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für Mathematik
in den Naturwissenschaften
Leipzig

Efficient long time computations of time-domain
boundary integrals for 2D and dissipative wave
equation

by

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Preprint no.: 65

2010



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October 28, 2010

Abstract

Linear hyperbolic partial differential equations in a homogeneous medium, e.g., the wave equation describing the propagation and scattering of acoustic waves, can be rewritten as a time-domain boundary integral equation. We propose an efficient implementation of a numerical discretization of such equations when the strong Huygens' principle does not hold.

For the numerical discretization, we make use of convolution quadrature in time and standard boundary element method in space. The quadrature in time results in a discrete convolution of weights W_j with the boundary density evaluated at equally spaced time points. If the strong Huygens' principle holds, W_j converge to 0 exponentially quickly for large enough j . If the strong Huygens' principle does not hold, e.g., in even space dimensions or when some damping is present, the weights are never zero, thereby presenting a difficulty for efficient numerical computation.

In this paper we prove that the kernels of the convolution weights approximate in a certain sense the time domain fundamental solution and that the same holds if both are differentiated in space. The tails of the fundamental solution being very smooth, this implies that the tails of the weights are smooth and can efficiently be interpolated. We discuss the efficient implementation of the whole numerical scheme and present numerical experiments.

1. Introduction

A variety of physical applications, such as the propagation or the scattering of electromagnetic or acoustic waves, lead to the problem of solving linear hyperbolic partial differential equations in two or three dimensional space. Since these problems are typically considered in an unbounded homogeneous domain, a method to tackle them is to reformulate the partial differential equation as an integral equation on the, usually bounded, surface of the domain.

In this paper, the discretization in time is done by using convolution quadrature. The most attractive feature, beside the excellent stability properties, is that, unlike numerical methods based purely on Galerkin discretization, it determines the weights using Laplace transform of the kernel function instead of the kernel function itself. This technique has been introduced by

Lubich [17, 18, 19] and has since then been successfully applied to many applications, see also the reviews [20] and [7].

In this work we will concentrate on solving the acoustic wave equation. For the case of three spatial dimensions in which Huygens' principle holds, Hackbusch, Kress and Sauter ([11]) present a cutoff strategy that helps to overcome the drawback of densely populated matrices arising from the spatial discretization of the convolution coefficients. They suggest to replace the system matrix by a sparse approximation, which is possible due to the finite propagation of waves and Huygens' principle.

Here, we focus on the cases where this strategy is not applicable due to the Huygens' principle failing to hold. We show that the convolution weight kernels approximate the tail of the fundamental solution in time domain to high accuracy. Additionally, we point out, that, since the tail of the fundamental solution is very smooth, interpolation of the weights can lead to a major reduction of storage and computational complexity. We show an algorithmic realisation for the solution of the wave equation by extending the algorithm given in [5] to the present case.

The plan of the paper is as follows. The section following this introduction is dedicated to a short description of the problem treated in this paper as well as to fixing the notation used in the forthcoming sections. In Section 3 we discuss the approximation result and describe the algorithm. Concluding, in Section 4, we give a detailed numerical example underlining the statement.

2. Notation and statement of the problem

Let Ω be a bounded Lipschitz subdomain of \mathbb{R}^n ($n = 2, 3$) with boundary Γ and complement $\Omega^+ := \mathbb{R}^n \setminus \bar{\Omega}$. The goal is to find a function $u(\cdot, t) \in H^1(\Omega)$ that solves the dissipative wave equation with velocity $c > 0$ and damping factor $\alpha \geq 0$ given as follows

$$\partial_t^2 u(x, t) + \alpha \partial_t u(x, t) - c^2 \Delta u(x, t) = 0, \quad (x, t) \in \Omega^+ \times (0, T), \quad (2.1a)$$

$$\text{with initial conditions} \quad u(x, 0) = \partial_t u(x, 0) = 0, \quad x \in \Omega^+, \quad (2.1b)$$

$$\text{and Dirichlet boundary condition} \quad u(x, t) = g(x, t), \quad (x, t) \in \Gamma \times (0, T), \quad (2.1c)$$

on a time interval $(0, T)$ for some $T > 0$. It is well-known that $u(x, t)$ exists and that it is unique for data $g(\cdot, t) \in H^{\frac{1}{2}}(\Gamma)$ vanishing near $t = 0$, see [4].

Since the Huygens' principle does not hold in two space dimensions even without damping, to simplify presentation we always set $\alpha = 0$ in this case. Otherwise, the damping factor α expresses a non-negative real number.

Employing a single layer potential ansatz we may write

$$u(x, t) = \int_0^t \int_{\Gamma} k(|x - y|, t - \tau) \varphi(y, \tau) d\Gamma_y d\tau, \quad (x, t) \in \Omega^+ \times (0, T),$$

for the solution of the partial differential equation (2.1). The density $\varphi(\cdot, t) \in H^{-\frac{1}{2}}(\Gamma)$ is unknown whereas $k(d, t)$ is the fundamental solution of the wave equation (2.1a). That is

$$k(d, t) = \begin{cases} \frac{H(t - \frac{d}{c})}{2\pi\sqrt{t^2 - \frac{d^2}{c^2}}}, & n = 2 \\ \frac{e^{-\alpha t/2}}{4\pi d} \left(\delta(t - \frac{d}{c}) + \frac{\alpha d}{2\sqrt{c^2 t^2 - d^2}} I_1 \left(\frac{\alpha}{2} \sqrt{t^2 - \frac{d^2}{c^2}} \right) H \left(t - \frac{d}{c} \right) \right), & n = 3. \end{cases} \quad (2.2)$$

Here, $\delta(t)$ denotes Dirac's delta distribution, $H(t)$ Heaviside's function, and $I_1(t)$ the modified Bessel function of order one, see [9].

For any density φ equation (2.1a) with condition (2.1b) is satisfied. The density φ can, hence, be obtained by applying the boundary condition (2.1c), and solving the resulting boundary integral equation

$$g(x, t) = \int_0^t \int_{\Gamma} k(|x - y|, t - \tau) \varphi(y, \tau) d\Gamma_y d\tau, \quad (x, t) \in \Gamma \times (0, T). \quad (2.3)$$

When discretizing (2.3) with respect to the time variable, we will make use of convolution quadrature; for more information on this approach see for instance [17], [18], [19], and [20]. This time-discretization method makes use not of $k(d, t)$ but of its Laplace transform $K(d, s) := \mathcal{L}k(d, t)$ which is given by

$$K(d, s) = \begin{cases} \frac{1}{2\pi} K_0 \left(\frac{sd}{c} \right), & n = 2 \\ \frac{e^{-\frac{d}{c}\sqrt{s^2 + \alpha s}}}{4\pi d}, & n = 3, \end{cases} \quad (2.4)$$

with $K_0(s)$ being the Macdonald function of order zero (see [14]). Here we already see a possible advantage of convolution quadrature: the time-domain fundamental solutions are distributional functions and in the case of the dissipative wave equation also given by a lengthy expression. In contrast, in the Laplace domain, these become simpler, analytic functions of s .

