Fast and Stable Contour Integration for High Order Divided Differences via Elliptic Functions *

M. Lopez-Fernandez† S. Sauter‡

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Abstract

In this paper, we will present a new method for evaluating high order divided differences for certain classes of analytic, possibly, operator valued functions. This is a classical problem in numerical mathematics but also arises in new applications such as, e.g., the use of generalized convolution quadrature to solve retarded potential integral equations. The functions which we will consider are allowed to grow exponentially to the left complex half plane, polynomially to the right half plane and have an oscillatory behaviour with increasing imaginary part. The interpolation points are scattered in a large real interval. Our approach is based on the representation of divided differences as contour integral and we will employ a subtle parameterization of the contour in combination with a quadrature approximation by the trapezoidal rule.

Keywords: Divided Differences, Numerical Approximation of Contour Integrals, Jacobi Elliptic Functions, Convolution Quadrature.

Mathematics Subject Classification (2000): 65D30, 30E20, 33B99, 39A70, 65R20.

1 Introduction

The numerical solution of time-space retarded potential integral equations for solving the wave equation in unbounded, exterior domains has become a new field of vivid research in the last years in numerical analysis and the convolution quadrature method is now one of the most popular solution method [12], [2], [23], [24], [15], [4], [3]. In the recent paper [22], the method has been generalized to allow for variable time stepping. In this context, the problem arises to evaluate

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

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

high-order divided differences $[x_j, x_{j+1}, \ldots, x_n]\, \mathcal{K}(\cdot)$ for all $1 \le j \le n \le N+1$ for a parameter-dependent integral operator $\mathcal{K}(\cdot)$.

Here, the nodes are related to the (adaptively) generated time steps $0 = t_0 < t_1 < \ldots < t_{N+1} = T$ (= final time) by means of $x_j = \Delta_j^{-1}$, where $\Delta_j = t_j - t_{j-1}$ are the step widths. For our application the spectral radius of the integral operator $\mathcal{K}(z)$ as well as its inverse has the qualitative behavior

$$f(z) = \left(1 + \mathrm{e}^{-d \operatorname{Re} z}\right)(1 + |z|)^p \tag{1}$$

for a parameter $d \in [0,1]$ and some degree $p \in \{1,2,3,4\}$.

As is common in numerical analysis new challenges arise from new applications and we are faced with the problem to evaluate a sequence of divided differences for a function whose analytic behavior can be characterized by (1). Note that the nodal points x_j, typically, are not given a priorily but they are generated in course of the time stepping scheme. Hence, they can have all kinds of multiplicities, they are, possibly, very densely clustered around some points and, in addition, their condition number $\frac{\max x_j}{\min x_j}$ can be very large.

It turns out that the application of Newton's table to compute a sequence of divided differences fails for this problem already for very small number of time steps $N \gtrsim 20$ due to severe roundoff errors; although we are re-ordering Newton's table according to increasing nodal values. We emphasize that, for the described application, the sequence of divided difference is needed but not the interpolating polynomial (cf. Remark 1) and, hence, the use of, e.g., Lagrangian interpolation in barycentric coordinates is not a remedy.

In this paper, we consider the stable and efficient evaluation of high order divided differences via contour integrals for a class of functions which includes functions of the type (1). With this method we were able to evaluate divided differences up to an order $N = 1000$ without stability problems.

To formulate the problem in an abstract way, we consider a real sequence x_i, $1 \le i \le N+1$, of nodal points with given function values f_i, $1 \le i \le N+1$ the interpolating polynomial of degree N can be written in the form

$$\sum_{i=1}^{N+1} \left([x_1, x_2, \ldots, x_i]\, f\right) \omega_{i-1}$$

with the Newton polynomials

$$\omega_i(x) = \prod_{k=1}^{i} (x - x_k)\,. \tag{2}$$

Its evaluation at some point x requires the accurate and efficient evaluation of the product $\left([x_1, x_2, \ldots, x_i]\, f\right) \omega_{i-1}(x)$ facing the before mentioned severe stability problems. The nodal points x_i, $1 \le i \le N+1$, for the divided differences of a function f are assumed to be positive and contained in an interval $\mathcal{I} = [m, M]$ with $0 < m < M$. The function f is assumed to be analytic in a half plane

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

for some $\sigma \in \mathbb{R}$ and may grow polynomially to the right half plane so that functions of the form (1) are contained in this class.

