Max-Planck-Institut für Mathematik in den Naturwissenschaften Leipzig

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Preprint no.: 72 2012

BIT manuscript No.
(will be inserted by the editor)

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Received: date / Accepted: date

Abstract Wave propagation problems in unbounded homogeneous domains can be formulated as time-domain integral equations. An effective way to discretize such equations in time are Runge-Kutta based convolution quadratures. In this paper the behaviour of the weights of such quadratures are investigated. In particular approximate sparseness of their Galerkin discretization is analyzed. Application of these results in the construction of fast algorithms for the construction of the fully discrete systems is also briefly described.

Keywords convolution quadrature · Runge-Kutta methods · time-domain boundary integral equations · wave equation

Mathematics Subject Classification (2000) 65R20 · 65L06 · 35L05 · 65M38

1 Introduction

In many physical applications, e.g. electromagnetic scattering, it is necessary to solve the exterior boundary value problem for three-dimensional wave equation. Such problems can be effectively treated with the use of time-domain boundary integral equations (TDBIE). The well-posedness of such formulations for the wave equation was analyzed in [2, 3].

Solution of time domain boundary integral equations is usually performed with Galerkin time-space methods [14], collocation methods [11], time-stepping techniques or Laplace-domain approaches. A review of these methods can be found in

A brief review of the main results of this paper has been published in the Proceedings of the 6th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2012).

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[10]. However, compared to the field of elliptic problems, fast solvers for time domain boundary integral equations are not that extensively developed. A particularly efficient approach for solution of retarded potential boundary integral equations is offered in [13].

One of the methods for solution of TDBIE, convolution quadrature [18–20], combines Laplace-domain and time-stepping techniques. It is stable, efficient and does not require underlying space quadratures to be evaluated with high accuracy, as e.g. Galerkin time-space methods. Applicability of the method to external boundary-value problems for wave equation was justified in [20, 8]. These results were supported by extensive numerical experiments in [4]. In the same work it was shown that the Runge-Kutta convolution quadrature [21] is preferable to the multistep convolution quadrature whenever the scattering domain is non-star-shaped. In [5] the theoretical justification of this fact was given.

In this paper we apply an m-stage A-stable Runge-Kutta convolution quadrature [21]. The weights of the convolution quadrature are integral operators. The main part of this paper is devoted to the investigation of the behaviour of the kernels of these weights. Estimates are proved that show the exponential decay of the kernels $w_n^h(d)$ away from $nh \approx d$. The paper ends with an illustration of how these results can be used to speed up existing algorithms for the computation of convolution weights.

2 Statement of the problem

Let $\Omega \subset \mathbb{R}^3$ be a bounded Lipschitz domain with boundary Γ and let $\Omega^c = \mathbb{R}^3 \setminus \overline{\Omega}$ be its complement.

We will consider the homogeneous wave equation set in Ω^c,

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \Delta u = 0 \qquad & \text{in} \quad [0,T] \times \Omega^c, \\ u(0,.) = \frac{\partial u}{\partial t}(0,.) = 0 \qquad & \text{in} \quad \Omega^c, \\ u(t,x) = g(t,x) \qquad & \text{on} \quad [0,T] \times \Gamma. \end{aligned} \tag{2.1}$$

For any boundary data g, the solution u of the above system can be represented as the single-layer potential of an unknown density λ

$$\begin{aligned} u(t,\tilde{x}) = (\mathscr{S}\lambda)(t,\tilde{x}) &= \int_0^t \int_\Gamma \frac{\delta(t-\tau-\|\tilde{x}-y\|)}{4\pi\|\tilde{x}-y\|} \lambda(\tau,y) d\Gamma_y d\tau, \\ &= \int_\Gamma \frac{\lambda\,(t-\|\tilde{x}-y\|)}{4\pi\|\tilde{x}-y\|} d\Gamma_y, \qquad (t,\tilde{x}) \in [0,T] \times \Omega^c, \end{aligned}$$

where $\delta(\cdot)$ denotes the Dirac delta function. Single layer potential $\mathscr{S}\lambda$ is also known as the *retarded potential*, the name being justified by the second expression above. For any density λ, the function $u = \mathscr{S}\lambda$ satisfies the first two equations in (2.1), therefore to solve (2.1) it remains to choose λ so that the boundary condition is also satisfied. Single layer potential $\mathscr{S}\lambda$ is continuous across Γ, so letting in the above equation

$\tilde{x} \to x \in \Gamma$ and using the boundary condition from (2.1), we obtain a *boundary integral equation* for the unknown density λ

$$g(t,x) = (\mathscr{V}\lambda)(t,x) = \int_0^t \int_\Gamma \frac{\delta(t-\tau-\|x-y\|)}{4\pi\|x-y\|}\lambda(\tau,y)d\Gamma_y d\tau, \quad \forall (t,x) \in [0,T]\times\Gamma. \tag{2.2}$$

Here, the operator $\mathscr{V}$ is called the single layer boundary integral operator. For existence and uniqueness of solutions of this equation see [2].

For further discussion we will require the Laplace transforms of $\mathscr{S}$ and $\mathscr{V}$. With the Laplace transform defined by

$$\mathscr{L}f(s) = \int_0^\infty e^{-st} f(t)dt, \quad \operatorname{Re} s > 0,$$

and causal f, i.e. $f(t) = 0$, for $t \le 0$, it holds that

$$\mathscr{L}(f(\cdot - r))(s) = \int_0^\infty e^{-st} f(t-r)dt = e^{-sr}\mathscr{L}f(s), \qquad r \ge 0. \tag{2.3}$$

Hence the Laplace transforms of $\mathscr{S}$ and $\mathscr{V}$ are given respectively by

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

and

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

Next, we address the time-discretization of retarded potentials.

2.1 Convolution quadrature based on backward differences

Let $h > 0$ denote the timestep and $t_j = jh$ the equally spaced time-points. Then the derivative of a causal function f can be approximated by

$$f'(t) \approx \tfrac{1}{h}(f(t) - f(t-h)). \tag{2.4}$$

Taking the Laplace transform of the above approximation and applying (2.3) gives

$$s\mathscr{L}f(s) \approx \frac{1-e^{-sh}}{h}\mathscr{L}f(s). \tag{2.5}$$

We can also reverse this procedure: approximate the differentiation symbol s in the Laplace domain by $\frac{1-e^{-sh}}{h} = s + sO((sh))$, see (2.5), and compute the inverse Laplace transform of the approximation to obtain the backward difference approximation of the derivative (2.4).

Convolution quadrature of $\mathscr{S}\lambda$ and $\mathscr{V}\lambda$ proceeds in a similar way. First the approximation in Laplace domain is made

$$V(s)\mathscr{L}\lambda \approx V\left(\tfrac{1-e^{-sh}}{h}\right)\mathscr{L}\lambda \tag{2.6}$$

and then the inverse Laplace transform of the approximation is computed and used as an approximation of $\mathscr{V}\lambda$. Let the following expansion hold

$$V\left(\tfrac{1-e^{-sh}}{h}\right) = \sum_{j=0}^{\infty} \omega_j(V)e^{-shj} = \sum_{j=0}^{\infty} \omega_j(V)e^{-st_j}, \qquad \operatorname{Re} s > 0.$$

Remark 2.1 Note that $V(s)$ is an analytic and bounded function of s for $\operatorname{Re} s > 0$,

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

see [2]. Also $1-e^{-sh}$ is an analytic function of e^{-sh} and $\operatorname{Re}(1-e^{-sh}) > 0$ for $\operatorname{Re} s > 0$. Hence, the above expansion is well defined and the linear operators $\omega_j(V) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ are bounded.

Using (2.3) again, we see that the inverse Laplace transform of the approximation in (2.6) is given by

$$\mathscr{V}\lambda(t) \approx \sum_{j=0}^{\infty} \omega_j(V)\lambda(t-t_j).$$

Assuming causality of λ we obtain the convolution quadrature approximation at $t = t_n$:

$$\sum_{j=0}^{n} \omega_j(V)\lambda(t_n - t_j) = \sum_{j=0}^{n} \omega_{n-j}(V)\lambda(t_j).$$

Error and stability analysis of this first order time-discretization method and of convolution quadrature based on other A-stable linear multistep methods can be found in [20].

2.2 Runge-Kutta based convolution quadrature

Since A-stable linear multistep methods have order restricted to $p \leq 2$, Runge-Kutta based methods need to be considered. For the importance of high order methods in wave propagation problems see [4] and for the analysis of the resulting discrete systems see [21] and [7].