Discretizing (2.3) by convolution quadrature at equally spaced points $t_j = j\Delta t$, with $j = 0, 1, \dots, N$ and $\Delta t = T/N > 0$, one needs to find the unknown densities $\varphi_j^{\Delta t}(y) := \varphi^{\Delta t}(y, t_j)$ satisfying the semi-discrete equivalent of (2.3) which with $g_n := g(x, t_n)$ reads

$$g_n(x) = \sum_{j=0}^n \int_{\Gamma} \omega_{n-j}(|x - y|) \varphi_j^{\Delta t}(y) d\Gamma_y, \quad n = 0, 1, \dots, N, \quad x \in \Gamma, \quad (2.5)$$

with kernels (weight functions) $\omega_{n-j}(d)$ implicitly defined by the generating function

$$K(d, \rho(\zeta)/\Delta t) = \sum_{n=0}^{\infty} \omega_n(d) \zeta^n. \quad (2.6)$$

Here, the function $\rho(\zeta)$ stands for the quotient of the generating polynomials of a linear multistep method. In this paper, the A-stable backward differentiation formulae of order $p = 1$ and $p = 2$ are used so that we in particular have

$$\rho(\zeta) = \sum_{i=0}^p \frac{1}{i} (1 - \zeta)^i. \quad (2.7)$$

The results of this paper can be extended to A-stable Runge-Kutta methods of arbitrary order, but to keep the paper at a reasonable length we do not perform this extension here.

3. Approximation of $k(d, t)$ by the weights $\omega_j(d)$

The aim of this section is to investigate more closely the functions $d \mapsto \omega_j(d)$. In [17] and [20] it has been shown that for a kernel $K(s)$ bounded polynomially in the complement of a sector with an acute angle to the negative real axis, the corresponding weights ω_j approximate $\Delta t k(t_j)$ to accuracy $O(\Delta t^{p+1})$; p being the order of the underlying linear multistep method. Here we wish to show a similar result for non-sectorial functions $K(s, d)$ of the previous section. The result will only hold for large enough j and has already been stated in [21] as a conjecture based on numerical experiments. In order to simplify the presentation, we set for the rest of the paper the speed of propagation of waves to $c = 1$.

Before we go in to more detail pertaining to the approximation of convolution weight functions, we will consider the weights for the shift operator e^{-sd} given by the generating function

$$e^{-d \frac{\rho(\zeta)}{\Delta t}} = \sum_{n=0}^{\infty} \hat{\omega}_n(d) \zeta^n,$$

which have a representation as a contour integral,

$$\hat{\omega}_n(d) = \frac{1}{2\pi i} \oint_C \frac{e^{-\frac{d}{\Delta t} \rho(\zeta)}}{\zeta^{n+1}} d\zeta, \quad (3.1)$$

where the contour C can be chosen as a circle with centre at the origin and radius smaller than one. When $\rho(\zeta) = 1 - \zeta$, i.e., when backward differentiation formula of order one is the underlying scheme, these weights are given by

$$\hat{\omega}_n(d) = e^{-\frac{d}{\Delta t}} \frac{1}{n!} \left(\frac{d}{\Delta t} \right)^n,$$

whereas they read

$$\hat{\omega}_n(d) = \frac{1}{n!} \left(\frac{d}{2\Delta t} \right)^{n/2} e^{-\frac{3}{2} \frac{d}{\Delta t}} H_n \left(\sqrt{\frac{2d}{\Delta t}} \right)$$

when $\rho(\zeta) = \frac{3}{2} - 2\zeta + \frac{1}{2}\zeta^2$, i.e., when backward differentiation formula of order two is used (see [6], [11]). In the last equation the functions $H_n(d)$ denote the Hermite polynomials of order n . Since the weights $\hat{\omega}(d)$ play an important role in the analysis of this section, we first state some of their properties.

Lemma 3.1. *Let $\Delta t > 0$, $\varepsilon > 0$, and $k \approx 1.086435$ as well as*

$$I_{n,\varepsilon} := \left[0, -t_n W \left(-\frac{1}{e} (\varepsilon k^{1-p})^{p/n} \right) \right],$$

where $p = 1, 2$ is the order of the underlying BDF multistep scheme and W is the principle branch of the Lambert W function.

Then there holds

(a) For any $n \geq 1$

$$|\widehat{\omega}_n(d)| < \varepsilon, \quad \forall d \in I_{n,\varepsilon}.$$

(b) For any $d > 0$

$$\left(\sum_{n=0}^{\infty} |\widehat{\omega}_n(d)|^p \right)^{1/p} \leq k^{p-1},$$

Proof. For BDF2, a similar result to (a) has appeared in [11]. We will give the proof for the refined bound (a) and for (b) in the appendix. \square

The Lambert W function $W(x)$ used in Lemma 3.1 is the multi-valued function $W(x)$ that satisfies $x = W(x)e^{W(x)}$. If its argument is real and positive then the function is single-valued. In the interval $(-1/e, 0)$, $W(x)$ has two real branches, the principal branch of $W(x)$ giving results from the interval $(-1, 0)$. A more detailed definition as well as a review of the history, theory and applications of the Lambert W function may be found in [8].

We show next that in a certain way the weights $\omega_n(d)$ given by (2.6) approximate the inverse Laplace transform $k(d, t)$ of the function $K(d, s)$ at discrete times $t_n = n\Delta t$ with order $p+1$, where p is the order of the underlying multistep method used for time discretization. The details are given in the following theorem.

Theorem 3.1. *Let $d \in (0, D]$ and $k(d, t)$ be the inverse Laplace transform of $K(d, s)$. Assume that $e^{ds}K(d, s)$ is analytic in the sector $|\arg(s)| < \pi - \beta$, for some $\beta < \pi/2$, and satisfies there the inequality $|e^{ds}K(d, s)| \leq M(d) \cdot |s|^\mu$ with $\mu > -p$. Furthermore, let $\omega_j(d)$ be the corresponding convolution weights based on BDF multistep scheme of order $p \in \{1, 2\}$. Then, for $\varepsilon < C \cdot \Delta t^{1+p+\max(0,\mu)}$,*

$$J = \min \left\{ j \in \mathbb{N} : -jW \left(-\frac{1}{e}(\varepsilon k^{1-p})^{p/j} \right) > D/\Delta t \right\}, \quad (3.2)$$

arbitrary $\delta > 0$, the inequality

$$|\omega_n(d) - \Delta t \cdot k(d, n\Delta t)| \leq C(\delta)M(d)\Delta t^{p+1}, \quad t_n \in [t_J + \delta, T] \quad (3.3)$$

holds with a constant $C(\delta)$ independent of Δt , d , and n .

