Generalized Convolution Quadrature with Variable Time Stepping. Part II: Algorithm and Numerical Results*

M. Lopez-Fernandez† S. Sauter‡

August 27, 2012

Abstract

In this paper, we will address the implementation of the Generalized Convolution Quadrature (GCQ) presented and analyzed in [M. López-Fernández, S. Sauter: A Generalized Convolution Quadrature with Variable Time Stepping, Preprint 17-2011, University of Zurich (2011)] for solving linear parabolic and hyperbolic evolution equations. Our main goal is to overcome the current restriction to uniform time steps of Lubich's Convolution Quadrature (CQ). A major challenge for the efficient realization of the new method is the evaluation of high-order divided differences for the transfer function in a fast and stable way. Our algorithm is based on contour integral representation of the numerical solution and quadrature in the complex plane. As the main application we will consider the wave equation in exterior domains which is formulated as a retarded boundary integral equation.

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

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

1 Introduction

In this paper, we will address the efficient algorithmic realization of the Generalized Convolution Quadrature (GCQ) as presented and analyzed in [15] for

*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

solving linear convolution equations of the form

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

where $*$ denotes convolution with respect to time, g is a given function, and k is some fixed kernel function/operator, i.e., the left-hand side in (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/operator* $\mathcal{K}$ in the Laplace domain and analyticity of $\mathcal{K}$ is assumed in a region containing the half plane $\operatorname{Re} z \geq \sigma_+ > 0$. For this type of problems, the convolution quadrature method (CQ) has been developed originally by Lubich, see [17, 18, 21, 20] for parabolic problems and [19] 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 ordinary differential equations (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 well-established theory of ODEs can be employed 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.

Since the derivation and algorithmic formulation of the CQ method strongly relies on uniform time steps, only recently the generalized convolution quadrature method has been presented (cf. [15]) which allows for variable time stepping. For the formulation of the algorithm and its error analysis, a new theory has been developed in [15] which avoids the use of the discrete Fourier transform, i.e., the reason for the restriction to uniform time steps. We will 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. The extension of both the analysis and the implementation of our method to high order versions is by no means straightforward and is the subject of future research. It is our opinion that fully understanding the first order method will open the way to further analytical and algorithmical developments.

The idea of the new GCQ method in [15] is to apply a time integrator for scalar ODEs $y' = zy + g$ and allow for variable time stepping. For *sectorial* convolution kernels this idea is already present in the fast and oblivious algorithm in [14]. However the algorithm in [14] is not applicable to wave equations and an error analysis has not been developed. 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.

Another approach for solving retarded potential integral equations with variable time steps has been introduced recently in [27] and is based on the partition of unity method in time for a direct space-time Galerkin discretization of the RPIE. This approach enjoys nice stability properties and avoids numerical dissipation of energy. On the other hand, challenging quadrature problems arise for the generation of the linear system – some quadrature methods have been developed in [27], [12].

The paper is organized as follows. In Section 2 we will 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 will be concerned with the temporal discretization of the convolution equation and the description of an algorithm for its practical realization. Our algorithm is based on contour integral representation of the numerical solution, quadrature and time integration of parameter-dependent ODEs in the Laplace domain. In Section 4 we will describe the new quadrature formula which is at the heart of the GCQ algorithm. The application to the boundary integral formulation of the wave equation will be considered in Section 5, where new estimates for the acoustic single layer potential operator will be derived for general complex frequencies. The results of numerical experiments will be presented in Section 6.

2 One-Sided Convolution Equations

We will consider the class of convolution operators as described in [19, 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 $g : \mathbb{R}_{\geq 0} \to D$, we consider the problem of finding $\phi : \mathbb{R}_{\geq 0} \to B$ 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 $\mathcal{K} : I_{\sigma_+} \to \mathcal{L}(B, D)$ be an analytic operator-valued function in a half-plane

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

which is bounded by

$$\|\mathcal{K}(z)\| \leq C_{\mathrm{op}} |z|^{\theta}, \qquad \forall z \in I_{\sigma_+}, \tag{3}$$

for some $C_{\mathrm{op}} > 0$ and $\theta \in \mathbb{R}$. For $\rho \in \mathbb{Z}$, we define

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

For any $\rho > \max\{-1, \theta + 1\}$, the Laplace inversion formula

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

for a contour $\gamma = \sigma + \mathrm{i}\,\mathbb{R}$, $\sigma \geq \sigma_+$, defines a continuous and exponentially bounded operator $k_\rho(t)$, which by Cauchy's integral theorem vanishes for $t < 0$. As in [19] we denote the convolution $k * \phi$ by

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

for sufficiently smooth functions ϕ which satisfy $\phi(x) = 0$ for $x \leq 0$.

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. [19, (2.3), (2.22)]) leads to

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

so that

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

for appropriately chosen ρ. 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 $C_{\mathrm{op}} > 0$ and $\mu \in \mathbb{R}$, a similar estimate[1] to (3) holds for $\mathcal{K}^{-1}$, namely

$$\left\|\mathcal{K}^{-1}(z)\right\| \leq C_{\mathrm{op}} |z|^\mu, \qquad \forall z \in I_{\sigma_+}. \tag{9}$$

In this way, ρ will be chosen according to

$$\rho > \max\{-1, \mu + 1, \theta + 1\}. \tag{10}$$

In [15], the GCQ method has been derived, where the assumptions on the transfer function/operator and its inverse were (3), (9). However, in order to apply the quadrature method developed in [16] in a stable way and develop a fast and stable algorithmic version of the GCQ we impose some additional assumptions on $\mathcal{K}$.

Assumption 1 *$\mathcal{K}$ is analytic in a half plane $\operatorname{Re} z > \sigma_-$, for some $\sigma_- < -1$, and satisfies there the growth estimate*

$$\|\mathcal{K}(z)\| \leq C_{\mathrm{op}} \left(1 + \mathrm{e}^{-\beta \operatorname{Re} z}\right) (\max\{1, |z|\})^\theta \qquad \operatorname{Re} z > \sigma_-. \tag{11}$$

Thus we require $\mathcal{K}$ to be analytic in a region entering the left half plane but allow for exponential growth in this region.

[1]For simplicity, we use the same notation for the multiplicative constants in (3) and (9).

3 Temporal Discretization and Formulation of the Algorithm

We recall here the definition of the generalized convolution quadrature as presented and analyzed in [15].

Definition 2 (Generalized Convolution Quadrature) *For a set of given time points $(t_n)_{n=1}^N$ the generalized convolution quadrature approximation based on the implicit Euler method of*

$$\mathcal{K}(\partial_t)\,\phi = g \tag{12}$$

at time points t_n is given by

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)\phi_n = g_n^{(\rho)} - \sum_{j=1}^{n-1}\omega_{n,j}(0)\left(\left[\frac{1}{\Delta_j},\frac{1}{\Delta_{j+1}},\ldots,\frac{1}{\Delta_n}\right]\mathcal{K}_{-\rho}\right)\phi_j, \tag{13}$$

for $n = 1,\ldots N$, $\mathcal{K}_{-\rho}(z) := z^\rho\mathcal{K}(z)$, cf. (4) *and*

$$\omega_{n,j}(z) := \prod_{\ell=j+1}^{n}(z-\Delta_\ell). \tag{14}$$

The expression $[\cdot,\ldots,\cdot]\,\mathcal{K}_{-\rho}$ denotes Newton's divided difference with respect to the arguments in the brackets with the standard generalization for repeated arguments.

The implementation of (13) is very challenging due to the presence of high order divided differences of the operator $K_{-\rho}$ at arbitrary positive arguments Δ_j^{-1}, which furthermore might appear repeatedly in an arbitrary order during a time stepping procedure. The direct evaluation of these quantities by building Newton's table of divided differences is a highly ill-conditioned problem and will likely become unreliable – we refer to [22], [4] for details and an improvement for the special case of the exponential function. However these techniques are not directly applicable for the class of functions described in Assumption 1. In order to overcome this drawback, we propose to use Cauchy's integral formula for the divided differences; see, e.g., [5, 28], [15]. This leads to the following representation of the summands in (13)

$$\omega_{n,j}(0)\left(\left[\frac{1}{\Delta_j},\frac{1}{\Delta_{j+1}},\ldots,\frac{1}{\Delta_n}\right]\mathcal{K}_{-\rho}\right) = \Delta_j\frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}}\frac{\mathcal{K}_{-\rho}(z)}{\prod_{\ell=j}^{n}(1-\Delta_\ell z)}\,dz \tag{15}$$

for a complex contour $\mathcal{C}$ located in the analyticity domain of $\mathcal{K}$ and surrounding the poles Δ_ℓ^{-1}, $\ell = 1,\ldots,n$.

