zeta))^{-1} = A(zA - \mathrm{I})^{-1} - \frac{\zeta}{1 - R(z)\zeta} (zA - \mathrm{I})^{-1} \mathbb{1} b^T (zA - \mathrm{I})^{-1}. \tag{2.12}$$

This readily implies (i). To see (ii), we combine (2.12) with (2.6) to get

$$\begin{aligned} b^T A^{-1} (z\,\mathrm{I} - \Delta(\zeta))^{-1} &= b^T (zA - \mathrm{I})^{-1} + \frac{(R(z) - R(\infty))\zeta}{1 - R(z)\zeta}\, b^T (zA - \mathrm{I})^{-1} \\ &= \frac{1 - R(\infty)\zeta}{1 - R(z)\zeta}\, b^T (zA - \mathrm{I})^{-1}. \end{aligned}$$

□

3 Runge-Kutta convolution quadrature

Runge-Kutta based convolution quadratures of (1.1) have been presented in [12]. While the error analysis of [12] assumed K to be analytic and polynomially bounded outside a sector with an acute angle to the negative real axis, the same algorithmic procedure can be used in the present case of kernels with Laplace transforms K that are analytic merely in a half-plane $\operatorname{Re} s > \sigma_0$. For a Runge-Kutta method satisfying Assumption 2.3, the convolution quadrature approximation to $u(t_{n+1})$ at time $t_{n+1} = (n+1)h$ is then given by

$$u_h(t_{n+1}) := b^T A^{-1} \sum_{j=0}^{n} W_{n-j}(K) \left(g(t_j + c_l h) \right)_{l=1}^{m} \tag{3.1}$$

where the ($m \times m$-matrix) convolution weights are defined by the power series expansion

$$K\left(\frac{\Delta(\zeta)}{h}\right) = \sum_{n=0}^{\infty} W_n(K)\zeta^n, \tag{3.2}$$

Here, the $m \times m$-matrix $\Delta(\zeta)$ has already been introduced in (2.11). The weights $W_n(K)$ can be efficiently computed using FFT as described in [12].

Remark 3.1. (2.11) shows that for A-stable Runge-Kutta methods and all ζ sufficiently small, the spectrum of $\Delta(\zeta)$ is contained in a fixed compact set S of the (open) right half-plane. Hence, for h_0 sufficiently small, the spectrum $\sigma(\Delta(\zeta)/h)$ is contained in the domain of analyticity of K for all $h \le h_0$ and therefore the map $\zeta \mapsto K(\Delta(\zeta)/h)$ is analytic on a sufficiently small ball centered at the origin. Thus, the matrices $W_n(K)$ defined by (3.2) are indeed well-defined. ∎

To extend the discrete solution u_h to all $t \ge 0$, we may use the zero extension of g to negative times, $g(t) \equiv 0$, for $t \le 0$, and define

$$u_h(t) := b^T A^{-1} \sum_{j=0}^{\infty} W_j(K) \left(g(t - t_j + c_l h - h)\right)_{l=1}^{m}.$$

The following theorem gives an error estimate for the Runge-Kutta convolution quadrature error and is the main result of the paper.

Theorem 3.2. *Let K satisfy Assumption 2.1 and the Runge-Kutta method Assumption 2.3. Let $r > \max(p + \mu_1, p, q + 1)$ and $g \in C^r([0,T])$ satisfy $g(0) = g'(0) = \cdots = g^{(r-1)}(0) = 0$. Then there exists $\bar{h} > 0$ such that for $0 < h \le \bar{h}$ and $t \in [0,T]$,*

$$|u_h(t) - u(t)| \le C\, h^{\min(p, q+1-\mu_2)} \left(|g^{(r)}(0)| + \int_0^t |g^{(r+1)}(\tau)| d\tau\right).$$

The constant C is independent of h and g, but does depend on the Runge-Kutta method, on $\bar{h}$, T, and the constants in Assumption 2.1.

