A Generalized Convolution Quadrature with Variable Time Stepping*

M. Lopez-Fernandez† S. Sauter‡

December 23, 2011

Abstract

In this paper, we will present a generalized convolution quadrature for solving linear parabolic and hyperbolic evolution equations. The original convolution quadrature method by Lubich works very nicely for equidistant time steps while the generalization of the method and its analysis to non-uniform time stepping is by no means obvious. We will introduce the generalized convolution quadrature allowing for variable time steps and develop a theory for its error analysis. This method opens the door for further development towards adaptive time stepping for evolution equations. As the main application of our new theory we will consider the wave equation in exterior domains which are formulated as retarded boundary integral equations.

Keywords: variable step size, convolution quadrature, convolution equations, retarded potentials, boundary integral equations, wave equation.

Mathematics Subject Classification (2000): 65M15, 65R20, 65L06, 65M38

1 Introduction

In this paper, we will present a numerical method for the discretization of linear convolution equations of the form

$$k * \phi = g, \tag{1}$$

*Part of this work has been carried out during a visit of the second author at the Department of Mathematics, University of California, San Diego, La Jolla. This support is gratefully acknowledged. The first author has been partially supported by the Spanish grant MTM 2010-19510.

†Institut für Mathematik, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland, e-mail: maria.lopez@math.uzh.ch

‡Institut für Mathematik, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland, e-mail: stas@math.uzh.ch

where $*$ denotes convolution with respect to time, g is a given function, and k is some fixed kernel function, in such a way that (1) is understood as a mapping of the function ϕ into some function space. In many applications such as partial differential equations of hyperbolic or parabolic type the kernel function k is defined as the inverse Laplace transform of the *transfer function* $\mathcal{K}$ in the Laplace domain and analyticity of $\mathcal{K}$ is assumed in a region containing the half plane $\operatorname{Re} z \geq \sigma_0 > 0$. For this type of problems, the convolution quadrature method has been developed originally by Lubich, see [6, 7, 10, 9] for parabolic problems and [8] for hyperbolic ones. The idea is to express the convolution kernel k as the inverse Laplace transform of $\mathcal{K}$ and reduce the problem to the solution of scalar ODEs of the form $y' = zy + g$, for z the variable in the Laplace domain. The temporal discretization then is based on the approximation of the solution of these ODEs by some time-stepping method and the transformation of the resulting equation back to the original time domain. This results in a discrete convolution in time which has very nice properties: a) It allows for FFT-type algorithms for solving the discrete convolution equation and b) the theory of ODEs can be employed nicely for deriving error estimates in the Laplace domain and, then, these estimates can be transformed back to the original time domain via Parseval's theorem.

On the other hand, there is also a drawback in the convolution quadrature method. Since it heavily employs the continuous *and* discrete Fourier-Laplace transforms for the formulation of the method and its analysis, the generalization to variable time-stepping is by no means obvious. However, if the right-hand side is not uniformly smooth and/or contains non-uniformly distributed variations in time, and/or consists of localized pulses, the use of adaptive time stepping becomes very important in order to keep the number of time steps reasonably small. Furthermore, the introduction of adaptivity is the first step in the development of strategies to control the step size in terms of the behavior of the solution to the integral equation.

In this paper, we will present a generalized convolution quadrature which allows for variable time stepping and develop a new theory for its error analysis. We restrict to the implicit Euler method for the time discretization. Note that the use of low order methods is justified for problems, where the solution, possibly, contains non-uniformly distributed irregularities. We emphasize that our derivation of the method can be extended to higher order Runge–Kutta methods, but the representation of the discrete solution becomes more complicated and the extension of the analysis is by no means straightforward. It is our opinion that fully understanding the first order method will open the way to further developments, both from the analytical and the algorithmic point of view.

Our idea is based on introducing adaptivity in the time integration of the scalar ODEs $y' = zy + g$. This idea is already present in the fast and oblivious algorithm developed in [5]. However this algorithm is restricted to *sectorial* convolution kernels and, thus, not applicable to wave equations. Furthermore, no error analysis is available. Our main application is the solution of retarded potential integral equations (RPIE) which arise if the wave equation in an unbounded exterior domain is formulated as a space-time integral equation on the boundary of the scatterer. The most popular numerical approaches for its discretization in the literature are: a) the direct space-time Galerkin discretization of the RPIE and b) the convolution quadrature. For the first class of methods only very recently a temporal discretization with variable time steps has been proposed [15], while for the convolution quadrature, to the best of our knowledge, such a generalization does not exist in the literature.

The paper is organized as follows. In Section 2 we introduce abstract one-sided convolution equations and formulate appropriate assumptions on the growth behavior of the transfer operator in some complex half plane. Section 3 is concerned with the temporal discretization of the convolution equation via the time integration of a parameter-dependent ODE in the Laplace domain. The error analysis for the discretization of this abstract equation is developed in Section 4. We apply this theory to the time-space discretization of retarded potential integral equations for solving the wave equation in Section 5 and give some concluding remarks in Section 6. Some technical estimates for the stability function for the implicit Euler method are postponed to the Appendix.

2 One-Sided Convolution Equations

We consider the class of convolution operators as described in [8, Sec. 2.1] and recall its definition. Let B and D denote some normed vector spaces and let $\mathcal{L}(B,D)$ be the space of continuous, linear mappings. As a norm in $\mathcal{L}(B,D)$ we take the usual operator norm

$$\|\mathcal{F}\| := \sup_{u\in B\backslash\{0\}} \frac{\|\mathcal{F}u\|_D}{\|u\|_B}.$$

For given right-hand side $g:\mathbb{R}_{\geq 0}\rightarrow D$, we consider the problem of finding $\phi:\mathbb{R}_{\geq 0}\rightarrow B$ such that for all $t\geq 0$

$$\int_0^t k(t-\tau)\,\phi(\tau)\,d\tau = g(t) \tag{2}$$

considered as an equation in D. The kernel operator k is defined via a *transfer operator* $\mathcal{K}$ as follows. Let $\mathcal{K}: I_{\sigma_0}\rightarrow\mathcal{L}(B,D)$ be an analytic operator-valued function in a half-plane

$$I_{\sigma_0} := \{z\in\mathbb{C} : \operatorname{Re} z \geq \sigma_0\}, \quad \text{for some } \sigma_0 > 0,$$

which is bounded by

$$\|\mathcal{K}(z)\| \leq M\,|z|^{\theta}, \qquad \forall z\in I_{\sigma_0}, \tag{3}$$

for some $M>0$ and $\theta\in\mathbb{R}$. For $m\in\mathbb{Z}$, we define

$$\mathcal{K}_m(z) := z^{-m}\mathcal{K}(z). \tag{4}$$

We choose $m > \max\{-1, \theta + 1\}$, so that the Laplace inversion formula

$$k_m(t) := \frac{1}{2\pi \mathrm{i}} \int_\gamma \mathrm{e}^{zt} \mathcal{K}_m(z)\, dz, \tag{5}$$

for a contour $\Gamma = \sigma + \mathrm{i}\,\mathbb{R}$, $\sigma \geq \sigma_0$, defines a continuous and exponentially bounded operator $k_m(t)$, which by Cauchy's integral theorem vanishes for $t < 0$. As in [8] we denote the convolution $k * \phi$ by

$$(\mathcal{K}(\partial_t)\phi)(t) := \left(\frac{d}{dt}\right)^m \int_{-\infty}^{t} k_m(t-\tau)\,\phi(\tau)\, d\tau = \int_0^\infty k_m(\tau)\,\phi^{(m)}(t-\tau)\, d\tau. \tag{6}$$

Our goal is to solve the convolution equation

$$\mathcal{K}(\partial_t)\,\phi = g, \tag{7}$$

where we always assume that the given right-hand side is temporarily smooth and vanishes near $t = 0$. Additional smoothness assumptions at $t = 0$ will be formulated later.

The composition rule for one-sided convolutions (cf. [8, (2.3), (2.22)]) leads to

$$\phi = \mathcal{K}^{-1}(\partial_t)\, g$$

so that

$$\phi(t) = \int_0^t \left(\frac{1}{2\pi \mathrm{i}} \int_\gamma \mathrm{e}^{z\tau} (\mathcal{K}^{-1})_m(z) dz\right) g^{(m)}(t-\tau)\, d\tau \tag{8}$$

for appropriately chosen m. This representation of the solution clearly shows that the growth behavior of $\left\|\mathcal{K}^{-1}(z)\right\|$ determines the smoothness requirements on the right-hand side g. We will assume that, for some $M > 0$ and $\mu \in \mathbb{R}$, a similar estimate to (3) holds for $\mathcal{K}^{-1}$, namely

$$\left\|\mathcal{K}^{-1}(z)\right\| \leq M\,|z|^\mu, \qquad \forall z \in I_{\sigma_0}. \tag{9}$$

In this way, m will be chosen $m > \max\{-1, \mu + 1\}$.