Remark 3.1. *Note that this extends Theorem 2.1 in [20] to the present special class of non-sectorial functions $K(d, s)$.*

Proof. At the first step of this proof we develop an equation that connects the weights $\omega_n(d)$ and the function $k(d, n\Delta t)$. At the second step we will derive (3.3).

We begin with the first part by introducing a shifted function

$$\tilde{k}(d, t) := k(d, t + d). \quad (3.4)$$

Transforming $\tilde{k}(d, t)$ into Laplace domain, we get $\tilde{K}(d, s) = e^{ds}K(d, s)$. Hence, recalling (2.6) and with

$$K \left(d, \frac{\rho(\zeta)}{\Delta t} \right) = \sum_{n=0}^{\infty} \omega_n(d)\zeta^n, \quad \tilde{K} \left(d, \frac{\rho(\zeta)}{\Delta t} \right) = \sum_{n=0}^{\infty} \tilde{\omega}_n(d)\zeta^n,$$

$$e^{-\frac{\rho(\zeta)}{\Delta t}d} = \sum_{n=0}^{\infty} \widehat{\omega}_n(d) \zeta^n,$$

we see that

$$\sum_{n=0}^{\infty} \omega_n(d) \zeta^n = \left(\sum_{n=0}^{\infty} \widehat{\omega}_n(d) \zeta^n \right) \left(\sum_{n=0}^{\infty} \widetilde{\omega}_n(d) \zeta^n \right) = \sum_{n=0}^{\infty} \left(\sum_{j=0}^n \widehat{\omega}_{n-j}(d) \widetilde{\omega}_j(d) \right) \zeta^n.$$

By comparing the coefficients above, we obtain

$$\omega_n(d) = \sum_{j=0}^n \widehat{\omega}_{n-j}(d) \widetilde{\omega}_j(d).$$

Due to the assumed analyticity and boundedness of $\widetilde{K}(d, s) = e^{ds} K(d, s)$ within the sector $|\arg(s)| < \pi - \beta$, we may use here the sectorial version of the result we want to prove [20, Theorem 2.1]. Thereby we obtain

$$\widetilde{\omega}_n(d) - \Delta t \widetilde{k}(d, n\Delta t) = t_n^{-\mu-1-p} \cdot \varepsilon_n(d) \quad (3.5)$$

with $|\varepsilon_n(d)| \leq CM(d)\Delta t^{p+1}$. This leads to

$$\begin{aligned} \omega_n(d) &= \sum_{j=0}^{n-J-1} \widehat{\omega}_{n-j}(d) \widetilde{\omega}_j(d) + \sum_{j=n-J}^n \widehat{\omega}_{n-j}(d) \left\{ \Delta t \widetilde{k}(d, j\Delta t) + t_j^{-\mu-1-p} \varepsilon_j(d) \right\} \\ &= \sum_{j=0}^{n-J-1} \widehat{\omega}_{n-j}(d) \widetilde{\omega}_j(d) + \sum_{j=n-J}^n \widehat{\omega}_{n-j}(d) t_j^{-\mu-1-p} \varepsilon_j(d) + \Delta t \sum_{j=n-J}^n \widehat{\omega}_{n-j}(d) \widetilde{k}(d, j\Delta t). \end{aligned} \quad (3.6)$$

We have split the sum into three terms in order to analyse each term separately.

Let us first focus on the final sum in (3.6). We introduce a cutoff function $\chi(t) \in C^\infty(\mathbb{R})$ satisfying

$$\chi(t) := \begin{cases} 0 & \text{if } t \leq \frac{\delta}{2}, \\ 1 & \text{if } t \geq \delta, \end{cases} \quad \text{and} \quad |\chi(t)| \leq 1 \quad (3.7)$$

for the constant $\delta > 0$ from the statement of the theorem. Furthermore, we define

$$f(d, t) := \begin{cases} \chi(t) \widetilde{k}(d, t) & \text{if } t > \frac{\delta}{2}, \\ 0 & \text{if } t \leq \frac{\delta}{2}. \end{cases} \quad (3.8)$$

For all n such that $t_n - t_J > \delta$ we therefore have

$$\Delta t \sum_{j=n-J}^n \widehat{\omega}_{n-j}(d) \widetilde{k}(d, j\Delta t) = \Delta t \sum_{j=n-J}^n \widehat{\omega}_{n-j}(d) \widetilde{k}(d, j\Delta t) \chi(j\Delta t)$$

$$= \Delta t \sum_{j=0}^n \widehat{\omega}_{n-j}(d) f(d, j\Delta t) + \bar{\varepsilon}(d), \quad (3.9)$$

and with the error term

$$|\bar{\varepsilon}(d)| = \Delta t \left| \sum_{j=0}^{n-J-1} \widehat{\omega}_{n-j}(d) f(d, j\Delta t) \right| \leq \Delta t \sum_{j=1}^{n-J-1} |\widehat{\omega}_{n-j}(d) \tilde{k}(d, j\Delta t)|.$$

Now, applying Lemma (3.1) which shows $|\widehat{\omega}_k(d)| \leq \varepsilon$ for $k > J$ and $d \in (0, D]$, remembering (3.2), and using the fact that the assumptions on $\tilde{K}(d, s)$ imply that $\tilde{k}(d, t)$ is bounded by $C \cdot M(d)t^{-1-\mu}$ for positive t , see Lemma B.1, it follows

$$\begin{aligned} |\bar{\varepsilon}(d)| &\leq \varepsilon \Delta t \sum_{j=1}^{n-J-1} |\tilde{k}(d, j\Delta t)| \leq \varepsilon \Delta t \cdot C \cdot M(d) \sum_{j=1}^{n-J-1} \frac{1}{(j\Delta t)^{1+\mu}} \\ &= C \cdot M(d) \varepsilon \sum_{j=1}^{n-J-1} \frac{1}{j} \frac{1}{(j\Delta t)^\mu} \leq \varepsilon C \cdot M(d) \log(3(n-J)) \begin{cases} \Delta t^{-\mu}, & \mu > 0 \\ T^{-\mu}, & \mu \leq 0 \end{cases}. \end{aligned} \quad (3.10)$$

The last step is derived from the bound in [10, (0.131)] for the harmonic sum.