Hence, the contour integral representation of (13) is given by

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)\phi_n = g_n^{(\rho)} - \frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}}\sum_{j=1}^{n-1}\Delta_j\frac{\mathcal{K}_{-\rho}(z)}{\prod_{\ell=j}^{n}(1-\Delta_\ell z)}\phi_j\,dz, \tag{16}$$

which is nothing but

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)\phi_n = g_n^{(\rho)} - \frac{1}{2\pi\mathrm{i}}\int_{\mathcal{C}} \frac{\mathcal{K}_{-\rho}(z)}{1-\Delta_n z} u_{n-1}(z)\,dz, \tag{17}$$

for u_{n-1} the approximation at time t_{n-1} of the scalar ODE problem

$$u_t(z,t) = z\,u(z,t) + \phi(t), \qquad u(z,0) = 0 \tag{18}$$

by the implicit Euler method applied with variable step sizes $\Delta_j = t_j - t_{j-1}$, $j = 1,\ldots,n-1$.

Assume now that a good quadrature rule with prescribed nodes z_ℓ and weights w_ℓ, $\ell = 1,\cdots,N_Q$, is available for (17). Then we are led to the computation of

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)\tilde{\phi}_n = g_n^{(\rho)} - \sum_{\ell=1}^{N_Q} w_\ell \frac{\mathcal{K}_{-\rho}(z_\ell)}{1-\Delta_n z_\ell}\tilde{u}_{n-1}(z_\ell), \tag{19}$$

where $\tilde{u}_{n-1}(z_\ell)$ is the implicit Euler approximation of (18) for z the quadrature point z_ℓ, $1 \le \ell \le N_Q$. The method is formulated in an algorithmic way as follows.

Algorithm 3 (GCQ with contour quadrature)

- ***Initialization.*** *Generate*[2] $\mathcal{K}_{-\rho}(z_\ell)$ *for all contour quadrature nodes* z_ℓ, $\ell = 1,2,\ldots,N_Q$. *Compute* $\tilde{\phi}_1$ *from*

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_1}\right)\tilde{\phi}_1 = g_1^{(\rho)}. \tag{20}$$

- ***For*** $n = 2,\ldots,N$

  1. ***Implicit Euler step.*** *Apply an implicit Euler step to (18) and compute*

  $$\tilde{u}_{n-1}(z_\ell) = \frac{\tilde{u}_{n-2}(z_\ell)}{1-\Delta_{n-1}z_\ell} + \frac{\Delta_{n-1}}{1-\Delta_{n-1}z_\ell}\tilde{\phi}_{n-1}$$

  for all contour quadrature nodes: $z = z_\ell$, $\ell = 1,\ldots,N_Q$.

  2. ***Generate linear system.*** *If* Δ_n *is a new time step, then, generate* $\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)$*; otherwise this operator was already generated in a previous step. Update the right-hand side*

  $$r_n = r_n(\tilde{u}_{n-1}) := g^{(\rho)}(t_n) - \sum_{\ell=1}^{N_Q} w_\ell \frac{\mathcal{K}_{-\rho}(z_\ell)}{1-\Delta_n z_\ell}\tilde{u}_{n-1}(z_\ell).$$

[2] For the numerical solution of the wave equation by GCQ (cf. Sec. 5), this requires the discretization of the operator $\mathcal{K}_{-m}\left(\frac{1}{\Delta_1}\right)$, e.g., by the Galerkin boundary element method.

3. ***Linear Solve.*** *Solve the linear system*

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)\tilde{\phi}_n = r_n.$$

Remark 4 *This new algorithm avoids the storage of the full history ϕ_i, $1 \leq i \leq n-1$: For the computation of the new ϕ_n only the solution u_{n-1} of the ODEs at time t_{n-1} is needed. Instead, the algorithm requires the pre-computation of the operators $K_{-\rho}(z_\ell)$, their storage and the solution of the (decoupled) ODEs at the quadrature nodes z_ℓ. The main part of the computational cost and the memory requirements will be spent in the computation and the storage of the $K_{-\rho}(z_\ell)$. We emphasize that, thanks to the results in the next section, the required number of quadrature nodes will not be much bigger than the corresponding number of nodes for the original convolution quadrature with uniform time stepping – which is $O(N)$ (see [18, 3]).*

Another important advantage of our algorithm is that the time steps do not need to be known in advance – only a lower and an upper bound of them are required, as we will see in the next Section.

The development of an efficient quadrature rule for the integrals in (15) is a challenging problem and depends on a subtle choice of the contour parametrization which is adapted to the class of functions considered in Assumption 1. For this class of functions such a quadrature approximation has been developed and analyzed recently by the authors (cf. [16]). In the following we will briefly describe this quadrature method and adapt it to the generalized convolution quadrature method.

4 Contour Quadrature

For the sake of simplicity and as explained in Remark 4, we will assume that the contour in (17) and the quadrature points z_ℓ are fixed during the time stepping. The choice of the contour will depend on the minimal and maximal mesh width $\Delta_{\min}$, $\Delta_{\max}$, which should be chosen in advance. Since the number of quadrature nodes will depend only very mildly on the ratio $\frac{\Delta_{\max}}{\Delta_{\min}}$, the choices $\Delta_{\min} = \Delta_{\max}^{\alpha}$ for some $1 \leq \alpha \leq 2$ or even stronger gradings $\alpha > 2$ will lead to an efficient algorithm.

4.1 The Quadrature Method

The contour and the quadrature will depend on[3]

$$m = \frac{1}{\Delta_{\max}}, \qquad M = \max\left(m^2, \frac{1}{\Delta_{\min}}\right) \tag{21}$$

[3] Our numerical experiments show that the choice $M := \Delta_{\min}^{-1}$ performs better in practice while the choice as in (21) allows to employ the error estimates in [16] without modifications.

and the ratio

$$q := \frac{M}{m}. \tag{22}$$

To avoid technicalities we always assume that $m \geq 2$ holds.

For $\lambda \in [0,1]$, we employ the usual notation

$$\mathrm{sn}\,(\sigma) = \mathrm{sn}\,(\sigma|\lambda), \qquad \mathrm{cn}\,(\sigma) = \mathrm{cn}\,(\sigma|\lambda), \qquad \mathrm{dn}\,(\sigma) = \mathrm{dn}\,(\sigma|\lambda)$$

for the Jacobi elliptic functions as defined, e.g., in [1] and denote by

$$K\,(\lambda) := \int_0^1 \frac{dx}{\sqrt{(1-x^2)\,(1-\lambda x^2)}} \qquad \text{(see [8, 8.112 (1.) and (2.)]} \tag{23}$$

$$K'\,(\lambda) := K\,(1-\lambda) \qquad \text{(see [8, 8.112 (3.) and 8.111 (2.)])} \tag{24}$$

the complete elliptic integrals of the first kind.

For

$$k = k(q) = \frac{q-\sqrt{2q-1}}{q+\sqrt{2q-1}} \qquad \text{and} \qquad \lambda = k^2 \tag{25}$$

we set

$$P = -K(\lambda) + \frac{\mathrm{i}}{2}K'(\lambda) \quad \text{and} \quad Q = P + 4K(\lambda). \tag{26}$$

Our choice for the integration contour $\mathcal{C}$ in (17) is

$$\overline{PQ} \to \mathcal{C} : \sigma \mapsto \gamma_M(\sigma) = \frac{M}{q-1}\left(\sqrt{2q-1}\frac{k^{-1}+\mathrm{sn}\,(\sigma)}{k^{-1}-\mathrm{sn}\,(\sigma)} - 1\right) \tag{27}$$

which is nothing but the circle in the complex plane of radius M centered at M parameterized in a subtle way (cf. [16, Lemma 15]. This parametrization is a modification of the one in [10], where the computation of matrix functions by quadrature in the complex plane was considered.

For fixed $N_Q \geq 1$, the quadrature weights and nodes in (19) are then given by

$$z_\ell = \gamma_M(\sigma_\ell), \quad w_\ell = \frac{4K(\lambda)}{2\pi\mathrm{i}}\gamma_M'(\sigma_\ell), \quad \text{with} \quad \sigma_\ell = -K(\lambda) + \left(\ell - \frac{1}{2}\right)\frac{4K(\lambda)}{N_Q}, \tag{28}$$

for $\ell = 1, \ldots, N_Q$, where

$$\gamma_M'(\sigma) = \frac{M\sqrt{2q-1}}{q-1}\frac{2\mathrm{cn}\,(\sigma)\mathrm{dn}\,(\sigma)}{k(k^{-1}-\mathrm{sn}\,(\sigma))^2}. \tag{29}$$

The choice of nodes in (28) corresponds to the composite mid-point formula. Notice that this is equivalent to the composite trapezoidal formula for $4K(\lambda)$-periodic functions, with quadrature nodes shifted to the right by $\frac{2K(\lambda)}{N_Q}$.