Let an m-stage Runge-Kutta method be given by its Butcher tableau:

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}.$$

In terms of A, b, and 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

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

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,

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

as $h \to 0$.

The corresponding stability function is defined by $R(z) = 1 + zb^T(I - Az)^{-1}\mathbb{1}$, where $\mathbb{1} = (1\ \dots\ 1)^T$ and the following approximation property holds

$$R(z) = \mathrm{e}^z + O(z^{p+1}). \tag{2.7}$$

We will only use Runge-Kutta methods with nonsingular matrix A whose stability function satisfies the following assumptions.

Assumption 2.1 *(a) A-stability, namely $|R(z)| \leq 1$ for all z, s.t.* $\mathrm{Re}\, z \leq 0$.
(b) stiff accuracy, i.e. $R(\infty) = 0$.
(c) for all $y \in \mathbb{R} \setminus \{0\}$, $|R(iy)| < 1$.

These assumptions are required by the theory of Runge-Kutta convolution quadrature representation, see [7].

Runge-Kutta methods work not just on equally spaced points $t_j = jh$, but also at stages $t_j + c_i h$, $i = 1,\dots,m$. For simplicity we will assume that $0 < c_1 < c_2 < \cdots < c_m = 1$. As in the previous section we will want to approximate the derivative of a function f, but this time at the vector of stages:

$$f(t + ch) = \begin{pmatrix} f(t + c_1 h) \\ \vdots \\ f(t + c_m h) \end{pmatrix}.$$

Using (2.3) and proceeding as in the previous section we see that an approximation in the Laplace domain of the form

$$s e^{csh} \mathscr{L} f(s) \approx \frac{\Delta(e^{-sh})}{h} e^{csh} \mathscr{L} f(s)$$

is required, where

$$e^{csh} = \begin{pmatrix} e^{c_1 sh} \\ \vdots \\ e^{c_m sh} \end{pmatrix}$$

and $\Delta(\zeta) : \mathbb{C} \to \mathbb{C}^{m\times m}$ is a matrix valued function with the property

$$\Delta(e^{-z})e^{cz} \approx ze^{cz}.$$

Next lemma gives a definition of such a function and proves some of its properties.

Lemma 2.1 *Let*

$$\Delta(\zeta) = \left(A + \frac{\zeta}{1-\zeta}\mathbb{1}b^T\right)^{-1} = A^{-1} - \zeta A^{-1}\mathbb{1}b^T A^{-1}. \tag{2.8}$$

Then the following hold:

(a) For $z \to 0$ it holds

$$\Delta(e^{-z})e^{cz} = ze^{cz} + O(z^{q+1}).$$

(b) If $\mu \notin \sigma(A^{-1})$, then $R(\mu) = \zeta^{-1}$ if and only if $\mu \in \sigma(\Delta(\zeta))$.

Proof The equality in (2.8) is readily proved by using the Sherman-Morrison formula and the assumption $b^T A^{-1}\mathbb{1} = 1$. Result (b) follows from the expression

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

proved in [21, Lemma 2.4].

Proof of (a) requires a few more steps. In [7, Lemma 2.5], it has been shown that

$$zb^T e^{cz} = e^z - 1 + O(z^{p+1}) \quad \text{and} \quad zAe^{cz} = e^{cz} - \mathbb{1} + O(z^{q+1}).$$

Hence,

$$\begin{aligned}\Delta(e^{-z})^{-1}ze^{cz} &= e^{cz} - \mathbb{1} + \frac{1}{1-e^{-z}}\mathbb{1} - \frac{e^{-z}}{1-e^{-z}}\mathbb{1} + O(z^{q+1}) \\ &= e^{cz} + O(z^{q+1}).\end{aligned}$$

□

Therefore we are in a similar position as in the previous section. The last step that we need to do is construct the expansion

$$V\left(\frac{\Delta(\zeta)}{h}\right) = \sum_{j=0}^{\infty} W_n^h(V)\zeta^j.$$

Remark 2.2 Note that A-stability and Lemma 2.1(b) imply that the eigenvalues of $\Delta(\zeta)$ for $|\zeta| < 1$ all lie in the right-half complex plane. Therefore the same arguments as in Remark 2.1 tell us that the above expansion is well defined and that the convolution weights $W_n^h(V)$ are $m \times m$ matrices of bounded linear operators mapping from $H^{-1/2}(\Gamma)$ to $H^{1/2}(\Gamma)$.

Recalling the definition of $V(s)$ we see that $W_n^h(V)$ are integral operators defined by

$$W_n^h\lambda(x) = \int_\Gamma w_n^h(\|x-y\|)\lambda(y)d\Gamma_y, \qquad x \in \Gamma,$$

where the kernels $w_n^h(d)$ are defined by the corresponding expansion

$$\frac{\exp\left(-\frac{\Delta(\zeta)}{h}d\right)}{4\pi d} = \sum_{n=0}^{\infty} w_n^h(d)\,\zeta^n. \tag{2.9}$$

Let us denote by g_n and $\mathbf{g}_n$ the following functions

$$g_n(x) = g(nh,x), \qquad \mathbf{g}_n(x) = \begin{pmatrix} g(nh+c_1h,x) \\ \vdots \\ g(nh+c_mh,x) \end{pmatrix}.$$

With this notation the Runge-Kutta convolution quadrature of (2.2) is given by

$$\mathbf{g}_n(x) = \sum_{i=0}^{n} \left(W_{n-i}^h \boldsymbol{\lambda}_i\right)(x),$$

where $\boldsymbol{\lambda}_n$ denotes

$$\boldsymbol{\lambda}_n(x) = \begin{pmatrix} \lambda(nh+c_1h,x) \\ \vdots \\ \lambda(nh+c_mh,x) \end{pmatrix}.$$

In the remainder of the paper we will require the scaled convolution kernels $\mathrm{w}_n(d) := 4\pi d w_n^h(hd)$. Notice that $\mathrm{w}_n(d)$ are the coefficients of the following expansion:

$$\exp(-\Delta(\zeta)d) = \sum_{n=0}^{\infty} \mathrm{w}_n(d)\,\zeta^n. \tag{2.10}$$

3 Sparsity of Runge-Kutta Convolution Weights

Our task in this section is to find the estimates for convolution weights $w_n^h(d)$ in terms of d and n. To do so, we first derive bounds for scaled convolution weights $\mathrm{w}_n(d)$ and next use these results to show that similar bounds hold also for $w_n^h(d)$.

The scaled convolution weight $\mathrm{w}_n(d)$ for $d > 0$ can also be expressed as

$$\mathrm{w}_n(d) = \frac{1}{2\pi i} \oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}\mathrm{e}^{-zd}dz, \tag{3.1}$$

see [21]. Here, γ represents a contour that encloses all the eigenvalues of A^{-1}.

To prove the main estimates, we will require to choose carefully the contour γ. First, we consider the domain Υ_r, $r > 0$:

$$\Upsilon_r = \{z \in \mathbb{C} \,:\, |R(z)| > r\}.$$

The contour γ_r is defined as the boundary this domain, i.e., $\gamma_r := \partial \Upsilon_r$. Hence, $|R(z)| = r$ holds for all $z \in \gamma_r$. Next, we prove some properties of domains Υ_r.

Let

$$A_+ = \{z \in \mathbb{C} \, : \, |R(z)| > |e^z|, \, \mathrm{Re}\, z > 0\}$$

denote the order star of R restricted to the right-half complex plane, see [17]. In fact A_+ denotes just the m bounded fingers containing the m, counting multiplicities, singularities of R. Since $|R(iy)| < 1$ for $y \neq 0$, the origin is the only point of intersection of the closure of the order star with the imaginary axis and hence

$$\overline{A}_+ \subset \Upsilon_1 \cup \{0\}.$$

We will need the following well-known lemma. Its proof can be found in Appendix.

Lemma 3.1 *There exist $q, \nu > 0$, such that the domain*

$$\{(x,y) \mid |y| < \nu x^{\frac{1}{\ell}}, \, 0 < x < q\}$$

belongs to Υ_1 (and intersects all the order star fingers). Here

$$\ell = \begin{cases} p+1, & \text{if } p \text{ is odd,} \\ 2s, & \text{if } p \text{ is even,} \end{cases}$$

where s is defined by

$$E(y) = |Q(iy)|^2 - |P(iy)|^2 = e_0 y^{2s} + O(y^{2s+2}), \; e_0 > 0.$$

Lemma 3.2 *Under Assumption 2.1, the domain Υ_1 is located in the open right-half plane and is bounded and connected (possibly multiply).*

Proof The boundedness follows directly from the assumption of stiff accuracy $R(\infty) = 0$. A-stability and the bound $|R(iy)| < 1$, $y \in \mathbb{R} \setminus 0$ imply that Υ_1 is located in the open right-half plane.