Convolution weights $\widehat{\omega}_j(d)$ are generated by the operator e^{-sd} , see ((3.1)), which corresponds to a shift by $-d$ in time domain. Therefore, we have from [19, Theorem 3.1] that

$$\Delta t \sum_{j=0}^n \widehat{\omega}_{n-j}(d) f(d, j\Delta t) = \Delta t f(d, n\Delta t - d) + \hat{\varepsilon}(d, \delta)$$

with $|\hat{\varepsilon}(d, \delta)| \leq \widehat{C}(d, \delta) \Delta t^{p+1}$. The constant $\widehat{C}(d, \delta)$ is bounded by $C(T) \max_{t \in [0, T]} |\partial_t^m f(d, t)|$, with $C(T)$ being a constant that depends on T and $m = p + 2 + \mu$. Note that

$$|\mathcal{L}(\partial_t^m f(d, \cdot))| = |s^m \mathcal{L} f(d, \cdot)| \leq C(\sigma) |s|^m, \quad \text{for all } \operatorname{Re} s \geq \sigma > 0,$$

the last step being valid since $f(d, \cdot)$ is a C^∞ function for $t \geq 0$ and increasing at most polynomially. Consequently, we can apply Lemma B.1 to obtain a bound for $\partial_t^m f(d, t)$:

$$\max_{t \in [0, T]} |\partial_t^m f(d, t)| = \max_{t \in [\delta/2, T]} |\partial_t^m f(d, t)| \leq CM(d) \delta^{-m-1}.$$

Let us now have a look at the second sum in (3.6). Denoting $\tilde{\varepsilon}(d) = \sup\{|\varepsilon_j(d)| : j = n - J, \dots, n\}$, so that $\tilde{\varepsilon}(d) \leq \tilde{C}M(d)\Delta t^{p+1}$, we have

$$\left| \sum_{j=n-J}^n \widehat{\omega}_{n-j}(d) t_j^{-\mu-1-p} \varepsilon_j(d) \right| \leq |\tilde{\varepsilon}(d)| \left(\sum_{j=n-J}^n t_j^{-(\mu+1+p)p} \right)^{1/p}.$$

Here we made use of Lemma 3.1 part (b). Therefore, using the assumptions $n - J > \delta/\Delta t$ and $\mu > -p$, we conclude that

$$\left| \sum_{j=n-J}^n \widehat{\omega}_{n-j}(d) t_j^{-\mu-1-p} \varepsilon_j(d) \right| \leq C(\delta) M(d) \Delta t^{p+1}. \quad (3.11)$$

Finally, we estimate the first sum of (3.6). We observe that as a consequence of [20, Theorem 2.1] and of the fact that $\tilde{k}(d, t)$ is bounded by $C \cdot M(d)t^{-1-\mu}$ for positive t , the modulus of the weights $\tilde{\omega}_n(d)$ for positive n is bounded by $CM(d)\Delta t \cdot t_n^{-1-\mu}$, and for $\tilde{\omega}_0 = K(\rho(0)/\Delta t)$ the condition $|\tilde{K}(d, s)| \leq M(d) \cdot |s|^\mu$ implies directly $|\tilde{\omega}_0(d)| \leq CM(d)\Delta t^{-\mu}$. Consequently, and by consulting Lemma (3.1) to bound $\hat{\omega}_n(d)$, we conclude

$$\begin{aligned}
\sum_{j=0}^{n-J-1} |\hat{\omega}_{n-j}(d)\tilde{\omega}_j(d)| &\leq \varepsilon \sum_{j=0}^{n-J-1} |\tilde{\omega}_j(d)| \\
&\leq \varepsilon \Delta t CM(d) \sum_{j=1}^{n-J-1} (j\Delta t)^{-\mu-1} + \varepsilon CM(d)\Delta t^{-\mu} \\
&\leq \varepsilon CM(d) \left(\sum_{j=1}^{n-J-1} \frac{1}{j} (j\Delta t)^{-\mu} + \Delta t^{-\mu} \right) \\
&\leq \varepsilon CM(d) (\log(3(n-J)) + 1) \begin{cases} \Delta t^{-\mu}, & \mu > 0 \\ T^{-\mu}, & \mu \leq 0 \end{cases}. \quad (3.12)
\end{aligned}$$

Combining the above analysis of the three terms in (3.6) gives the required result. \square

Now we show that the kernel functions of the wave equation in two and three space dimensions, given in (2.2), and their Laplace transforms, given in (2.4), satisfy the assumptions of Theorem (3.1).

Lemma 3.2. *For any $\alpha > 0$ and $d > 0$ the following holds:*

- (a) *Function $s \mapsto e^{ds} \left(\frac{\partial^m}{\partial d^m} e^{-d\sqrt{s^2+\alpha s}} \right)$ is analytic and bounded by $C|s|^m$, $m = 0, 1, \dots$, on the cut plane $\mathbb{C} \setminus (-\infty, 0]$.*
- (b) *For any $\beta > 0$, there exists a constant $M > 0$, such that for $|\arg(s)| < \pi - \beta$ and $|s| > 0$ it holds*

$$\left| e^{ds} K_0(sd) \right| \leq M \begin{cases} 1 + \log \frac{1}{|sd|}, & |sd| < 1, \\ |sd|^{-1/2}, & |sd| \geq 1. \end{cases}$$

and for any $m \in \mathbb{N}$ with a constant $M_m > 0$

$$\left| e^{ds} \frac{\partial^m}{\partial d^m} K_0(sd) \right| \leq M_m |s|^m \begin{cases} |sd|^{-m}, & |sd| < 1, \\ |sd|^{-1/2}, & |sd| \geq 1. \end{cases}$$

Proof. Part (a) follows from the inequality

$$\operatorname{Re}(s) \leq \operatorname{Re} \left(\sqrt{s^2 + \alpha s} \right),$$

which we prove next. Consider the function $f(s) := s - \sqrt{s^2 + \alpha s}$. Taking the interval $[-\alpha, 0]$ as the branch cut, the function $f(s)$ is analytic in $\mathbb{C} \setminus [-\alpha, 0]$, and so the real part $\operatorname{Re}(f)$ is

harmonic. Since $\operatorname{Re}(f) \rightarrow -\alpha/2$ as $|s| \rightarrow \infty$ and $\operatorname{Re}(f(s)) \leq 0$ for all $s \in [-\alpha, 0]$ it follows by the maximum principle, see [3], that $\operatorname{Re}(f) \leq 0$.

We now address part (b). According to [1], the function $K_0(z)$ is analytic throughout the complex plane cut along the negative real axis and consequently so is $e^{ds}K_0(ds)$ as a function of s .