3 Temporal Discretization

Our main application will be the time discretization of retarded potentials associated to wave equations. In this context, (9) will typically holds for some $\mu > 0$. As we have seen in the previous section, *solving* the convolution equation (7) is equivalent to the *evaluation* of the convolution with the inverse transfer function applied to the right-hand side (cf. (8)), which can be written in compact form as

$$\phi = (\mathcal{K}^{-1})_m(\partial_t) g^{(m)}.$$

In an abstract setting, we are concerned with the approximation of the mapping

$$f \mapsto \mathcal{C}(\partial_t) f \tag{10}$$

in prescribed time points for a given transfer operator $\mathcal{C}$ which satisfies a bound like (9) for some $\mu < 0$. To discretize (10) we express the mapping in (10) as the inverse Laplace transform of the transfer operator:

$$\left(\mathcal{C}\left(\partial_t\right) f\right)(t) = \frac{1}{2\pi\,\mathrm{i}} \int_0^t \left(\int_\gamma \mathrm{e}^{z(t-\tau)}\, \mathcal{C}\left(z\right)\, dz \right) f(\tau)\, d\tau.$$

By interchanging the order of integration, we can write

$$\left(\mathcal{C}\left(\partial_t\right) \phi\right)(t) = \frac{1}{2\pi\,\mathrm{i}} \int_\gamma \mathcal{C}\left(z\right) u\left(z,t\right) dz, \tag{11}$$

where

$$u\left(z,t\right) := \int_0^t \mathrm{e}^{z(t-\tau)}\, f(\tau)\, d\tau.$$

Note that the function u in (11) is the solution of the initial value problem

$$u_t(z,t) = z\, u(z,t) + f(t), \qquad u(z,0) = 0. \tag{12}$$

We will consider the implicit Euler method with variable mesh width for the discretization of (12). For a time mesh $t_0 = 0 < t_1 < t_2 \cdots < t_N = T$ with variable step sizes $\Delta_j = t_j - t_{j-1}$, $j = 1, \ldots, N$, the implicit Euler method for (12) is given by

$$u_n\left(z\right) = \frac{1}{1-\Delta_n z} u_{n-1}\left(z\right) + \frac{\Delta_n}{1-\Delta_n z} f_n, \quad u_0\left(z\right) = 0. \tag{13}$$

This recursion can be resolved and we obtain

$$u\left(z,t_n\right) \approx u_n(z) = \sum_{j=1}^{n} \Delta_j f_j \prod_{k=j}^{n} \frac{1}{1-\Delta_k z}. \tag{14}$$

By considering (11) at time point t_n and replacing $u\left(z,t_n\right)$ by the approximation $u_n\left(z\right)$ we obtain the approximation to the convolution $\left(\mathcal{C}\left(\partial_t\right)\phi\right)\left(t_n\right)$:

$$\left(\mathcal{C}\left(\partial_t\right) \phi\right)\left(t_n\right) \approx \frac{1}{2\pi\,\mathrm{i}} \int_\gamma \mathcal{C}\left(z\right) u_n\left(z\right)\, dz. \tag{15}$$

By solving the recursion (13) and using Cauchy's integral formula for the divided differences of an analytic function (see for instance [2, Formula (51)]) we conclude from the combination of (14) and (15) that the approximation in (15) can be written in the form

$$\left(\mathcal{C}\left(\partial_t\right) \phi\right)\left(t_n\right) \approx \sum_{j=1}^{n} \omega_{n,j}\left(0\right) \left(\left[\frac{1}{\Delta_j}, \frac{1}{\Delta_{j+1}}, \ldots, \frac{1}{\Delta_n} \right] \mathcal{C} \right) f_j, \tag{16}$$

where $\omega_{n,j}\left(z\right) = \prod_{\ell=j+1}^{n} \left(z - \Delta_\ell^{-1}\right)$ and $\left[\frac{1}{\Delta_j}, \frac{1}{\Delta_{j+1}}, \ldots, \frac{1}{\Delta_n}\right] \mathcal{C}$ denotes Newton's divided difference with respect to the nodes Δ_k^{-1}, $j \leq k \leq n$.

For $\mathcal{C} = (\mathcal{K}^{-1})_m$ and $f = g^{(m)}$, formula (16) defines an approximation $\phi_n \approx \phi(t_n)$ to the *solution* of the convolution equation (7). In order to define a recursive method based on $\mathcal{K}$ rather than $\mathcal{K}^{-1}$ we need the following lemma.

Lemma 1 (Inverse formula) *Let $(x_i)_{i\in\mathbb{N}} \subset \mathbb{R}$ denote a sequence of points and let $f : \mathbb{R} \to E$ denote some function into a set E of linear mappings. We assume that $f(x_i)$ is invertible for all $i \in \mathbb{N}_{\geq 1}$. Let $\tilde{\omega}_{n,j}(x) := \prod_{\ell=j+1}^{n} (x - x_\ell)$. A mapping of the form*

$$q_n := \sum_{j=1}^{n} \tilde{\omega}_{n,j}(0) \left([x_j, x_{j+1}, \ldots, x_n] f \right) u_j, \quad n \in \mathbb{N}_{\geq 1} \tag{17}$$

can be inverted and it holds

$$u_n = \sum_{j=1}^{n} \tilde{\omega}_{n,j}(0) [x_j, x_{j+1}, \ldots, x_n] f^{-1} q_j, \quad n \in \mathbb{N}_{\geq 1}. \tag{18}$$

Proof. We denote the left-hand side in (18) by $\tilde{u}_n$ and prove that $\tilde{u}_n = u_n$ if we replace q_j by the definition (17). By inserting (17) into the right-hand side of (18) we obtain

$$\tilde{u}_n = \sum_{j=1}^{n} \tilde{\omega}_{n,j}(0) [x_j, x_{j+1}, \ldots, x_n] f^{-1} \sum_{k=1}^{j} \tilde{\omega}_{j,k}(0) \left([x_k, x_{k+1}, \ldots, x_j] f \right) u_k.$$

Observe that $\tilde{\omega}_{n,j}(0)\, \tilde{\omega}_{j,k}(0) = \tilde{\omega}_{n,k}(0)$ so that after interchanging the ordering of the summations

$$\tilde{u}_n = \sum_{k=1}^{n} \tilde{\omega}_{n,k}(0) \left(\sum_{j=k}^{n} [x_j, x_{j+1}, \ldots, x_n] f^{-1} \left([x_k, x_{k+1}, \ldots, x_j] f \right) \right) u_k. \tag{19}$$

The Leibniz rule for divided differences [2, Corollary 28] leads to

$$\begin{aligned} \sum_{j=k}^{n} [x_j, x_{j+1}, \ldots, x_n] f^{-1} \left([x_k, x_{k+1}, \ldots, x_j] f \right) &= [x_k, x_{k+1}, \ldots, x_n] \left(f^{-1} f \right) \\ &= [x_k, x_{k+1}, \ldots, x_n] I = \delta_{k,n} I. \end{aligned}$$

Here, I is the identity mapping considered as a constant function in x. Hence, only the summand with $k = n$ in (19) is different from zero and the assertion follows. ■

Definition 2 (Generalized Convolution Quadrature) *For a set of given time points $(t_i)_{i=1}^{N}$ the generalized convolution quadrature approximation of*

$$\mathcal{K}(\partial_t)\, \phi = g$$

is given by

$$\mathcal{K}_{-m}\left(\frac{1}{\Delta_n}\right)\phi_n = g_n^{(m)} - \sum_{j=1}^{n-1}\omega_{n,j}\left(0\right)\left(\left[\frac{1}{\Delta_j},\frac{1}{\Delta_{j+1}},\ldots,\frac{1}{\Delta_n}\right]\mathcal{K}_{-m}\right)\phi_j, \quad (20)$$

where $\mathcal{K}_{-m}(z) := z^m\mathcal{K}(z)$, *cf.* (4).