Let $\widetilde{\Upsilon}_1$ be a connected (possibly multiply) component of Υ_1. Then, by the maximum principle, $\widetilde{\Upsilon}_1$ must contain a singularity of $R(z)$ and the closure of the corresponding finger (minus the origin). According to Lemma 3.1, the intersection of $\widetilde{\Upsilon}_1$ with the all the other fingers is nonempty. Since $\widetilde{\Upsilon}_1$ contains all the singularities of Υ_1, by the maximum modulus principle applied to $R(z)$, it coincides with Υ_1. □

Remark 3.1 The domain Υ_1 is not necessarily simply connected: it can have a hole, namely, there can exist a bounded domain Υ', s.t. $R(z)$ vanishes in one of its interior points, $|R(z)| < 1$ inside Υ' and $\partial \Upsilon' \subset \partial \Upsilon_1$.

Remark 3.2 Note that in a small enough vicinity of $r = 1$, Υ_r stays bounded and connected. This follows from the fact that $z \in \partial \Upsilon_r$ is equivalent to

$$P(z) - \frac{1}{re^{i\phi}} Q(z) = 0, \qquad \phi \in [0, \, 2\pi), \; Q(z) \neq 0.$$

The roots of the polynomial depend continuously on its coefficients, and hence there exists δ_* s.t.

$$\text{the domain } \Upsilon_r \text{ is bounded and connected for } |r - 1| < \delta_*. \tag{3.2}$$

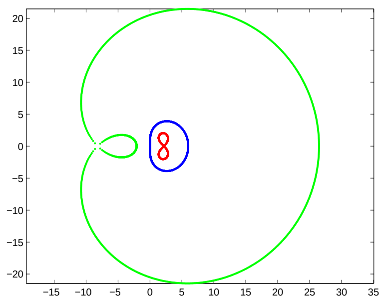

Fig. 3.1 Curves γ_r, for the 2-stage Radau IIA method, are plotted for $r = 1$ (middle curve in blue) and the critical values $r = r_1 = 5+3\sqrt{3}$ (outer curve in green) and $r = r_2 = 3\sqrt{3}-5$ (inner curve in red). For $r > r_1$ and $r < r_2$ the curve splits into two disjoint curves.

Corollary 3.1 *If the stability function of a Runge-Kutta method coincides with Padé approximant for the exponential, the domain Υ_1 is simply connected.*

Proof For the proof we need two ingredients:

1. Ehle's Conjecture [22, Theorem 7]. Any Padé approximation $R(z) = \frac{P(z)}{Q(z)}$, $\deg P = k$, $\deg Q = m$ is A-stable iff $m-2 \leq k \leq m$.
2. All zeros of such Padé approximants lie in the open left-half plane, see [12].

Hence, the existence of a bounded domain Υ', s.t. $|R(z)| < 1$ inside Υ' and $\partial\Upsilon' \subset \partial\Upsilon_1$ (i.e. a hole in Υ_1), contradicts the maximum modulus principle applied to the analytic function $\frac{1}{R(z)}$, $z \in \mathbb{C}_+$. □

Lemma 2.1(b) provides us with an easy way to draw the curves $\gamma_r = \partial\Upsilon_r$, i.e., by plotting the eigenvalues of $\Delta(\zeta)$ for all $|\zeta| = 1/r$.

In [4] the multiplicity of the eigenvalues of $\Delta(\zeta)$ for the 2- and 3-stage Radau IIA Runge-Kutta methods was discussed. In both cases $\Delta(\zeta)$ has only simple eigenvalues for $|\zeta| = 1$, as explained also by Corollary 3.1. For the 2-stage version, eigenvalues of multiplicity greater than 1 occur only for $\zeta = -5 \pm 3\sqrt{3}$. For a plot of these curves at the critical values and $r = 1$ see Figure 3.1.

Let us fix $r > 0$ satisfying (3.2) and choose a positively oriented contour $\gamma = \gamma_r$. For the rest of the paper we will assume that the domain Υ_1 is simply connected. However, all the arguments can be trivially extended to the case when it is multiply connected. By Remark 3.2, Υ_r, for sufficiently small $|r-1|$, is then also simply connected.

Remark 3.3 Note that the length of the curve γ_r is bounded, see [1, Lemma 3], by:

$$|\gamma_r| \leq 4md(\gamma_r),$$

where $d(\gamma_r)$ is a diameter of the curve.

From (3.1) the following bound on the Euclidean norm of $\mathrm{w}_n(d)$ follows:

$$\begin{aligned}\|\mathrm{w}_n(d)\| &\leq \frac{1}{2\pi}\left\|\int_{\gamma_r} R(z)^{n-1}\mathrm{e}^{-zd}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}dz\right\| \\ &\leq \frac{1}{2\pi}|\gamma_r|r^{n-1}\max_{z\in\gamma_r}\|\mathrm{e}^{-zd}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}\|.\end{aligned}$$

Denoting by $Q_A(z)=(I-Az)^{-1}$, one can deduce the bound

$$\begin{aligned}\max_{z\in\gamma_r}\|(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}\| &\leq \max_{z\in\gamma_r}\|(I-Az)^{-1}\|^2\|\mathbb{1}b^T\| \\ &\leq \max_{z\in\gamma_r}\|Q_A(z)\|^2\|b\|\sqrt{m},\end{aligned}$$

which implies that

$$\|\mathrm{w}_n(d)\| \leq \frac{1}{2\pi}r^{n-1}|\gamma_r|\|b\|\sqrt{m}\max_{z\in\gamma_r}|\mathrm{e}^{-zd}|\max_{z\in\gamma_r}\|Q_A(z)\|^2. \tag{3.3}$$

To understand the behaviour of a scaled convolution weight $\mathrm{w}_n(d)$ we need to find a bound on $\max_{z\in\gamma_r}|\mathrm{e}^{-zd}|$. To do so, we use the fact that the stability function $R(z)$ is an approximant to e^z, see (2.7), and thus $\max_{z\in\gamma_r}|\mathrm{e}^{-zd}|$ can be expressed via the value of $|R(z)|$ on γ_r.

For a Runge-Kutta method of order p we can write

$$R(z)=\mathrm{e}^z+f(z),$$

where $f(z)=O(z^{p+1})$.

Let us consider $z\in\gamma_r$ and $d\in\mathbb{R}_{>0}$. Multiplying the last equation by $\mathrm{e}^{-z}R(z)^{-1}$, taking modulus and raising to the dth power both sides of the equation we obtain

$$\begin{aligned}\max_{z\in\gamma_r}|\mathrm{e}^{-zd}| &= \max_{z\in\gamma_r}|R(z)^{-1}\left(1+f(z)\mathrm{e}^{-z}\right)|^d \\ &= r^{-d}\max_{z\in\gamma_r}|1+f(z)\mathrm{e}^{-z}|^d.\end{aligned}$$

On the other hand,

$$\max_{z\in\gamma_r}|\mathrm{e}^{-zd}|=\mathrm{e}^{-x_0 d},$$

where $x_0=\min_{z\in\gamma_r}\operatorname{Re}z$.

Hence

$$\mathrm{e}^{-x_0 d}=r^{-d}\left|1+f(z_0)\mathrm{e}^{-z_0}\right|^d, \tag{3.4}$$

where $z_0=x_0+iy_0$ is a point, such that

$$\operatorname{Re}z'\geq\operatorname{Re}z_0, \qquad \text{for all} \quad z'\in\gamma_r. \tag{3.5}$$

In order to bound this product we need to understand how x_0 and x_0+iy_0 behave. This question has been studied in [16] examining the behaviour of $R(z)$ in the order star [22]. Namely, when $r\to 1$, such x_0 is close to $r-1$ and $|z_0|=|x_0+iy_0|$ is close to $|r-1|$. This and the fact that $f(z)=O(z^{p+1})$ will allow us to obtain the required bounds on scaled convolution weights. Here we will employ the results from [16].

Definition 3.1 ([16]) Given a rational function $R(z)$ we define the error growth function as the real-valued function $\phi(x) := \sup_{\operatorname{Re} z<x} |R(z)|$.