Splitting the proof of boundedness, we first consider $|ds| < 1$. Using the power series expansion given in [1, (9.6.13)] for $K_0(z)$, $|z| < 1$, we have with the Euler constant $\gamma = 0.5772157\dots$

$$K_0(z) = - \left(\log\left(\frac{z}{2}\right) + \gamma \right) \sum_{n=0}^{\infty} \left(\frac{z}{2}\right)^{2n} \frac{1}{n!^2} + \sum_{n=1}^{\infty} \left(\frac{z}{2}\right)^{2n} \frac{1}{n!^2} \sum_{k=1}^n \frac{1}{k}.$$

The bounds in (b) for $0 < |sd| < 1$ and $m = 0$ follow directly from the above expansion, whereas the bound for $m = 1, 2, \dots$ can be obtained by first differentiating the expansion term by term.

From the asymptotic expansion [1, (9.7.2)]

$$K_0(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z} \left\{ 1 - \frac{1}{8z} + \frac{(-1)(-9)}{2!(8z)^2} + \frac{(-1)(-9)(-25)}{3!(8z)^3} + \dots \right\},$$

valid for $|z| \rightarrow \infty$ and $|\arg z| < \frac{3}{2}\pi$, we see that

$$|K_0(z)| = \sqrt{\frac{\pi}{2}} |z|^{-1/2} e^{-\operatorname{Re} z} + O(|z|^{-3/2} e^{-\operatorname{Re} z}).$$

Therefore $|K_0(z)| \leq \text{const} |z|^{-1/2} e^{-\operatorname{Re} z}$ and since $K_0(z)$ is analytic in the cut plane, by Cauchy integral formula the same bound holds, with a possibly different constant also for the derivatives $K_0^{(m)}(z)$. With this the proof of (b) is complete. \square

Corollary 3.1. *With $\mu = m$ and under the conditions of Theorem 3.1 the following holds for $d \in (0, D]$, $\delta > 0$, $t_n \in (t_J + \delta, T]$, and J defined as in Theorem 3.1:*

(a) For $K(s, d) = \mathcal{L}k = K_0(sd)$

$$\left| \frac{\partial^m}{\partial d^m} \omega_n(d) - \Delta t \cdot \frac{\partial^m}{\partial d^m} k(d, n\Delta t) \right| \leq C(d, \delta) \Delta t^{p+1}.$$

(b) For $K(s, d) = \mathcal{L}k = e^{-d\sqrt{s^2 + \alpha s}}/d$, $\alpha \geq 0$,

$$\left| \frac{\partial^m}{\partial d^m} [d\omega_n(d)] - \Delta t \cdot \frac{\partial^m}{\partial d^m} [dk(d, n\Delta t)] \right| \leq C(d, \delta) \Delta t^{p+1}.$$

The constant $C(d, \delta)$ is bounded by $C(\delta)(1 + \log d)$ in the 2D case and by a constant $C(\delta)$ independent of d in the 3D case.

4. Interpolating the weights and efficient implementation

4.1. Interpolating the weights

Let us consider the introductory example (2.1). We have shown that for a fixed time t_n , if n is greater than J for some $J > D/\Delta t$, the kernels $\omega_n(d)$ defined in (2.6) approximate the scaled fundamental solution in time. Additionally, Corollary 3.1 states that a similar approximation result with same order of convergence also holds for the (spatial) derivatives of the weight functions. This means that the spatial derivatives of $\omega_n(d)$ are bounded by spatial derivatives of $k(d, t_n)$ when t_n is sufficiently larger than d . Since $k(d, t)$ is very smooth for $t > d$, i.e., after the wave front has passed, both $\omega_n(d)$ and $k(d, t_n)$ can be approximated to high accuracy in space with only a few interpolation points in the interval $d \in [0, D]$ if t_n is sufficiently larger than D . Next, we will focus on this interpolation.

Consider a fixed time step $t_j \leq T$. Let $r + 1$ distinct interpolation points $d_k \in [0, \text{diam}(\Gamma)]$, $k = 0, \dots, r$, be given, together with corresponding values $\kappa_{k,j} = \omega_j(d_k)$. We introduce an interpolation operator $\mathcal{I}_r : C([0, \text{diam}(\Gamma)]) \rightarrow \mathcal{P}_r$ which maps a continuous function on $[0, \text{diam}(\Gamma)]$ to a polynomial of order r that interpolates $\omega_j(d)$ at the points d_k . Namely, we define

$$(\mathcal{I}_r \omega_j)(d) := \sum_{k=0}^r \kappa_{k,j} \cdot \ell_k(d), \quad (4.1)$$

where $\ell_k(d)$, $k = 0, \dots, r$, denote the interpolating polynomials. For numerical realization, we use Lagrange fundamental polynomials that are given by

$$\ell_j(d) = \prod_{k=0, k \neq j}^n \frac{d - d_k}{d_j - d_k}.$$

We turn our attention to the convolutional sum (2.5) and apply (4.1) to get

$$\begin{aligned} \sum_j \int_{\Gamma} \omega_{n-j}(|x - y|) \varphi_j^{\Delta t}(y) d\Gamma_y &\approx \sum_j \int_{\Gamma} (\mathcal{I}_r \omega_{n-j})(|x - y|) \varphi_j^{\Delta t}(y) d\Gamma_y \\ &= \sum_{k=0}^r \int_{\Gamma} \ell_k(|x - y|) \left(\sum_j \kappa_{k,n-j} \varphi_j^{\Delta t}(y) \right) d\Gamma_y \\ &= \sum_{k=0}^r I_k \left(\sum_j \kappa_{k,n-j} \varphi_j^{\Delta t}(\cdot) \right) (x), \end{aligned} \quad (4.2)$$

where

$$I_k \varphi(x) = \int_{\Gamma} \ell_k(|x - y|) \varphi(y) d\Gamma_y.$$

The advantage of this approach comes from the fact, that, instead of storing all operators $W_j : \varphi \mapsto \int_{\Gamma} \omega_j(|x - y|) \varphi(y) d\Gamma_y$, $j > J$, we just need to know the corresponding coefficients and $r + 1$ additional operators. We also remark, that the inner sum over j in (4.2) can be evaluated in a fast manner applying the fast Fourier transform.

4.2. Algorithmic realization

We consider the semi-discrete convolutional system (2.5) which has to be satisfied by the unknown densities $\varphi_n^{\Delta t}$, $n = 0, \dots, N$. The corresponding matrix of this linear system then has the structure of a lower triangular Toeplitz matrix whose first column is given by the vector $(W_0, W_1, \dots, W_N)^T$. In our case the convolution weights are boundary integral operators $W_n : H^{-\frac{1}{2}}(\Gamma) \rightarrow H^{\frac{1}{2}}(\Gamma)$ defined by

$$(W_j \varphi)(x) = \int_{\Gamma} \omega_j(|x - y|) \varphi(y) d\Gamma_y, \quad x \in \Gamma.$$

To solve the lower triangular Toeplitz system we will use the recursive algorithm as introduced in [13] and modified in [5]. The resulting algorithm has complexity $O(N \log^2 N)$, uses only the Laplace domain kernel functions, and requires only the operator W_0 to be inverted.