The proof of this theorem covers the remainder of this section. Applying the Laplace transformation $\mathscr{L}$ to the error $e_h = u_h - u$ yields, again with the notation $e^{csh} = (e^{c_1 sh}, \ldots, e^{c_m sh})^T$,

$$\mathscr{L}e_h(s) = \left\{ b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh} e^{-sh} - K(s) \right\} \mathscr{L}g(s). \tag{3.3}$$

The key ingredient of our error analysis is the following representation of the expression in curly brackets in (3.3):

Lemma 3.3. *Let K satisfy Assumption 2.1 and let the Runge-Kutta method satisfy Assumption 2.3. For every $\sigma_1 > \sigma_0$, there exist constants $\rho_1 > 0$ and $h_1 > 0$ such that for $0 < h \le h_1$ and all s with $\operatorname{Re} s \ge \sigma_1$ and $|sh| < \rho_1$,*

$$b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh} e^{-sh} = K(s) + s^{\mu_1 + p}\, \mathrm{O}(h^p) + s^{q+1}\, \mathrm{O}(h^{q+1-\mu_2}).$$

The implied constants in the O*-notation are independent of h and s.*

Proof. We start from the Cauchy integral formula, with $\zeta = e^{-sh}$,

$$b^T A^{-1} K\left(\frac{\Delta(\zeta)}{h}\right) = \frac{1}{2\pi\,\mathrm{i}} \int_\Gamma K\left(\frac{z}{h}\right) b^T A^{-1} (z\,\mathrm{I} - \Delta(\zeta))^{-1}\, dz$$

with a contour Γ in the right half-plane that encloses the spectrum of $\Delta(\zeta)$. By Lemma 2.6, we thus have

$$b^T A^{-1} K\left(\frac{\Delta(\zeta)}{h}\right) = \frac{1}{2\pi\,\mathrm{i}} \int_\Gamma K\left(\frac{z}{h}\right) \frac{1}{1 - R(z)\zeta}\, b^T A^{-1} (z\,\mathrm{I} - A^{-1})^{-1}\, dz. \tag{3.4}$$

For $|sh|$ sufficiently small, i.e., for $\zeta = e^{-sh}$ in a sufficiently small neighbourhood of 1, Assumption 2.3 implies that there is a unique solution to the equation $R(z) = 1/\zeta$ that lies in the vicinity of the origin and which we denote by

$$\widehat{z} = \widehat{s}h \quad \text{satisfying} \quad R(\widehat{s}h) = e^{sh}.$$

Since $R(z) = e^z + \mathrm{O}(z^{p+1})$, we obtain

$$\widehat{s}h = sh\Big(1 + \mathrm{O}\big((sh)^p\big)\Big). \tag{3.5}$$

We take the residue at $\widehat{z}$ out of the above contour integral, so that

$$\begin{aligned} b^T A^{-1} K\left(\frac{\Delta(\zeta)}{h}\right) &= -K\left(\frac{\widehat{z}}{h}\right) \frac{1}{R'(\widehat{z})\zeta}\, b^T A^{-1} (\widehat{z}\,\mathrm{I} - A^{-1})^{-1} \\ &\quad + \frac{1}{2\pi\,\mathrm{i}} \int_{\Gamma_A} K\left(\frac{z}{h}\right) \frac{1}{1 - R(z)\zeta}\, b^T A^{-1} (z\,\mathrm{I} - A^{-1})^{-1}\, dz, \end{aligned}$$

where Γ_A is a contour that encloses the eigenvalues of A^{-1} (which have positive real part by assumption) and all solutions of $R(z) = 1/\zeta$ other than $\widehat{z}$. This contour can be chosen to lie within a fixed sector $|\arg z| \le \frac{\pi}{2} - \theta$ with $\theta > 0$, since for sufficiently small $|sh|$, the set $\{z\colon R(z) = 1/\zeta\} \backslash \{\widehat{z}\}$ is contained in a fixed compact subset of the open right half plane. We have, since $e^{sh} = 1/\zeta = R(\widehat{z})$ and $R(\widehat{z}) = e^{\widehat{z}} + \mathrm{O}(\widehat{z}^{p+1})$ and applying Lemma 2.5,

$$b^T A^{-1} (\widehat{z}\,\mathrm{I} - A^{-1})^{-1} e^{csh} = -b^T (\mathrm{I} - \widehat{z}A)^{-1} R(\widehat{z})^c = -b^T (\mathrm{I} - \widehat{z}A)^{-1} \big(e^{c\widehat{z}} + \mathrm{O}(\widehat{z}^{p+1})\big) = -e^{\widehat{z}} + \mathrm{O}(\widehat{z}^{p+1}).$$