Theorem 3.1 *(Theorem 7 in [16]) Let $R(z) = \frac{P(z)}{Q(z)}$ be an A-stable approximation to e^z of exact order $p \geq 1$, namely:*

$$R(z) = \frac{P(z)}{Q(z)} = \mathrm{e}^z + C_{p+1}z^{p+1} + O(z^{p+2}), \qquad \text{for} \quad z \to 0,\ C_{p+1} \neq 0. \tag{3.6}$$

Furthermore, assume $|R(iy)| < 1$ for $y \neq 0$, and $|R(\infty)| < 1$. Then we have for $x \to 0$:

– *if p is odd,*
$$\phi(x) = \mathrm{e}^x + O(x^{p+1}),$$
– *if p is even and $(-1)^{p/2}C_{p+1}x > 0$,*
$$\phi(x) = \mathrm{e}^x + O(x^{p+1}).$$
– *if p is even and $(-1)^{p/2}C_{p+1}x < 0$,*
$$\phi(x) = \mathrm{e}^x + O(x^{1+p/(2s-p)}),$$
where s is defined by
$$E(y) = |P(iy)|^2 - |Q(iy)|^2 = e_0 y^{2s} + O(y^{2s+2}),\ e_0 > 0. \tag{3.7}$$

Remark 3.4 ([16]) For $x < \operatorname{Re}\lambda_{min}$, with λ_{min} being an eigenvalue of A^{-1} with the smallest real part, $\phi(x)$ is a strictly monotonically increasing continuous function.

The following proposition shows that for $r \to 1$ $x_0 = \min_{z\in\gamma_r} \operatorname{Re} z$ is close to $r-1$.

Proposition 3.1 *Let $R(z)$ be the stability function of the Runge-Kutta method satisfying Assumption 2.1, let (3.6) hold and let $x_0 = \min_{z\in\gamma_r} \operatorname{Re} z$. Then for $r \to 1$:*

– *if p is odd,*
$$x_0 = r - 1 + O((r-1)^2).$$
– *if p is even and $(-1)^{p/2}C_{p+1}x_0 > 0$,*
$$x_0 = r - 1 + O((r-1)^2).$$
– *if p is even and $(-1)^{p/2}C_{p+1}x_0 < 0$,*
$$x_0 = r - 1 + o(|r-1|).$$

Proof On the contour γ_r $|R(z)| = r$. Since the error growth function $\phi(x)$ is a strictly monotonically increasing continuous function, see Remark 3.4, $\phi(x_0) = r$. The statement of the proposition follows from the application of the implicit function theorem to the 3 cases of Theorem 3.1 and the fact that $\phi(0) = 1$, $\frac{d\phi}{dx}(0) = 1$. □

Next proposition shows that when $r \approx 1$, the point z_0 defined by (3.5) lies in a small circle centered at the origin.

Proposition 3.2 *Let $R(z)$ be the stability function of the Runge-Kutta method satisfying Assumption 2.1 and (3.6). Then there exists $\delta_0 > 0$ and $K > 0$, s.t. for all $r: \ |r-1| < \delta_0$ the point $z_0 \in \gamma_r$ defined by (3.5) lies inside one of the circles specified below:*

1. *for p odd:*

$$|z_0| \leq K|r-1|.$$

2. *for p even:*
   (a) *if $r > 1$ and $(-1)^{\frac{p}{2}} C_{p+1} > 0$ or $r < 1$ and $(-1)^{\frac{p}{2}} C_{p+1} < 0$,*

$$|z_0| \leq K|r-1|.$$

   (b) *if $r > 1$ and $(-1)^{\frac{p}{2}} C_{p+1} < 0$ or $r < 1$ and $(-1)^{\frac{p}{2}} C_{p+1} > 0$,*

$$|z_0| \leq K|r-1|^{\frac{1}{2s-p}},$$

   where s is defined by (3.7).

Proof The proof of this statement closely follows the proof of Theorem 7 in [16]. As argued in the proof, for $x \to 0$ the maximum of $|R(x+iy)|$, $y \in \mathbb{R}$ has to lie inside the order star close to the origin. We consider the following cases (for $x \to 0$):

1. p is odd.
   As shown in the proof of Theorem 7 in [16], for $z = x+iy \to 0$, the local extrema of $|R(x+iy)|$ for a fixed x lie asymptotically on the lines $y = x\tan(k\pi/p)$, $k = 0,1,\cdots,p-1$. Since $|R(z)|$ achieves extremum at z_0, $|z_0| \leq C|x_0|$, where $C > 0$ and depends on the Runge-Kutta method.
   Proposition 3.1 gives an expression for x_0 (using $\phi(x_0) = r$):

$$x_0 = r - 1 + O((r-1)^2).$$

   Hence,

$$|z_0| \leq K|r-1|,$$

   for some $K > 0$.
2. p is even.
   (a) As proved in Theorem 7 in [16], for $(-1)^{p/2} C_{p+1} x_0 < 0$, $|z_0|$ is asymptotically ($z_0 \to 0$) bounded: $|z_0| \leq C|x_0|$, $C > 0$. The statement of the proposition is obtained with the help of the same arguments as in the previous case and the fact that $\operatorname{sgn} x_0 = \operatorname{sgn}(r-1)$.

(b) For the last case, namely $(-1)^{p/2}C_{p+1}x > 0$, in the proof of Theorem 7 in [16] it was shown that the maximum of $|R(x+iy)|$, for $x \to 0$, is achieved near the imaginary axis and lies on the curve $y^{2s-p} = Dx$, where $D \in \mathbb{R}$ and s is defined by (3.7).
Then, for x_0 being sufficiently small:

$$\begin{aligned}
|z_0| &= |x_0|^{1/(2s-p)} \left| x_0^{1-\frac{1}{2s-p}} + iD \right| \\
&= |D||x_0|^{1/(2s-p)} \left(1 + \frac{|x_0|^{2-2/(2s-p)}}{D^2} \right)^{1/2} \\
&\leq |D||x_0|^{1/(2s-p)} \left(1 + \frac{|x_0|^{2-2/(2s-p)}}{2D^2} + \cdots \right).
\end{aligned}$$

According to Proposition 3.4 in [17] $2s \geq p+1$, therefore, for even p, $2s \geq p+2$. This implies that $|x_0|^{2-1/(2s-p)} = o(|x_0|)$ and

$$|z_0| \leq K|r-1|^{\frac{1}{2s-p}},$$

for some $K > 0$. □

Now we have all the estimates necessary to prove the next proposition on the decay of scaled convolution weights.

Proposition 3.3 *Let $R(z)$ be the stability function of an m-stage Runge-Kutta method of order p satisfying Assumption 2.1 and (3.6).*

Let s be defined by (3.7). Then there exist positive constants G, G', C, C' and $\bar{\delta} \in (0,\,1)$, such that for $n \geq 1$ and $0 < \delta < \bar{\delta}$ the following estimates hold:

1. *p is odd*

$$\begin{aligned}
\|\mathrm{w}_n(d)\| &\leq G(1-\delta)^{n-d}(1+C\delta^{p+1})^d \qquad \textit{for} \quad d \leq n, \\
\|\mathrm{w}_n(d)\| &\leq G'(1+\delta)^{n-d}(1+C'\delta^{p+1})^d \qquad \textit{for} \quad d > n;
\end{aligned} \tag{3.8}$$

2. *p is even*
   (a) $C_{p+1}(-1)^{\frac{p}{2}} > 0$

$$\begin{aligned}
\|\mathrm{w}_n(d)\| &\leq G(1-\delta)^{n-d}(1+C\delta^{p+1})^d \qquad \textit{for} \quad d \leq n, \\
\|\mathrm{w}_n(d)\| &\leq G'(1+\delta)^{n-d}(1+C'\delta^{\frac{p+1}{2s-p}})^d \qquad \textit{for} \quad d > n;
\end{aligned} \tag{3.9}$$

   (b) $C_{p+1}(-1)^{\frac{p}{2}} < 0$

$$\begin{aligned}
\|\mathrm{w}_n(d)\| &\leq G(1-\delta)^{n-d}(1+C\delta^{\frac{p+1}{2s-p}})^d \qquad \textit{for} \quad d \leq n, \\
\|\mathrm{w}_n(d)\| &\leq G'(1+\delta)^{n-d}(1+C'\delta^{p+1})^d \qquad \textit{for} \quad d > n.
\end{aligned} \tag{3.10}$$

The convolution weight $\mathrm{w}_0(d)$ *satisfies:*

$$\|\mathrm{w}_0(d)\| \leq \exp(-\mu d), \tag{3.11}$$

for some $\mu > 0$.

Constants G, G', C, C', $\bar{\delta}$, μ *depend only on the Runge-Kutta method and do not depend on* n *and* d.

