Generalized convolution quadrature with variable time stepping.
Part II: algorithm and numerical results

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Abstract

In this paper we address the implementation of the Generalized Convolution Quadrature (gCQ) presented and analyzed by the authors in a previous paper for solving linear parabolic and hyperbolic convolution 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 consider the wave equation in exterior domains, which is formulated as a retarded boundary integral equation. We provide numerical experiments to illustrate the theoretical results.

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 [14] for solving linear convolution equations of the form

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

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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 it is the Laplace transform $\mathcal{K}$ of the convolution kernel k what is known or convenient to evaluate. For these problems the Convolution Quadrature (CQ) developed originally by Lubich is an excellent method, see [17, 18, 21, 20] for parabolic problems and [19] for hyperbolic ones. However both, the derivation of the CQ and its implementation, are strongly restricted to fixed time step integration. The Generalized Convolution Quadrature (gCQ) presented in [14] provides a remedy to this limitation when the time discretization is based on the implicit Euler method. In the recent work [16] the method in [14] has been extended to high order Runge–Kutta methods. An alternative approach which also allows variable time steps for solving *retarded potential integral equations* can be found in [26], [28].

In [14], the gCQ has been introduced and formulated via high order divided differences of the *transfer function/operator* $\mathcal{K}$, in a way which was appropriate for the stability and error analysis but less suited for the efficient algorithmic realization. Here, we will present an efficient algorithmic formulation of the gCQ which is based on the approximation of the divided differences by quadrature in the complex plane, following [15]. The algorithm is easy to implement and allows for a high level of parallelism.

In the present paper we impose weaker assumptions on the transfer operator $\mathcal{K}$ compared to those in [14, Section 2] and, thus, allow for more general operators $\mathcal{K}$ which are analytic in the half plane

$$\mathbb{C}_\sigma := \{z \in \mathbb{C} \mid \operatorname{Re} z > \sigma\}$$

for some $\sigma \in \mathbb{R} \cup \{-\infty\}$ and have some algebraic growth behaviour in $\mathbb{C}_\sigma$. 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. We generalize here the estimate of the continuity constant for the acoustic single layer operator to frequencies in the whole complex plane which simplifies the choice of the contour for the quadrature approximation.

The paper is organized as follows. In Section 2 we will introduce the class of problems 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 by means of the implicit Euler method with variable step size, what we call Generalized Convolution Quadrature (gCQ). An algorithm for the practical realization of the gCQ is presented in Section 4. Our algorithm is based on contour integral representation of the numerical solution and quadrature in the complex plane. The quadrature method is described in Section 5. In Section 6 we analyze the error introduced by the contour quadrature discretization. The application to the boundary integral formulation of the wave equation is considered in Section 7, where new estimates for the acoustic single layer potential operator are derived for general complex frequencies. Numerical experiments are shown in Section 8.

2 The class of problems

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 its inverse Laplace transform, the *transfer operator* $\mathcal{K}$. The class of problems under consideration is defined as follows.

Assumption 1 *Let $\theta,\mu \in \mathbb{R}$, $\sigma_+ > 0$ and $\sigma_- < \sigma_+$. The class $\mathcal{A}^{\theta,\mu}_{\sigma_-,\sigma_+}(B,D)$ of transfer operators consists of operator valued mappings $\mathcal{K} : \mathbb{C}_{\sigma_-} \to \mathcal{L}(B,D)$ which satisfy:*

1. *$\mathcal{K} : \mathbb{C}_{\sigma_-} \to \mathcal{L}(B,D)$ is analytic.*
2. *$\mathcal{K}$ satisfies the estimate*

$$\|\mathcal{K}(z)\| \leq C_{\mathrm{op}} (\max\{1,|z|\})^{\theta}, \qquad \forall z \in \mathbb{C}_{\sigma_-}, \tag{3}$$

   for a fixed constant $C_{\mathrm{op}} > 0$.

3. *The inverse operator $\mathcal{K}^{-1} : \mathbb{C}_{\sigma_+} \to \mathcal{L}(D,B)$ exists and hence is analytic.*
4. *$\mathcal{K}^{-1}$ satisfies the estimate*

$$\left\|\mathcal{K}^{-1}(z)\right\| \leq C_{\mathrm{inv}} |z|^{\mu}, \qquad \forall z \in \mathbb{C}_{\sigma_+}, \tag{4}$$

   for fixed $C_{\mathrm{inv}} > 0$. [1]

For $\rho \in \mathbb{N}_0$ we define

$$\mathcal{K}_\rho(z) := z^{-\rho}\mathcal{K}(z). \tag{5}$$

For any $\rho > \theta + 1$, the Laplace inversion formula

$$k_\rho(t) := \frac{1}{2\pi\,\mathrm{i}} \int_\gamma \mathrm{e}^{zt}\,\mathcal{K}_\rho(z)\,dz, \tag{6}$$

[1]The generic constant C in the following estimates will depend on C_{op} and C_{inv} but not explicitly on σ_-, σ_+. Hence, if $C_{\mathrm{op}}, C_{\mathrm{inv}}$ are independent of σ_-, σ_+ so is the constant C.

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

$$(\mathcal{K}(\partial_t)\phi)(t) := \left(\frac{d}{dt}\right)^\rho \int_{-\infty}^t k_\rho(t-\tau)\,\phi(\tau)\,d\tau = \int_0^\infty k_\rho(\tau)\,\phi^{(\rho)}(t-\tau)\,d\tau \quad (7)$$

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

By the composition rule for one-sided convolutions (cf. [19, (2.3), (2.22)]) the solution of the convolution equation

$$\mathcal{K}(\partial_t)\,\phi = g, \quad (8)$$

for g being smooth enough and having sufficiently many vanishing moments at $t = 0$ (cf. Theorem 15), is given by

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

Then

$$\phi(t) = \int_0^t \left(\frac{1}{2\pi\,\mathrm{i}}\int_\gamma \mathrm{e}^{z\tau}(\mathcal{K}^{-1})_\rho(z)dz\right) g^{(\rho)}(t-\tau)\,d\tau, \quad (9)$$

for $\rho \in \mathbb{N}_0$ with $\rho > \mu + 1$. In this way, ρ will be chosen as

$$\rho := \min\{s \in \mathbb{N}_0 \mid s > \max\{\mu+1, \theta+1\}\}. \quad (10)$$

3 Generalized convolution quadrature based on implicit Euler

In [14], the generalized convolution quadrature has been presented via high order divided differences which are well suited for the stability and error analysis but suffer from strong roundoff instabilities for the practical implementation. In this paper, we will introduce a new (but equivalent) formulation via contour integrals which will play the key role for its algorithmic realization.