The evaluation of the Jacobi elliptic functions and the elliptic integrals at complex arguments can be performed very efficiently in MATLAB by means of Driscoll's Schwarz–Christoffel Toolbox [6] which is freely available online. In particular the functions `ellipkkp` and `ellipjc` are needed to compute (28), cf. [10].

As we have already mentioned in Remark 4, in our main applications the evaluation of the quadrature rule will be the most expensive part of the procedure. Thus, it will be important to exploit the symmetry in (28). In this way, in cases where the transfer operator $\mathcal{K}(z)$ is real on the real axis (so that $\mathcal{K}(\overline{z}) = \overline{K(z)}$ by the Schwarz reflection principle), we can halve the evaluations of the operators $\mathcal{K}(\sigma_\ell)$ to those σ_ℓ belonging to $\overline{PH}$ with

$$H = P + 2K(\lambda).$$

This corresponds to evaluate $\mathcal{K}$ only along the upper semicircle centered at M with radius M.

4.2 Error Analysis

In [15], the generalized convolution quadrature (based on the implicit Euler method) without quadrature approximation (cf. (13)) has been introduced and analyzed. We recall here the convergence theorem for the corresponding error $\phi(t_n) - \phi_n$ and will derive in this section estimates for the perturbation $\phi_n - \tilde{\phi}_n$, i.e., for the error between the solution ϕ_n of the unperturbed GCQ method (13) and the solution $\tilde{\phi}_n$ of Algorithm 3 with the contour quadrature as in Section 4.1 – needless to say that an estimate of the total error $\phi(t_n) - \tilde{\phi}_n$ then follows from a triangle inequality.

Theorem 5 *Let (9) be satisfied and let $\Delta_{\max}$ be sufficiently small such that $1 - \Delta_{\max}\sigma_+ \geq \alpha_0$ for some $\alpha_0 > 0$. Let $N \geq 1$ be the total number of time steps and ρ in (13) be chosen such that (10) holds. Let the right-hand side in (12) satisfy $g \in C^{\rho+3}([0,T])$ and $g^{(\ell)}(0) = 0$ for all $0 \leq \ell \leq \rho + 2$. We denote by ϕ_n, for $1 \leq n \leq N$, the solution of (13). Then, the error estimate holds*

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

with

$$\delta_0 := \sigma_+/\alpha_0 \quad \text{and} \quad c_\nu(\Delta) = \begin{cases} 1 + \log \frac{1}{\Delta}, & \text{if } \nu = 1, \\ 1, & \text{if } \nu > 1. \end{cases} \tag{30}$$

The proof of this theorem is given in [15].

The exact solution $(\phi_j)_{j=0}^N$ of the generalized convolution quadrature (based on the implicit Euler method) has the contour integral representation (cf (16))

$$\sum_{j=1}^{n} \Delta_j I_{j,n} \phi_j = g_n^{(\rho)} \quad \text{with} \quad I_{j,n} := \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \frac{\mathcal{K}_{-\rho}(z)}{\prod_{\ell=j}^{n}(1 - \Delta_\ell z)} dz. \tag{31a}$$

The solution $\left(\tilde{\phi}_j\right)_{j=0}^{N}$ of the system where the contour integral is replaced by our contour quadrature (cf. Algorithm 3) is given by

$$\sum_{j=1}^{n} \Delta_j Q_{j,n} \tilde{\phi}_j = g_n^{(\rho)} \quad \text{with} \quad Q_{j,n} := \begin{cases} \sum_{\ell=1}^{N_Q} w_\ell \frac{\mathcal{K}_{-\rho}(z_\ell)}{\prod_{k=j}^{n}(1-\Delta_k z_\ell)} & j < n, \\ \frac{1}{\Delta_n} \mathcal{K}\left(\frac{1}{\Delta_n}\right) & j = n, \end{cases} \tag{31b}$$

where the weights and nodes are chosen by (28). The proof of the following error estimate follows from [16, Theorem 10] with the choice (21) for m and M and $c_0 \leftarrow 1/2$ therein.

Lemma 6 *Let q be defined as in (22), λ and k as in* (25). *Let $N \geq 1$ be the total number of time steps in* (13) *and define the ratio (cf. (21))*

$$R := N\left(m^{-1} + M^{-1/2}\right).$$

Let $\mathcal{K}$ satisfy Assumption 1. Then there exist constants $C_1, C_2 > 0$ depending only on C_{op} and θ but not on the discretization parameters such that

$$\Delta_j \left\| I_{j,n} - Q_{j,n} \right\| \leq \varepsilon_{\text{quad}} := C_1 \left(M^{\theta+1} \log q\right) \frac{\mathrm{e}^{2\max(1,\beta)R}}{\mathrm{e}^{N_Q \tau} - 1} \tag{32}$$

with

$$\tau := C_2 \frac{\min\left\{m^{-1}, M^{-1/2}\right\}}{\log q}. \tag{33}$$

The systems (31) can be rewritten in matrix form by setting $\mathbf{g}^{(\rho)} = \left(g_n^{(\rho)}\right)_{n=1}^{N}$, $\boldsymbol{\phi} = (\phi_n)_{n=1}^{N}$, $\mathbf{M} = (M_{j,n})_{j,n=1}^{N}$ and $\tilde{\mathbf{M}} = \left(\tilde{M}_{j,n}\right)_{j,n=1}^{N}$ with

$$M_{j,n} := \Delta_j \begin{cases} I_{j,n} & j \geq n, \\ 0 & \text{otherwise,} \end{cases} \quad \text{and} \quad \tilde{M}_{j,n} := \Delta_j \begin{cases} Q_{j,n} & j \geq n, \\ 0 & \text{otherwise,} \end{cases}$$

i.e.,

$$\mathbf{M}\boldsymbol{\phi} = \mathbf{g}^{(\rho)} \quad \text{and} \quad \tilde{\mathbf{M}}\widetilde{\boldsymbol{\phi}} = \mathbf{g}^{(\rho)}. \tag{34}$$

Hence,

$$\widetilde{\boldsymbol{\phi}} = \left(\left(\mathbf{I} - \mathbf{M}^{-1}\boldsymbol{\delta}\right)^{-1}\right)\mathbf{M}^{-1}\mathbf{g} \quad \text{with} \quad \boldsymbol{\delta} = \mathbf{M} - \tilde{\mathbf{M}}. \tag{35}$$

In order to derive consistency, stability, and convergence of the GCQ with contour quadrature we will introduce some appropriate norms.

Definition 7 *Let F and G denote normed vector spaces. For any $\mathbf{f} = (f_n)_{n=1}^{N} \in F^N$ we set*

$$\|\mathbf{f}\|_{0,\infty,F} := \max_{1 \leq n \leq N} \|f_n\|_F \quad \textit{and} \quad \|\mathbf{f}\|_{0,1,F} := \sum_{n=1}^{N} \Delta_n \|f_n\|_F.$$

A norm which is related to the second order divided differences is given by[4]

$$\|\mathbf{f}\|_{2,1,F} := \sum_{n=1}^{N} (\Delta_n + \Delta_{n-1}) \|[t_{n-2}, t_{n-1}, t_n]\, \mathbf{f}\|_F .$$

For an operator $\mathbf{H} : F^N \to G^N$ *we denote the operator norm by*

$$\|\mathbf{H}\|_{(i,j,G)\leftarrow(k,\ell,F)} := \sup_{\mathbf{v}\in F^N\setminus\{\mathbf{0}\}} \frac{\|\mathbf{H}\mathbf{v}\|_{i,j,G}}{\|\mathbf{v}\|_{k,\ell,F}}$$

for any $(i,j), (k,\ell) \in \{(0,1), (0,\infty), (2,1)\}$.