Moreover, we note $R'(\widehat{z}) = e^{\widehat{z}} + \mathrm{O}(\widehat{z}^p)$. Hence we obtain, recalling $\zeta = e^{-sh}$ and $\widehat{z} = \widehat{s}h$,

$$\begin{aligned} b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh} e^{-sh} &= K(\widehat{s})\big(1 + \mathrm{O}((\widehat{s}h)^p\big) \\ &\quad + \frac{1}{2\pi\,\mathrm{i}} \int_{\Gamma_A} K\left(\frac{z}{h}\right) \frac{1}{1 - R(z)e^{-sh}}\, b^T A^{-1} (z\,\mathrm{I} - A^{-1})^{-1} e^{csh} e^{-sh}\, dz. \end{aligned}$$

For the first term on the right-hand side we note, using the bounds (3.5) and $|K'(s)| \le M|s|^{\mu_1 - 1}$ (which is obtained from the Cauchy integral formula for derivatives),

$$K(\widehat{s}) = K(s) + \mathrm{O}(s^{\mu_1}(sh)^p).$$

¿From Lemma 2.5 we have, uniformly for $z \in \Gamma_A$,

$$b^T (\mathrm{I} - zA)^{-1} e^{csh} = \frac{e^{sh} - R(z)}{sh - z} + \alpha(z, sh) \quad \text{with} \quad \alpha(z, sh) = \mathrm{O}((sh)^{q+1}),$$

so that the contour integral reduces to

$$\frac{1}{2\pi\,\mathrm{i}}\int_{\Gamma_A} K\left(\frac{z}{h}\right)\frac{1}{sh-z}\,dz + \frac{1}{2\pi\,\mathrm{i}}\int_{\Gamma_A} K\left(\frac{z}{h}\right)\frac{\alpha(z,sh)}{e^{sh}-R(z)}\,dz.$$

The first integral vanishes by Cauchy's integral theorem, and by Assumption 2.1 the second integral is bounded by $\mathrm{O}(h^{-\mu_2}(sh)^{q+1})$. All taken together, we have obtained the stated result. □

Proof. (of Theorem 3.2). We proceed along the lines of [10, Theorem 3.1]. Let $\sigma_1 \geq \sigma_0$ be given by Lemma 3.3. The Laplace transform of the error $e_h(t) = u(t) - u_h(t)$ is

$$\mathscr{L}e_h(s) = \left\{b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh}e^{-sh} - K(s)\right\}\mathscr{L}g(s).$$

Hence, if this expression is integrable along $\sigma_1 + \mathrm{i}\,\mathbb{R}$, we have by the inverse Laplace transform

$$e_h(t) = \frac{1}{2\pi\,\mathrm{i}}\int_{\sigma_1+\mathrm{i}\,\mathbb{R}} e^{st}\left\{b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh}e^{-sh} - K(s)\right\}\mathscr{L}g(s)ds.$$

Note that along the integration contour, $|e^{st}| = e^{\sigma_1 t} \leq e^{\sigma_1 T}$.

Let us first consider the special case $\mathscr{L}g\,(s) = s^{-r-1}$, i.e., $g(t) = t^r/r!$, and study the integral

$$I = \int_{-\infty}^{\infty}\left|\left\{b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh}e^{-sh} - K(s)\right\} s^{-r-1}\right| d\omega, \quad s = \sigma_1 + \mathrm{i}\,\omega.$$

We split the integral into three parts:

$$\begin{aligned} I \leq I_1 + I_2 + I_3 := &\int_{|sh|<\rho_1}\left|\left\{b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh}e^{-sh} - K(s)\right\} s^{-r-1}\right| d\omega \\ &+ \int_{|sh|\geq\rho_1}\left|b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) e^{csh}e^{-sh}\, s^{-r-1}\right| d\omega \\ &+ \int_{|sh|\geq\rho_1}|K(s)\, s^{-r-1}|d\omega, \end{aligned}$$

with the constant $\rho_1 > 0$ of Lemma 3.3.