Proof Let us start with the case $\mathrm{w}_0(d)$. From the definition of scaled convolution weights

$$\exp\left(-\Delta(\zeta)d\right) = \sum_{n=0}^{\infty} \mathrm{w}_n(d)\,\zeta^n,$$
$$\Delta(\zeta) = A^{-1} - \zeta A^{-1}\mathbb{1}b^T A^{-1},$$

it follows that $\mathrm{w}_0(d) = \exp(-A^{-1}d)$. All the eigenvalues of A lie on the right from the imaginary axis (due to A-stability of the Runge-Kutta method) and hence the same hold for the eigenvalues of A^{-1}. The bound on $\mathrm{w}_0(d)$ can then be obtained from the definition of the matrix exponential.

For a general case $\mathrm{w}_n(d)$, $n \geq 1$, we use the bounds derived before, inserting (3.4) into (3.3):

$$\begin{aligned}\|\mathrm{w}_n(d)\| &\leq \frac{1}{2\pi} r^{n-1}\|b\|\sqrt{m}|\gamma_r| \max_{z\in\gamma_r} |\mathrm{e}^{-zd}| \max_{z\in\gamma_r} \|Q_A(z)\|^2 \\ &= \frac{1}{2\pi} r^{n-d-1}|\gamma_r| \max_{z\in\gamma_r} \|Q_A(z)\|^2 \|b\|\sqrt{m}|1+f(z_0)\mathrm{e}^{-z_0}|^d,\end{aligned} \tag{3.12}$$

where z_0 is such that for all $z' \in \gamma_r$ $\operatorname{Re} z' \geq \operatorname{Re} z_0$ and $f(z) = R(z) - \mathrm{e}^z$.

Let us first derive the bound for $|1 + f(z_0)\mathrm{e}^{-z_0}|$. For $|z| < \frac{1}{\lambda_0}$, where λ_0 is the spectral radius of A, we can expand $R(z) = 1 + zb^T(I - Az)^{-1}\mathbb{1}$ with the help of Neumann series to obtain an explicit expression for $f(z)$:

$$f(z) = R(z) - \mathrm{e}^z = z\sum_{l=p}^{\infty} b^T A^l \mathbb{1} z^l - \sum_{l=p+1}^{\infty} \frac{z^l}{l!}.$$

For $|z| < \frac{1}{\|A\|}$, we can trivially bound

$$|1 + f(z)\mathrm{e}^{-z}|^d \leq \left(1 + C|z|^{p+1}\right)^d, \tag{3.13}$$

where C depends on the Runge-Kutta method, but does not depend on z or d.

Now let $n > d$. We choose $r < 1$, $r = 1 - \delta$, $0 < \delta < \min\left\{\delta_*, \frac{1}{\|A\|}\right\}$. Here δ_* is a constant from (3.2), which allows to choose the contour γ_r, s.t. $|R(z)| = r$ for all $z \in \gamma_r$.

Then the bound (3.12), using (3.13), can be rewritten as:

$$\|\mathrm{w}_n(d)\| \leq \frac{1}{2\pi}(1-\delta)^{n-d-1}|\gamma_{1-\delta}| \max_{z\in\gamma_{1-\delta}} \|Q_A(z)\|^2 \|b\|\sqrt{m}\left(1 + C|z_0|^{p+1}\right)^d,$$

where z_0 is such that $\operatorname{Re} z_0 < \operatorname{Re} z$ for all $z \in \gamma_{1-\delta}$.

The length of the curve $\gamma_{1-\delta}$ as well as $\max_{z\in\gamma_{1-\delta}} \|Q_A(z)\|$ can be bounded by constants that depend on the Runge-Kutta method, see also Lemma 3.2 and Remarks 3.2 and 3.3. Applying Proposition 3.2 to estimate $\left(1+C|z_0|^{p+1}\right)^d$, we obtain the required expressions for the case $n > d$.

The bound for $n < d$ can be obtained similarly setting $r = 1+\delta$, with $0 < \delta < \min\left\{\delta_*, \frac{1}{\|A\|}\right\}$. □

Remark 3.5 Note that for even p the above bounds imply that when $2s - p < p+1$ scaled convolution weights decay exponentially. However, $2s \le 2m$ (m is a number of stages and the degree of the denominator in $R(z) = \frac{P(z)}{Q(z)}$), and thus for exponential decay it suffices that $p \ge m$.

Remark 3.6 From the proof it can be seen that the effect of dispersion of convolution weights is due to the term $|1 + f(z_0)e^{-z_0}|$ which was bounded by a constant greater than 1. We have not observed in the numerical experiments any case when this term is noticeably smaller than 1, which would force the norm of the convolution weights $\mathrm{w}_n(d)$ decay exponentially with increasing $n \approx d$.

We have shown that scaled convolution weights $\mathrm{w}_n(d)$ exhibit exponential decay outside of a neighborhood of $n \approx d$, which is an expression of Huygens principle and finite speed of wave propagation.

Our estimates also reflect some other properties of scaled convolution weights that are observed in numerical experiments. For example, inequalities (3.8) predict that for Runge-Kutta methods of odd orders with increasing n the size of the support of a convolution weight $\mathrm{w}_n(d)$ increases, however, with the rate of increase smaller for higher orders. An illustration of this effect is shown in Figure 3.2. We depicted the norms of scaled convolution weights $\mathrm{w}_n(d)$ on the semilogarithmic axis for three methods: BDF1 (1-stage Radau IIA of 1st order), 2-stage Radau IIA of 3rd order and 3-stage Radau IIA of 5th order. Particularly, one can see that for BDF1 the width of a convolution weight increases with n and is also quite large in comparison to the width of a convolution weight for 3-stage Radau IIA method of 5th order. The rate at which the width increases is also larger for BDF1, in agreement to what our estimates predict.

For Runge-Kutta methods of even orders the obtained estimates predict that for larger n and d the width of a convolution weight gets larger in a non-symmetric manner: the part of the support of a convolution weight $\mathrm{w}_n(d)$ corresponding to $d < n$ can get larger with increasing n faster than the part corresponding to $n > d$ or vice versa. For larger n, d the nonsymmetricity will become more and more visible. This can be illustrated through an example of Lobatto IIIC method of 6th order. Numerical experiments indicate that with increasing n the part of the support of the convolution weight $\mathrm{w}_n(d)$ of Lobatto IIIC method corresponding to $d < n$ increases slower than the part of the support $d > n$. This effect can be explained by estimates (3.9) as follows. It is known that the stability function of 4-stage Lobatto IIIC method is the $(2,4)$-Padé approximation to e^z. For such approximants the sign of the error term C_{p+1} is negative (see, for example, [9]); then the sign of $C_{p+1}(-1)^{\frac{p}{2}}$ is positive.

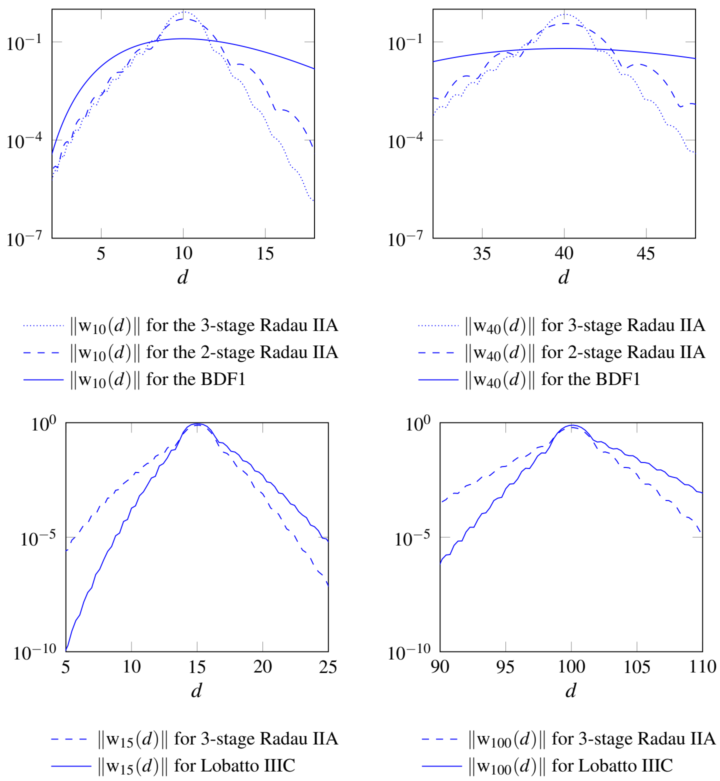

Fig. 3.2 Scaled convolution weights $\mathrm{w}_n(d)$ for BDF1, 2-stage and 3-stage Radau IIA methods and 4-stage Lobatto IIIC method.