Definition 2 (Generalized Convolution Quadrature) *For a set of given time points $\Theta := (t_n)_{n=0}^N$ and corresponding time steps $\Delta_j = t_j - t_{j-1}$, $1 \leq j \leq N$, the generalized convolution quadrature approximation based on the implicit Euler method of*

$$\mathcal{K}(\partial_t)\,\phi = g \quad (11)$$

at time points t_n is given by the solution $\boldsymbol{\phi} = (\phi_n)_{n=1}^N$ of

$$\mathcal{K}_{-\rho}\left(\partial_t^\Theta\right)\boldsymbol{\phi} = \mathbf{g}^{(\rho)}, \quad (12)$$

where $\mathbf{g}^{(\rho)} = \left(g^{(\rho)}(t_n)\right)_{n=1}^N$ and the operator $\mathcal{K}_{-\rho}\left(\partial_t^\Theta\right)$ applied to a vector $\boldsymbol{\phi}$ is given by

$$\left(\mathcal{K}_{-\rho}\left(\partial_t^\Theta\right)\boldsymbol{\phi}\right)_n = \frac{1}{2\pi\,\mathrm{i}}\int_{\mathcal{C}} \mathcal{K}_{-\rho}(z)\,u_n(z)dz. \quad (13)$$

Here u_n is the approximation of the scalar ODE problem

$$\partial_t u(z,t) = z\, u(z,t) + \phi(t), \qquad u(z,0) = 0 \tag{14}$$

at time t_n by the implicit Euler method, this is

$$u_n(z) = \frac{1}{1-\Delta_n z} u_{n-1}(z) + \frac{\Delta_n}{1-\Delta_n z}\phi_n; \quad u_0(z) = 0. \tag{15}$$

$\mathcal{C}$, in (13), is any closed contour lying in $\mathbb{C}_{\sigma_-}$ and enclosing all poles Δ_n^{-1}, $1 \le n \le N$, of the integrand in (13).

Remark 3 *The solution of equation (12) can be written in the form*[2] *[4, 14]*

$$\phi_n = \left(\mathcal{K}^{-1}\right)_\rho \left(\partial_t^\Theta\right) \mathbf{g}^{(\rho)} = \sum_{j=1}^{n} \omega_{n,j}(0) \left(\left[\frac{1}{\Delta_j}, \frac{1}{\Delta_{j+1}}, \ldots, \frac{1}{\Delta_n} \right] \left(\mathcal{K}^{-1}\right)_\rho \right) g_j^{(\rho)}, \tag{16}$$

where

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

and $[y_1, \ldots, y_n]\, f$ denotes Newton's divided difference for a (operator-valued) function f with respect to the arguments in the brackets, with the standard generalization for repeated arguments. For some $\mathbf{f} = (f_i)_{i=1}^n$, we will use the notation $[y_1, \ldots, y_n]\, \mathbf{f}$ for the divided difference associated to the pairs $(y_i, f_i)_{i=1}^n$. Representation (16) *was used in [14] for the error analysis.*

In general, for any transfer operator $\mathcal{V}$ the action of $\mathcal{V}\left(\partial_t^\Theta\right)$ to a vector $\boldsymbol{\phi} = (\phi_n)_{n=1}^N$ is nothing but the application of a block triangular matrix $(\mathcal{V}_{n,j})_{n,j=1}^N$ to $\boldsymbol{\phi}$ by setting

$$\mathcal{V}_{n,j} := \begin{cases} \dfrac{\Delta_j}{2\pi\,\mathrm{i}} \displaystyle\int_{\mathcal{C}} \frac{\omega_{n,j}(0)}{\omega_{n,j}(z)} \mathcal{V}(z)\, dz & j \le n, \\ 0 & \textit{otherwise}. \end{cases} \tag{17}$$

4 Algorithm for gCQ

From (15), definition (13) and Cauchy's formula, equation (12) can be written in the form

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)\phi_n = g_n^{(\rho)} - \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \frac{\mathcal{K}_{-\rho}(z)}{1-\Delta_n z} u_{n-1}(z)\, dz, \tag{18}$$

for u_{n-1} being the approximation at time t_{n-1} of the scalar ODE (14). In [15] an efficient quadrature rule for (18) has been proposed, with nodes z_ℓ and weights

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

w_ℓ, $\ell = 1, \cdots, N_Q$, given explicitly in (29). The application of this quadrature to (18) leads to the computation of

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

where $u_{n-1}(z_\ell)$ is the implicit Euler approximation of (14) with $z \leftarrow z_\ell$. The reduction of (1) to the solution of scalar ODEs in the Laplace domain and the application of quadrature in the complex plane are also key ingredients in the algorithm presented in [13]. However the complexity and storage estimates in [13] do not apply directly to our setting due to different properties of the integrands in the Laplace transforms and the different performance of the quadrature formula.

Our method is formulated in an algorithmic way as follows.

Algorithm 4 (gCQ with contour quadrature)

- ***Initialization.*** *Generate*[3] $\mathcal{K}_{-\rho}(z_\ell)$ *for all contour quadrature nodes* z_ℓ, $\ell = 1, 2, \ldots, N_Q$. *Compute* $\phi_1^{\mathcal{C}}$ *from*

$$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_1}\right)\phi_1^{\mathcal{C}} = g_1^{(\rho)}. \tag{20}$$

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

  1. ***Implicit Euler step.*** *Apply an implicit Euler step to (14) and compute*

  $$u_{n-1}(z_\ell) = \frac{u_{n-2}(z_\ell)}{1-\Delta_{n-1}z_\ell} + \frac{\Delta_{n-1}}{1-\Delta_{n-1}z_\ell}\phi_{n-1}^{\mathcal{C}}$$

  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*

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

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

  $$\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_n}\right)\phi_n^{\mathcal{C}} = r_n.$$

[3] For the numerical solution of the wave equation by gCQ (cf. Sec. 7), this requires the discretization of the operator $\mathcal{K}_{-\rho}\left(\frac{1}{\Delta_1}\right)$, e.g., by the Galerkin boundary element method.

Remark 5 *The algorithm above requires the pre-computation of the operators $\mathcal{K}_{-\rho}(z_\ell)$, 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 $\mathcal{K}_{-\rho}(z_\ell)$. 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]). For example, if $\Delta \sim N$ and $\Delta_{\min} \sim \Delta^2$, as in Section 8, the number of required quadrature nodes is $O(N \log(N))$. Furthermore, it is to be expected that the use of variable steps can significantly reduce N for the same target accuracy, see Figures 3 and 4, with the corresponding savings in the number of evaluations and storage of $\mathcal{K}$ in comparison with a uniform step implementation.*

Another important advantage of our algorithm is that the time steps do not need to be known in advance – only an upper bound of their total number as well as lower and upper bounds of their sizes are required, as we will see in the next section.