Our approach will be based on the representation as contour integrals of the divided differences and a discretization by the trapezoidal rule. The choice of the contour and its parametrization is very delicate if the ratio M/m is large. As our contour, we choose here a circle about M with radius M. The simple parametrization by $M(1+\exp(\mathrm{i}\,\theta))$, $\theta \in [0, 2\pi)$, results in a very slow convergence if the ratio M/m becomes large. A much better behavior is obtained by using a translation and dilation of a composition of a Jacobi elliptic function with a Möbius transform – this idea was used in [16] to compute matrix functions via contour integrals. The theory will be based on classical quadrature estimates for the trapezoidal rule for periodic functions which can be extended analytically to some complex strip around the integration interval. Since a Jacobi elliptic function is involved the error analysis requires some technical estimates of this function. The good results of our numerical experiments show that the choice of our integration contour avoids roundoff errors which often arise when integrating highly oscillatory functions.

The evaluation of divided differences is a classical problem in numerical analysis. However the accurate evaluation of *high order* divided differences for quite general and, possibly, adaptively selected nodal points with changing multiplicities is still a challenging problem. For the evaluation of divided differences for the exponential function this is well known; in [25] an improved procedure is presented which combines the traditional recurrence with special properties of the exponential function. This method has been further developed in [6] for the matrix exponential propagator, while fast versions of the traditional recurrence are presented, e.g., in [28] an [11]. However, as explained above, our applications [22, 21] involve more general functions and quite general, possibly, highly non-uniform and adaptively selected nodal points with varying multiplicities and do not fit into the classes of functions which are considered in these references.

Remark 1 (Stability) *The general question of the stability of a numerical method for computing high order divided differences is challenging since the dependence on the number of nodal points, their condition number, and their distribution is quite involved. For specific, (nearly) optimal sets of nodal points such an analysis exist and we refer to [19], [26], [5] for further details. However for most applications, the computation of high order divided differences is not the final goal. To illustrate this, we consider the before mentioned application of retarded potential integral equations with variable time stepping. In this context a triangular block system of the form* $\mathbf{K}\boldsymbol{\phi} = \mathbf{g}$ *has to be solved with*

$$\mathbf{K} := \begin{bmatrix} \mathcal{K}(x_1) & 0 & \dots & 0 \\ \omega_{2,1}(0)[x_1, x_2]\,\mathcal{K} & \mathcal{K}(x_2) & \ddots & \vdots \\ \omega_{3,1}(0)[x_1, x_2, x_3]\,\mathcal{K} & \omega_{3,2}(0)[x_2, x_3]\,\mathcal{K} & \mathcal{K}(x_3) & \\ \vdots & \ddots & \ddots & \ddots\ 0 \\ \omega_{N,1}(0)[x_1, x_2, \dots, x_N]\,\mathcal{K} & \dots & & \mathcal{K}(x_N) \end{bmatrix}$$

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and $\mathcal{K}$ is some integral operator which depends analytically on a complex variable. Hence, the stability of the arising system does not directly depend on the stability of the computed divided differences but on the boundedness (stability) of the inverse operator $\mathbf{K}^{-1}$. In [22, Sect. 4.1] we proved that this inverse is bounded in appropriate norms independent on the number N of nodal points and their ratio M/m. This is related to the fact that the diagonal blocks in $\mathbf{K}$ contain the integral operator $\mathcal{K}$, simply evaluated at the nodal points without any roundoff errors, and these operator $\mathcal{K}(x_i)$ are strongly elliptic.

However, we emphasize that the general question concerning the dependence of the condition number of our proposed method for computing a high-order divided difference on the number N of nodal points, their ratio M/m, and their distribution is challenging but beyond the scope of this paper.