Lemma 8 *The norms* $\|\cdot\|_{0,\infty,F}$, $\|\cdot\|_{0,1,F}$, $\|\cdot\|_{2,\infty,F}$ *are equivalent and the constants of equivalence depend on the final time* $T = \sum_{n=1}^{N} \Delta_n$ *and the minimal mesh width* $\Delta_{\min}$*:*

$$\begin{aligned} \Delta_{\min} \|\mathbf{f}\|_{0,\infty,F} \leq \|\mathbf{f}\|_{0,1,F} &\leq T \|\mathbf{f}\|_{0,\infty,F} , \\ \|\mathbf{f}\|_{2,1,F} &\leq 4\frac{N}{\Delta_{\min}} \|\mathbf{f}\|_{0,\infty,F} . \end{aligned} \tag{36}$$

Lemma 9 (Consistency) *Let the assumptions of Lemma 6 be valid. Then, the consistency estimate*

$$\|\boldsymbol{\delta}\|_{(0,\infty,D)\leftarrow(0,\infty,B)} \leq N\varepsilon_{\text{quad}}. \tag{37}$$

holds with $\varepsilon_{\text{quad}}$ *as in (32).*

Proof. Let $\boldsymbol{\psi} = (\psi_n)_{n=1}^{N} \in B^N$. Then from (32) we conclude that

$$\|\delta_{j,n}\psi_n\|_D \leq \varepsilon_{\text{quad}} \|\psi_n\|_B$$

holds so that

$$\|\boldsymbol{\delta\psi}\|_{0,\infty,D} = \max_{0\leq n\leq N} \left\| \sum_{j=1}^{n-1} \delta_{n,j}\psi_j \right\|_D \leq \varepsilon_{\text{quad}} \max_{0\leq n\leq N} \sum_{j=1}^{n-1} \|\psi_j\|_B \leq \varepsilon_{\text{quad}} N \|\boldsymbol{\psi}\|_{0,\infty,B} .$$

■

The stability of the GCQ as in Definition 2 is proved in [15, Theorem 6] and implies the stability of the GCQ with contour quadrature.

Lemma 10 (Stability) *Let* q *be defined as in (22),* λ *and* k *as in* (25). *Let* $N \geq 1$ *be the total number of time steps in* (13). *Let the maximal mesh width* $\Delta_{\max}$ *be sufficiently small such that* $1 - \Delta_{\max}\sigma_+ \geq \alpha_0$ *for some* $\alpha_0 > 0$. *Let* $\mathcal{K}$ *and its inverse satisfy Assumption 1 and (9) for some* μ *and* σ_+ *as in (9) and let* ρ *be chosen according to (10). The solution of Algorithm 3 with contour*

[4] Formally we set $t_{-1} := -t_1$ and $f_{-1} = f_0 := 0$.

quadrature as in Section 4 is denoted $\tilde{\phi}_n$, $1 \leq n \leq N$. *Let the number of quadrature points* N_Q *be chosen such that*

$$C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\,\frac{N^2}{\Delta_{\min}}\varepsilon_{\text{quad}} \leq 1/8$$

with $\varepsilon_{\text{quad}}$ *as in (32). Then, the following stability estimate holds*

$$\left\|\tilde{\boldsymbol{\phi}}\right\|_{0,\infty,B} \leq 2C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D}. \tag{38}$$

with δ_0 *as in (30).*

Proof. In [15, Theorem 6] the stability estimate for the GCQ *without* contour quadrature is proved which is the first inequality in

$$\|\boldsymbol{\phi}\|_{0,\infty,B} = \left\|\mathbf{M}^{-1}\mathbf{g}^{(\rho)}\right\|_{0,\infty,B} \leq C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D} \tag{39}$$

$$\overset{(36)}{\leq} 4C_{\text{stab}}^{\text{I}}\frac{N}{\Delta_{\min}}\,\mathrm{e}^{\delta_0 T}\left\|\mathbf{g}^{(\rho)}\right\|_{0,\infty,D}. \tag{40}$$

The GCQ *with* contour quadrature (cf. (19)) has a unique solution since the operators $\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)$ are invertible (cf. (9)). Hence,

$$\begin{aligned}
\left\|\tilde{\boldsymbol{\phi}}\right\|_{0,\infty,B} &\overset{(35),\,(39)}{\leq} C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\left\|\left(\mathbf{I}-\mathbf{M}^{-1}\boldsymbol{\delta}\right)^{-1}\right\|_{0,\infty,B\leftarrow 0,\infty,B}\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D}\\
&\leq C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\,\frac{\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D}}{1-\left\|\mathbf{M}^{-1}\boldsymbol{\delta}\right\|_{(0,\infty,B)\leftarrow(0,\infty,B)}}\\
&\overset{(40)}{\leq} C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\,\frac{\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D}}{1-4C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\,\frac{N}{\Delta_{\min}}\left\|\boldsymbol{\delta}\right\|_{(0,\infty,D)\leftarrow(0,\infty,B)}}.
\end{aligned}$$

The combination of the consistency estimate and (38) gives the assertion. ■

We finally formulate the convergence theorem for the GCQ with contour quadrature.

Theorem 11 *Let* q *be defined as in (22),* λ *and* k *as in* (25). *Let* $N \geq 1$ *be the total number of time steps in* (13). *Let the maximal mesh width* $\Delta_{\max}$ *be sufficiently small such that* $1-\Delta_{\max}\sigma_+ \geq \alpha_0$ *for some* $\alpha_0 > 0$. *Let* $\mathcal{K}$ *and its inverse satisfy Assumption 1 and (9), respectively, for some* μ *and* σ_+ *as in (9) and let* ρ *satisfy (10). The solution of Algorithm 3 with contour quadrature as in Section 4 is denoted* $\tilde{\phi}_n$, $1 \leq n \leq N$. *Let the number of quadrature points* N_Q *be chosen such that* $\varepsilon_{\text{quad}}$ *in (32) satisfies*

$$C_{\text{stab}}^{\text{I}}\,\mathrm{e}^{\delta_0 T}\,\frac{N^2}{\Delta_{\min}}\varepsilon_{\text{quad}} \leq 1/8.$$

Then, the following error estimate holds

$$\left\| \boldsymbol{\phi} - \widetilde{\boldsymbol{\phi}} \right\|_{0,\infty,B} \leq C_{\text{stab}}^{\text{II}} \frac{N^2}{\Delta_{\min}} \varepsilon_{\text{quad}} \left\| \mathbf{g}^{(\rho)} \right\|_{2,1,D}, \tag{41}$$

with $C_{\text{stab}}^{\text{II}} := 2C_1 \left(2C_{\text{stab}}^{\text{I}} \mathrm{e}^{\delta_0 T}\right)^2$.

Proof. From (34) we obtain the error representation

$$\boldsymbol{\phi} - \widetilde{\boldsymbol{\phi}} = -\mathbf{M}^{-1} \boldsymbol{\delta} \widetilde{\boldsymbol{\phi}}$$

and hence, the result follows from (40), Lemma 9, and Lemma 10 via

$$\begin{aligned}
\left\| \boldsymbol{\phi} - \widetilde{\boldsymbol{\phi}} \right\|_{0,\infty,B} &\overset{(39)}{\leq} 4C_{\text{stab}}^{\text{I}} \frac{N}{\Delta_{\min}} \mathrm{e}^{\delta_0 T} \left\| \boldsymbol{\delta} \widetilde{\boldsymbol{\phi}} \right\|_{0,\infty,D} \\
&\overset{(\text{Lem.9})}{\leq} 4C_{\text{stab}}^{\text{I}} \mathrm{e}^{\delta_0 T} \frac{N^2}{\Delta_{\min}} \varepsilon_{\text{quad}} \left\| \widetilde{\boldsymbol{\phi}} \right\|_{0,\infty,B} \\
&\overset{(\text{Lem. }10)}{\leq} 2 \left(2C_{\text{stab}}^{\text{I}} \mathrm{e}^{\delta_0 T}\right)^2 \frac{N^2}{\Delta_{\min}} \varepsilon_{\text{quad}} \left\| \mathbf{g}^{(\rho)} \right\|_{2,1,D}.
\end{aligned}$$

■

Finally, we will formulate a simplified version of Theorem 11 under some mild assumptions on the step sizes and the mesh grading. Note that $\Delta_{\max} \geq \frac{T}{N}$ always holds. We assume in addition the following two (mild) assumptions on the mesh grading: There exist $C_{\text{uni}} > 0$, $\alpha \geq 1$, and $c_{\text{grad}} > 0$ such that

$$\Delta_{\max} \leq C_{\text{uni}} \frac{T}{N} \quad \text{and} \quad \Delta_{\min} \geq c_{\text{grad}} \Delta_{\max}^{\alpha}. \tag{42}$$

The subsequent constants depend on the time mesh only via the constants C_{uni}, c_{grad}, and α but not on the size of $\Delta_{\max}$. Condition (42) implies for the ratio $q = M/m$ and the quantities R, τ in Lemma 6 the estimates

$$\begin{aligned}
q &\leq C_3 \left(N + N^{\alpha-1}\right), & R &\leq 4N\Delta_{\max} =: C_4, \\
\tau &\geq \frac{c_5}{N^{\gamma} \log N} & &\text{with} \quad \gamma := \max\left\{1, \tfrac{\alpha}{2}\right\},
\end{aligned}$$

where the positive constants C_3, C_4, c_5 only depend on T, c_{grad}, C_{uni}, and α.