Remark 6 (Complexity for the wave equation) *In the case of constant time stepping for the boundary integral formulation of the wave equation, the* solution *of the arising block triangular Toeplitz system can be accelerated by FFT techniques (cf. [9]). The resulting CPU time is of order $\mathcal{O}\left(L^3 + L^2 N\right)$ up to logarithmic terms, where L is the dimension of the boundary element space for the spatial discretization. A straightforward implementation of the new gCQ algorithm requires the generation of $\mathcal{O}(N)$ $L \times L$ boundary element matrices (up to logarithmic factors) while the solution of the integro-differential equation requires $\mathcal{O}\left(L^3 n_{\#} + L^2 N^2\right)$ arithmetic operations, with $n_{\#} \leq N$ being the number of different time steps. We emphasize that updates involved in each step of our algorithm can be performed in parallel and, in addition, that the number of time steps N for the gCQ can be much smaller than for the CQ method. For certain applications, these facts may compensate the quadratic scaling with respect to N for the gCQ. It is a topic of future research to develop a fast version of this algorithm which scales log-linear with respect to N.*

For a general transfer operator $\mathcal{V}$ and quadrature rule with nodes z_ℓ and weights w_ℓ we denote the discretization of the blocks in (17) by

$$
\left(Q_{\mathcal{C}}\left(\mathcal{V}\right)\right)_{n,j} := \begin{cases} \frac{\Delta_j}{2\pi \mathrm{i}} \sum_{\ell=1}^{N_Q} w_\ell \frac{\omega_{n,j}(0)}{\omega_{n,j}(z_\ell)} \mathcal{V}(z_\ell) & j < n, \\ \mathcal{V}\left(\frac{1}{\Delta_n}\right) & j = n, \\ 0 & \text{otherwise.} \end{cases} \tag{21}
$$

5 Contour quadrature

The development of an efficient quadrature rule for the integrals in (12) is a challenging problem due to the presence of poles $\Delta_j^{-1} \in [m, M]$ with possibly $M/m \gg 1$, [10, 15]. A subtle choice of the contour parametrization is required, which must be adapted to the class of functions satisfying Assumption 1. For this class of functions such a quadrature approximation has been developed and analyzed recently by the authors in [15]. In the following we will develop this quadrature method for the gCQ.

The case $\sigma_- < -1$.

We first consider the case $\sigma_- < -1$ while the modifications for the case $\sigma_- \geq -1$ are explained in Remark 7.

For the sake of simplicity and as explained in Remark 5, we will assume that the contour in (18) and the quadrature points z_ℓ are fixed during the time stepping. The choice of the contour will depend on the maximal and the minimal time steps, which are denoted by

$$\Delta := \max_{1\leq j\leq N} \Delta_j \quad \text{and} \quad \Delta_{\min} := \min_{1\leq j\leq N} \Delta_j$$

and should be chosen in advance. Since the number of quadrature nodes will depend only very mildly on the ratio $\frac{\Delta}{\Delta_{\min}}$, the choices $\Delta_{\min} = \Delta^\alpha$ for some $1 \leq \alpha \leq 2$ or even stronger gradings $\alpha > 2$ will lead to an efficient algorithm.

The contour and the quadrature will depend on[4]

$$m = \Delta^{-1}, \qquad M = \max\left(m^2, \frac{1}{\Delta_{\min}}\right), \tag{22}$$

and the ratio

$$q := \frac{M}{m}. \tag{23}$$

To avoid technicalities we always assume that $\Delta^{-1} > \frac{8}{3}$ holds, which guarantees that a certain neighborhood of the contour which will be relevant for the error analysis has a proper distance from the interval $[m, M]$.

For $\lambda \in [0, 1]$, we employ the usual notation $\operatorname{sn}(\eta|\lambda)$, $\operatorname{cn}(\eta|\lambda)$, $\operatorname{dn}(\eta|\lambda)$ for the Jacobi elliptic functions as defined, e.g., in [1] and denote by

$$K(\lambda) := \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-\lambda x^2)}} \qquad \text{(see [7, 8.112 (1.) and (2.)]} \tag{24}$$

$$K'(\lambda) := K(1-\lambda) \qquad \text{(see [7, 8.112 (3.) and 8.111 (2.)])} \tag{25}$$

the complete elliptic integrals of the first kind.

For q as is (23) we compute

$$k = k(q) = \frac{q - \sqrt{2q-1}}{q + \sqrt{2q-1}} \qquad \text{and} \qquad \lambda = k^2 \tag{26}$$

[4] Our numerical experiments show that the choice $M := \Delta_{\min}^{-1}$ performs better in practice while the choice as in (22) allows to employ the error estimates in [15] without modifications.

and set

$$P = -K(\lambda) + \frac{\mathrm{i}}{2}K'(\lambda) \quad \text{and} \quad Q = P + 4K(\lambda). \tag{27}$$

Our choice for the integration contour $\mathcal{C}$ in (18) is then

$$\overline{PQ} \to \mathcal{C} : \eta \mapsto \gamma_M(\eta) := \frac{M}{q-1}\left(\sqrt{2q-1}\frac{k^{-1} + \mathrm{sn}\,(\eta|\lambda)}{k^{-1} - \mathrm{sn}\,(\eta|\lambda)} - 1\right) \tag{28}$$

which is nothing but the circle in the complex plane of radius M centered at M parameterized in a subtle way (cf. [15, 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

$$z_\ell = \gamma_M(\eta_\ell) \quad \text{and} \quad w_\ell = \frac{4K(\lambda)}{2\pi\mathrm{i}}\gamma_M'(\eta_\ell), \tag{29}$$

with

$$\eta_\ell = -K(\lambda) + \left(\ell - \frac{1}{2}\right)\frac{4K(\lambda)}{N_Q} + \frac{\mathrm{i}}{2}K'(\lambda), \tag{30}$$

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

$$\gamma_M'(\eta) = \frac{M\sqrt{2q-1}}{q-1}\frac{2\mathrm{cn}\,(\eta|\lambda)\mathrm{dn}\,(\eta|\lambda)}{k(k^{-1} - \mathrm{sn}\,(\eta|\lambda))^2}. \tag{31}$$

The choice of nodes in (29) 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 [5] which is freely available online. In particular the functions `ellipkkp` and `ellipjc` are needed to compute (29), cf. [10].

As we have already mentioned in Remark 5, 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 (29). 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 $\mathcal{K}(\eta_\ell)$ to those η_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.

The case $\sigma_- \geq -1$.

If $\sigma_- \geq -1$ we can shift the integration contour $\mathcal{C}$ to the right as explained in the following remark.