Here, we want to describe how to combine the interpolation approach with the recursive algorithm. We have the time discretized convolutional system (2.5) as a starting point and assume that for $n > J$ the kernels $\omega_n(d)$ of the integral operators W_n may be interpolated to high accuracy with few interpolation polynomials ℓ_k , $k = 0, 1, \dots, r$. Since the n th lower diagonal of the Toeplitz-matrix is given by W_n , all the kernels which may be replaced by an interpolation are located below the J th lower diagonal. The solution of (2.5) then follows the idea described below and graphically illustrated in Figure 1.

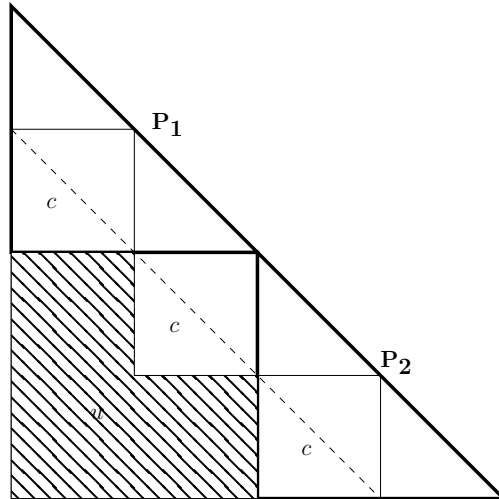


Figure 1: Schematic illustration of the recursive solution

We recall the problem (2.5)

$$\text{Solve: } g_n = \sum_{j=0}^n W_{n-j} \varphi_j^{\Delta t}, \quad n = 0, 1, \dots, N, \quad t_n = n\Delta t,$$

and divide it into two subproblems P_1 and P_2 . These read like this

$$\begin{aligned}
P_1 \quad & \text{Solve: } \sum_{j=0}^n W_{n-j} \varphi_j^{\Delta t} = g_n \text{ for } n = 0, 1, \dots, \left\lfloor \frac{N}{2} \right\rfloor \\
P_2 \quad & \text{Solve: } \sum_{j=\left\lfloor \frac{N}{2} \right\rfloor + 1}^n W_{n-j} \varphi_j^{\Delta t} = g_n - v_n \text{ for } n = \left\lfloor \frac{N}{2} \right\rfloor + 1, \dots, N \\
& \text{with } v_n = \sum_{j=0}^{\left\lfloor \frac{N}{2} \right\rfloor} W_{n-j} \varphi_j^{\Delta t}.
\end{aligned} \tag{4.3}$$

The subproblems P_1 and P_2 result from splitting the whole problem (2.5) into problems with half the size. The dashed line in Figure 1 indicates the J th diagonal. Thus, the convolution weights, whose kernels we want to interpolate, are concentrated in the lower left triangle.

We assume at this point, that P_1 is already solved, and hence the densities $\varphi_j^{\Delta t}$, $j = 0, \dots, \lfloor N/2 \rfloor$, are known. This solution is obtained in a recursive way using the algorithm of [5] in an unchanged way. Once the right-hand side $g_n - v_n$, $n = \lfloor N/2 \rfloor + 1, \dots, N$, is computed, we can solve P_2 in the same way as P_1 . To compute the right-hand side a matrix-vector product with the matrix u in Figure 1 needs to be computed. We observe that, on the one hand we have already computed the block c , i.e., the upper right part of u , when we solved P_1 and can therefore use the information of this block to evaluate the corresponding part of the sums giving v_n , $n = \lfloor N/2 \rfloor + 1, \dots, N$. On the other hand, in the remaining part of u , represented by the shaded L-shaped domain in Figure 1, only operators W_j , where j is greater than J , are involved, so that here we can apply the interpolation approach of the previous section and obtain v_n without computing further operators, provided I_k , $k = 0, \dots, r$ have already been computed. For larger problems, in the picture Figure 1 a further triangular block P_3 can be added, solved recursively with a right-hand side that can again be computed using purely the block c and operators W_j with $j \geq J$.

5. Numerical Results

5.1. Approximation property of weights $\omega_j(d)$

In this section we want to illustrate the statement of Theorem 3.1. Therefore, we consider the problem (2.1) in 3D with damping parameter $\alpha = 2$ and velocity $c = 1$. Since we are interested in a comparison of the weight functions $\omega_n(d)$ (see (2.6)) and the time domain kernel function $k(d, t)$ (see (2.2)), let us note that the weight functions are given implicitly as the contour integral

$$\omega_n(d) = \frac{1}{2\pi i} \oint_C \frac{1}{4\pi d} \frac{e^{-\frac{d}{\Delta t} \sqrt{\rho(\zeta)^2 + \alpha \Delta t \cdot \rho(\zeta)}}}{\zeta^{n+1}} d\zeta,$$

with contour C being a circle in the complex plane centered at the origin of radius less than one and the function $\rho(\zeta)$ being the ratio of generating polynomials of the multistep method used for

time discretization, see (2.7). These weight functions can numerically be computed by applying the trapezoidal quadrature rule.

To show convergence for $\Delta t \rightarrow 0$, we set $d = 1$ and fix time at $t = n\Delta t = 4$. The absolute error $|\omega_n(d) - \Delta t k(d, n\Delta t)|$ is plotted against Δt in Figure 2.

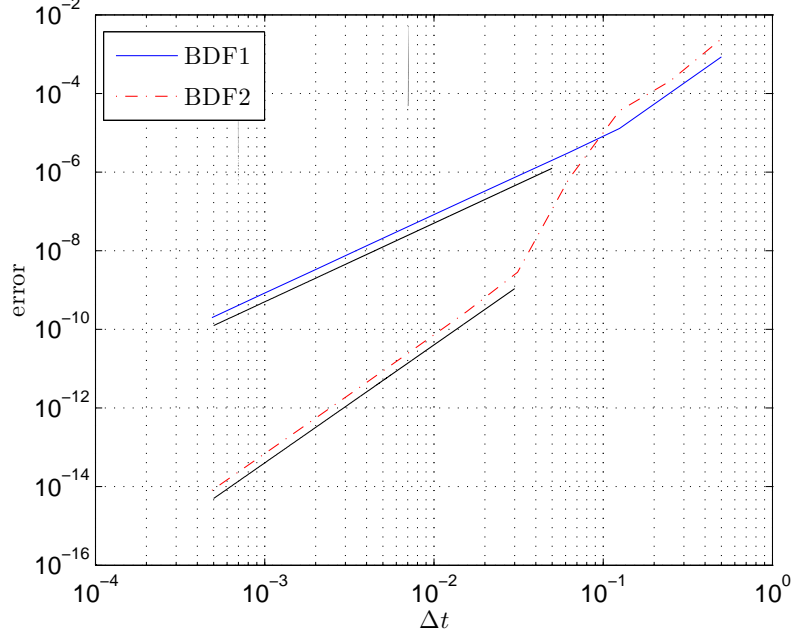


Figure 2: Error $|\omega_j(1) - \Delta t k(1, t_j)|$ for $t_j = 4$ plotted against Δt for the wave equation in three dimensions with damping parameter $\alpha = 2$.