4 Error Analysis

For some fixed $N \geq 1$, we consider the discrete approximations ϕ_n defined by (20), for $1 \leq n \leq N$. We set

$$\Delta := \max\left\{\Delta_j : 1 \leq j \leq N\right\}.$$

From (20), we are interested in the solution of the equation

$$\sum_{j=1}^{n}\omega_{n,j}\left(0\right)\left[\frac{1}{\Delta_j},\frac{1}{\Delta_{j+1}},\ldots,\frac{1}{\Delta_n}\right]\mathcal{K}_{-m}\phi_j = g_n^{(m)} \qquad 1 \leq n \leq N. \quad (21)$$

4.1 Discrete Stability

Lemma 3 (Summation by parts) *Let ϕ_n be the solution of (21) and assume that $g \in C^m\left([0,T]\right)$ and $g_{-1}^{(m)} = g_0^{(m)} = 0$. Then ϕ_n has the representation*

$$\phi_n = \sum_{j=1}^{n}\left(\Delta_j + \Delta_{j-1}\right)Q_j^{(m+2,n)}\left[t_{j-2},t_{j-1},t_j\right]g^{(m)}, \quad (22)$$

where $t_{-1} < 0$ can be chosen arbitrary[1] *and* $\Delta_0 := t_0 - t_{-1}$.

$$Q_j^{(k,n)} := \frac{1}{2\pi\,\mathrm{i}}\int_\gamma \frac{\mathcal{K}^{-1}\left(z\right)}{z^k\prod_{\ell=j}^{n}\left(1-\Delta_\ell z\right)}\,dz, \qquad \forall 1 \leq j \leq n. \quad (23)$$

Proof. As a consequence of Lemma 1 we obtain from (21)

$$\begin{aligned}\phi_n &= \sum_{j=1}^{n}\omega_{n,j}\left(0\right)\left[\frac{1}{\Delta_j},\frac{1}{\Delta_{j+1}},\ldots,\frac{1}{\Delta_n}\right](\mathcal{K}^{-1})_m g_j^{(m)} \\ &= (\mathcal{K}^{-1})_m\left(\frac{1}{\Delta_n}\right)g_n^{(m)} + \sum_{j=1}^{n-1}\Delta_j Q_j^{(m,n)}g_j^{(m)}.\end{aligned} \quad (24)$$

Applying twice the relation

$$\Delta_j Q_j^{(k,n)} = -\left(Q_{j+1}^{(k+1,n)} - Q_j^{(k+1,n)}\right),$$

[1] For simplicity we fix $t_{-1} := -t_1$.

which can be verified straightforwardly, we obtain from (24) and following the notation[2] in (4)

$$\phi_n = (\mathcal{K}^{-1})_m \left(\frac{1}{\Delta_n}\right) g_n^{(m)} - Q_n^{(m+1,n)} g_{n-1}^{(m)} - Q_n^{(m+2,n)} [t_{n-2}, t_{n-1}]\, g^{(m)} \qquad (25)$$
$$+ \sum_{j=1}^{n-1} (\Delta_j + \Delta_{j-1})\, Q_j^{(m+2,n)} [t_{j-2}, t_{j-1}, t_j]\, g^{(m)}.$$

Using the relation $Q_n^{(k,n)} = (\mathcal{K}^{-1})_{k-1}\left(\frac{1}{\Delta_n}\right)$ for $1 \leq j \leq n$, we obtain

$$\phi_n = \sum_{j=1}^{n} (\Delta_j + \Delta_{j-1})\, Q_j^{(m+2,n)} [t_{j-2}, t_{j-1}, t_j]\, g^{(m)}.$$

■

We next estimate the operators in the representation formula (22) for ϕ.

Assumption 4 *For all $\sigma_0 > 0$ and $z \in I_{\sigma_0}$ the transfer operator $\mathcal{K}(z) : B \to D$ is invertible and satisfies the bound for some $\mu \in \mathbb{R}$*

$$\left\|\mathcal{K}^{-1}(z)\right\| \leq M\, |z|^{\mu} \quad \forall z \in I_{\sigma_0},$$

where M depends on σ_0.

Lemma 5 *Let Assumption 4 be satisfied and let Δ be sufficiently small that $1 - \Delta\sigma_0 \geq \alpha_0$ for some $\alpha_0 > 0$. Let m in (20) be the smallest integer such that $m > \mu - 1$, with μ in (9). Then, there exists a constant C depending only on σ_0, α_0, and on the transfer operator $\mathcal{K}^{-1}$ through the constants M and μ in Assumption 4 such that for all $g \in D$ it holds*

$$\left\|Q_j^{(m+2,n)} g\right\|_B \leq C\, \mathrm{e}^{\delta_0 (t_n - t_{j-1})} \|g\|_D \quad \textit{with} \quad \delta_0 := \frac{\sigma_0}{1 - \Delta\sigma_0}. \qquad (26)$$

Proof. From Assumption 4 we conclude that

$$\left\|Q_j^{(m+2,n)} g\right\|_B \leq \frac{1}{2\pi} \frac{1}{\prod_{\ell=j}^{n} |1 - \Delta_\ell \sigma_0|} \left| \int_\gamma \left\|\mathcal{K}_{m+2}^{-1}(z)\, g\right\|_B dz \right|$$
$$\leq \frac{1}{2\pi} \frac{M}{\prod_{\ell=j}^{n} |1 - \Delta_\ell \sigma_0|} \left| \int_\gamma |z|^{\mu - m - 2} dz \right| \|g\|_D . \qquad (27)$$

Note that for $m > \mu - 1$, the integral in (27) is bounded by a constant C_{σ_0}. The product can be estimated by means of Lemma 14 in the Appendix and the assertion follows.

[2] Note that $(\mathcal{K}^{-1})_m(z)$ is understood as $z^{-m}\mathcal{K}^{-1}(z)$ and **not** as $(\mathcal{K}_m(z))^{-1}$.

■

The combination of the representation formula in Lemma 3 and the estimates in Lemma 5 directly leads to the following stability estimate of the discrete convolution.

Theorem 6 *Let Assumption 4 be satisfied and let* Δ *be sufficiently small that* $1 - \Delta\sigma_0 \geq \alpha_0$ *for some* $\alpha_0 > 0$*. Let* m *in* (20) *be the smallest integer such that* $m > \mu - 1$*. Let* ϕ_n*, for* $1 \leq n \leq N$*, denote the solution of (21). Then, there exists a constant* C *depending only on* σ_0*,* α_0*, and* c_{qu} *such that*

$$\|\phi_n\|_B \leq C \sum_{j=1}^{n} (\Delta_j + \Delta_{j-1}) \, \mathrm{e}^{\delta_0 (t_n - t_{j-1})} \left\| [t_{j-2}, t_{j-1}, t_j] \, g^{(m)} \right\|_D$$

with δ_0 *as in (26).*

4.2 Convergence

By assuming that g is $(m+2)$-times differentiable and has $(m+1)$ vanishing derivatives at the origin the exact solution can be written

$$\phi(t_n) = \frac{1}{2\pi\,\mathrm{i}} \int_\gamma (\mathcal{K}^{-1})_{m+2}(\zeta)\, d\zeta \int_0^{t_n} \mathrm{e}^{\zeta(t_n - \tau)}\, g^{(m+2)}(\tau)\, d\tau,$$

cf. (8). By interchanging above the ordering of integration we obtain

$$\phi(t_n) = \int_0^{t_n} Q^{(m+2,n)}(\tau)\, g^{(m+2)}(\tau)\; d\tau \tag{28}$$

with

$$Q^{(k,n)}(\tau) := \frac{1}{2\pi\,\mathrm{i}} \int_\gamma (\mathcal{K}^{-1})_k(\zeta)\, \mathrm{e}^{\zeta(t_n - \tau)}\, d\zeta, \qquad \text{for} \quad k \in \mathbb{N}. \tag{29}$$

Theorem 7 *Let Assumption 4 be satisfied and let* Δ *be sufficiently small that* $1 - \Delta\sigma_0 \geq \alpha_0$ *for some* $\alpha_0 > 0$*. Let* $N \geq 1$ *be the total number of time steps and* m *in* (20) *be the smallest integer such that* $m \geq 1 + \mu$*. Let the right-hand side in (21) satisfy* $g \in C^{m+3}([0,T])$ *and* $g^{(\ell)}(0) = 0$ *for all* $0 \leq \ell \leq m+2$*. We denote by* ϕ_n*, for* $1 \leq n \leq N$*, the solution of (21). Then, the error estimate holds*

$$\|\phi(t_n) - \phi_n\|_B \leq C\Delta^{m-\mu} c_{\mu-m}(\Delta) \left(\sum_{j=1}^{n} \frac{\Delta_j + \Delta_{j-1}}{2}\, \mathrm{e}^{-\delta_0 t_{j-1}} \max_{\substack{\tau \in [t_{j-2}, t_j] \\ \ell \in \{2,3\}}} \left\| g^{(m+\ell)}(\tau) \right\|_D \right),$$

with

$$c_\nu(\Delta) = \begin{cases} 1 + \log \frac{1}{\Delta}, & \textit{if} \;\; \nu = 1, \\ 1, & \textit{if} \;\; \nu > 1. \end{cases} \tag{30}$$

Proof. The combination of (28) with (22) leads to the error representation

$$\phi(t_n) - \phi_n = I_1 + I_2 + I_3, \tag{31}$$

where we set

$$I_1 := \int_0^{t_n} Q^{(m+2,n)}(\tau)\, g^{(m+2)}(\tau)\, d\tau - \sum_{j=1}^{n} \frac{\Delta_j + \Delta_{j-1}}{2} Q^{(m+2,n)}(t_{j-1})\, g^{(m+2)}(t_{j-1}), \tag{32}$$

$$I_2 := \sum_{j=1}^{n} \frac{\Delta_j + \Delta_{j-1}}{2} \left(Q^{(m+2,n)}(t_{j-1}) - Q_j^{(m+2,n)} \right) g^{(m+2)}(t_{j-1}) \tag{33}$$

$$I_3 := \sum_{j=1}^{n} \frac{\Delta_j + \Delta_{j-1}}{2} Q_j^{(m+2,n)} \left(g^{(m+2)}(t_{j-1}) - 2[t_{j-2}, t_{j-1}, t_j] g^{(m)} \right).$$

In the following, we will estimate these terms separately.