Remark 7 *For $\sigma_- \geq -1$ in Assumption 1, we shift the contour to the right by choosing $\gamma_{M,\mu} := \mu + \gamma_M$ as the parametrization, for some $\mu \geq 0$ whose choice is explained next, and by imposing the mild condition* (33) *on the maximal time step. For $\kappa \geq 0$, we introduce the contour neighborhood*

$$\mathcal{C}_{M,\kappa} := \left\{ \gamma_M \left(t + \mathrm{i}\, v \right) : t \in \overline{PQ} \wedge -\kappa \leq v \leq \kappa \right\}. \tag{32}$$

The condition $\mu > \sigma_- + 1$ ensures the shifted contour neighborhood $\mu + \mathcal{C}_{M,\kappa}$ is contained in the analyticity region $\mathbb{C}_{\sigma_-}$ for $0 \leq \kappa \leq c_1 \min \left\{ M^{-1/2}, m^{-1} \right\}$ and some fixed constant $c_1 > 0$ (see [15, Theorem 8]). To ensure that the shifted contour $\mu + \mathcal{C}_{M,\kappa}$ encircles $[m, M]$ we assume, as a first condition on the maximal time step, that $\mu < m$. From [15, Theorem 8], we then conclude that

$$\max \left\{ |z| : z \in \mu + \mathcal{C}_{M,\rho} \right\} \leq c_2 M$$

and also that, for all $x \in [m, M]$, it holds

$$\operatorname{dist}\left(x, \mu + \mathcal{C}_{M,\rho} \right) \geq \left(1 - 2M^{-1/2} - \left(\frac{2}{3} + \mu \right) m^{-1} \right) x. \tag{33}$$

As the final condition on the maximal time step we assume that

$$\Delta^{-1} > \frac{8}{3} + \mu \tag{34}$$

holds which implies that the right-hand side in (32) is positive.

6 Error analysis

In this section we estimate the difference between the solution $\boldsymbol{\phi}$ of the "exact" gCQ (12) and the solution $\boldsymbol{\phi}^{\mathcal{C}}$ of the contour quadrature based gCQ for the weights and nodes in (29). Throughout this section we assume that the contour quadrature is applied as described in Section 5: If $\sigma_- < -1$, we set $\mu = 0$ while, for $\sigma_- \geq -1$, the shift parameter μ is chosen as explained in Remark 7. The condition (33) on the maximal time step is always assumed to be satisfied.

The gCQ with and without contour quadrature can be written in the form

$$\mathcal{K}_{-\rho}(\partial_t^{\Theta})\boldsymbol{\phi} = \mathbf{g}^{(\rho)} \qquad \text{and} \qquad Q_{\mathcal{C}}(\mathcal{K}_{-\rho})\boldsymbol{\phi}^{\mathcal{C}} = \mathbf{g}^{(\rho)},$$

according to definition (21). It follows that

$$\boldsymbol{\phi}^{\mathcal{C}} = \left(\left(\mathbf{I} - \mathcal{K}_{\rho}^{-1}(\partial_t^{\Theta})\mathcal{D} \right)^{-1} \right) \mathcal{K}_{\rho}^{-1}(\partial_t^{\Theta})\mathbf{g}^{(\rho)} \quad \text{with} \quad \mathcal{D} = \mathcal{K}_{\rho}(\partial_t^{\Theta}) - Q_{\mathcal{C}}(\mathcal{K}_{\rho}) \tag{35}$$

and

$$\boldsymbol{\phi} - \boldsymbol{\phi}^{\mathcal{C}} = -\mathcal{K}_{\rho}^{-1}(\partial_t^{\Theta})\mathcal{D}\boldsymbol{\phi}^{\mathcal{C}} \tag{36}$$

Remark 8 *The conditions and estimates in Remark 7 allow a straightforward generalization of the quadrature error analysis in [15] to the case $\sigma_- \geq -1$.*

Lemma 9 *Let q be defined as in (23), λ and k as in* (26)*. Let $N \geq 1$ be the total number of time steps in* (12) *and define the quantity*

$$R := N\left(\frac{1}{M^{1/2}} + \frac{2+3\mu}{6m}\right),$$

which is related with the mesh grading (cf. (22)), where $\mu = 0$ if $\sigma_- \leq -1$ and is otherwise chosen as explained in Remark 7. Assume that $m > \frac{8}{3} + \mu$ and let $\mathcal{K}$ satisfy (3)*. Then there exist constants $C_1, C_2 > 0$ independent of the discretization parameters such that*

$$\left\| \mathcal{K}_{n,j} - \left(Q_{\mathcal{C}}(\mathcal{K})\right)_{n,j} \right\| \leq \varepsilon_{\text{quad}} := C_{\text{op}} C_1 \left(M^{\theta+1} \log q\right) \frac{\mathrm{e}^{2R}}{\mathrm{e}^{N_Q \tau} - 1} \tag{37}$$

with $\mathcal{K}_{n,j}$ as in (17)*, $Q_{\mathcal{C}}(\mathcal{K}))_{n,j}$ as in* (21)*, C_{op} as in (3), and*

$$\tau := C_2 \frac{\min\left\{m^{-1}, M^{-1/2}\right\}}{\log q}. \tag{38}$$

Proof. It follows from [15, Theorem 10] with the choice (22) for m and M and $c_0 \leftarrow 1/2$ therein. Notice that for fixed $\sigma_- < -1$, every $K \in A^{\theta,\mu}_{\sigma_-,\sigma_+}(B, D)$ belongs also to the class $A(\sigma_-, \theta, C_{\text{op}} + 1)$ defined in [15, Definition 3]. ■

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

Definition 10 *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 (cf. Remark 3) is given by[5]

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

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

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

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

Notice that the first subindex in the norm stands for the order of the divided differences which are involved in its definition.

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

Lemma 11 *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* $\Delta_{\min}$*:*

$$\begin{aligned}\Delta_{\min}\|\mathbf{f}\|_{0,\infty,F} \leq \|\mathbf{f}\|_{0,1,F} \leq T\|\mathbf{f}\|_{0,\infty,F}\,,\\ \|\mathbf{f}\|_{2,1,F} \leq 4\frac{N}{\Delta_{\min}}\|\mathbf{f}\|_{0,\infty,F}\,.\end{aligned} \tag{39}$$

The simple proof is left to the interested reader.

Lemma 12 (Consistency) *Let the assumptions of Lemma 9 be valid. Then, the consistency estimate*

$$\|\mathcal{D}\|_{(0,\infty,D)\leftarrow(0,\infty,B)} \leq N\varepsilon_{\mathrm{quad}}. \tag{40}$$

holds with $\varepsilon_{\mathrm{quad}}$ *as in (36).*

Proof. Let $\boldsymbol{\psi}=(\psi_n)_{n=1}^{N}\in B^N$. Then from (36) we conclude that

$$\|\mathcal{D}_{j,n}\psi_n\|_D \leq \varepsilon_{\mathrm{quad}}\|\psi_n\|_B$$

holds so that

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

■

The stability of the gCQ as in Definition 2 (without contour quadrature) is proved in [14, Theorem 6]. Here, we will generalize these results and derive the stability of the gCQ *with* contour quadrature.