The paper is organized as follows. In Section 2 we will present the new method for computing divided differences via contour integrals and the particular choice of the contour. Section 3 is devoted to the error analysis for the approximation of contour integrals by the trapezoidal rule and will be based on analytic function theory. In Section 4 we will analyze the width of the complex neighborhood of the contour where the function f can be extended analytically. This involves some technical estimates for Jacobi elliptic functions. Finally, in Section 5 we will present some numerical experiments which show the efficiency of our approximation method.

2 Divided Differences via Contour Integrals

Let a finite sequence of real and positive points $(x_i)_{i=1}^N$ be given which satisfies[1]

$$1 \leq m := \min_{1\leq i\leq N} x_i. \tag{3a}$$

For fixed $c_0 \in (0,1)$, we choose

$$M \geq \max\left\{\max_{1\leq i\leq N} x_i, \frac{1}{1-c_0}m\right\} \tag{3b}$$

such that the interval $\mathcal{I} := [m, M]$ contains all points x_i. We denote by $q := M/m$ the condition number of the points $(x_i)_i$.

Remark 2 *The definition (3b) allows in most cases the intuitive choice $M := \max x_i$. However, our quadrature error estimates will contain a factor $q/(q-1)$ which becomes large if the condition number q is close to 1. To circumvent this theoretical artifact, we have therefore taken the freedom to choose M large enough such that all nodal points are contained in $[m, M]$ and this ratio $q/(q-1)$*

[1]We have chosen here the condition $m \geq 1$ instead of $m > 0$ to reduce technicalities.

is bounded from above by the fixed constant c_0^{-1}*. We emphasize that (3b) obviously covers also the case that all nodal points are equal since the choice* $M = m/(1 - c_0)$ *is then admissible. Note that (3b) implies*

$$q - 1 \geq c_0 q. \tag{3c}$$

For a function $f : \mathcal{I} \to V$ with values in some normed linear space V we denote by

$$\delta_N(f) := [x_1, x_2, \ldots, x_N] f \tag{4}$$

the divided difference of f with respect to these points with standard modifications for points with multiplicities larger than 1 (see, e.g., [29]). Our goal is to present a fast and stable method to evaluate $\delta_N(f)$ for a certain class of functions, which we define below.

Definition 3 *For* $\sigma < -1$*,* $p \in \mathbb{R}$*,* $\alpha > 0$*, the set* $\mathcal{A}(\sigma, p, \alpha)$ *contains all functions* $f : \mathbb{C}_\sigma \to V$ *that satisfy*

1. f *is analytic in* $\mathbb{C}_\sigma$
2. f *satisfies the growth estimate*

$$|f(z)| \leq \alpha \left(\max\{1, |z|\}\right)^p \qquad \forall z \in \mathbb{C}_\sigma.$$

Remark 4

1. *We assume that the function* f *is explicitly given in* $\mathbb{C}_\sigma$ *and the problem of analytic continuation from real values of* f *to complex ones does not arise.*
2. *Functions of the form (1) belong to* $\mathcal{A}(-\infty, p, 1)$*.*
3. *The condition* $\sigma < \sigma_0$ *with* $\sigma_0 = -1$ *can be relaxed: if a function* g *satisfies the conditions in (3) for some different* $\sigma_0 \neq -1$ *then* $g(\cdot + 1 + \sigma_0) \in \mathcal{A}(\sigma, p, \alpha)$ *holds and the algorithm can be applied to the shifted function.*

For the set of points $(x_i)_{i=1}^N$, the Newton polynomial is defined (cf. (2)) by

$$\omega_N(z) = \prod_{i=1}^{N} (z - x_i).$$

We use the contour integral representation for the divided difference [13, 17], see also [8], namely

$$\delta_N(f) = \frac{1}{2\pi \mathrm{i}} \int_{\mathcal{C}} \frac{f(z)}{\omega_N(z)} dz, \tag{5}$$

where $\mathcal{C}$ is any closed contour in $\mathbb{C}_\sigma$ which contains $\mathcal{I}$ and is oriented counterclockwise. Our approach for approximating divided differences is based on the approximation of the contour integral by a trapezoidal rule.