Corollary 12 *Let the assumptions of Theorem 11 be valid and let the mesh satisfy (42). For given $\varepsilon > 0$, let the number of quadrature points for the approximation of the contour integral satisfy*

$$N_Q \geq C_6 N^{\gamma} \log N \left(\log N + \log \left(\frac{1}{\varepsilon} \right) \right)$$

for some $C_6 > 0$ depending only on T, on the constants in (11), and (42). Then, the solution $\tilde{\phi}_n$, $1 \leq n \leq N$, of Algorithm 3 with contour quadrature as in Section 4 is well defined and satisfies the error estimate

$$\left\| \boldsymbol{\phi} - \widetilde{\boldsymbol{\phi}} \right\|_{0,\infty,B} \leq \varepsilon \left\| \mathbf{g}^{(\rho)} \right\|_{2,1,D}.$$

For $\varepsilon = C_{\mathrm{uni}} \frac{T}{N}$ we obtain: The choice $N_Q \geq \tilde{C}_6 N^{\gamma} \log^2 N$ implies the following estimate for the total error at time points t_n :

$$\left\| \phi(t_n) - \tilde{\phi}_n \right\|_B \leq C_g \Delta_{\max} c_{\rho-\mu}(\Delta_{\max}) \quad \forall 1 \leq n \leq N.$$

Remark 13 *Our numerical experiments indicate that for a grading exponent $\alpha = 2$, the choice*

$$N_Q = N \log N$$

already leads to sufficiently small contour quadrature errors. Note that for a transfer operator which is symmetric with respect to the real axis (as it is the case in our applications) this implies

$$N_Q = \frac{1}{2} N \log N.$$

5 Application to the Wave Equation

In this section we will show that the boundary integral formulation for the wave equation can be efficiently solved by the GCQ method by using the contour integral representation (16) in combination with the quadrature method, i.e., (19) with the choice of quadrature points and nodes as in (28). For this, we will prove in this section that the transfer operator for the retarded potential boundary integral equation belongs to the class which is described in Assumption 1 with properly chosen constants α, β, p, σ_-.

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

$$\partial_t^2 u = \Delta u \qquad \text{in } \Omega \times (0,T) \tag{43a}$$

with initial conditions

$$u(\cdot, 0) = \partial_t u(\cdot, 0) = 0 \qquad \text{in } \Omega \tag{43b}$$

and boundary conditions

$$u = g \quad \text{on } \Gamma \times (0,T) \tag{43c}$$

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* (cf. [7],[2])

$$\forall t \in (0,T) \quad u(x,t) = \int_0^t \int_\Gamma \frac{\delta(t - \|x-y\|)}{4\pi \|x-y\|} \phi(y,\tau) \, d\Gamma_y \, d\tau \quad \forall x \in \Omega, \tag{44}$$

with the Dirac delta distribution $\delta(\cdot)$.

The ansatz (44) satisfies the homogeneous equation (43a) and the initial conditions (43b). The extension $x \to \Gamma$ is continuous and hence, the unknown density ϕ in (44) is determined via the boundary conditions (43c), $u(x,t) = g(x,t)$. This results in the boundary integral equation for ϕ,

$$\forall t \in (0,T) \quad \int_0^t k(t-\tau)\phi(\tau)\,d\tau = g(t) \quad \text{in } H^{1/2}(\Gamma), \tag{45}$$

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

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

The Sobolev spaces $H^s(\Gamma)$, $s \geq 0$, are defined in the usual way (see, e.g., [9] or [23]) and the spaces with negative order $s < 0$ by duality. The norm is denoted by $\|\cdot\|_{H^s(\Gamma)}$.

Existence and uniqueness results for the solution of the continuous problem (45) are proven in [2].

The Laplace transformed integral operator, i.e., the transfer operator for $k(t)$, is given by

$$\mathcal{K}(z)\,\phi := \int_\Gamma \frac{\mathrm{e}^{-z\|\cdot - y\|}}{4\pi \|\cdot - y\|} \phi(y)\,d\Gamma_y. \tag{46}$$

It is well known (see [2, Prop. 3]) that $\mathcal{K}(z) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is an isomorphism for all z with $\operatorname{Re} z > 0$ and also for $z = 0$. More precisely, the following continuity estimates hold [2].

Proposition 14 *Let $z \in \mathbb{C}$ with $\operatorname{Re} z = \sigma_+ > 0$. Then*

$$\|\mathcal{K}(z)\|_{H^{1/2}(\Gamma) \leftarrow H^{-1/2}(\Gamma)} \leq C \frac{1 + \sigma_+^2}{\sigma_+^3} |z|$$

and

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

5.1 The Continuity Constant of the Acoustic Single Layer Operator

In this section, we will generalize the existing estimates of the continuity constant of $\mathcal{K}(z)$ for $\operatorname{Re} z > \sigma_+ > 0$ to the whole complex plane. The proof uses similar arguments as in [24, Lemma 3.5 and 3.7].

For $z \in \mathbb{C}$, the acoustic single layer boundary integral operator with complex frequency $z \in \mathbb{C}$ is defined (cf. (46)) by

$$(\mathcal{K}(z))\,\phi(x) := \int_\Gamma G_z(x-y)\,\phi(y)\,d\Gamma_y,$$

where $G_z : \mathbb{R}^3 \backslash \{0\} \to \mathbb{C}$ denotes the fundamental solution for the operator $\mathcal{L}_z := -\Delta + z^2$, i.e., $G_z(x) = g_z(\|x\|)$ with $g_z(r) = \frac{\mathrm{e}^{-zr}}{4\pi r}$. Our goal is to estimate the continuity constant $C_c(z)$ of the operator $\mathcal{K}(z)$, i.e.,

$$C_c(z) := \|\mathcal{K}(z)\|_{H^{1/2}(\Gamma) \leftarrow H^{-1/2}(\Gamma)}$$

in terms of z. For the estimate of $\mathcal{K}(z)$ we will employ the Newton potential $N(z) : H^{-1}_{\text{comp}}\left(\mathbb{R}^3\right) \to H^1_{\text{loc}}\left(\mathbb{R}^3\right)$ which is defined by

$$(N(z)f)(x) := \int_{\mathbb{R}^3} \frac{\mathrm{e}^{-z\|x-y\|}}{4\pi\|x-y\|} f(y)\, dy \quad \forall f \in H^{-1}_{\text{comp}}\left(\mathbb{R}^3\right).$$

Let $\gamma_0 : H^1_{\text{loc}}\left(\mathbb{R}^3\right) \to H^{1/2}(\Gamma)$ denote the standard trace operator and $\gamma_0' : H^{-1/2}(\Gamma) \to H^{-1}_{\text{comp}}\left(\mathbb{R}^3\right)$ its dual, i.e.,

$$\langle \gamma_0'(\varphi), v\rangle_{H^{-1}_{\text{comp}}(\mathbb{R}^3)\times H^1_{\text{loc}}(\mathbb{R}^3)} = \langle \varphi, \gamma_0(v)\rangle_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} \qquad \forall v \in H^1_{\text{loc}}\left(\mathbb{R}^3\right).$$

Then, we have $\mathcal{K}(z) := \gamma_0 N(z)\gamma_0'$ (cf. [26, Def. 3.15 and (3.1.6); see also: p.146, l 5]).

Note that for $\varphi \in H^{-1/2}(\Gamma)$, the functional $\gamma_0'(\varphi)$ is a distribution in $H^{-1}_{\text{comp}}\left(\mathbb{R}^3\right)$ with $\operatorname{supp}\gamma_0'(\varphi) \subset \Gamma$. Hence, we may choose an open ball B_Γ with radius $R = O(\operatorname{diam}\Gamma)$ such that $\operatorname{supp}\gamma_0'(\varphi) \subset \Gamma \subset B_\Gamma$. The combination of Lemma 16 below with standard mapping properties of the trace operator and its dual leads to

$$\begin{aligned}
\|K(z)\varphi\|_{H^{1/2}(\Gamma)} &= \|\gamma_0 N(z)\gamma_0'(\varphi)\|_{H^{1/2}(\Gamma)} \leq C_\Gamma \|N(z)\gamma_0'(\varphi)\|_{H^1(B_\Gamma)} \\
&\overset{\text{(Lem. 16)}}{\leq} C_\Gamma C_R \max\{1,|z|\}\left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right)\|\gamma_0'(\varphi)\|_{H^{-1}(\mathbb{R}^3)} \\
&\leq C_\Gamma' C_\Gamma C_R \max\{1,|z|\}\left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right)\|\varphi\|_{H^{-1/2}(\Gamma)}.
\end{aligned}$$

This is summarized as the following theorem.