The bound (2.1) on $K(s)$ implies $I_3 = \mathrm{O}(h^{r-\mu_1})$. Starting from (3.4) and proceeding along the lines of the proof of Lemma 3.3, one can show

$$b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) = \mathrm{O}(h^{-\max(0,\mu_1)}) \tag{3.6}$$

if one observes that by periodicity of the exponential function, one may assume that $|\operatorname{Im} sh| \leq \pi$ and then distinguishes the cases of $\left|e^{-sh} - 1\right|$ being small and not small. The bound (3.6) then implies

$$I_2 \leq Ch^{-\max(0,\mu_1)}\int_{|s|>\rho_1/h}|s|^{-r-1}d\omega = \mathrm{O}(h^{r-\max(0,\mu_1)}).$$

With the estimate of Lemma 3.3, if $r > p + \mu_1$ and $r > q + 1$,

$$I_1 \leq Ch^p\int_{|sh|\leq\rho_1}|s|^{p+\mu_1-r-1}d\omega + Ch^{q+1-\mu_2}\int_{|sh|\leq\rho_1}|s|^{q-r}d\omega = \mathrm{O}(h^p) + \mathrm{O}(h^{q+1-\mu_2}).$$

The generalization from the special case $\mathscr{L}g(s) = s^{-r-1}$ to that of general g is achieved with the observation

$$\sup_{\operatorname{Re} s=\sigma_1} \left| s^{r+1} \left(\mathscr{L}g(s) - s^{-r-1} g^{(r)}(0) \right) \right| = \sup_{\operatorname{Re} s=\sigma_1} \left| \mathscr{L}g^{(r+1)}(s) \right| \le \int_0^\infty e^{-\sigma_1 t} \left| g^{(r+1)}(t) \right| dt.$$

Finally, by extending g as the rth degree Taylor polynomial at t we can see that the above integration interval can be reduced to $[0, t]$. □

Remark 3.4. The proof of Theorem 3.2 shows that condition (2.2) could be weakened slightly: The bound (2.2) merely needs to hold on a *fixed* sector that depends on the Runge-Kutta method employed. While the condition $R(\infty) = 0$ in Assumption 2.3 covers the practically relevant cases, Theorem 3.2 also holds under the weakened condition $|R(\infty)| < 1$, if the convolution weights W_n in (3.2) are defined by the relation $K(\Delta(\zeta)/h) = (1 - \zeta R(\infty)) \sum_{n=0}^{\infty} W_n(K)\zeta^n$. ∎

4 A scalar numerical example

Let us consider the functions

$$K_1(s) = \mathrm{i} \tan(\sqrt{-\mathrm{i}\, s}) = \frac{1 - e^{-2\mathrm{i}\, w}}{1 + e^{-2\mathrm{i}\, w}}, \qquad \operatorname{Re} s > 0, \tag{4.1}$$

$$K_2(s) = K_1(s) - 1 \tag{4.2}$$

where the principal branch of the square root is used; hence, $w = \sqrt{-\mathrm{i}\, s}$ belongs to the fourth quadrant, i.e., $\operatorname{Re} w > 0$ and $\operatorname{Im} w < 0$. It is easy to check that K_1 has singularities located on the imaginary axis at the points $s_n = \mathrm{i}\, \pi^2 (n + 1/2)^2$, $n \in \mathbb{Z}_0$. Fairly straightforward analysis shows that the functions K_1 and K_2 satisfy Assumption 2.1:

Lemma 4.1. *(i) For every fixed $\sigma_0 > 0$ the function K_1 satisfies Assumption 2.1 with $\mu_1 = 1/2$ and $\mu_2 = 0$.*