Estimate of I_2. For I_2 we start with

$$Q^{(m+2,n)}(t_{j-1}) - Q_j^{(m+2,n)} = \frac{1}{2\pi\,\mathrm{i}} \int_\gamma (\mathcal{K}^{-1})_{m+2}(\zeta)\, d^{(j,n)}(\zeta)\, d\zeta, \tag{34}$$

where

$$d^{(j,n)}(\zeta) := \mathrm{e}^{\zeta(t_n - t_{j-1})} - \frac{1}{\prod_{\ell=j}^{n} (1 - \Delta_\ell \zeta)}. \tag{35}$$

We split the contour $\gamma = \sigma_0 + \mathrm{i}\,\mathbb{R}$ into

$$\gamma^{\text{near}} := \left\{ \zeta \in \gamma : |\zeta \Delta| < \hat{C} \right\} \quad \text{and} \quad \gamma^{\text{far}} := \gamma \backslash \gamma^{\text{near}} \tag{36}$$

for some $\hat{C} = O(1)$. From Lemma 14 in the Appendix we conclude

$$\left| d^{(j,n)}(\zeta) \right| \leq 2\,\mathrm{e}^{\delta_0 (t_n - t_{j-1})}$$

with δ_0 as in (26). Hence, for the farfield part of the integral in (34) we obtain the estimate

$$\left\| \frac{1}{2\pi\,\mathrm{i}} \int_{\gamma^{\text{far}}} (\mathcal{K}^{-1})_{m+2}(\zeta)\, d^{(j,n)}(\zeta)\, d\zeta \right\|_{B \leftarrow D} \leq C_T\, \mathrm{e}^{-\delta_0 t_{j-1}} \int_{\frac{c}{\Delta}}^{\infty} \frac{1}{\left(\sqrt{\sigma_0^2 + \theta^2} \right)^{m+2-\mu}} d\theta$$

$$\leq C_T\, \mathrm{e}^{-\delta_0 t_{j-1}} \int_{\frac{c}{\Delta}}^{\infty} \frac{1}{\theta^{m+2-\mu}} d\theta \leq C_T\, \mathrm{e}^{-\delta_0 t_{j-1}}\, \Delta^{m-(\mu-1)},$$

where c only depends on $\hat{C}$. Since $m \geq 1 + \mu$, we conclude that $\Delta^{m-(\mu-1)} \leq \Delta^2$.

For the nearfield part of the integral in (34) we conclude from Lemma 15 that

$$|d_{n,j}(\zeta)| \leq C_3 \Delta\, |\zeta|^2\, \mathrm{e}^{-\delta_0 t_{j-1}}$$

and hence

$$\left\| \frac{1}{2\pi \mathrm{i}} \int_{\gamma^{\mathrm{near}}} (\mathcal{K}^{-1})_{m+2} (\zeta)\, d^{(j,n)} (\zeta)\, d\zeta \right\|_{B \leftarrow D} \leq C \Delta\, \mathrm{e}^{-\delta_0 t_{j-1}} \int_0^{\frac{c}{\Delta}} |\zeta|^{\mu - m}\, d\zeta.$$

An easy calculation shows that

$$\int_0^{\frac{c}{\Delta}} |\zeta|^{\mu-m}\, d\zeta \leq C c_{m-\mu} (\Delta)$$

with $c_{m-\mu}(\Delta)$ as in (30). Thus,

$$\left\| \frac{1}{2\pi \mathrm{i}} \int_{\gamma^{\mathrm{near}}} (\mathcal{K}^{-1})_{m+2} (\zeta)\, d^{(j,n)} (\zeta)\, d\zeta \right\|_{B \leftarrow D} \leq C \Delta c_{m-\mu} (\Delta)\, \mathrm{e}^{-\delta_0 t_{j-1}}.$$

In summary, we have proved

$$\|I_2\|_B \leq C \Delta c_{m-\mu} (\Delta) \sum_{j=1}^{n} \frac{\Delta_j + \Delta_{j-1}}{2}\, \mathrm{e}^{-\delta_0 t_{j-1}} \left\| g^{(m+2)} (t_{j-1}) \right\|_D .$$

Estimate of I_1. Note that the difference I_1 is the error of the composite trapezoidal rule applied to the integral on the right-hand side in (32). We use only the fact that the trapezoidal rule is exact for constant functions to obtain the error estimate

$$\|I_1\|_B \leq C \sum_{j=1}^{n} \Delta_j^2 \max_{\tau \in [t_{j-1}, t_j]} \left\| \left(Q^{(m+2,n)} (\tau)\, g^{(m+2)} (\tau) \right)' \right\|_B .$$

We get

$$\left(\frac{d}{d\tau} \right)^{\ell} Q^{(m+2,n)} (\tau) = \frac{1}{2\pi \mathrm{i}} \int_{\gamma} (-\zeta)^{\ell} (\mathcal{K}^{-1})_{m+2} (\zeta)\, \mathrm{e}^{\zeta (t_n - \tau)}\, d\zeta.$$

This leads to the norm estimate for $\ell = 0, 1$

$$\begin{aligned} \max_{\tau \in [t_{j-1}, t_j]} \left\| \left(\frac{d}{d\tau} \right)^{\ell} Q^{(m+2,n)} (\tau) \right\|_{B \leftarrow D} &\leq C\, \mathrm{e}^{\sigma_0 (t_n - t_{j-1})} \int_{\gamma} |\zeta|^{\ell + \mu - (m+2)}\, d\zeta \\ &\leq \tilde{C}\, \mathrm{e}^{\sigma_0 (t_n - t_{j-1})}, \end{aligned}$$

since $\ell + \mu - (m+2) \leq -2$. The Leibniz rule leads to

$$\|I_1\|_B \leq C \Delta \sum_{j=1}^{n} \Delta_j\, \mathrm{e}^{-\sigma_0 t_{j-1}} \max_{\substack{\tau \in [t_{j-1}, t_j] \\ \ell \in \{2,3\}}} \left\| g^{(m+\ell)} (\tau) \right\|_D .$$

Estimate of I_3.

A well-known property of divided differences is that there exists some $\tau \in [t_{j-2}, t_j]$ such that

$$2\left[t_{j-2}, t_{j-1}, t_j\right] g^{(m)} = g^{(m+2)}(\tau)$$

so that

$$\left\| g^{(m+2)}(t_{j-1}) - g^{(m+2)}(\tau) \right\|_D \leq (\Delta_j + \Delta_{j-1}) \max_{\tau \in [t_{j-2}, t_j]} \left\| g^{(m+3)}(\tau) \right\|_D .$$

By means of Lemma 5 we finally obtain

$$\|I_3\|_B \leq C\Delta \sum_{j=1}^{n} \frac{\Delta_j + \Delta_{j-1}}{2} \mathrm{e}^{-\delta_0 t_{j-1}} \max_{\tau \in [t_{j-2}, t_j]} \left\| g^{(m+3)}(\tau) \right\|_D .$$

■

5 Application to the Wave Equation

Let $\Omega^- \subset \mathbb{R}^3$ be a bounded Lipschitz domain with boundary Γ. The unbounded complement is denoted by $\Omega^+ := \mathbb{R}^3 \backslash \overline{\Omega^-}$. In the following $\Omega \in \{\Omega^-, \Omega^+\}$. Our goal is to numerically solve the homogeneous wave equation

$$\partial_t^2 u = \Delta u \qquad \text{in } \Omega \times (0, T) \tag{37a}$$

with initial conditions

$$u(\cdot, 0) = \partial_t u(\cdot, 0) = 0 \qquad \text{in } \Omega \tag{37b}$$

and boundary conditions

$$u = g \quad \text{on } \Gamma \times (0, T) \tag{37c}$$

on a time interval $(0, T)$ for some $T > 0$ and given sufficiently smooth and compatible boundary data. For its solution, we employ an ansatz as a *retarded single layer potential*

$$\forall t \in (0, T) \quad u(t) = \int_0^t k(t - \tau)\, \phi(\tau) d\tau \quad \text{in } H^{1/2}(\Gamma) \tag{38}$$

where $k(t) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is the kernel operator

$$k(t)\, \phi = \int_\Gamma \frac{\delta(t - \|\cdot - y\|)}{4\pi \|\cdot - y\|} \phi(y)\, d\Gamma_y$$

and $\delta(\cdot)$ denotes the Dirac delta distribution. The Sobolev space $H^s(\Gamma)$, $s \geq 0$, are defined in the usual way (see, e.g., [4] or [11]). The range of s for which $H^s(\Gamma)$ is defined may be limited, depending on the global smoothness of the surface Γ. Throughout, we let $[-k, k]$ denote the range of Sobolev indices for which $H^s(\Gamma)$ is defined, with the negative order spaces defined by duality in the usual way. The norm is denoted by $\|\cdot\|_{H^s(\Gamma)}$.