Figure 2 shows the results for backward differentiation formulas of order one and two. The numerical results confirm the theorem's statement: we see that convergence rate is Δt^{p+1} for BDF scheme of order p . We also see, that for BDF1 the asymptotic rate of convergence is obtained earlier, than for BDF2, where, a faster pre-asymptotic regime seems to exist.

5.2. A large-scale experiment

This example focuses on the three dimensional case. Let Γ be the unit ball in \mathbb{R}^3 , i.e. $\Gamma = \mathbb{S}^2 = \{x \in \mathbb{R}^3 : |x| = 1\}$ and let us consider the homogeneous wave equation (2.1). For convenience, we set the wave speed $c = 1$. After having employed the ansatz as a single layer potential and the boundary condition, the problem is reduced to identifying the unknown density $\varphi(x, t)$ in the integral equation

$$g(x, t) = \int_0^t \int_{\Gamma} k(|x - y|, t - \tau) \varphi(y, \tau) d\Gamma_y d\tau \quad (x, t) \in \Gamma \times (0, T). \quad (5.1)$$

For our experiment, we arrange the right-hand side $g(x, t)$ to be separable in time and spatial variables, so that we have $g(x, t) = g(t)e(x)$ with $e(x)$ an eigenfunction of the single layer

potential $V(s)$. As pointed out in [6], this choice allows to reduce (5.1) to a problem depending only on time since also the solution will have a separable form $\varphi(x, t) = \varphi(t)e(x)$. The simplest choice of right-hand side is to pick $g(x, t)$ to be constant for a fixed time. In particular, we let $g(t) = \sin^5(t)$ and $e(x) = 2\sqrt{\pi}Y_0^0 = 1$, where Y_0^0 a spherical harmonic: an eigenfunction of the single layer potential. Finally, we fix the damping factor and take $\alpha = 2$ and use step size $\Delta t = 0.1$ for time discretization.

In this experiment we will discuss the influence on the solution when taking perturbed convolution weights, coming from an interpolation of the weights' kernel function in question, instead of taking original weights.

In this numerical example, we take backward differentiation formula of order two for time discretization and ε of Lemma 3.1 to be 10^{-6} . Furthermore, we observe that the domain's diameter is two. The condition (3.2) then gives $J = 62$. We make use of Lagrange interpolation with Chebyshev knots of the second kind. The interpolating polynomials are chosen to be of order $r = 6$ and $r = 10$, respectively. This means, that we need to compute the operators I_k and the interpolation coefficients $\kappa_{k,j}$ for $j = J + 1, \dots, N$ and $k = 0, 1, \dots, r$; see also (4.2).

Although the problem could be solved without any approximation in space, in order to test our algorithms for the space discretization we have used standard Galerkin boundary element method with piecewise constant boundary element basis. The matrices coming from this discretization were computed and stored in \mathcal{H} -matrix format using the HLIBpro library of Ronald Kriemann ([15], [16]). The computation of all the matrices was done in parallel.

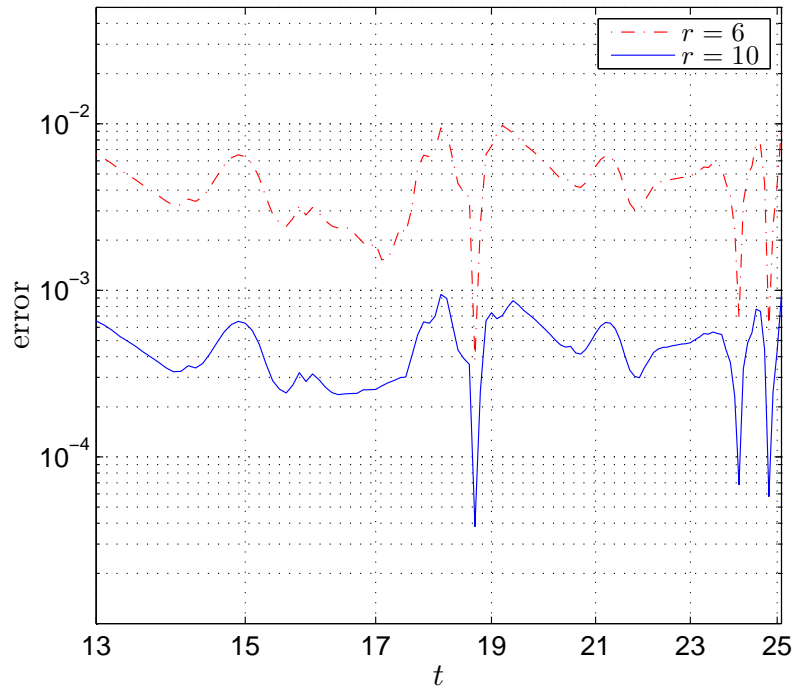


Figure 3: Absolute error $|\varphi^{\Delta t}(x, t) - \tilde{\varphi}(x, t)|$ for $\Delta t = 0.1$ and $\alpha = 2$

Figure 3 shows for fixed $x \in \Gamma$ and for different number of interpolation points r the abso-

lute error $|\varphi^{\Delta t}(x, t) - \tilde{\varphi}(x, t)|$. Here, $\varphi^{\Delta t}(x, t)$ is the discrete solution obtained by unperturbed convolution quadrature and $\tilde{\varphi}(x, t)$ is the solution obtained with weights approximated by interpolation. Note, that the right-hand side was chosen the way, that the solution is constant for a fixed time, therefore the error is similar for all x on the boundary of the sphere. The implementation was done according to the algorithm presented in Section 4.2. For the numerical realization we approximate the weights at time $t > 13$. So the difference $|\varphi^{\Delta t}(x, t) - \tilde{\varphi}(x, t)|$ vanishes for $t \leq 13$ and a change of accuracy can be detected for $t > 13$. The plot indicates that the error does not increase significantly with increasing t .

6. Conclusion

The fact, that, regarding the wave equation, in two space dimensions as well as in three space dimensions if a dissipative term gets involved, Huygens' principle does not hold is well-known ([12],[2]). It follows that a cutoff strategy as recommended in [11] is not applicable since the tail of the convolution weight functions $\omega_n(d)$ does not vanish not longer for large $t_n = n\Delta t$.