According to the estimates (3.9) for larger n the part of the support of the convolution weights $\mathrm{w}_n(d)$ of Lobatto IIIC method corresponding to $d < n$ should increase slower than the part of the support $d > n$. To demonstrate these effects we depicted $\mathrm{w}_{15}(d)$ and $\mathrm{w}_{100}(d)$ for the Lobatto IIIC of 6th order and Radau IIA of 5th order in Figure 3.2.

The next proposition is a corollary of Proposition 3.3 and shows that (non-scaled) convolution weights $w_n^h(d)$ also experience exponential decay away from $\frac{d}{h} \approx n$.

Proposition 3.4 *Let $R(z)$ be the stability function of an m-stage Runge-Kutta method of order p satisfying Assumptions 2.1 and (3.6).*

Let s be defined by (3.7). Then there exist positive constants G, G', C, C' and $\bar{\delta} \in (0,\, 1)$, such that for $n \geq 1$ and $0 < \delta < \bar{\delta}$ the following estimates hold:

1. *p is odd*

$$\begin{aligned} \|w_n^h(d)\| &\leq \frac{G}{h}(1-\delta)^{n-\frac{d}{h}}(1+C\delta^{p+1})^{\frac{d}{h}} && \text{for} \quad \frac{d}{h} \leq n, \\ \|w_n^h(d)\| &\leq \frac{G'}{d}(1+\delta)^{n-\frac{d}{h}}(1+C'\delta^{p+1})^{\frac{d}{h}} && \text{for} \quad \frac{d}{h} > n; \end{aligned} \tag{3.14}$$

2. *p is even*
   (a) $C_{p+1}(-1)^{\frac{p}{2}} > 0$

$$\begin{aligned} \|w_n^h(d)\| &\leq \frac{G}{h}(1-\delta)^{n-\frac{d}{h}}(1+C\delta^{p+1})^{\frac{d}{h}} && \text{for} \quad \frac{d}{h} \leq n, \\ \|w_n^h(d)\| &\leq \frac{G'}{d}(1+\delta)^{n-\frac{d}{h}}(1+C'\delta^{\frac{p+1}{2s-p}})^{\frac{d}{h}} && \text{for} \quad \frac{d}{h} > n; \end{aligned} \tag{3.15}$$

   (b) $C_{p+1}(-1)^{\frac{p}{2}} < 0$

$$\begin{aligned} \|w_n^h(d)\| &\leq \frac{G}{h}(1-\delta)^{n-\frac{d}{h}}(1+C\delta^{\frac{p+1}{2s-p}})^{\frac{d}{h}} && \text{for} \quad \frac{d}{h} \leq n, \\ \|w_n^h(d)\| &\leq \frac{G'}{d}(1+\delta)^{n-\frac{d}{h}}(1+C'\delta^{p+1})^{\frac{d}{h}} && \text{for} \quad \frac{d}{h} > n. \end{aligned} \tag{3.16}$$

The convolution weight $w_0^h(d)$ satisfies:

$$\|w_0^h(d)\| \leq \frac{\exp(-\mu\frac{d}{h})}{4\pi d},$$

for some $\mu > 0$.

Constants G, G', C, C', $\bar{\delta}$, μ depend only on the Runge-Kutta method and do not depend on n, d and h.

Proof Let us again start with the case $w_0^h(d)$. From the definition of scaled convolution weights it follows that $w_0^h(d) = \frac{\mathrm{w}_0(\frac{d}{h})}{4\pi d}$, and the required bound can be obtained from (3.11). Note, however, that the convolution weight $w_0^h(d)$ has a singularity at $d = 0$.

Bounds for the case $\frac{d}{h} > n$ can be obtained straightforwardly from expressions (3.8, 3.9, 3.10) applied to $w_n^h(d) = \frac{\mathrm{w}_n(\frac{d}{h})}{4\pi d}$.

The case $\frac{d}{h} \leq n$ has to be treated separately: we cannot directly apply Proposition 3.3 for bounding $w_n^h(d) = \frac{\mathrm{w}_n(\frac{d}{h})}{4\pi d}$, since for small d this bound would be far from optimal. We will proceed as follows. First, we will show that a scaled convolution weight $\mathrm{w}_n(d)$ has a zero at $d = 0$ of multiplicity at least n. Next, this fact and ideas from the proof of Proposition 3.3 will be used to demonstrate that away from n convolution weights $w_n^h(d)$ decay exponentially.

Let us first expand the generating function of scaled convolution weights $\mathrm{e}^{-\Delta(\zeta)d}$, see (2.10), into Taylor series in ζ and then into series in d:

$$\exp\left(-\Delta(\zeta)d\right) = \sum_{n=0}^{\infty} \mathrm{w}_n(d)\zeta^n,$$
$$\exp\left(-\Delta(\zeta)d\right) = \sum_{n=0}^{\infty} \frac{(-\Delta(\zeta))^n}{n!} d^n.$$

Matching the powers of ζ we obtain the following expansion for $\mathrm{w}_n(d)$, $n \geq 0$:

$$\mathrm{w}_n(d) = \sum_{m=n}^{\infty} d^m f_m^n(A,b,h),$$

where $f_m^n(A,b,h)$ are matrix-valued functions of A, b and h.

Therefore, $\mathrm{w}_n(0) = 0$, $n \geq 1$. Let us recall the representation of scaled convolution weights (3.1):

$$\mathrm{w}_n(d) = \frac{1}{2\pi i} \oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}\mathrm{e}^{-zd}dz, \tag{3.17}$$

where γ is a contour that encloses all the eigenvalues of A^{-1}, $n \geq 1$. From this it follows that

$$\mathrm{w}_n(0) = \frac{1}{2\pi i} \oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}dz = 0. \tag{3.18}$$

The above implies as well that convolution weights $w_n^h(d)$, $n \geq 1$, have a zero at $d=0$ of order at least $n-1$.

Now let us prove the bounds (3.14, 3.15, 3.16) for $\frac{d}{h} < n$. Let $d \neq 0$. We express $\mathrm{e}^{-z\frac{d}{h}}$ in terms of an integral of a parameter $0 \leq \rho \leq 1$:

$$\mathrm{e}^{-z\frac{d}{h}} = 1 - \frac{zd}{h}\int_0^1 \mathrm{e}^{-z\frac{d}{h}\rho}d\rho.$$

Then the definition (3.17) can be rewritten:

$$\begin{aligned}
w_n^h(d) &= \frac{1}{2\pi i d}\oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}\mathrm{e}^{-z\frac{d}{h}}dz \\
&= \frac{1}{2\pi i d}\oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}dz - \\
&- \frac{1}{2\pi i h}\int_0^1\oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}z\mathrm{e}^{-z\frac{d}{h}\rho}dzd\rho.
\end{aligned}$$

The first term in the above sum equals 0, due to (3.18). The modulus of the second term, namely,

$$\frac{1}{2\pi ih}\int_0^1 \oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}z\mathrm{e}^{-z\frac{d}{h}\rho}dzd\rho,$$

can be estimated using the mean value theorem. We first bound the value of the integral

$$I(\rho,d)=\frac{1}{2\pi ih}\oint_\gamma R(z)^{n-1}(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}z\mathrm{e}^{-z\frac{d}{h}\rho}dz$$

repeating the arguments of the proof of Proposition 3.3. Note that two changes have to be made. First, d has to be substituted with $\frac{d}{h}$. And second, instead of bounding $\|(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}\|$ we now bound $\|(I-Az)^{-1}\mathbb{1}b^T(I-Az)^{-1}z\|$, for z lying on a contour $\gamma=\gamma_r$, by a constant that does not depend neither on d, nor on h or n, but only on the Runge-Kutta method.

It is not difficult to see that there exist positive constants G, C, $\bar{\delta}\in(0,\,1)$, $q>0$ such that for $n\geq 1$ and $0<\delta<\bar{\delta}$ the following estimate holds:

$$|I(\rho,d)|\leq\frac{1}{h}G(1-\delta)^{n-\frac{d}{h}\rho}(1+C\delta^q)^{\frac{d}{h}\rho},$$

for $\frac{d}{h}\rho\leq n$. In the above expression q is either $p+1$ or $\frac{p+1}{2s-p}$, as in Proposition 3.3. Clearly this estimate is valid for all $d:\frac{d}{h}<n$ and $\rho\in[0,\,1]$.