Lemma 13 (Stability) *Let* q *be defined as in (23),* λ *and* k *as in* (26)*. Let* $N\geq 1$ *be the total number of time steps in* (12)*. Let the maximal mesh width* Δ *be sufficiently small such that* $1-\Delta\sigma_+\geq\alpha_0$ *for some* $\alpha_0>0$*. Let* $\mathcal{K}$ *and its inverse satisfy Assumption 1 for some* μ *and* σ_+ *as in (4) and let* ρ *be chosen according to (10). The solution of Algorithm 4 with contour quadrature as in Section 5 is denoted* $\phi_n^{\mathcal{C}}$, $1\leq n\leq N$*. Let the number of quadrature points* N_Q *be chosen such that*

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

with $\varepsilon_{\mathrm{quad}}=\varepsilon_{\mathrm{quad}}(N_Q)$ *as in (36). Then, the following stability estimate holds*

$$\left\|\boldsymbol{\phi}^{\mathcal{C}}\right\|_{0,\infty,B}\leq 2C_{\mathrm{stab}}^{\mathrm{I}}\,\mathrm{e}^{\delta_0 T}\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D} \tag{41}$$

with

$$\delta_0=\frac{\sigma_+}{\alpha_0}. \tag{42}$$

Proof. In [14, Theorem 6] the stability estimate for the gCQ *without* contour quadrature is proved which is the first inequality in

$$\|\boldsymbol{\phi}\|_{0,\infty,B} = \left\|\mathcal{K}_\rho^{-1}(\partial_t^\Theta)\mathbf{g}^{(\rho)}\right\|_{0,\infty,B} \le C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T} \left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D} \tag{43}$$

$$\overset{(38)}{\le} 4C_{\text{stab}}^{\text{I}} \frac{N}{\Delta_{\min}} \, \mathrm{e}^{\delta_0 T} \left\|\mathbf{g}^{(\rho)}\right\|_{0,\infty,D}. \tag{44}$$

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. (4)). Hence,

$$\begin{aligned}
\left\|\boldsymbol{\phi}^{\mathcal{C}}\right\|_{0,\infty,B} &\overset{(34),\,(42)}{\le} C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T} \left\|\left(\mathbf{I} - \mathcal{K}_\rho^{-1}(\partial_t^\Theta)\mathcal{D}\right)^{-1}\right\|_{0,\infty,B\leftarrow 0,\infty,B} \left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D} \\
&\le C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T} \frac{\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D}}{1 - \left\|\mathcal{K}_\rho^{-1}(\partial_t^\Theta)\mathcal{D}\right\|_{(0,\infty,B)\leftarrow(0,\infty,B)}} \\
&\overset{(43)}{\le} C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T} \frac{\left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D}}{1 - 4C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T} \frac{N}{\Delta_{\min}} \|\mathcal{D}\|_{(0,\infty,D)\leftarrow(0,\infty,B)}}.
\end{aligned}$$

The combination of the consistency estimate and (40) gives the assertion. ■

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

Theorem 14 (Convergence) *Let q be defined as in* (23), *λ and k as in* (26). *Let $N \ge 1$ be the total number of time steps in* (12). *Let the maximal mesh width Δ be sufficiently small such that $1 - \Delta\sigma_+ \ge \alpha_0$ for some $\alpha_0 > 0$. Let $\mathcal{K}$ and its inverse satisfy* (3) *and* (4), *respectively, for some μ and σ_+ as in (4) and let ρ satisfy (10). The solution of Algorithm 4 with contour quadrature as in Section 5 is denoted $\phi_n^{\mathcal{C}}$, $1 \le n \le N$. Let the number of quadrature points N_Q be chosen such that $\varepsilon_{\text{quad}}$ in (36) satisfies*

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

Then, the following error estimate holds

$$\left\|\boldsymbol{\phi} - \boldsymbol{\phi}^{\mathcal{C}}\right\|_{0,\infty,B} \le C_{\text{stab}}^{\text{II}} \frac{N^2}{\Delta_{\min}} \varepsilon_{\text{quad}} \left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D} \tag{45}$$

with $C_{\text{stab}}^{\text{II}} := 2C_1 \left(2C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T}\right)^2$ and δ_0 as in (41).

Proof. By using the error representation in (35), the result follows from (43), Lemma 12, and Lemma 13 via

$$\begin{aligned}
\left\|\boldsymbol{\phi} - \boldsymbol{\phi}^{\mathcal{C}}\right\|_{0,\infty,B} &\overset{(42)}{\le} 4C_{\text{stab}}^{\text{I}} \frac{N}{\Delta_{\min}} \, \mathrm{e}^{\delta_0 T} \left\|\mathcal{D}\boldsymbol{\phi}^{\mathcal{C}}\right\|_{0,\infty,D} \\
&\overset{\text{(Lem.12)}}{\le} 4C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T} \frac{N^2}{\Delta_{\min}} \varepsilon_{\text{quad}} \left\|\boldsymbol{\phi}^{\mathcal{C}}\right\|_{0,\infty,B} \\
&\overset{\text{(Lem. 13)}}{\le} 2\left(2C_{\text{stab}}^{\text{I}} \, \mathrm{e}^{\delta_0 T}\right)^2 \frac{N^2}{\Delta_{\min}} \varepsilon_{\text{quad}} \left\|\mathbf{g}^{(\rho)}\right\|_{2,1,D}.
\end{aligned}$$

■

The total error in our approximation of (1) is $\phi(t_n) - \phi_n^{\mathcal{C}}$. We recall here the convergence theorem from [14] for the error $\phi(t_n) - \phi_n$. We notice that in [14, Theorem 4.3] an exponential factor $e^{\delta_0 T}$ is included in the error constant C. In the statement below we have opted for a sharper version of the estimate with a j-dependent factor $e^{\delta_0(t_n - t_{j-1})}$.

Theorem 15 *Let (4) be satisfied and let Δ be sufficiently small such that $1 - \Delta\sigma_+ \geq \alpha_0$ for some $\alpha_0 > 0$. Let $N \geq 1$ be the total number of time steps and ρ in (12) be chosen such that (10) holds. Let the right-hand side in (11) 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 (12). Then, the error estimate holds*

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

with

$$c_\nu(\Delta) := \begin{cases} 1 + \log \frac{1}{\Delta}, & \textit{if } \nu = 1, \\ 1, & \textit{if } \nu > 1, \end{cases} \tag{46}$$

and δ_0 as in (41).