Nevertheless, in this paper we have shown, that instead of cutoff, the tail can efficiently be interpolated. Numerical experiments for the wave equation have illustrated the effectiveness of this approach. The same procedure is possible for a wider class of linear hyperbolic equations arising in, e.g., viscoelastodynamics and electromagnetics [7], since there the kernel functions have a similar form and will satisfy the conditions of Theorem 3.1.

A. Proof of Lemma 3.1

Proof. We recall the representation of the weight functions $\hat{\omega}_n(d)$. They read

$$\hat{\omega}_n(d) = e^{-\frac{d}{\Delta t}} \frac{1}{n!} \left(\frac{d}{\Delta t} \right)^n, \quad (\text{A.1})$$

in the case of BDF1 and

$$\hat{\omega}_n(d) = \frac{1}{n!} \left(\frac{d}{2\Delta t} \right)^{n/2} e^{-\frac{3}{2} \frac{d}{\Delta t}} H_n \left(\sqrt{\frac{2d}{\Delta t}} \right) \quad (\text{A.2})$$

in the case of BDF2.

In order to get an estimate for the modulus of the weight functions, we make use the bound $e^{x^2/2} 2^{n/2} \sqrt{n!} k$, where $k = 1.086435 \dots$, for Hermite polynomials $H_n(x)$ of order n appearing in (A.2), see [1, 22.14.17]. Therefore

$$|\hat{\omega}_n(d)|^p \leq k^{p(p-1)} \frac{1}{n!} \left(\frac{d}{\Delta t} \right)^n e^{-\frac{d}{\Delta t}}. \quad (\text{A.3})$$

From this part (b) follows immediately.

Next, we apply Stirling's formula, $n! \geq (n/e)^n \cdot (2\pi n)^{1/2}$, that is valid for $n \geq 1$, to (A.3) to obtain

$$|\hat{\omega}_n(d)| \leq \frac{1}{(2\pi n)^{1/2p}} \left(\frac{de}{t_n} \right)^{n/p} e^{-d/(p\Delta t)} k^{p-1} < \left(\frac{de}{t_n} \right)^{n/p} e^{-d/(p\Delta t)} k^{p-1} \leq \varepsilon.$$

We rewrite the last relation and end up with

$$\frac{d}{t_n} e^{-d/t_n} \leq \frac{1}{e} (\varepsilon k^{1-p})^{p/n},$$

that we solve for d using Lambert's W function $W(x)$.

$$d \leq -t_n W \left(-\frac{1}{e} (\varepsilon k^{1-p})^{p/n} \right).$$

This proves part (a). □

B. A bound on sectorial operators

Lemma B.1. *Let $K(s)$ be analytic in $|\arg(s)| < \pi - \beta$ for some $\beta < \pi/2$, and bounded there as $|K(s)| \leq M|s|^\mu$. Then, there exists a unique $k \in C^\infty(\mathbb{R}_{>0})$ such that $K = \mathcal{L}k = \int_0^\infty e^{-st} k(t) dt$. Further,*

$$|k(t)| \leq C \cdot M t^{-\mu-1}, \quad \text{for all } t > 0.$$

Proof. We observe that function k is given by the inverse Laplace transform

$$k(t) := \frac{1}{2\pi i} \int_{\Gamma} e^{st} K(s) ds,$$

with contour $\Gamma = \Gamma_{1,\delta} + \Gamma_{2,\delta} + \Gamma_{3,\delta}$ where

$$\Gamma_{1,\delta} = (\infty e^{i(\pi+\beta')}, \delta e^{i(\pi+\beta')}], \quad \Gamma_{2,\delta} = \{\delta e^{i\varphi} : \varphi \in [-\pi+\beta', \pi-\beta']\}, \quad \Gamma_{3,\delta} = [\delta e^{-i(\pi+\beta')}, \infty e^{-i(\pi+\beta')}),$$

with $\beta < \beta' < \pi/2$ and $\delta > 0$.

We split the proof and concentrate first on the case $\mu > -1$. Here, we will make use of the identity

$$\int_0^\infty s^\mu e^{-ts} ds = \Gamma(\mu+1) t^{-\mu-1},$$

that holds for $t > 0$; see [10, (3.381)]. Concerning the first part of the contour we get

$$\frac{1}{2\pi} \left| \int_{\Gamma_{1,\delta}} e^{st} K(s) ds \right| \leq \frac{M}{2\pi} \int_\delta^\infty e^{-rt \cos(\beta')} r^\mu dr \leq \frac{M}{2\pi \cos(\beta')^{\mu+1}} \Gamma(\mu+1) t^{-\mu-1}.$$

Concerning the second part of the contour we have

$$\frac{1}{2\pi} \left| \int_{\Gamma_{2,\delta}} e^{st} K(s) ds \right| \leq \frac{M}{2\pi} \delta^{\mu+1} \int_{-\pi+\beta'}^{\pi-\beta'} e^{t\delta \cos(\varphi)} d\varphi \leq M \delta^{\mu+1} e^{t\delta}.$$

Taking the symmetry of the contours $\Gamma_{1,\delta}$ and $\Gamma_{3,\delta}$ into consideration and letting δ tend to zero we have the result.

Let us now focus on the special case $\mu = -1$. With the same contour Γ we get for $\Gamma_{1,\delta}$

$$\frac{1}{2\pi} \left| \int_{\Gamma_{1,\delta}} e^{st} K(s) ds \right| \leq \frac{M}{2\pi} \int_{\delta}^{\infty} \frac{e^{-rt \cos(\beta')}}{r} dr \leq \frac{M}{2\pi} \int_{\delta t \cos(\beta')}^{\infty} \frac{e^{-r}}{r} dr = \frac{M}{2\pi} \Gamma(0, \delta t \cos(\beta')),$$

where we made use of the incomplete Gamma function. The treatment of the circular part of the contour Γ follows the case $\mu > -1$. Choosing $\delta = 1/t$ we see that $|k(t)|$ is bounded by a constant independent of t .

Finally we turn our attention to the case $\mu < -1$. We have $k(0) = \int_{\Gamma} K(s) ds$ and from the Cauchy integral formula it hence follows that $k(0) = 0$ and $\mathcal{L}(k'(t))(s) = sK(s) - k(0) = sK(s)$.

Let us now assume that the statement of the lemma holds for $\mu+1$. We show that the statement then also holds for μ , i.e., for $|K(s)| \leq M|s|^{\mu}$ within the sector:

$$|k(t)| = \left| \int_0^t k'(\tau) d\tau \right| \leq CM \left| \int_0^t \tau^{-\mu-2} d\tau \right| = MCt^{-\mu-1}.$$

□

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