Next, we bound $\int_0^1 I(\rho,d)d\rho$ as:

$$\begin{aligned}\left|\int_0^1 I(\rho,d)d\rho\right| &\leq \max_{\rho\in[0,\,1]}|I(\rho,d)|\\ &\leq \frac{1}{h}G(1-\delta)^n\max_{\rho\in[0,\,1]}\left(\frac{1+C\delta^q}{1-\delta}\right)^{\frac{d}{h}\rho}\\ &\leq \frac{1}{h}G(1-\delta)^{n-\frac{d}{h}}(1+C\delta^q)^{\frac{d}{h}}.\end{aligned}$$

This finishes the proof of the statement. □

4 Computation of convolution weights

Let us write

$$\mathscr{K}_d(\zeta)=\frac{\exp\left(-\Delta(\zeta)\frac{d}{h}\right)}{4\pi d}.$$

The expansion (2.9) shows that $w_n^h(d)$ is the the nth Taylor coefficient of $\mathscr{K}_d(\zeta)$. Therefore, Cauchy integral formula gives another representation of $w_n^h(d)$,

$$w_n^h(d) = \frac{1}{2\pi i}\oint_{\mathscr{C}} \mathscr{K}_d(\zeta)\zeta^{-n-1}d\zeta.$$

Let us choose the contour $\mathscr{C}$ to be the circle centred at the origin with radius $\rho < 1$. Discretizing this integral with the composite Trapezoid rule gives the approximation

$$w_n^h(d) = \rho^{-n}\sum_{j=0}^{N}\mathscr{K}_d\left(\rho e^{ij\frac{2\pi}{N+1}}\right)e^{-ijn\frac{2\pi}{N+1}} + O(\rho^{N+1}), \qquad n = 0,1,\ldots,N. \quad (4.1)$$

In practice, the parameter $\rho > 0$ cannot be chosen arbitrarily small in finite precision arithmetic. If eps denotes the machine precision the best accuracy that can be achieved is $\sqrt{\text{eps}}$ with the choice $\rho = \text{eps}^{\frac{1}{2N}}$, see [19]. Using FFT, $w_n^h(d)$ can be computed in $O(N\log N)$ time for all $n = 0,1,\ldots,N$. However, if d is restricted, it is possible to avoid the scaling parameter ρ as described in the next proposition.

Proposition 4.1 *Given $D = Ch > 0$, the following holds true:*

1. *There exists a finite term approximation to the convolution kernel $\mathscr{K}_d(z) = \frac{\exp\left(-\Delta(z)\frac{d}{h}\right)}{4\pi d}$. Namely, given $\varepsilon > 0$ there exists $L = L(\log\frac{1}{\varepsilon h}, C) \in \mathbb{N}$ such that*

$$\left|\mathscr{K}_d(z) - \sum_{\ell=0}^{L} w_\ell^h(d)z^\ell\right| \le \varepsilon$$

   for all $z \in \mathbb{C}$ with $|z| \le 1$ and $0 < d \le D$.
2. *The convolution weights can be approximated with an arbitrary accuracy ε by an $L(\log\frac{1}{\varepsilon h}, \frac{D}{h}) + 1$-term discrete Fourier transform of the convolution kernel. Namely, given $\varepsilon > 0$ there exists $L = L(\log\frac{1}{\varepsilon h}, \frac{D}{h}) \in \mathbb{N}$ such that:*

$$\left|w_n^h(d) - \frac{1}{L+1}\sum_{\ell=0}^{L}\mathscr{K}_d(\mathrm{e}^{i\ell\frac{2\pi}{L}})\mathrm{e}^{-i\ell n\frac{2\pi}{L+1}}\right| \le \varepsilon$$

   for all $n \le L$ and $0 < d \le D$.
   Here $L = L(\log\frac{1}{\varepsilon h}, C)$ is the same as in the first statement and depends on $\log\frac{1}{\varepsilon h}$ and C at most linearly.

Proof The proof of the first statement trivially follows from the bounds on convolution weights derived in Proposition 3.4. The proof of the second statement can be obtained by sampling $\mathscr{K}_d(z)$ in $L(\log\frac{1}{\varepsilon h}, \frac{D}{h}) + 1$ points on unit circle and applying the inverse discrete Fourier transform to the resulting sequence. □

Remark 4.1 Note that in the above statement the dependence of L on $\log\frac{1}{h}$ cannot be removed. To illustrate this fact, in Figure 4.1 we plot $n_* = \sup\{n \in \mathbb{N} \mid \|w_\ell^h(d)\| < \varepsilon$, for all $\ell \ge n,\ d \le D\}$ for different values of h and ε and fixed $\frac{D}{h} = 10$, for 3-stage Radau IIA method of the fifth order.

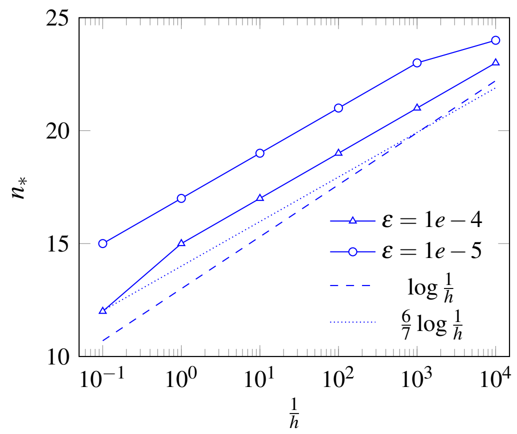

Fig. 4.1 Dependence of $n_* = \sup\{n \in \mathbb{N} \mid \|w_\ell^h(d)\| < \varepsilon$, for all $\ell \geq n$, $d \leq D\}$ on $\frac{1}{h}$, for $\varepsilon = 1e-4$, $1e-5$ and fixed $\frac{D}{h} = 10$, for 3-stage Radau IIA method.

5 Applications

The idea of use of sparsity of convolution weights to speed up calculations is not new. Most straightforward way of using the sparsity is to notice that for large enough n, the weights W_j^h, $j > n$, need not be computed but can be approximated by zero. In order to describe more advanced algorithms we need to briefly introduce the Galerkin boundary element discretization of convolution weights.

Let the boundary Γ be split into M disjoint panels $\tau_1, \ldots, \tau_M$ so that $\Gamma = \cup_i \bar{\tau}_i$. The span of piecewise constant basis functions

$$b_i(x) = \begin{cases} 1 & x \in \tau_i \\ 0 & x \notin \tau_i \end{cases}, \qquad i = 1, 2, \ldots, M,$$

defines a finite dimensional subspace $X \subset H^{-1/2}(\Gamma)$.

The corresponding Galerkin discretization of a convolution weight W_n^h is given by

$$\begin{aligned} \left(\mathbf{W}_n^h\right)_{ij} &= \int_\Gamma \left(W_n^h b_i\right)(x) b_j(x) d\Gamma_x \\ &= \int_\Gamma \int_\Gamma w_n^h(\|x-y\|) b_i(y) b_j(x) d\Gamma_y d\Gamma_x \\ &= \int_{\tau_i} \int_{\tau_j} w_n^h(\|x-y\|) d\Gamma_y d\Gamma_x. \end{aligned}$$

Remark 5.1 Convolution weights W_n^h are $m \times m$-matrices of operators bounded as mappings from $H^{-1/2}(\Gamma)$ to $H^{1/2}(\Gamma)$. Therefore if

$$W_n^h = \begin{pmatrix} W_n^{11} & \cdots & W_n^{1m} \\ \vdots & \cdots & \vdots \\ W_n^{m1} & \cdots & W_n^{mm} \end{pmatrix},$$

then $\mathbf{W}_n^h$ should be understood as a matrix of matrices (a tensor) and

$$\left(\mathbf{W}_n^h\right)_{ij} = \begin{pmatrix} \int_\Gamma \left(W_n^{11} b_i\right)(x) b_j(x) d\Gamma_x & \cdots & \int_\Gamma \left(W_n^{1m} b_i\right)(x) b_j(x) d\Gamma_x \\ \vdots & \cdots & \vdots \\ \int_\Gamma \left(W_n^{m1} b_i\right)(x) b_j(x) d\Gamma_x & \cdots & \int_\Gamma \left(W_n^{mm} b_i\right)(x) b_j(x) d\Gamma_x \end{pmatrix}.$$

For the understanding of this section it is however sufficient to consider the scalar case, $m = 1$.

The sparsity of convolution weights shows that many entries in the Galerkin matrices need not be computed. This fact, though only for linear multistep based methods, has been used in [15] to construct and analyse an efficient algorithm.