The ansatz (38) satisfies the homogeneous equation (37a) and the initial conditions (37b). The extension $x \to \Gamma$ is continuous and hence, the unknown density ϕ in (38) is determined via the boundary conditions (37c), $u(x,t) = g(x,t)$. This results in the boundary integral equation for ϕ,

$$\forall t \in (0,T) \quad \int_0^t k(t-\tau)\phi(\tau)d\tau = g\left(t\right) \quad \text{in } H^{1/2}\left(\Gamma\right). \tag{39}$$

Existence and uniqueness results for the solution of the continuous problem are proven in [1], [8]. The generalized convolution quadrature for (39) with the implicit Euler method then is given by

$$\mathcal{K}_{-m}\left(\frac{1}{\Delta_n}\right)\phi_n = g_n^{(m)} - \sum_{j=1}^{n-1}\omega_{n,j}\left(0\right)\left(\left[\frac{1}{\Delta_j},\frac{1}{\Delta_{j+1}},\ldots,\frac{1}{\Delta_n}\right]\mathcal{K}_{-m}\right)\phi_j, \quad \text{in } H^{1/2}\left(\Gamma\right), \tag{40}$$

where the error analysis will justify the choice $m = 3$.

Note that (40) is only semi-discrete since it is formulated in the infinite-dimensional space $H^{1/2}\left(\Gamma\right)$. The fully discrete space-time discretization will be introduced in Section 5.2.

5.1 Analysis of the Semi-Discrete Method

The Laplace transformed integral operator is given by

$$\mathcal{K}_m\left(\zeta\right)\phi := \int_\Gamma \frac{\mathrm{e}^{-\zeta\|\cdot-y\|}}{4\pi\zeta^m\|\cdot-y\|}\phi\left(y\right)d\Gamma_y.$$

It is well-known (see [1, Prop. 3] and [8, Prop. 2.3]) that $\mathcal{K}_0\left(\zeta\right): H^{-1/2}\left(\Gamma\right) \to H^{1/2}\left(\Gamma\right)$ is an isomorphism for all ζ with $\operatorname{Re}\zeta > 0$ and also for $\zeta \in \mathbb{R}_{\geq 0}$. More precisely, the following continuity estimates hold.

Proposition 8 *Let* $\zeta \in \mathbb{C}$ *with* $\operatorname{Re}\zeta = \sigma_0 > 0$. *Then*

$$\|\mathcal{K}_0\left(\zeta\right)\|_{H^{1/2}(\Gamma)\leftarrow H^{-1/2}(\Gamma)} \leq C\frac{1+\sigma_0^2}{\sigma_0^3}\left|\zeta\right| \quad \text{and} \quad \left\|\mathcal{K}_0^{-1}\left(\zeta\right)\right\|_{H^{-1/2}(\Gamma)\leftarrow H^{+1/2}(\Gamma)} \leq C\frac{1+\sigma_0}{\sigma_0}\left|\zeta\right|^2.$$

Proof. The first estimate follows from [1, Prop. 3] and [8, Prop. 2.3]. Note that the second estimate is a consequence of the coercivity estimate [1, Prop. 3]

$$\operatorname{Re}\left(\zeta\mathcal{K}_0\left(\zeta\right)\psi,\psi\right)_\Gamma \geq c\frac{\min\left(1,\sigma\right)}{\left|\zeta\right|}\left\|\psi\right\|_{H^{-1/2}(\Gamma)}^2, \ \forall\psi \in H^{-1/2}\left(\Gamma\right), \ \forall\zeta \in \mathbb{C} \text{ with } \operatorname{Re}\zeta = \sigma > 0, \tag{41}$$

where $\left(\cdot,\cdot\right)_\Gamma$ denotes the continuous extension of the $L^2\left(\Gamma\right)$-scalar product to the anti-linear dual pairing $\langle\cdot,\cdot\rangle_{H^{1/2}(\Gamma)\times H^{-1/2}(\Gamma)}$. ■

Proposition 8 implies that Assumption 4 holds with $\mu = 2$ so that Theorem 7 can be applied in the following form.

Theorem 9 *We consider the generalized convolution quadrature (40) for the wave equation. Let* Δ *be sufficiently small that* $1-\Delta\sigma_0 \geq \alpha_0$ *for some* $\alpha_0 > 0$*. Let* $N \geq 1$ *be the number of time steps and* $m = 3$*. Let the boundary data in (37) satisfy* $g \in C^{m+3}([0,T])$ *and* $g^{(\ell)}(0) = 0$ *for all* $0 \leq \ell \leq m+2$*. Let* ϕ_n*, for* $1 \leq n \leq N$*, denote the solution of (21). Then, the error estimate holds*

$$\|\phi(t_n) - \phi_n\|_{H^{-1/2}(\Gamma)}$$

$$\leq C\Delta\left(1+\log\frac{1}{\Delta}\right)\left(\sum_{j=1}^{n}\frac{\Delta_j+\Delta_{j-1}}{2}\,\mathrm{e}^{-\delta_0 t_{j-1}}\max_{\substack{\tau\in[t_{j-2},t_j]\\ \ell\in\{2,3\}}}\left\|g^{(m+\ell)}(\tau)\right\|_{H^{1/2}(\Gamma)}\right).$$

In the following we will prove a shift theorem for the case that both, the boundary Γ of Ω^- is analytic and the data $g(t)$ is analytic. The frequency variable is always assumed to be in a half plane

$$I_{\sigma_0} := \{z \in \mathbb{C} : \operatorname{Re} z \geq \sigma_0\} \quad \text{for some } \sigma_0 > 0.$$

Tubular neighborhoods $\mathcal{N}$ of Γ are open sets which satisfy

$$\mathcal{N} \supset \left\{x \in \mathbb{R}^d \mid \operatorname{dist}(x,\Gamma) < \varepsilon\right\},$$

for some $\varepsilon > 0$.

Definition 10 *For an open set* $\mathcal{N} \subset \mathbb{R}^3$ *and constants* C*,* $\gamma > 0$ *we set*

$$\mathcal{A}(C,\gamma,\mathcal{N}) := \left\{f \in L^2(\mathcal{N}) \mid \|\nabla^n f\|_{L^2(\mathcal{N})} \leq C\gamma^n \max\{n+1,|\zeta|\}^n \quad \forall n \in \mathbb{N}_0\right\}.$$

Here, $|\nabla^n u(x)|^2 := \sum_{\alpha\in\mathbb{N}_0^3:|\alpha|=n}\frac{n!}{\alpha!}|D^\alpha u(x)|^2$.

For $s \in \{+,-\}$, we will need the standard trace operator $\gamma_0^s : H^1(\mathcal{N}\cap\Omega^s) \to H^{1/2}(\Gamma)$ and the one-sided normal derivative $\gamma_1^s : H^1(\mathcal{N}\cap\Omega^s) \to H^{-1/2}(\Gamma)$, where the normal vector is oriented in both cases Ω^+, Ω^- into the unbounded domain Ω^+.