Theorem 15 *Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with diameter R. It holds*

$$\|\mathcal{K}(z)\|_{H^{1/2}(\Gamma)\leftarrow H^{-1/2}(\Gamma)} \leq C_{\Gamma,R}\max\{1,|z|\}\left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right) \qquad \forall z \in \mathbb{C}.$$

Thus, the transfer function $\mathcal{K}(z)$ for the retarded potential of the wave equation satisfies Assumption 1 with $C_{\text{op}} = C_\Gamma$, $\theta = 1$, any $\sigma_- < 0$, and some $\beta > 0$ depending only on $\operatorname{diam}\Gamma$.

The proof of Theorem 15 follows from the next lemma, which provides explicit bounds for the solution operator $N(z)$.

Lemma 16 *For any $R > 0$, there exists a constant*[5] *$C_R > 0$ such that for any $f \in H^{-1}_{\text{comp}}\left(\mathbb{R}^3\right)$ with support contained in a ball B_R with some diameter R it holds*

$$\|\nabla N(z) f\|_{L^2(B_R)} + \|N(z) f\|_{L^2(B_R)} \leq C_R \max\{1,|z|\}\left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right)\|f\|_{H^{-1}(\mathbb{R}^3)}$$

for all $z \in \mathbb{C}$.

[5]In the following, the constant C_R may change in every occurance – however it will always be positive and depend only on $R > 0$.

Proof. We start by recalling the definition of the Fourier transform for functions with compact support

$$\hat{u}(\xi) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\langle \xi, x\rangle} u(x)\, dx \qquad \forall \xi \in \mathbb{R}^3$$

and the inversion formula

$$u(x) = (2\pi)^{-3/2} \int_{\mathbb{R}^3} \mathrm{e}^{\mathrm{i}\langle x, \xi\rangle} \hat{u}(\xi)\, d\xi \qquad \forall x \in \mathbb{R}^3.$$

Let $f \in H^{-1}_{\mathrm{comp}}(\mathbb{R}^3)$ be given and let $B_R \subset \mathbb{R}^3$ be an open ball of radius R containing $\operatorname{supp} f$. Let $\nu \in C^\infty(\mathbb{R}_{\geq 0})$ be a cutoff function such that

$$\begin{aligned}
&\operatorname{supp} \nu \subset [0, 4R], && \nu|_{[0,2R]} = 1, \quad |\nu|_{W^{1,\infty}(\mathbb{R}_{\geq 0})} \leq \frac{C}{R}, \\
&\forall x \in \mathbb{R}_{\geq 0} : 0 \leq \nu(x) \leq 1, && \nu|_{[4R,\infty[} = 0, \quad |\nu|_{W^{2,\infty}(\mathbb{R}_{\geq 0})} \leq \frac{C}{R^2}.
\end{aligned} \tag{47}$$

Let $\mathcal{M}(z) := \nu(\|z\|)$ and

$$w_\nu(x) := \int_{B_R} G(z, x-y)\, \mathcal{M}(x-y)\, f(y)\, dy \qquad \forall x \in \mathbb{R}^3.$$

Since $\operatorname{supp} f \subset B_R$ we may define

$$w := G(z, \cdot) \star f \quad \text{and write} \quad w_\nu = (G(z,\cdot)\,\mathcal{M}) \star f. \tag{48}$$

The properties of ν guarantee $w_\nu|_{B_R} = w|_{B_R}$ so that we may restrict our attention to the function w_ν. We compute the Fourier transform of $G(z,\cdot)\,\mathcal{M}$:

$$\begin{aligned}
(G\widehat{(z,\cdot)\,\mathcal{M}})(\xi) &= (2\pi)^{-3/2} \int_{\mathbb{R}^3} \mathrm{e}^{-\mathrm{i}\langle \xi, x\rangle} G(z,x)\, \mathcal{M}(x)\, dx \\
&= (2\pi)^{-3/2} \int_0^\infty g(z,r)\, \nu(r)\, r^2 \left(\int_{\mathbb{S}_2} \mathrm{e}^{-\mathrm{i}\, r \langle \xi, \zeta\rangle} dS_\zeta \right) dr \\
&= (2\pi)^{-3/2} I(z,\xi).
\end{aligned}$$

The inner integral in $I(z,\xi)$ can be evaluated analytically (cf. [24, p. 1882]) and $I(z,\xi) = \iota(z, \|\xi\|)$ with

$$\iota(z,s) = 4\pi \int_0^\infty g(z,r)\, \nu(r)\, r^2 \frac{\sin(rs)}{(rs)} dr. \tag{49}$$

Applying the Fourier transform to the convolution (48) leads to

$$\widehat{w_\nu} = (2\pi)^{3/2} (G\widehat{(z,\cdot)\,\mathcal{M}}) \widehat{f}.$$

By using standard properties of the Fourier transformation and its relation to Sobolev norms we obtain

$$\|w\|_{H^1(B_R)} \leq \|w_\nu\|_{H^1(\mathbb{R}^3)} = (2\pi)^{3/2} \left\| \sqrt{1+\|\xi\|^2} (\widehat{G(z,\cdot)\mathcal{M})}\widehat{f} \right\|_{L^2(\mathbb{R}^3)} \tag{50}$$

$$\leq \left(\max_{\xi\in\mathbb{R}^3} \left| \left(1+\|\xi\|^2\right) I(z,\xi) \right| \right) \left\| \frac{1}{\sqrt{1+|\xi|^2}} \widehat{f} \right\|_{L^2(\mathbb{R}^3)}$$

$$\leq \left(\max_{s\geq 0} \left| \left(1+s^2\right) \iota(z,s) \right| \right) \|f\|_{H^{-1}(\mathbb{R}^3)}.$$

Hence, Lemma 17 below implies

$$\|w\|_{H^1(B_R)} \leq C_R \max\{1,|z|\} \left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right) \|f\|_{H^{-1}(\mathbb{R}^3)}.$$

■

Lemma 17 *The function $\iota(z,\cdot)$ defined in (49) can be estimated by*

$$\max_{s\geq 0} \left| \left(1+s^2\right) \iota(z,s) \right| \leq C_R \max\{1,|z|\} \left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right) \qquad \forall z\in\mathbb{C}.$$

Proof. Applying integration by parts we obtain

$$|\iota(z,s)| = \frac{C}{|z|} \left| \int_0^\infty \mathrm{e}^{-zr} \left(\nu'(r) \frac{\sin(rs)}{s} + \nu(r)\cos(rs) \right) dr \right|$$

$$\leq C \frac{1+\mathrm{e}^{-4R\operatorname{Re}(z)}}{|z|} \int_0^{4R} \left(\frac{C}{R} r + 1 \right) dr = CR \frac{1+\mathrm{e}^{-4R\operatorname{Re}(z)}}{|z|}.$$

On the other hand for $|z| \leq 1$

$$|\iota(z,s)| = \left| \int_0^\infty \mathrm{e}^{-zr} \nu(r) \frac{\sin(rs)}{s} dr \right| \leq \left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right) \int_0^{4R} \left| \frac{\sin rs}{s} \right| dr$$

$$\leq \left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right) \int_0^{4R} r dr = 8R^2 \left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right)$$

so that

$$|\iota(z,s)| \leq C_R \frac{1+\mathrm{e}^{-4R\operatorname{Re}(z)}}{1+|z|}.$$

For the product $s^2\iota_k(s)$, we get

$$\left|s^2\iota(z,s)\right| = C \left| \int_0^\infty \mathrm{e}^{-zr} \nu(r)\, s\sin(rs)\, dr \right| = C \left| \int_0^\infty \mathrm{e}^{-zr} \nu(r)\, \partial_r \cos(rs)\, dr \right|$$

$$\leq C \left(\left| \int_0^\infty \cos(rs)\, \partial_r \left(\mathrm{e}^{-zr}\nu(r)\right) dr \right| + 1 \right)$$

$$\leq C|z| \left| \int_0^\infty \cos(rs)\, \mathrm{e}^{-zr} \nu(r)\, dr \right| + C \left(\left| \int_0^\infty \cos(rs)\, \mathrm{e}^{-zr} \nu'(r)\, dr \right| + 1 \right)$$

$$\leq C(1+R|z|) \left(1+\mathrm{e}^{-4R\operatorname{Re}(z)}\right). \qquad ■$$

6 Numerical Experiments

6.1 Decoupled, purely time-depending example

In [27] analytical solutions for the acoustic potential in (45) have been computed for the case $\partial\Omega = \mathbb{S}^2$, assuming that $g(x,t) = g(t)Y_n^m$, for Y_n^m the spherical harmonic of degree n and order m. It is well known (cf. [13], [25]) that