By the triangle inequality, an estimate for the global error $\phi(t_n) - \phi_n^{\mathcal{C}}$ follows straightforwardly from Theorems 15 and 14.

Finally, we will formulate a simplified version of Theorem 14 under some mild assumptions on the step sizes and the mesh grading. Note that $\Delta \geq \frac{T}{N}$ 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

$$\Delta \leq C_{\text{uni}} \frac{T}{N} \quad \text{and} \quad \Delta_{\min} \geq c_{\text{grad}} \Delta^\alpha. \tag{47}$$

The subsequent constants depend on the time mesh only via the constants C_{uni}, c_{grad}, and α but not on the size of Δ. Condition (46) implies for the ratio $q = M/m$ and the quantities R, τ in Lemma 9 the estimates

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

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

Corollary 16 *Let the assumptions of Theorem 14 be valid and let the mesh satisfy (46). 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 Assumption 1, and (46). Then, the solution $\phi_n^{\mathcal{C}}$, $1 \leq n \leq N$, of Algorithm 4 with contour quadrature as in Section 5 is well defined and satisfies the error estimate

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

For $\varepsilon = C_{\text{uni}} \frac{T}{N}$ 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

$$\left\| \phi(t_n) - \phi_n^{\mathcal{C}} \right\|_B \leq C_g \Delta c_{\rho-\mu}(\Delta) \quad \forall 1 \leq n \leq N,$$

where c_ν is as in (45).

Remark 17 *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

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

7 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. For this, we will prove that the transfer operator for the retarded potential boundary integral equation satisfies Assumption 1 with properly chosen constants C_{op}, C_{inv}, θ, μ, σ_- and 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

$$\partial_t^2 u = \Delta u \qquad \text{in } \Omega \times (0,T) \tag{47a}$$

with initial conditions

$$u(\cdot, 0) = \partial_t u(\cdot, 0) = 0 \qquad \text{in } \Omega \tag{47b}$$

and boundary conditions

$$u = g \quad \text{on } \Gamma \times (0,T) \tag{47c}$$

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. [6],[2])

$$\forall t \in (0,T) \quad u(x,t) = \int_0^t \int_\Gamma \frac{\delta(t - \|x-y\|)}{4\pi \|x-y\|} \phi(y,\tau)\, d\Gamma_y\, d\tau \quad \forall x \in \Omega \tag{49}$$

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

The ansatz (48) satisfies the homogeneous equation (47a) and the initial conditions (47b). The extension $x \to \Gamma$ is continuous and hence, the unknown density ϕ in (48) is determined via the boundary conditions (47c), $u(x,t) = g(x,t)$. This results in the boundary integral equation for ϕ,

$$\forall t \in (0,T) \quad \int_0^t k(t-\tau)\phi(\tau)\, d\tau = g(t) \quad \text{in } H^{1/2}(\Gamma), \tag{50}$$

where $k(t) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is the boundary integral operator for the single layer potential of the wave equation (47),

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

The Sobolev space $H^s(\Gamma)$, $s \in [-1,1]$, is defined in the usual way (see, e.g., [8] or [22]) and the corresponding norm is denoted by $\|\cdot\|_{H^s(\Gamma)}$. Existence and uniqueness results for the solution of the continuous problem (49) are proven in [2].

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

$$\mathcal{K}(z)\phi := \int_\Gamma \frac{\mathrm{e}^{-z\|\cdot - y\|}}{4\pi \|\cdot - y\|} \phi(y)\, d\Gamma_y. \tag{51}$$

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 18 *Let $\sigma > 0$. For all $z \in \mathbb{C}_\sigma$ it holds*

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

and

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

In the following section, we will generalize the existing estimates (Proposition 18) 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 [23, Lemma 3.5 and 3.7]. This allows to avoid the shift of the integration contour since we will prove $\sigma_- = -\infty$.

7.1 The continuity constant of the acoustic single layer operator

For $z \in \mathbb{C}$, the acoustic single layer boundary integral operator with complex frequency $z \in \mathbb{C}$ is defined (cf. (50)) 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 $\mathcal{N}(z) : H^{-1}_{\text{comp}}(\mathbb{R}^3) \to H^1_{\text{loc}}(\mathbb{R}^3)$ which is defined by

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

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

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

Then, we have $\mathcal{K}(z) := \gamma_0 N(z) \gamma_0'$ (cf. [25, 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 $H^{-1}_{\text{comp}}(\mathbb{R}^3)$ with $\operatorname{supp} \gamma_0'(\varphi) \subset \Gamma$. Hence, we may choose an open ball B_Γ with radius $d = O(\operatorname{diam} \Gamma)$ such that $\operatorname{supp} \gamma_0'(\varphi) \subset \Gamma \subset B_\Gamma$. The combination of Lemma 20 below with standard mapping properties of the trace operator and its dual leads to

$$\begin{aligned}
\|\mathcal{K}(z)\varphi\|_{H^{1/2}(\Gamma)} &= \|\gamma_0 \mathcal{N}(z) \gamma_0'(\varphi)\|_{H^{1/2}(\Gamma)} \le C_\Gamma \|\mathcal{N}(z) \gamma_0'(\varphi)\|_{H^1(B_\Gamma)} \\
&\overset{\text{(Lem. 20)}}{\le} C_\Gamma C_d \max\{1, |z|\} \left(1 + \mathrm{e}^{-4d \operatorname{Re}(z)}\right) \|\gamma_0'(\varphi)\|_{H^{-1}(\mathbb{R}^3)} \\
&\le C_\Gamma' C_\Gamma C_d \max\{1, |z|\} \left(1 + \mathrm{e}^{-4d \operatorname{Re}(z)}\right) \|\varphi\|_{H^{-1/2}(\Gamma)}.
\end{aligned}$$

This is summarized as the following theorem.

Theorem 19 *Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with diameter d. It holds*

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

Thus, the transfer function $\mathcal{K}(z)$ for the retarded potential of the wave equation satisfies Assumption 1 with $C_{\text{op}} = C_{\Gamma,d}(1 + \mathrm{e}^{-4d\sigma_-})$, $\theta = 1$ and any $\sigma_- \in \mathbb{R}$.

The proof of Theorem 19 follows from the next lemma, which provides explicit bounds for the solution operator $\mathcal{N}(z)$.