Remark 5 *The choice of the contour and its parametrization is a very delicate problem if the quotient $q = M/m$ becomes large. If $\mathcal{C}$ is "too" close to the interval $\mathcal{I}$ then the denominator in (5) becomes very small and numerical quadrature will suffer.*

We have chosen $\mathcal{C}$ as the circle $\mathcal{C}_M$ about M with radius M. For an interval $J = \overline{AB} \subset \mathbb{C}$ with length $|J| := |B - A|$, let $\gamma_M : J \to \mathcal{C}_M$ denote a $|J|$-periodic parametrization of $\mathcal{C}_M$ which can be extended analytically in a complex neighborhood of J. Then the approximation of the divided difference is given by applying the trapezoidal rule for periodic functions to the parametrized integral

$$\begin{aligned}\delta_N(f) &= \frac{1}{2\pi\,\mathrm{i}} \int_J \frac{f \circ \gamma_M(\sigma)}{\omega_N(\gamma_M(\sigma))} \gamma_M'(\sigma)\, d\sigma \\ &\approx \frac{|J|}{2\pi\,\mathrm{i}\, N_Q} \sum_{\ell=0}^{N_Q-1} \frac{f \circ \gamma_M(t_\ell)}{\omega_N(\gamma_M(t_\ell))} \gamma_M'(t_\ell) =: \tilde{\delta}_N(f), \end{aligned} \tag{6}$$

where $t_\ell = A + \frac{\ell}{N_Q}(B - A)$.

Next, we will introduce the concrete choice of the parametrization γ_M being motivated by the quadrature error analysis for analytic periodic functions. For the sake of simplicity we assume that $\operatorname{Im} A = \operatorname{Im} B$ and, for $\rho > 0$, we define the extension of the parameter interval $J = \overline{AB}$ to a complex horizontal strip

$$\mathfrak{s}_\rho(J) := \{t + \mathrm{i}\, v : t \in J \wedge -\rho \le v \le \rho\}. \tag{7}$$

We assume that γ_M can be extended analytically to $\mathfrak{s}_\rho(J)$ for some $\rho > 0$ and we define the mapped region under γ_M by

$$\mathcal{C}_{M,\rho} := \{\gamma_M(\sigma) : \sigma \in \mathfrak{s}_\rho(J)\}. \tag{8}$$

An important quantity in the error estimate is the modulus

$$\mathfrak{M}_{M,\rho}(f) := \sup_{z \in \mathcal{C}_{M,\rho}} \left| \frac{f(z)}{\omega_N(z)} \right|. \tag{9}$$

Our assumptions on f (cf. (3)) imply analyticity and polynomial growth for all $z \in \mathbb{C}_\sigma$ for some $\sigma < -1$. Hence, we will choose the parametrization γ_M such that

$$\mu(M,\rho) := \min\{\operatorname{Re} z : z \in \mathcal{C}_{M,\rho}\} \ge -1. \tag{10}$$

Note that the standard parametrization of $\mathcal{C}_M$ by $\gamma(t) := M\left(1 + \mathrm{e}^{2\pi\,\mathrm{i}\, t}\right)$, $t \in [0,1]$ leads to a prohibitive large number of quadrature points if the ratio M/m is large. This is due to the restricted width ρ of the analyticity strip $\mathfrak{s}_\rho(J)$, which turns out to be limited by m/M, and to the "too" fast growth of $\mu(M,\rho)$ to the left half of the complex plane as ρ increases (for details see Remark 15 and Section 5).

A much better behavior is obtained by using a translation and dilation of a composition of a Jacobi elliptic function with a Möbius transform – this idea was used in [16] to compute matrix functions via contour integrals. The definition needs some preparatory steps.