$$\mathcal{K}(z)Y_n^m = \lambda_n(z)Y_n^m,$$

where $\lambda_n(z)$ can be expressed in terms of modified Bessel functions I_κ and K_κ (see [1]) by

$$\lambda_n(z) = I_{n+\frac{1}{2}}(z)K_{n+\frac{1}{2}}(z).$$

The ansatz

$$\phi(x,t) = \phi(t)Y_n^m$$

leads to the one-dimensional problem: Find $\phi(t)$ such that

$$\int_0^t \mathcal{L}^{-1}[\lambda_n](t-\tau)\phi(\tau)\,d\tau = g(t).$$

For $n = 0$, the first spherical harmonic Y_0^0 is constant so that $g(x,t) = g(t)$ and

$$\lambda_0(z) = \frac{1 - \mathrm{e}^{-2z}}{2z}.$$

The exact solution in this case is given by

$$\phi(t) = 2\sum_{k=0}^{\lfloor t/2 \rfloor} g'(t-2k). \tag{51}$$

Remark 18 *The full wave-equation is particularly important to model electric or acoustic systems shortly after they are "switched on", i.e., before the system has reached a time-harmonic steady state which then can be modeled in the frequency domain by a Helmholtz-type equation. The problem becomes very challenging if the right-hand side g is not* very *smooth at $t = 0$, i.e., has only, say, one or two vanishing derivatives at $t = 0$. These are the kind of applications, where the GCQ becomes advantageous.*

To test the performance of the GCQ for such kinds of applications we have chosen the following model problem as our first numerical example

$$g(t) = t^{3/2}\mathrm{e}^{-t}, \quad \mathcal{K}(z) = \lambda_0(z) = \frac{1-\mathrm{e}^{-2z}}{2z}, \quad \mathcal{K}^{-1}(z) = \frac{2z}{1-\mathrm{e}^{-2z}}, \tag{52}$$

where g and g' vanish at the origin but g'' already has a singularity for $t = 0$.

Remark 19 (Choice of Regularization Parameter) *In our numerical experiments it turns out that the simplest choice $\rho = 0$ of the regularization parameter in (19) performs very well and indicate that the theoretical condition $\rho \geq 3$ in [15] might be too strong. It is an open problem whether there exist examples where $\rho > 0$ is necessary or whether this condition is an artifact of the theory.*

We have approximated ϕ for $t \in [0, 1]$ by applying (13) with $\rho = 0$. Note that the non-smoothness of g at $t = 0$ is inherited to an irregularity of the solution ϕ of strength $O\left(t^{1/2}\right)$ due to (51). This justifies to use a time mesh which is algebraically graded towards $t = 0$. As a grading exponent we have chosen (heuristically) a quadratic grading, i.e., $\alpha = 2$ in

$$t_j = \left(\frac{j}{N}\right)^{\alpha}, \qquad j = 1, \ldots, N \tag{53}$$

and compared this in our numerical experiment to constant time stepping, i.e., $\alpha = 1$ in (53). As expected we observe numerically (cf. Figure 3) an order reduction from 1 to 1/2 for the error associated to the implicit Euler method with *constant* time steps while the optimal (linear) convergence order is preserved by using the graded mesh.

In order to compute the approximation with $\alpha = 1$ we employed the CQ algorithm as presented in [18]. For the approximation with $\alpha = 2$ we applied the algorithm described in Section 3 with the quadrature formula (28). In this case, the choice of parameters for the quadrature is given by

$$\Delta_{\max} = N^{-1}, \quad \Delta_{\min} = N^{-2}, \quad q = N, \quad \theta = -1.$$

From Corollary 12 we deduce that, by choosing the number of contour quadrature points according to $N_Q = O\left(N \log^2 N\right)$, the GCQ *with* contour quadrature converges at the same rate as the unperturbed GCQ method. In practice a better behavior is observed and the results displayed in Figure 3 are computed with $N_Q = N \log N$.

Figure 1 shows the numerical and the exact solution for $N = 20$ time steps and the two values of the grading power $\alpha = 1, 2$. The corresponding evolution of the absolute error is shown in Figure 2. The maximal error appears at the first time steps due to the lack of regularity at the origin and is much smaller for the graded mesh than for constant time stepping. More precisely, Figure 3 shows that the convergence is optimal (linear) for the graded mesh while the convergence speed is reduced to $O\left(\Delta_{\max}^{1/2}\right)$ for constant time steps.

6.2 The full wave equation

Let again $\partial\Omega$ be the unit sphere. We solve numerically the full wave equation (43) with right-hand side

$$g(x, t) = g(t) Y_1^1(x), \tag{54}$$

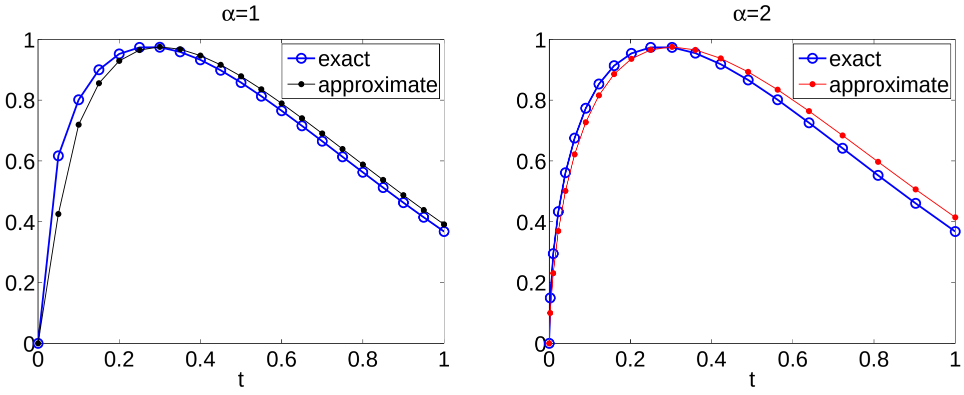

Figure 1: Exact and approximation of the potential for the data in (52) with 20 steps. *Left:* With uniform time steps ($\alpha = 1$ in (53)). *Right:* With quadratically graded time steps ($\alpha = 2$ in (53))

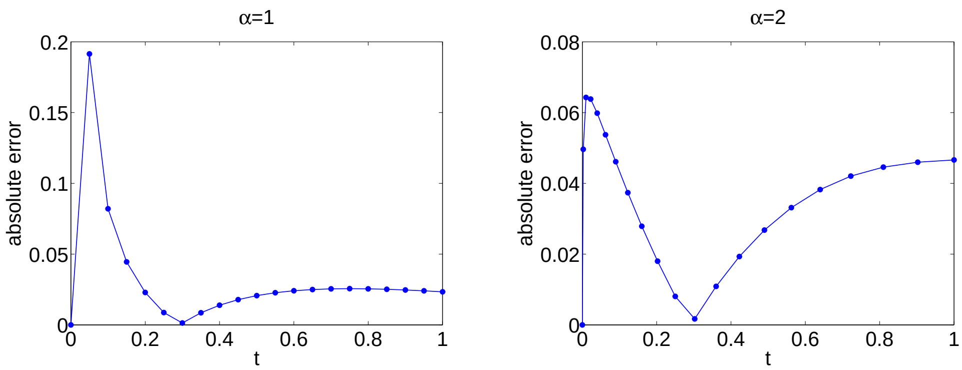

Figure 2: Pointwise error in the approximation of the potential for the data in (52) with 20 steps. *Left:* With uniform time steps ($\alpha = 1$ in (53)). *Right:* With quadratically graded time steps ($\alpha = 2$ in (53))

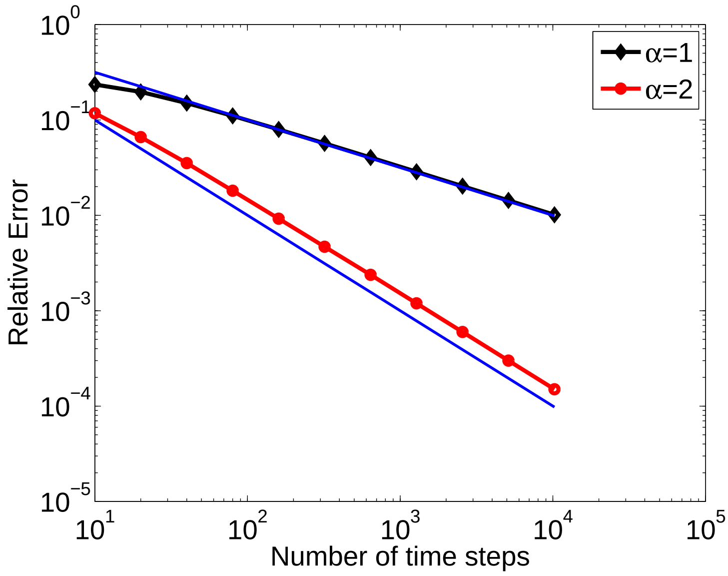

Figure 3: Error with respect to the number of steps for g in (52). The straight lines indicate slopes 1/2 and 1, respectively.