Lemma 20 *For any $d > 0$, there exists a constant[6] $C_d > 0$ such that for any $f \in H^{-1}_{\text{comp}}(\mathbb{R}^3)$ with support contained in a ball B_d with some diameter d it holds*

$$\|\nabla \mathcal{N}(z) f\|_{L^2(B_d)} + \|\mathcal{N}(z) f\|_{L^2(B_d)} \le C_d \max\{1, |z|\} \left(1 + \mathrm{e}^{-4d \operatorname{Re}(z)}\right) \|f\|_{H^{-1}(\mathbb{R}^3)}$$

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

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

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

$$\begin{aligned} &\operatorname{supp} \nu \subset [0, 4d], \qquad && \nu|_{[0,2d]} = 1, \qquad && |\nu|_{W^{1,\infty}(\mathbb{R}_{\geq 0})} \leq \frac{C}{d}, \\ &\forall x \in \mathbb{R}_{\geq 0} : 0 \leq \nu(x) \leq 1, \quad && |\nu|_{W^{2,\infty}(\mathbb{R}_{\geq 0})} \leq \frac{C}{d^2}. && \end{aligned} \tag{52}$$

Let $v(x) := \nu(\|x\|)$ and

$$w_\nu(x) := \int_{B_d} G_z(x-y)\, v(x-y)\, f(y)\, dy \qquad \forall x \in \mathbb{R}^3.$$

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

$$w := G_z \star f \quad \text{and write} \quad w_\nu = (G_z v) \star f. \tag{53}$$

The properties of ν guarantee $w_\nu|_{B_d} = w|_{B_d}$ so that we may restrict our attention to the function w_ν. We compute the Fourier transform of $G_z v$:

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

The inner integral in $I(z,\xi)$ can be evaluated analytically (cf. [23, p. 1882]) and gives $I(z,\xi) = \iota(z, \|\xi\|)$ with

$$\iota(z, s) = 4\pi \int_0^\infty g_z(r)\, \nu(r)\, r^2 \frac{\sin(rs)}{(rs)}\, dr. \tag{54}$$

Applying the Fourier transform to the convolution (52) leads to

$$\widehat{w}_\nu = (2\pi)^{3/2}\, \widehat{(G_z v)}\, \widehat{f}.$$

It is well known that Sobolev norms in the full space can be expressed as weighted L^2-norms in the Fourier domain so that we obtain

$$\begin{aligned}
\|w\|_{H^1(B_d)} &\leq \|w_\nu\|_{H^1(\mathbb{R}^3)} = (2\pi)^{3/2} \left\| \sqrt{1+\|\xi\|^2}\,\widehat{(G_z v)}\,\widehat{f} \right\|_{L^2(\mathbb{R}^3)} \qquad (55)\\
&\leq \left(\max_{\xi\in\mathbb{R}^3} \left| \left(1+\|\xi\|^2\right) I(z,\xi) \right| \right) \left\| \frac{1}{\sqrt{1+|\xi|^2}} \widehat{f} \right\|_{L^2(\mathbb{R}^3)}\\
&\leq \left(\max_{s\geq 0} \left| \left(1+s^2\right) \iota(z,s) \right| \right) \|f\|_{H^{-1}(\mathbb{R}^3)}.
\end{aligned}$$

Hence, Lemma 21 below implies

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

■

Lemma 21 *The function $\iota(z,\cdot)$ defined in (53) can be estimated by*

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

Proof. Applying integration by parts we obtain

$$\begin{aligned}
|\iota(z,s)| &= \frac{C}{|z|} \left| \int_0^\infty \mathrm{e}^{-zr} \left(\nu'(r) \frac{\sin(rs)}{s} + \nu(r)\cos(rs) \right) dr \right|\\
&\leq C \frac{1+\mathrm{e}^{-4d\,\mathrm{Re}(z)}}{|z|} \int_0^{4d} \left(\frac{C}{d} r + 1 \right) dr = Cd \frac{1+\mathrm{e}^{-4d\,\mathrm{Re}(z)}}{|z|}.
\end{aligned}$$

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

$$\begin{aligned}
|\iota(z,s)| &= \left| \int_0^\infty \mathrm{e}^{-zr} \nu(r) \frac{\sin(rs)}{s} dr \right| \leq \left(1+\mathrm{e}^{-4d\,\mathrm{Re}(z)}\right) \int_0^{4d} \left| \frac{\sin rs}{s} \right| dr\\
&\leq \left(1+\mathrm{e}^{-4d\,\mathrm{Re}(z)}\right) \int_0^{4d} r dr = 8d^2 \left(1+\mathrm{e}^{-4d\,\mathrm{Re}(z)}\right)
\end{aligned}$$

so that

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

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

$$\begin{aligned}
\left|s^2\iota(z,s)\right| &= C \left| \int_0^\infty \mathrm{e}^{-zr} \nu(r)\, s\sin(rs)\, dr \right| = C \left| \int_0^\infty \mathrm{e}^{-zr} \nu(r)\, \partial_r \cos(rs)\, dr \right|\\
&\leq C \left(\left| \int_0^\infty \cos(rs)\, \partial_r \left(\mathrm{e}^{-zr}\nu(r)\right) dr \right| + 1 \right)\\
&\leq C|z| \left| \int_0^\infty \cos(rs)\, \mathrm{e}^{-zr} \nu(r)\, dr \right| + C \left(\left| \int_0^\infty \cos(rs)\, \mathrm{e}^{-zr} \nu'(r)\, dr \right| + 1 \right)\\
&\leq C(1+d|z|) \left(1+\mathrm{e}^{-4d\,\mathrm{Re}(z)}\right). \qquad ■
\end{aligned}$$

8 Numerical experiments

The 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 $t = 0$. For these types of applications, gCQ has its strengths and can become advantageous to CQ (convolution quadrature with constant time stepping).

To test the performance of the gCQ for such kinds of applications we have chosen the following data for our numerical examples

$$g(t) = t^{3/2}\mathrm{e}^{-t}, \quad \mathcal{K}(z) = \frac{1-\mathrm{e}^{-2z}}{2z}, \quad \mathcal{K}^{-1}(z) = \frac{2z}{1-\mathrm{e}^{-2z}}, \tag{56}$$

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

Remark 22 (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 [14] 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.*

8.1 Decoupled, purely time-depending example

In [26], analytical solutions for the acoustic potential in (49) 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. [12], [24]) 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 $\mathcal{K}(z) := \lambda_0(z)$ is like in (55). As proved in [27], the exact solution in this case is given by

$$\phi(t) = 2\sum_{k=0}^{\lfloor t/2 \rfloor} g'(t-2k). \tag{57}$$

We have approximated ϕ for $t \in [0,1]$ by applying (12) 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 (56). 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

$$t_j = \left(\frac{j}{N}\right)^{\alpha}, \qquad j = 1, \ldots, N \tag{58}$$

and compared this in our numerical experiment to constant time stepping, i.e., $\alpha = 1$ in (57). 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 (29). In this case, the choice of parameters for the quadrature is given by

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

From Corollary 16 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 $O\left(\Delta^{1/2}\right)$ for constant time steps.