Theorem 11 *Assume that the boundary* Γ *is analytic and star-shaped. Let* $g = \gamma_0^- G$ *for some* $G \in \mathcal{A}(C_G,\gamma_G,\mathcal{N}_G\cap\Omega^-)$*. For* $\zeta \in \mathbb{C}$ *with* $\operatorname{Re}\zeta = \sigma_0 > 0$*, let* $\varphi = \mathcal{K}_0^{-1}(\zeta) g$*. Then,* $\varphi \in H^{q-1/2}(\Gamma)$ *for any* $q \geq 0$ *and*

$$\|\varphi\|_{H^{q-1/2}(\Gamma)} \leq C_g \begin{cases} |\zeta|^2 & q = 0, \\ |\zeta|^{q+3/2} & q \geq 1/2. \end{cases}$$

Proof. Let $\zeta \in \mathbb{C}$ with $\operatorname{Re}\zeta = \sigma_0 > 0$. For g as in the assumption of the theorem, let $\varphi = \mathcal{K}^{-1}(\zeta) g$. We define the potential

$$u(x) := (\mathcal{S}\varphi)(x) = \int_\Gamma \frac{\mathrm{e}^{-\zeta\|x-y\|}}{4\pi\|x-y\|}\varphi(y)\,d\Gamma_y \qquad \forall x \in \mathbb{R}^3.$$

Note that

$$-\Delta u + \zeta^2 u = 0 \quad \text{in } \Omega^- \cup \Omega^+, \qquad (42)$$
$$u = g \quad \text{on } \Gamma.$$

From [14, Lemma 3.1.9, Theorem 3.1.16] we conclude that $u \in H^1\left(\mathbb{R}^d\right)$. The well-known jump relation are

$$[\gamma_0 u]_\Gamma = 0 \quad \text{and} \quad [\gamma_1 u]_\Gamma = -\varphi.$$

From [13, Theorem B.2] we conclude that the solution of (42) satisfies $u \in \mathcal{A}\left(C_1, \gamma, \mathcal{N} \cap \Omega^s\right)$, where $C_1 \leq C\left(C_G + |\zeta|^{-1} \|u\|_{1,|\zeta|,\Omega^s}\right)$, where, for $\rho > 0$, the indexed norm $\|\cdot\|_{1,\rho,\Omega}$ is given by

$$\|f\|_{1,\rho,\Omega} := \sqrt{\|\nabla f\|^2_{L^2(\Omega)} + \rho^2 \|f\|^2_{L^2(\Omega)}}.$$

From [12, Remark 4.19], we conclude that

$$\|u\|_{1,|\zeta|,\Omega^s} \leq C|\zeta|\left(|g|_{H^{1/2}(\Gamma)} + |\zeta|^{1/2}\|g\|_{L^2(\Gamma)}\right)$$

so that

$$\|\nabla^n u\|_{L^2(\mathcal{N})} \leq C\left(C_G + |g|_{H^{1/2}(\Gamma)} + |\zeta|^{1/2}\|g\|_{L^2(\Gamma)}\right)\gamma^n \max\{n+1, |\zeta|\}^n. \qquad (43)$$

We have by Green's formula

$$\|\gamma_1^s u\|_{H^{-1/2}(\Gamma)} = \sup_{\psi \in H^{1/2}(\Gamma)\backslash\{0\}} \frac{|\langle \gamma_1^s u, \psi\rangle_\Gamma|}{\|\psi\|_{H^{1/2}(\Gamma)}} \leq \sup_{\psi \in H^{1/2}(\Gamma)\backslash\{0\}} \frac{\|u\|_{1,|\zeta|,\Omega^s}\|Z\psi\|_{1,|\zeta|,\Omega^s}}{\|\psi\|_{H^{1/2}(\Gamma)}};$$

from [1, Lemma 1] we conclude that there exists an extension operator $Z : H^{1/2}(\Gamma) \to H^1(\Omega^s)$ such that

$$\|Z\psi\|_{1,|\zeta|,\Omega^s} \leq C|\zeta|^{1/2}\|\psi\|_{H^{1/2}(\Gamma)}.$$

Thus,

$$\begin{aligned}
\|\varphi\|_{H^{-1/2}(\Gamma)} &\leq \sum_{s\in\{+,-\}} \|\gamma_1^s u\|_{H^{-1/2}(\Gamma)} \leq C|\zeta|^{1/2}\|u\|_{1,|\zeta|,\Omega^+\cup\Omega^-} \\
&\leq C|\zeta|^{3/2}\left(|g|_{H^{1/2}(\Gamma)} + |\zeta|^{1/2}\|g\|_{L^2(\Gamma)}\right) \\
&\leq C|\zeta|^2\|g\|_{H^{1/2}(\Gamma)}.
\end{aligned}$$

For $q \geq 1/2$, we obtain from standard trace inequalities and (43)

$$\|\varphi\|_{H^{q-1/2}(\Gamma)} \leq \sum_{s\in\{+,-\}} \|\gamma_1^s u\|_{H^{q-1/2}(\Gamma)} \leq C\|u\|_{H^{q+1}(\Omega^+\cup\Omega^-)} \leq C_q|\zeta|^{q+3/2}\|g\|_{H^{1/2}(\Gamma)}.$$

■

5.2 Generalized Convolution Quadrature and Spatial Galerkin Discretization for Retarded Potential Integral Equations

We assume that $S_{\mathcal{G}}^{p}$ is a finite-dimensional boundary element space subordinate to a shape-regular surface mesh $\mathcal{G} = \left\{ \tau_i : 1 \leq i \leq \tilde{M} \right\}$ of $\partial\Omega$, consisting of affine or possibly curved triangles (for the details we refer to [14, Chap. 4]).

The basis functions b_i of the corresponding boundary element space

$$S_{\mathcal{G}}^{p} = \operatorname{span}\left\{ b_i : 1 \leq i \leq M \right\} \subset H^{-1/2}\left(\partial\Omega\right), \tag{44}$$

are the usual Lagrange nodal basis functions, i.e., lifted piecewise polynomials of degree p with local support. We write short S for $S_{\mathcal{G}}^{p}$ if $\mathcal{G}$ and p are clear from the context. The maximal mesh width is denoted by

$$h_{\mathcal{G}} := \max\left\{ h_\tau : \tau \in \mathcal{G} \right\} \quad \text{with} \quad h_\tau := \operatorname{diam} \tau.$$

The Galerkin discretization of the semi-discrete equation (40) is given by seeking functions $\phi_{n,S}$, $1 \leq n \leq N$, such that for all $\psi \in S$

$$\begin{aligned} \left(\mathcal{K}_{-m}\left(\frac{1}{\Delta_n} \right) \phi_{n,S}, \psi \right)_\Gamma &= \left(g_n^{(m)}, \psi \right)_\Gamma \\ &-: \sum_{j=1}^{n-1} \omega_{n,j}\left(0\right) \left(\left(\left[\frac{1}{\Delta_j}, \frac{1}{\Delta_{j+1}}, \ldots, \frac{1}{\Delta_n} \right] \mathcal{K}_{-m} \right) \phi_{j,S}, \psi \right)_\Gamma, \end{aligned} \tag{45}$$

where, again, $m = 3$.

We denote by $P_S : L^2\left(\Gamma\right) \to S$ the $L^2\left(\Gamma\right)$-orthogonal projection onto S. The discrete Galerkin operator is given by

$$\mathcal{K}_{-m,S}\left(\zeta\right) := P_S \mathcal{K}_{-m}\left(\zeta\right) P_S^{\star} \quad \text{with} \quad P_S^{\star} \text{ denoting the adjoint of } P_S.$$

Then, (45) can be written in operator form

$$\sum_{j=1}^{n} \omega_{n,j}\left(0\right) \left(\left[\frac{1}{\Delta_j}, \frac{1}{\Delta_{j+1}}, \ldots, \frac{1}{\Delta_n} \right] \mathcal{K}_{-m,S} \right) \phi_{j,S} = P_S g_n^{(m)}.$$

For the following we need a generalization of Definition 10 to time-depending functions.