5.1 FFT and sparsity

The use of FFT, as in (4.1), usually destroys any sparsity, but in [6] it has been shown that both in this case advantage can be made of sparsity. Here we will just briefly explain the main idea.

In (4.1) we have seen that the convolution kernels can be approximated by a discrete Fourier transform and hence the same is true of the convolution weights

$$\mathbf{W}_n^h \approx \rho^{-n} \frac{1}{N+1} \sum_{\ell=0}^{N} \mathbf{V}(\rho e^{i\ell \frac{2\pi}{N+1}}) e^{-i\ell n \frac{2\pi}{N+1}},$$

for $m = 0, 1, \ldots, N$. This shows that N convolution weights can be computed in $O(N \log N)$ time. Recall that for a fixed time interval $[0, T]$, $N = T/h$.

From Proposition 3.4 we know that for a fixed $n_0 > 0$

$$\|w_n^h(d)\| \leq \frac{C}{h}(1-\delta)^{n-\frac{d}{h}} \leq \frac{\widetilde{C}}{h}(1-\delta)^{n-n_0},$$

for all $d \in (0, n_0 h)$ and $n > n_0$ with C and $\widetilde{C}$ constants. Hence there exists $n_1 \propto \log \varepsilon^{-1} + \log h^{-1}$ such that

$$\|w_n^h(d)\| \leq \varepsilon, \qquad \text{for all } 0 < d < n_0 h \text{ and } n > n_1.$$

Therefore for $n > n_1$, the "near-field" in matrices $\mathbf{W}_n^h$ can be approximated by zero:

$$\left(\mathbf{W}_n^h\right)_{ij} = \int_{\tau_i} \int_{\tau_j} w_n^h(\|x-y\|) d\Gamma_y d\Gamma_x \approx 0, \quad \text{if } \operatorname{dist}(\tau_i, \tau_j) < n_0 h,\ n > n_1.$$

Unfortunately this is not true for the $N+1$ matrices $\mathbf{V}(\mathrm{e}^{i\ell\frac{2\pi}{N+1}})$, further problem being that the near-field forms the part of the matrix which fast methods such as hierarchical matrices and the fast multipole method cannot be applied to. To reduce considerably the computational costs, we show next how to reduce the number of matrices for which the near-field needs to be computed from $O(N)$ to $O(\log N)$ and still make effective use of FFT. First we compute the n_1 weights $\mathbf{W}_n^h$, $n = 0, 1, \dots, n_1$ using

$$\mathbf{W}_n^h \approx \frac{\rho^{-n}}{n_1+1} \sum_{\ell=0}^{n_1} \mathbf{V}(\rho \mathrm{e}^{i\ell\frac{2\pi}{n_1+1}}) \mathrm{e}^{-i\ell n_1 \frac{2\pi}{N+1}}, \quad n = 0, 1, \dots, n_1.$$

This is not an expensive operation since n_1 depends only logarithmically on N. The remaining weights are computed using a similar formula as before in $O(N \log N)$ time

$$\mathbf{W}_n^h \approx \frac{\rho^{-n}}{N+1} \sum_{\ell=0}^{N} \widetilde{\mathbf{V}}(\rho \mathrm{e}^{i\ell\frac{2\pi}{N+1}}) \mathrm{e}^{-i\ell n \frac{2\pi}{N+1}}, \qquad n = n_1+1, \dots, N,$$

where

$$(\widetilde{\mathbf{V}}(s))_{ij} = \begin{cases} 0 & \text{if } \operatorname{dist}(\tau_i, \tau_j) < n_0 h \\ (\widetilde{\mathbf{V}}(s))_{ij} & \text{otherwise.} \end{cases}$$

Thereby N convolution weights can still be computed in $O(N \log N)$ time, but only for a $O(\log N)$ number of evaluations of $\mathbf{V}(s)$ is it necessary to compute the near-field.

For a more thorough explanation of how to use such ideas in a full algorithm for *solving* the discretized equations see [6].

6 Conclusions

In the present work the behaviour of the convolution weights of Runge-Kutta convolution quadrature has been analyzed. It was proved that convolution weights $w_n^h(d)$ decay exponentially away from $nh \approx d$. The obtained estimates on convolution weights explain the dependence of the size of approximate support of a convolution weight on the order of the underlying Runge-Kutta method. The results of this work can be used for design of the fast algorithms for solution of TDBIE for three-dimensional wave equation.

A Proof of Lemma 3.1

Lemma A.1 *(Lemma 3.1) There exist $q, \nu > 0$, such that the domain*

$$\{(x,y) \mid |y| < \nu x^{\frac{1}{\ell}},\ 0 < x < q\} \tag{A.1}$$

belongs to Υ_1 (and intersects all the order star fingers). Here

$$\ell = \begin{cases} p+1, & p \text{ is odd,} \\ 2s, & p \text{ is even,} \end{cases}$$

where s is defined by

$$E(y) = |Q(iy)|^2 - |P(iy)|^2 = e_0 y^{2s} + O(y^{2s+2}),\ e_0 > 0.$$

Proof We rewrite the stability function as

$$R(z) = \mathrm{e}^z + C_{p+1} z^{p+1} + r(z), \qquad C_{p+1} \neq 0,$$

where $r(z) = O(z^{p+2})$.

Let us consider the following cases.

1. p is odd. For a fixed $x \to 0$,

$$\begin{aligned} |R(x+iy)|^2 &= \mathrm{e}^{2x} + 2C_{p+1}\,\mathrm{Re}\left(\mathrm{e}^{x+iy}(x-iy)^{p+1}\right) + \\ &+ 2\,\mathrm{Re}\left(\mathrm{e}^{x+iy} r(x-iy)\right) + C_{p+1}^2 (x^2+y^2)^{p+1} + |r(x+iy)|^2 \\ &= 1 + 2x + 2C_{p+1}(-1)^{\frac{p+1}{2}} y^{p+1} + O(y^{p+2}). \end{aligned} \tag{A.2}$$

Note that $|R(iy)| < 1$, hence it is necessary that

$$C_{p+1}(-1)^{\frac{p+1}{2}} < 0.$$

From the above and (A.2) it follows that there exists $q, \nu > 0$, s.t. $|R(x+iy)| > 1$ for all

$$\left\{(x,\ y) \mid 0 < x < q,\ |y| < \nu x^{\frac{1}{p+1}}\right\}.$$

2. p is even. In this case we will make use of properties of an E-polynomial, see [17, Chapter IV]:

$$E(y) = |Q(iy)|^2 - |P(iy)|^2 = e_0 y^{2s} + O(y^{2s+2}), \tag{A.3}$$

where $2s \geq p+1$. For the Runge-Kutta methods with $|R(iy)| \leq 1$, $y \in \mathbb{R}$,

$$E(y) \geq 0.$$

Clearly, $E(y) \equiv 0$ implies that $|R(iy)| = 1$ for all $y \in \mathbb{R}$; for Runge-Kutta methods satisfying assumption (2.1), $e_0 > 0$.

Let us define

$$\psi_y(x) = |R(x+iy)|^2.$$

For a fixed y we can expand the above expression into Taylor series in x:

$$\psi_y(x) = |R(iy)|^2 + x\frac{d\psi_y}{dx}(0) + O(x^2).$$

Using (A.3), we can rewrite the first term:

$$|R(iy)|^2 = 1 - e_0 y^{2s} + O(y^{2s+2}).$$

For even p,

$$|R(x+iy)|^2 = \mathrm{e}^{2x} + 2C_{p+1}(-1)^{\frac{p}{2}} \mathrm{e}^x x y^p + r_1(x,y) + \mathrm{e}^x r_2(x,y) + \mathrm{e}^x x r_3(x,y) + O(x^2),$$

where $r_1(x,y) = O(x^2)$, $r_2(x,y) = O(y^{p+2})$, $r_3(x,y) = O(y^{p+2})$.

Then,

$$\psi_y(x) = 1 - e_0 y^{2s}\left(1 - \frac{x}{e_0 y^{2s}} - 2C_{p+1}(-1)^{\frac{p}{2}} \frac{x y^p}{e_0 y^{2s}} - \frac{x}{e_0 y^{2s}} r_2(x,y)\right) + O(x^2).$$

From the above expression we can see that there exists $q,\ \nu > 0$, s.t. $|R(x+iy)| > 1$ for all

$$\left\{(x,\ y) \mid 0 < x < q,\ |y| < \nu x^{\frac{1}{2s}}\right\}.$$

Since the bounds derived are asymptotically optimal, the domain (A.1) indeed intersects all the order star fingers. □

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