for the same time-dependent part $g(t)$ as in (52). Y_1^1 denotes the spherical harmonic of degree 1 and order 1. In spherical coordinates, Y_1^1 is given by

$$Y_1^1(\theta, \varphi) = -\sqrt{\frac{3}{8\pi}}\sin(\theta)\mathrm{e}^{\mathrm{i}\varphi}.$$

For $t \in [0, 2]$ the analytical solution for the potential is

$$\phi(x,t) = \left(2g'(t) + 2\int_0^t \sinh(\tau)g'(t-\tau)\,d\tau\right)\cdot Y_1^1(x).$$

For the spatial discretization we use Martin Huber's BEM implementation in MATLAB (cf. [11]) of the Galerkin boundary element method with continuous, piecewise linear boundary elements on surface triangulations – for details of the boundary element method we refer, e.g., to [26]. At every spatial node, the behavior of the solution in time is the same as in the scalar example in Section 6.1. Thus, we choose again the time steps as in (53) and compare the performance for $\alpha = 1.01$ (almost uniform time stepping) and $\alpha = 2$.

Once the problem is discretized in space, we integrate in time the semidiscrete problem by applying the algorithm in Section 3 for both values of α. Note that every summand in (19) involves a boundary element matrix. If the spatial boundary element mesh is unchanged during the time stepping, these matrices can be pre-computed in parallel.

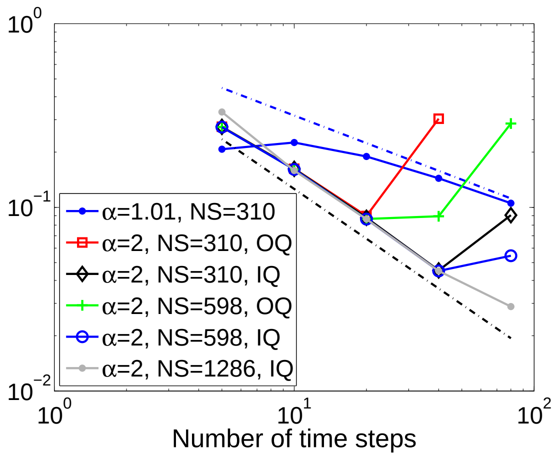

Figure 4: Error with respect to the number of time steps for g as in (54). NS is the number of degrees of freedom in the spatial discretization. The abbreviation "OQ" stands for "original quadrature" for approximating the entries of the boundary element matrices (cf. [26]), where the order is chosen as in the case of constant time stepping. "IQ" stands for "improved quadrature" where the quadrature order is significantly increased. The straight dashed lines depict the slopes 1/2 and 1, respectively.

In Figure 4, the maxima $\max_{1\leq n\leq N} \left\| \phi\left(t_n\right) - \tilde{\phi}_n \right\|_{L^2(\Gamma)}$ of the spatial L^2-errors for the two considered grading exponents, $\alpha = 1.01$ and $\alpha = 2$, are depicted. For the Galerkin boundary element discretization with continuous, piecewise linear shape functions we employed a boundary element mesh on the sphere consisting of 616 ($NS = 310$), 1192 ($NS = 598$) and 2568 ($NS = 1286$) triangles. As in the purely time-dependent problem of the previous section we observe an improvement of the order of convergence with respect to the number of time steps from $1/2$ to 1. In this plot we can also observe that the accuracy which is required for the quadrature approximation being involved for the generation of the boundary element matrices has to take into account the size (smallness) of the time steps: We can eliminate this pollution effect by either refining in space (crosses) or by increasing the number of quadrature nodes in the matrix assembly process (diamonds) or, of course, by doing both (circles and grey dots). A careful analysis in order to optimize the quadrature in space with respect to the time steps and the spatial discretization is the subject of future research.

References

[1] M. Abramowitz and I. A. Stegun. *Handbook of Mathematical Functions.* Applied Mathematics Series 55. National Bureau of Standards, U.S. Department of Commerce, 1972.

[2] A. Bamberger and T. H. Duong. Formulation Variationnelle Espace-Temps pur le Calcul par Potientiel Retardé de la Diffraction d'une Onde Acoustique. *Math. Meth. in the Appl. Sci.*, 8:405–435, 1986.

[3] L. Banjai. Multistep and multistage convolution quadrature for the wave equation: Algorithms and experiments. *SIAM J. Sci. Comput.*, 32(5):2964–2994, 2010.

[4] M. Caliari. Accurate evaluation of divided differences for polynomial interpolation of exponential propagators. *Computing*, 80(2):189–201, 2007.

[5] C. de Boor. Divided differences. *Surv. Approx. Theory*, 1:46–69, 2005.

[6] T. A. Driscoll. The Schwarz–Christoffel toolbox. *available online at http://www.math. udel.edu/˜driscoll/software/SC/.*

[7] M. Friedman and R. Shaw. Diffraction of pulses by cylindrical obstacles of arbitrary cross section. *J. Appl. Mech*, 29:40–46, 1962.

[8] I. S. Gradshteyn and I. Ryzhik. *Table of Integrals, Series, and Products.* Academic Press, New York, London, 1965.

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

[10] N. Hale, N. J. Higham, and L. N. Trefethen. Computing $\mathbf{A}^{\alpha}$, $\log(\mathbf{A})$, and related matrix functions by contour integrals. *SIAM J. Numer. Anal.*, 46(5):2505–2523, 2008.

[11] M. Huber. *Numerical Solution of the Wave Equation in Unbounded Domains.* Master Thesis. University of Zurich, 2011.

[12] B. Khoromskij, S. Sauter, and A. Veit. Fast Quadrature Techniques for Retarded Potentials Based on TT/QTT Tensor Approximation. *Comp. Meth. Appl. Math.*, 11(3):342–362, 2011.

[13] R. Kress. Minimizing the Condition Number of Boundary Integral Operators in Acoustics and Electromagnetic Scattering. *Q. Jl. Mech. appl. Math.*, 38:323–341, 1985.

[14] M. Lopez-Fernandez, C. Lubich, and A. Schädle. Adaptive, fast, and oblivious convolution in evolution equations with memory. *SIAM J. Sci. Comput.*, 30(2):1015–1037, 2008.

[15] M. Lopez-Fernandez and S. A. Sauter. A Generalized Convolution Quadrature with Variable Time Stepping. Technical Report 17-2011, Institut für Mathematik, Univ. Zürich, 2011.

[16] M. Lopez-Fernandez and S. A. Sauter. Fast and Stable Contour Integration for High Order Divided Differences via Elliptic Functions. Technical Report 08-2012, Institut für Mathematik, Univ. Zürich, 2012.

[17] C. Lubich. Convolution Quadrature and Discretized Operational Calculus I. *Numerische Mathematik*, 52:129–145, 1988.

[18] C. Lubich. Convolution Quadrature and Discretized Operational Calculus II. *Numerische Mathematik*, 52:413–425, 1988.

[19] C. Lubich. On the multistep time discretization of linear initial-boundary value problems and their boundary integral equations. *Numerische Mathematik*, 67(3):365–389, 1994.

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

[21] C. Lubich and A. Ostermann. Runge-Kutta methods for parabolic equations and convolution quadrature. *Math. Comp.*, 60(201):105–131, 1993.

[22] A. McCurdy, K. C. Ng, and B. N. Parlett. Accurate computation of divided differences of the exponential function. *Math. Comp.*, 43(168):501–528, 1984.

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

[24] J. Melenk and S. Sauter. Convergence Analysis for Finite Element Discretizations of the Helmholtz equation with Dirichlet-to-Neumann boundary condition. *Math. Comp*, 79:1871–1914, 2010.

[25] J. Nédélec. *Acoustic and Electromagnetic Equations*. Springer-Verlag, 2001.

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

[27] S. Sauter and A. Veit. A Galerkin Method for Retarded Boundary Integral Equations with Smooth and Compactly Supported Temporal Basis Functions. *Numer. Math.*, electronic.

[28] J. L. Walsh. *Interpolation and Approximation by Rational Functions in the Complex Domain*. American Mathematical Society, New York City, 1935.