Definition 12 *For an open set $\mathcal{N} \subset \mathbb{R}^3$ and constants C, γ, $\sigma_0 > 0$ we set*

$$\mathcal{A}\left(C, \gamma, \mathcal{N}, m, \sigma_0, T\right) := \left\{ f \in C^m\left(\left[0, T\right], L^2\left(\mathcal{N}\right)\right) : \int_0^\infty \mathrm{e}^{-\sigma_0 \tau} \left\| \nabla^n f\left(\tau\right) \right\|_{L^2(\mathcal{N})} d\tau \leq C \gamma^n \max\left\{ n+1, \left|\zeta\right| \right\}^n, \ \forall n \in \mathbb{N}_0 \right\}.$$

The subset of $\mathcal{A}\left(C, \gamma, \mathcal{N}, m, \sigma_0, T\right)$ with vanishing initial derivatives up to some order $k \leq m$ is given by

$$\mathcal{A}_0\left(C, \gamma, \mathcal{N}, k, m, \sigma_0, T\right) := \left\{ f \in \mathcal{A}\left(C, \gamma, \mathcal{N}, m, \sigma_0, T\right) \mid \forall 0 \leq \ell \leq m : f^{(\ell)}\left(0\right) = 0 \right\}.$$

Theorem 13 *Assume that the boundary Γ is analytic and star-shaped. Let $g(t) = \gamma_0 G(t)$ for some $G \in \mathcal{A}_0(C, \gamma, \mathcal{N}, p+9, p+10, \sigma_0, T)$ and we choose $m = 3$ in (20), (45). Let $S^p_{\mathcal{G}}$ denote the boundary element space with mesh $\mathcal{G}$ and local polynomial degree p. Let $N \geq 1$ the total number of time steps and Δ be sufficiently small that $1 - \Delta\sigma_0 \geq \alpha_0$ for some $\alpha_0 > 0$. Let $\phi_{n,S}$, for $1 \leq n \leq N$, denote the solution of (45). Then, the error estimate holds*

$$\|\phi(t_n) - \phi_{n,S}\|_{H^{-1/2}(\Gamma)} \leq C_g h_{\mathcal{G}}^{p+3/2} + C\Delta\left(1 + \log\frac{1}{\Delta}\right)\left(\sum_{j=1}^{n} \frac{\Delta_j + \Delta_{j-1}}{2} \mathrm{e}^{-\delta_0 t_{j-1}} \max_{\substack{\tau\in[t_{j-2},t_j] \\ \ell\in\{2,3\}}} \left\|g^{(m+\ell)}(\tau)\right\|_{H^{1/2}(\Gamma)}\right).$$

Proof. Lemma 3 can be applied and we obtain

$$\phi_{n,S} = \sum_{j=1}^{n} (\Delta_j + \Delta_{j-1}) Q_{j,S}^{(m+2,n)}[t_{j-2}, t_{j-1}, t_j] P_S g_j^{(m)},$$

where

$$Q_{j,S}^{(k,n)} := \frac{1}{2\pi\,\mathrm{i}} \int_\gamma \frac{(\mathcal{K}_S^{-1})_k(z)}{\prod_{\ell=j}^{n}(1 - \Delta_\ell z)} dz \qquad \forall 1 \leq j \leq n+1.$$

To estimate $\phi_{n,S} - \phi(t_n)$ we write

$$\phi(t_n) - \phi_{n,S} = I_0 + I_1 + I_2 + I_3,$$

where

$$I_0 := \int_0^\infty \left(Q^{(m+2,n)}(\tau) g^{(m+2)}(\tau) - Q_S^{(m+2,n)}(\tau) P_S g^{(m+2)}(\tau)\right) d\tau$$

with

$$Q_S^{(k,n)}(\tau) := \frac{1}{2\pi\,\mathrm{i}} \int_\gamma (\mathcal{K}_S^{-1})_k(\zeta) \mathrm{e}^{\zeta(t_n - \tau)} d\zeta.$$

I_1, I_2, I_3 are defined as in (32), where $Q^{(m+2,n)}(\tau)$ has to be replaced by $Q_S^{(m+2,n)}(\tau)$, and $Q_j^{(m+2,n)}$ by $Q_{j,S}^{(m+2,n)}$.

Estimate of I_0:

We apply $(p+5)$-times partial integration and use $g^{(\ell)}(0) = 0$ for all $\ell \leq m+p+6$ to obtain

$$I_0 = \int_0^\infty \left(Q^{(m+p+7,n)}(\tau) g^{(m+p+7)}(\tau) - Q_S^{(m+p+7,n)}(\tau) P_S g^{(m+p+7)}(\tau)\right) d\tau.$$

Let $\psi := (\mathcal{K}^{-1})_{m+p+7}(z) g^{(m+p+7)}$ and $\psi_S := (\mathcal{K}_S^{-1})_{m+p+7}(z) P_S g^{(m+p+7)}$. The $H^{-1/2}(\Gamma)$-orthogonal projection onto S is denoted by $\Pi_S : H^{-1/2}(\Gamma) \to S$. Then

$$\psi - \psi_S = (\psi - \Pi_S\psi) + (\Pi_S\psi - \psi_S).$$

By applying $(\mathcal{K}_S)_{-m}(z)$ to the second term and using Galerkin's orthogonality leads to

$$(\mathcal{K}_S)_{-m}(z)(\Pi_S\psi - \psi_S) = P_S\mathcal{K}_{-m}(z)(\Pi_S\psi - \psi).$$

Since the coercivity estimate (41) holds for all $\varphi \in S$ we conclude that[3] $(\mathcal{K}_S)_{-m}(z)P_S$ exists and satisfies the same bound as the continuous operator

$$\left\|(\mathcal{K}_S^{-1})_m(z)P_S\right\|_{H^{-1/2}(\Gamma)\leftarrow H^{+1/2}(\Gamma)} \leq C\frac{1+\sigma_0}{\sigma_0}|z|^{2-m}.$$

Using this estimate and Proposition 8 we obtain

$$\|\Pi_S\psi - \psi_S\|_{H^{-1/2}(\Gamma)} \leq C|z|^{2-m}\|\mathcal{K}_{-m}(z)((\Pi_S\psi - \psi))\|_{H^{1/2}(\Gamma)} \leq \tilde{C}|z|^3\|\Pi_S\psi - \psi\|_{H^{-1/2}(\Gamma)}.$$

In total, we have proved

$$\|\psi - \psi_S\|_{H^{-1/2}(\Gamma)} \leq \tilde{C}\left(1+|z|^3\right)\|\Pi_S\psi - \psi\|_{H^{-1/2}(\Gamma)}.$$

Hence,

$$\begin{aligned}&\|I_0\|_{H^{-1/2}(\Gamma)}\\ &\leq \tilde{C}_T\frac{1}{2\pi}\int_0^\infty \mathrm{e}^{-\sigma_0\tau}\left|\int_\gamma\left(1+|\zeta|^3\right)\left\|(\Pi_S - I)(\mathcal{K}^{-1})_{m+p+7}(\zeta)g^{(m+p+7)}(\tau)\right\|_{H^{-1/2}(\Gamma)}d\zeta\right|d\tau.\end{aligned}$$

Standard approximation properties of the space $S_{\mathcal{G}}^p$ leads to

$$\left\|(\Pi_S - I)(\mathcal{K}^{-1})_{m+p+7}(\zeta)g^{(m+p+7)}(\tau)\right\|_{H^{-1/2}(\Gamma)} \leq Ch_{\mathcal{G}}^{p+3/2}\left\|(\mathcal{K}^{-1})_{m+p+7}(\zeta)g^{(m+p+7)}(\tau)\right\|_{H^{p+1}(\Gamma)}.$$

We apply Theorem 11 to obtain

$$\int_0^\infty \mathrm{e}^{-\sigma_0\tau}\left(1+|\zeta|^3\right)\left\|(\mathcal{K}^{-1})_{m+p+7}(\zeta)g^{(m+p+7)}(\tau)\right\|_{H^{p+1}(\Gamma)} \leq C_g|\zeta|^{-2}.$$

The integral over ζ is bounded so that we obtain the required bound for I_0.

The estimates of I_1, I_2, I_3 are just a repetition of the arguments in the proof of Theorem 7 since also the Galerkin operator satisfies $\left\|\mathcal{K}_S^{-1}(\zeta)P_S\right\| \leq C|\zeta|^2$. ■

6 Conclusion

In this paper we have developed a generalized convolution quadrature method with variable time stepping for solving one-sided convolution equations. As in the original convolution quadrature the continuous equation is transformed to the Laplace domain and the transformed solution can be characterized as the solution of an ODE. In contrast to the original method we introduce a

[3] Note that $(\mathcal{K}^{-1})_{m,S}(\zeta) = \zeta^{-m}\mathcal{K}_{0,S}^{-1}(\zeta) = (\mathcal{K}_{-m,S}(\zeta))^{-1}$.

variable time stepping for the solution of the ODE. The discrete equation are transformed back to the time domain resulting in the generalized convolution quadrature method. The operators involved in this equation can be computed as Newton's divided differences applied to the transfer operator. Although the convolution structure is not inherited to the discrete level we expect that for problems with non-uniformly distributed irregularities in the right-hand side the savings in the number of time steps by adaptive time stepping can be very significant. Future work will be devoted to the development of a fast generalized convolution quadrature.

We have developed a new theory for the analysis of the generalized convolution quadrature which is different from the theory of the original convolution quadrature. The reason is that the discrete equation is no longer a proper discrete convolution and, hence, cannot be transformed to the Fourier-Laplace domain by the discrete Fourier transform. Instead, we have developed direct estimates for Newton's divided differences of the transfer operator which allows us to stay on the "time-domain side". As an important application of this theory we consider the formulation of the wave equation in unbounded domains as retarded potential integral equations and prove that the generalized convolution quadrature converges at an optimal rate (up to a logarithmic term).

Future research will be devoted to the implementation of the method and the development of a fast algorithmic version.