(ii) For every fixed $\sigma_0 > 0$ the function K_2 satisfies Assumption 2.1 with $\mu_1 = 1/2$ and arbitrary *$\mu_2 < 0$.*

We omit the details of the proof. We point out here that K_2 decays exponentially on sectors $|\arg s| \le \pi/2 - \theta_0 < \pi/2$, which is the reason for our being able to select any μ_2 in Assumption 2.1: Let $s = |s| e^{\mathrm{i}\, \theta}$ with $|\theta| \le \pi/2 - \theta_0$ for some $\theta_0 > 0$. Then $\operatorname{Im} w = |s|^{1/2} \sin(\theta/2 - \pi/2) \le -|s|^{1/2} \sin(\theta_0/2)$ and inspection of (4.1) shows that $K_2(s) = K_1(s) - 1 = O(e^{-\theta_0 |s|^{1/2}})$.

We apply the 3-stage Radau IIA method (stage order $q = 3$, classical order $p = 5$) to the convolution (1.1) with

$$g(t) = e^{-\frac{1}{2}t} \sin^7 t.$$

and kernel $K(s) = K_1(s) s^\mu$ with $\mu \in \{-1/2, 0, 1/2\}$. In Table 1 we present the maximum error of the convolution quadrature on the interval $t \in [0, T]$ with $T = 2.5$ and N steps. Theorem 3.2 predicts a convergence behaviour $\mathrm{O}(h^{4-\mu})$ and the numerical results for $\mu = -1/2$ and $\mu = 1/2$ confirm this. However, for $\mu = 0$ the results indicate a full order convergence $\mathrm{O}(h^5)$. This can be explained by writing $K_1(s) = 1 + K_2(s)$. For $K(s) \equiv 1$, the convolution quadrature gives the exact result, whereas $K_2(s) = K_1(s) - 1$ satisfies Assumption 2.1 with $\mu_1 = 1/2$ and any $\mu_2 < 0$. Since convolution quadrature is linear, Theorem 3.2 therefore asserts an $\mathrm{O}(h^5)$-convergence. This shows that our theory predicts also this, at first sight, exceptional case.

	$\mu=-1/2$		$\mu=0$		$\mu=1/2$	
N	error	rate	error	rate	error	rate
4	4.0×10^{-2}	0.0	6.2×10^{-2}	0.0	9.7×10^{-2}	0.0
8	1.5×10^{-3}	4.8	2.3×10^{-3}	4.8	7.7×10^{-3}	3.6
16	6.0×10^{-5}	4.6	1.6×10^{-4}	3.9	1.5×10^{-3}	2.3
32	1.8×10^{-6}	5.0	4.5×10^{-6}	5.1	1.2×10^{-4}	3.6
64	8.4×10^{-8}	4.4	1.2×10^{-7}	5.2	1.0×10^{-5}	3.6
128	3.6×10^{-9}	4.5	4.0×10^{-9}	4.9	9.0×10^{-7}	3.5

Table 1: Convergence of the 3-stage Radau IIA based convolution quadrature of $K(\partial_t)g$ for $K(s)=K_1(s)s^\mu$. The function K satisfies Assumption 2.1 with $\mu_1=\mu+1/2$ and $\mu_2=\mu$.

	$\mu=1/2$		$\mu=1$		$\mu=3/2$	
N	error	rate	error	rate	error	rate
4	3.9×10^{-2}	0.0	1.8×10^{-1}	0.0	4.3×10^{-1}	0.0
8	1.8×10^{-3}	4.4	1.2×10^{-2}	3.9	4.7×10^{-2}	3.2
16	1.1×10^{-4}	4.0	5.0×10^{-4}	4.6	2.4×10^{-3}	4.3
32	3.8×10^{-6}	4.9	2.0×10^{-5}	4.6	1.6×10^{-4}	3.9
64	1.3×10^{-7}	4.9	7.1×10^{-7}	4.8	6.9×10^{-6}	4.6
128	4.0×10^{-9}	5.0	2.2×10^{-8}	5.0	2.8×10^{-7}	4.6

Table 2: Convergence of the 3-stage Radau IIA based convolution quadrature of $K(\partial_t)g$ for $K(s)=K_1(s)s^\mu e^{-s}$. The function $s\mapsto K(s)$ satisfies Assumption 2.1 with $\mu_1=\mu+1/2$ and any $\mu_2<0$.