8.2 The three-dimensional wave equation

Let again $\partial\Omega$ be the unit sphere. We solve numerically the full wave equation (47) with right-hand side

$$g(x,t) = g(t)Y_1^1(x), \tag{59}$$

for the same time-dependent part $g(t)$ as in (55). 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

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

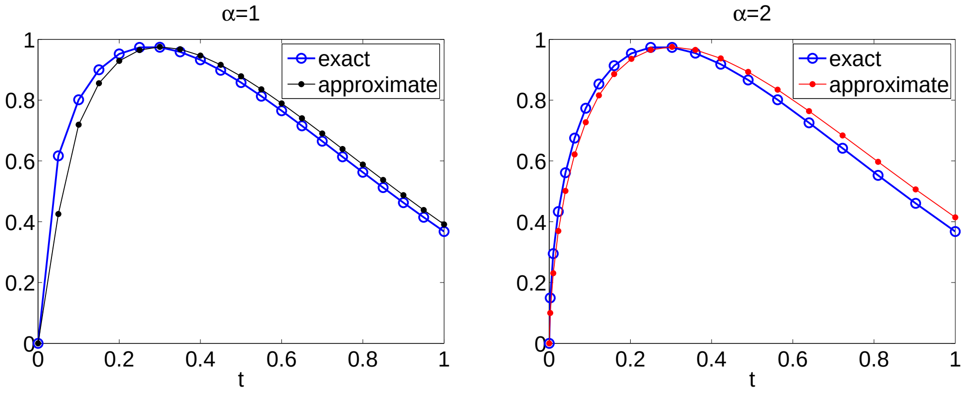

Figure 1: Exact and approximation of the potential for the data in (55) with 20 steps. *Left:* With uniform time steps ($\alpha = 1$ in (57)). *Right:* With quadratically graded time steps ($\alpha = 2$ in (57))

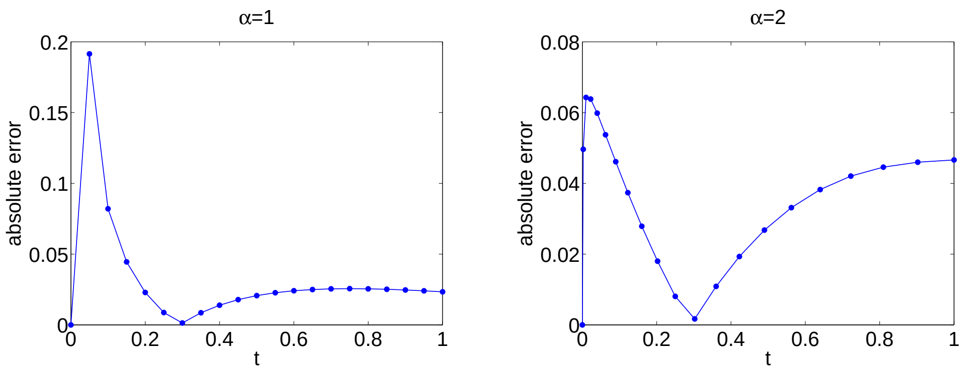

Figure 2: Pointwise error in the approximation of the potential for the data in (55) with 20 steps. *Left:* With uniform time steps ($\alpha = 1$ in (57)). *Right:* With quadratically graded time steps ($\alpha = 2$ in (57))

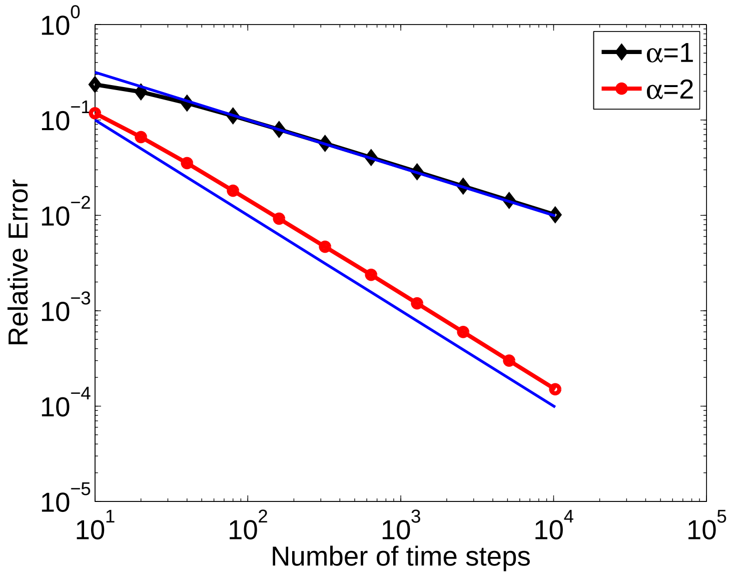

Figure 3: Error with respect to the number of steps for g in (55). The straight lines indicate slopes 1/2 and 1, respectively.

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 [25]. At every spatial node, the behavior of the solution in time is the same as in the scalar example in Section 8.1. Thus, we choose again the time steps as in (57) 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.

In Figure 4, the maxima $\max_{1\leq n\leq N} \left\|\phi(t_n) - \phi_n^{\mathcal{C}}\right\|_{L^2(\Gamma)}$ 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, where NS denote the dimension of the corresponding boundary element space. 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

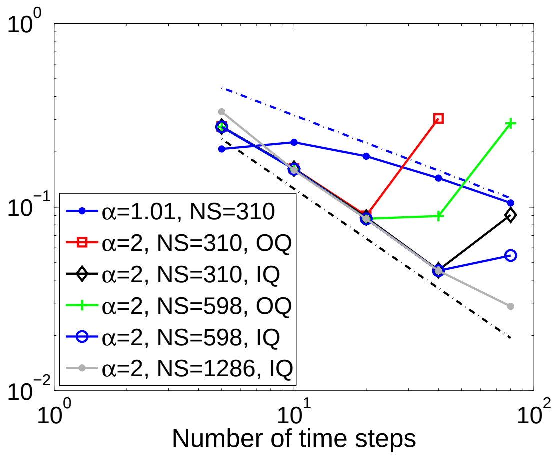

Figure 4: Error with respect to the number of time steps for g as in (58). NS is the number of degrees of freedom in the spatial discretization. The abbreviation “OQ” stands for “original quadrature” for approximating the entries of the boundary element matrices (cf. [25]), where the order is chosen as in the case of constant time stepping. “IQ” stands for “improved quadrature” where the quadrature order in the assembly of the boundary element matrices is significantly increased. The straight dashed lines depict the slopes $1/2$ and 1, respectively.

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.

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