For any parameter $\lambda \in [0,1]$, let $\operatorname{pr}(\cdot \mid \lambda)$ denote the Jacobi elliptic function according to the definition in [1, Section 16.1], where p, r is any two of the letters s, c, d, n. We write short

$$\operatorname{sn}(\sigma) = \operatorname{sn}(\sigma \mid \lambda), \qquad \operatorname{cn}(\sigma) = \operatorname{cn}(\sigma \mid \lambda), \qquad \operatorname{dn}(\sigma) = \operatorname{dn}(\sigma \mid \lambda).$$

The complete elliptic integrals of the first kind are defined by

$$K(\lambda) := \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-\lambda x^2)}} \qquad \text{(see [14, 8.112 (1.) and (2.)])} \tag{11a}$$

$$K'(\lambda) := K(1-\lambda) \qquad \text{(see [14, 8.112 (3.) and 8.111 (2.)])}. \tag{11b}$$

Remark 6 *Let $0 < m < M < \infty$ and $q = \frac{M}{m} \in (1,\infty)$. We will consider λ as a function of q, more precisely,*

$$\lambda = k^2 \qquad \textit{with} \qquad k = k(q) = \frac{q - \sqrt{2q-1}}{q + \sqrt{2q-1}}. \tag{12}$$

Note that k is strictly monotonously increasing and $0 = k(1) \le k(q) \le k(\infty) = 1$.

For later use we note that the choice of $\lambda = k^2(q)$ allows the following estimate

$$\frac{1}{\sqrt{q}} \le \left|1 - \lambda^{1/2}\right| \le 2\sqrt{\frac{2}{q}} \quad \textit{and} \quad \frac{1}{2\sqrt{q}} \le \left|1 - \lambda^{1/4}\right| \le 2\sqrt{\frac{2}{q}}. \tag{13}$$

We introduce the parameter interval

$$J_\lambda := \overline{P_\lambda Q_\lambda} \quad \text{with } P_\lambda = -K(\lambda) + \frac{\mathrm{i}}{2} K'(\lambda) \text{ and } Q_\lambda = 3K(\lambda) + \frac{\mathrm{i}}{2} K'(\lambda). \tag{14}$$

Definition 7 *Let λ and k be the functions of $q = M/m$ as in (12). The parametrization of the integration contour $\mathcal{C}_M$ is given by $\gamma_M(\sigma) = (z \circ u)(\sigma)$, where*

$$z(u) := \frac{M}{q-1}\left(\sqrt{2q-1}\,\frac{\lambda^{-1/2}+u}{\lambda^{-1/2}-u} - 1\right), \quad u(\sigma) := \operatorname{sn}(\sigma,\lambda), \quad \sigma \in J_\lambda. \tag{15}$$

Remark 8 *The function γ_M as in Definition 7 is a parametrization of the circle $\mathcal{C}_M$ (cf. Lemma 18). Note that the orientation of γ_M is clockwise, which by* (6) *leads to an approximation of $-\delta_N$.*

With this choice of contour our quadrature approximation reads

$$\delta_N(f) \approx \sum_{\ell=0}^{N_Q-1} w_\ell \frac{f(z_\ell)}{\omega_N(z_\ell)}, \tag{16}$$

with

$$z_\ell = \gamma_M(\sigma_\ell), \quad w_\ell = \frac{4K(\lambda)}{2\pi \mathrm{i} N_Q}\gamma_M'(\sigma_\ell), \quad \text{and} \quad \sigma_\ell = -K(\lambda) + \ell\frac{4K(\lambda)}{N_Q}, \tag{17}$$

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

$$\gamma_M'(\sigma) = \frac{M\sqrt{2q-1}}{q-1}\frac{2\mathrm{cn}\,(\sigma)\mathrm{dn}\,(\sigma)}{k(k^{-1} - \mathrm{sn}\,(\sigma))^2}. \tag{18}$$

The evaluation of the Jacobi elliptic functions and the elliptic integrals at complex arguments can be performed very efficiently and accurately in MATLAB by means of Driscoll's Schwarz–Christoffel Toolbox [9, 10] which is freely available online. In particular the functions `ellipkkp` and `ellipjc` are needed to compute (17), cf. [16].

3 Error Analysis

The error analysis is based on classical estimates of the trapezoidal rule when applied to periodic functions which can be extended analytically to a certain strip around the integration interval.