Next, we consider the case $K(s)=K_1(s)s^\mu e^{-s}$ for which our theory, under the stated smoothness assumptions on g, predicts optimal convergence $\mathrm{O}(h^5)$ irrespective of μ. This is seen in Table 2 for $\mu=1/2$ and $\mu=1$. For $\mu=3/2$ a reduced order convergence is observed. This is a consequence of g not having sufficiently many zero derivatives at $t=0$. Setting $g(t)=e^{-t/2}\sin^8(t)$ recovers the optimal order convergence.

5 Application to acoustic scattering

5.1 Boundary integral operators

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

$$S(s)\varphi(x):=\int_\Gamma \frac{e^{-s|x-y|}}{4\pi|x-y|}\varphi(y)d\Gamma_y,\quad x\in\mathbb{R}^3\setminus\Gamma.$$

We denote its boundary trace 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 terms of the standard Sobolev spaces $H^{1/2}(\Gamma)$ and $H^{-1/2}(\Gamma)$, these operators have the following properties:

Lemma 5.1. *Let $\sigma > 0$.*

(i) $V(s) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is boundedly invertible with

$$\|V^{-1}(s)\|_{H^{-1/2}(\Gamma)\leftarrow H^{1/2}(\Gamma)} \leq C(\sigma)\frac{|s|^2}{\operatorname{Re} s}, \qquad \operatorname{Re} s \geq \sigma > 0. \tag{5.1}$$

(ii) For $x \in \mathbb{R}^3 \setminus \Gamma$ the point evaluation of the single layer potential at x is a bounded linear operator with norm bounded as

$$\|S(s)\cdot(x)\|_{\mathbb{C}\leftarrow H^{-1/2}(\Gamma)} \leq C(\sigma, \operatorname{dist}(x,\Gamma))e^{-\operatorname{Re} s \operatorname{dist}(x,\Gamma)}|s|, \qquad \operatorname{Re} s \geq \sigma > 0. \tag{5.2}$$

Proof. Assertion (i) is shown in [1]. To see (ii), let $x \in \Omega^+$ with $\delta = \operatorname{dist}(x,\Gamma) > 0$ and $\Omega^+ = \mathbb{R}^3 \setminus \overline{\Omega}$. Let $d_x(y) = |x - y|$. Then,

$$\begin{aligned}
|S(s)\varphi(x)| &\leq \left\| \frac{e^{-sd_x}}{4\pi d_x} \right\|_{H^{1/2}(\Gamma)} \|\varphi\|_{H^{-1/2}(\Gamma)} \leq C \left\| \frac{e^{-sd_x}}{d_x} \right\|_{H^1(\Omega)} \|\varphi\|_{H^{-1/2}(\Gamma)} \\
&\leq C \left\| \frac{e^{-sd_x}}{d_x} \left(1 + |s| + \frac{1}{d_x}\right) \right\|_{L^2(\Omega)} \|\varphi\|_{H^{-1/2}(\Gamma)} \leq C(\sigma,\delta)|s|\,|e^{-s\delta}|\,\|\varphi\|_{H^{-1/2}(\Gamma)}.
\end{aligned}$$

Hence, the operator $\varphi \mapsto S(s)\varphi(x) : H^{-1/2}(\Gamma) \to \mathbb{C}$ is bounded as stated in (5.2) for $x \in \Omega^+$. A similar estimate is obtained for $x \in \Omega$ by writing

$$\left\| \frac{e^{-sd_x}}{4\pi d_x} \right\|_{H^{1/2}(\Gamma)} \leq C \left\| \frac{e^{-sd_x}}{4\pi d_x} \right\|_{H^1(\Omega_R)},$$

with $\Omega_R = \Omega^+ \cap B_R$, with $B_R = \{x \in \mathbb{R}^3 : |z| < R\}$ and R chosen such that $\Omega \subset B_R$. □

As has been demonstrated in [1], the operators S and V can be used to solve sound-soft scattering problems. More precisely, given $g(\cdot,t) \in H^{1/2}(\Gamma)$, we can define the convolution integral

$$\psi = V^{-1}(\partial_t)g \tag{5.3}$$

and observe that $u = S(\partial_t)\psi = SV^{-1}(\partial_t)g$ 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.