A Estimate of $d^{(j,n)}$

In this appendix we will derive some estimates for the function $d^{(j,n)}$ as in (35).

Lemma 14 *Let $\gamma = \sigma_0 + \mathrm{i}\,\mathbb{R}$ for some $\sigma_0 > 0$. For the maximal mesh width Δ, we assume $1 - \sigma_0 \Delta > 0$. For all $\zeta \in \gamma$, it holds*

$$\frac{1}{\prod_{\ell=j}^{n} |1 - \Delta_\ell \zeta|} \leq \mathrm{e}^{\delta_0 (t_n - t_{j-1})} \quad \text{with} \quad \delta_0 := \frac{\sigma_0}{1 - \sigma_0 \Delta}.$$

Proof. The assertion follows from

$$\frac{1}{\prod_{\ell=j}^{n} |1 - \Delta_\ell \zeta|} \leq \frac{1}{\prod_{\ell=j}^{n} |1 - \sigma_0 \Delta_\ell|} = \exp \left\{ \sum_{\ell=j}^{n} \log \left(1 + \frac{\Delta_\ell \sigma_0}{1 - \Delta_\ell \sigma_0} \right) \right\} \leq \mathrm{e}^{\delta_0 (t_n - t_{j-1})}.$$

■

Next, we will derive an estimate for $d_{n,j}$ for all $\zeta \in \gamma^{\mathrm{near}}$ (cf. (36)).

Lemma 15 *Let $\gamma = \sigma_0 + \mathrm{i}\,\mathbb{R}$ for some $\sigma_0 > 0$ and let γ^{near} be as in (36). For the maximal mesh width Δ, we assume $1 - \sigma_0 \Delta > 0$. Then, for all $\zeta \in \gamma^{\mathrm{near}}$ it holds*

$$|d_{n,j}(\zeta)| \leq C_3 \min \left\{ 1, \Delta |\zeta|^2 \right\} \mathrm{e}^{-\delta_0 t_{j-1}},$$

where C_3 depends on the final time T and the parameter σ_0.

Proof. Let

$$c_\ell := \frac{1}{1-\zeta\Delta_\ell}$$

and observe $|c_\ell| \geq (1-\sigma_0\Delta)^{-1} > 0$. Further let

$$\varepsilon_\ell := \mathrm{e}^{\Delta_\ell\zeta} - \frac{1}{1-\zeta\Delta_\ell} \qquad \text{and} \qquad \varepsilon := (\varepsilon_\ell)_{\ell=j}^n .$$

Then, it is easy to see that there is a constant C_2 depending only on C such that

$$|\varepsilon_\ell| \leq C_2 |\zeta\Delta_\ell|^2 \qquad \forall\zeta \in I_{\sigma_0,\Delta}.$$

We write

$$d_{n,j}(\zeta) = \prod_{\ell=j}^n (c_\ell + \varepsilon_\ell) - \prod_{\ell=j}^n c_\ell.$$

Taylor expansion of the function $g_{n,j}(\varepsilon) := \prod\limits_{\ell=j}^n (c_\ell + \varepsilon_\ell)$ about $\varepsilon = 0$ yields

$$g_{n,j}(\varepsilon) = g_{n,j}(0) + \langle \nabla g_{n,j}(\theta\varepsilon), \varepsilon\rangle \tag{46}$$

for some $\theta \in [0,1]$. For the derivatives of $g_{n,j}$ we obtain

$$\frac{\partial g_{n,j}}{\partial \varepsilon_k}(\theta\varepsilon) = \prod_{\substack{\ell=j \\ \ell\neq k}}^n (c_\ell + \theta\varepsilon_\ell).$$

From

$$\left|\prod_{\substack{\ell=j \\ \ell\neq k}}^n (c_\ell + \theta\varepsilon_\ell)\right| = \left|\prod_{\substack{\ell=j \\ \ell\neq k}}^n \left(\frac{1-\theta}{1-\zeta\Delta_\ell} + \theta\,\mathrm{e}^{\Delta_\ell\zeta}\right)\right|.$$

and

$$\left|\frac{1}{1-\Delta_\ell\zeta}\right| \leq \frac{1}{1-\Delta_\ell\sigma_0} \leq \mathrm{e}^{\delta_0\Delta_\ell} \quad \text{with} \quad \delta_0 := \frac{\sigma_0}{1-\Delta\sigma_0}$$

we obtain

$$\left|\prod_{\substack{\ell=j \\ \ell\neq k}}^n (c_\ell + \theta\varepsilon_\ell)\right| \leq \left|\prod_{\substack{\ell=j \\ \ell\neq k}}^n \left((1-\theta)\,\mathrm{e}^{\delta_0\Delta_\ell} + \theta\,\mathrm{e}^{\Delta_\ell\delta_0}\right)\right| \leq \prod_{\substack{\ell=j \\ \ell\neq k}}^n \mathrm{e}^{\Delta_\ell\delta_0} \leq \mathrm{e}^{\delta_0(t_n-t_{j-1})}.$$

From (46) we derive

$$\begin{aligned}
|\langle \nabla g_{n,j}(\theta\varepsilon), \varepsilon\rangle| &\leq C_2 \textstyle\sum_{\ell=j}^n \mathrm{e}^{\delta_0(t_n-t_{j-1})} |\zeta\Delta_\ell|^2 \\
&\leq C_2\Delta |\zeta|^2 |t_n - t_{j-1}| \,\mathrm{e}^{\delta_0(t_n-t_{j-1})} \\
&\leq \left(C_2 T\,\mathrm{e}^{\delta_0 T}\right)\Delta |\zeta|^2 \,\mathrm{e}^{-\delta_0 t_{j-1}}
\end{aligned}$$

and the estimate

$$|d_{n,j}(\zeta)| \leq C_3 \Delta |\zeta|^2 \, \mathrm{e}^{-\delta_0 t_{j-1}}$$

follows. The other estimate directly follows from Lemma 14:

$$|d_{n,j}(\zeta)| \leq \left| \mathrm{e}^{\zeta(t_n - \tau_{j-1})} \right| + \frac{1}{\prod_{\ell=j}^{n} |1 - \Delta_\ell \zeta|} \leq C_T \, \mathrm{e}^{-\delta_0 t_{j-1}} .$$

The combination of these two estimates leads to the assertion. ■

References

[1] A. Bamberger and T. Ha-Duong. Formulation variationelle espace-temps pour le calcul par potentiel retardé d'une onde acoustique. *Math. Meth. Appl. Sci.*, 8:405–435 and 598–608, 1986.

[2] C. de Boor, *Divided Differences*, Surveys in Approximation Theory 1 (2005), 46–69.

[3] T. Ha-Duong. On Retarded Potential Boundary Integral Equations and their Discretization. In M. Ainsworth, P. Davies, D. Duncan, P. Martin, and B. Rynne, editors, *Computational Methods in Wave Propagation*, volume 31, pages 301–336, Heidelberg, 2003. Springer.

[4] W. Hackbusch. *Elliptic Differential Equations*. Springer Verlag, 1992.

[5] M. López-Fernández, C. Lubich and A. Schädle. Adaptive, fast and oblivious convolution in evolution equations with memory. *SIAM J. Sci. Comput.*, 30:1015-1037, 2008.

[6] C. Lubich, Convolution quadrature and discretized operational calculus. I. *Numer. Math.*, 52:129–145, 1988.

[7] C. Lubich, Convolution quadrature and discretized operational calculus. II. *Numer. Math.*, 52:413–425, 1988.

[8] C. Lubich. On the multistep time discretization of linear initial-boundary value problems and their boundary integral equations. *Numer. Math.*, 67:365–389, 1994.

[9] C. Lubich, Convolution quadrature revisited. *BIT*, 44:503–514, 2004.

[10] C. Lubich and A. Ostermann, Runge-Kutta methods for parabolic equations and convolution quadrature. *Math. Comput.*, 60:105-131, 1993.

[11] W. McLean. *Strongly Elliptic Systems and Boundary Integral Equations.* Cambridge, Univ. Press, 2000.

[12] J. M. Melenk and S. A. Sauter. Wave-Number Explicit Convergence Analysis for Galerkin Discretizations of the Helmholtz Equation. *SIAM J. Numer. Anal.*, 49(3):1210–1243, 2011.

[13] J. Melenk. Mapping Properties of Combined Field Helmholtz Boundary Integral Operators. Technical Report 01-2010, ASC Report, 2010.

[14] S. Sauter and C. Schwab. *Boundary Element Methods.* Springer, Heidelberg, 2010.

[15] S. Sauter and A. Veit. Adaptive Time Discretization for Retarded Potentials. Technical Report 04-2011, Universität Zürich, 2011. submitted.