Remark 9 *The derivation of the estimates in this and the next section is rather technical. We emphasize that all constants are positive real numbers – independent of the function f and the parameters m, M, α, σ, p, λ, q, ρ. They are chosen to simplify the expressions which are involved in the statements and proofs. We have avoided to optimize their choice in order* not *to further increase technicalities and they should be regarded as a proof that "*such constants exists*".*

In Figure 1 we show how the conformal transformation γ_M maps parallel horizontal lines within the analyticity strip.

The following theorem estimates the width of the region $\mathcal{C}_{M,\rho}$.

Theorem 10 *Let $c_0 \in (0,1)$, m, and M be as in (3) and set $C_0 := \frac{370}{c_0}$. For any*

$$0 \le \rho \le (3C_0)^{-1} \min\left\{M^{-1/2}, m^{-1}\right\} \tag{19}$$

it holds

$$\mu(M,\rho) := \min\{\mathrm{Re}\, z : z \in \mathcal{C}_{M,\rho}\} \ge -1 \tag{20a}$$

and, for all $x \in \mathcal{I}$, we have

$$\mathrm{dist}\,(x, \mathcal{C}_{M,\rho}) \ge \left(1 - 2M^{-1/2} - \frac{2}{3}m^{-1}\right)x. \tag{20b}$$

For the modulus of $z \in \mathcal{C}_{M,\rho}$ it holds

$$\max\{|z| : z \in \mathcal{C}_{M,\rho}\} \le C_1 M \quad \textit{with} \quad C_1 = 10/3.$$

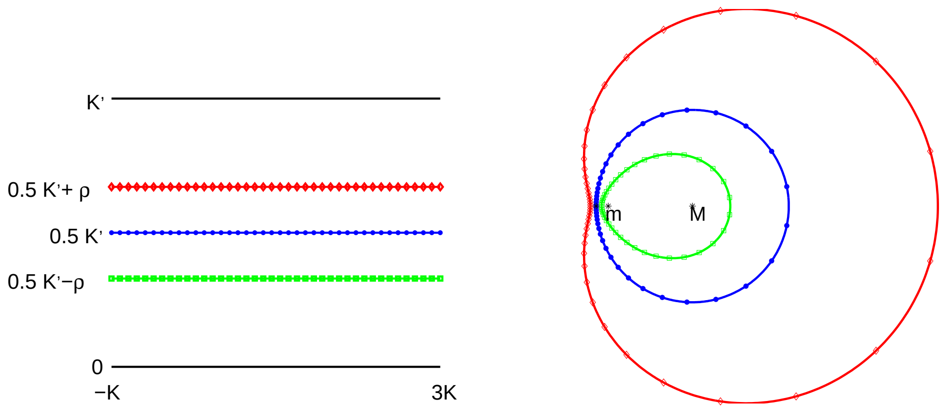

Figure 1: Illustration of the parametrization γ_M in Definition 7. *Left:* Horizontal lines in the σ-domain. *Right:* The corresponding images in the z-domain. The outer contour is kidney-shaped while the inner one is egg-shaped.

The proof of this theorem relies on some technical estimates of Jacobi's elliptic functions and will be postponed to Section 4 (cf. Theorem 23, Theorem 24, and Corollary 25).

We employ the following quadrature estimate for periodic functions.

Theorem 11 *Let $J = \overline{AB} \subset \mathbb{C}$ and $\mathfrak{s}_\rho(J)$ be as in (7) and let V be a normed linear space. For a periodic function $g : J \to V$ which can be extended to an analytic function in $\mathfrak{s}_\rho(J)$ for some $\rho > 0$ the quadrature error*

$$E_{N_Q}(g) := \int_J g(\sigma)\, d\sigma - \frac{|J|}{N_Q} \sum_{\ell=0}^{N_Q-1} g(t_\ell) \quad \textit{with} \quad t_\ell := A + \frac{\ell}{N_Q}(B-A)$$

can be estimated by

$$\left\| E_{N_Q}(g) \right\|_V \leq |J| \frac{2}{\mathrm{e}^{\frac{2\pi}{|J|} N_Q \rho} - 1} \sup_{\sigma \in \mathfrak{s}_\rho(J)} \| g(\sigma) \|_V .$$