5.2 Numerical results

Convolution quadrature can also be done in an operator-valued setting. Lemma 5.1 informs us that $s \mapsto V^{-1}(s)$ (viewed as an operator $H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$) satisfies Assumption 2.1 with $\mu_1 = 2$ and $\mu_2 = 1$. For fixed $x \notin \Gamma$, we have furthermore

$$\left|S(s)V^{-1}(s)g(x)\right| \leq C(\sigma, \operatorname{dist}(x,\Gamma))\frac{|s|^3}{\operatorname{Re} s}e^{-\operatorname{Re} s \operatorname{dist}(x,\Gamma)}$$

N	5	10	15	20	30
$e_{N,\Gamma}$	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
$e_{N,x}$	2.3×10^{-1}	1.7×10^{-2}	3.0×10^{-3}	8.5×10^{-4}	1.3×10^{-4}
order:	–	3.8	4.3	4.4	4.6

Table 3: Convergence of the 3-stage Radau IIA convolution quadrature of a time-domain boundary integral operator. The error on the boundary Γ in appropriate norm is denoted by $e_{N,\Gamma}$, whereas $e_{N,x}$ denotes the error at the point $x \notin \Gamma$.

so that in this case Assumption 2.1 is satisfied with $\mu_1 = 3$ and any μ_2. Hence, Theorem 3.2 yields that, if g vanishes to sufficient order near $t = 0$, Runge-Kutta convolution quadrature leads to convergence $O(h^q)$ for the approximation of $\psi = V^{-1}(\partial_t)g$ (in the $\|\cdot\|_{H^{-1/2}(\Gamma)}$ norm) and to optimal convergence $O(h^p)$ for the point evaluation away from the boundary. Detailed numerical experiments that support these conclusions are given next.

We have performed numerical experiments with the right-hand side

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

a non-convex domain Ω contained in a ball of radius 1 centred at the origin and defined in [2], and a time interval of length $T = 6$. Note that although $g(x,0)$ is not exactly zero, it is almost so: $|g(x,0)| \leq 7.2 \times 10^{-10}$, for $|x| \leq 1$, and also its higher derivatives are small at time $t = 0$. This discrepancy does not seem to have any influence on the results of the numerical experiments.

We have used a piecewise-constant Galerkin discretization in space with 1.4×10^4 triangular panels discretizing Γ. All the computations were done with the techniques described in [2]. Since no analytic solution is known we have estimated the error on the boundary by

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

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 does not significantly affect the results, we have computed $e_{N,\Gamma}$ 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 3, suggest a convergence order $\mathrm{O}(h^3)$ when computing (5.3) using the 3-stage Radau IIA method. The 3-stage Radau IIA method being of stage order $q = 3$, this is exactly as the theory predicts. We mention that the results of this experiment have already appeared in [3]. They were the original motivation for the present work.

Another interesting numerical experiment motivated by the theory is to investigate the convergence of the numerical solution at a point outside the domain; the results of this experiment have not previously appeared in print. We have computed the error

$$e_{N,x} := \|u_N(x,\cdot) - u_{2N}(x,\cdot)\|_{\ell^2} = \left(h \sum_{j=0}^{N} (u_N(x,t_j) - u_{2N}(x,t_j))^2 \right)^{1/2}$$

for $x = (1.5, 0, 0)^T \in \Omega^+$. Here, u_N is the Runge-Kutta convolution quadrature approximation to $SV^{-1}(\partial_t)g$, which is computed using the internal stage values in the approximation of $\psi = V^{-1}(\partial_t)g$. The theory predicts optimal order convergence and the numerically obtained estimate of the order given in Table 3 supports this.

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