Proof. The proof goes back to [7] – concretely the estimate follows from [20, (28)] by employing the affine pullback

$$\chi : [0, 2\pi] \to J, \qquad \chi(t) := A + \frac{t}{2\pi}(B-A).$$

■

Theorem 12 *Let $c_0 \in (m, M)$, $0 < m < M$ be as in (3). Let N be the number of points for the divided difference in (4) and let us define the ratio R by*[2]

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

[2]We can always assume $R \leq 2N/m$ since we have the freedom (cf. (3b)) to choose $M \geq m^2$.

Let λ, k be the functions of $q = M/m$ as in (12) and let the function $f \in \mathcal{A}(\sigma, p, \alpha)$ for some $\sigma < -1$. Then, for the divided difference approximation (6) via quadrature with the contour as in Definition 7 it holds

$$|\omega_N(0)| \left\| \delta_N(f) - \tilde{\delta}_N(f) \right\|_V \leq \alpha \frac{C_1^p C_2}{\pi} (10 + 2\log q) M^{p+1} \frac{\mathrm{e}^{2R}}{\mathrm{e}^{N_Q \tau} - 1} \tag{21}$$

with $\tau := \frac{\pi}{3C_0} \frac{\min\left\{M^{-1/2}, m^{-1}\right\}}{10+2\log q}$.

Proof. In view of (6) we introduce the function $g : J_\lambda \to V$ by

$$g(\sigma) := \frac{1}{2\pi\,\mathrm{i}} \frac{f \circ \gamma_M(\sigma)}{\omega_N(\gamma_M(\sigma))} \gamma_M'(\sigma).$$

Let $\rho = (3C_0)^{-1} \min\left\{M^{-1/2}, m^{-1}\right\}$ (cf. (19)). Then, Theorem 10 directly implies an estimate of $\mathfrak{M}_{M,\rho}(f)$ in (9). Note that (20a) yields

$$\sup_{z\in\mathcal{C}_{M,\rho}} |f(z)| \leq \sup_{z\in\mathcal{C}_{M,\rho}} \alpha \left(\max\{1, |z|\}\right)^p \leq \alpha (C_1 M)^p.$$

To estimate the denominator in (9) we start with

$$\inf_{z\in\mathcal{C}_{M,\rho}} |z - x_i| \overset{(20b)}{\geq} (1-\varepsilon) x_i \quad \text{with} \quad \varepsilon := 2\left(\frac{1}{\sqrt{M}} + \frac{1}{m}\right).$$

Thus,

$$\sup_{z\in\mathcal{C}_{M,\rho}} \omega_N^{-1}(z) \leq \left|\omega_N^{-1}(0)\right| (1-\varepsilon)^{-N} = \left|\omega_N^{-1}(0)\right| \mathrm{e}^{\sum_{i=1}^N \log(1-\varepsilon)} = \left|\omega_N^{-1}(0)\right| \mathrm{e}^{2R}.$$

Hence,

$$|\omega_N(0)|\, \mathfrak{M}_{M,\rho}(f) \leq \alpha (C_1 M)^p \mathrm{e}^{2R}.$$

It remains to estimate γ_M' in the strip $\mathfrak{s}_\rho(J_\lambda)$. We use Corollary 20 below, the choice of ρ, and $q^{1/2} M^{-1/2} \leq 1$ (which follows from (3a)) to obtain for all $\sigma \in \mathfrak{s}_\rho(J_\lambda)$ the estimate

$$|\gamma_M'(\sigma)| \leq C_2 M \quad \text{with} \quad C_2 := \frac{65}{c_0}\sqrt{2}.$$

Hence,

$$|\omega_N(0)| \sup_{\sigma\in\mathfrak{s}_\rho(J)} \|g(\sigma)\|_V \leq \frac{C_1^p C_2}{2\pi} \alpha M^{p+1} \mathrm{e}^{2R}.$$

To apply Theorem 11 we have to estimate the interval length $|J_\lambda| = 4K(\lambda)$ and employ Lemma 26 to obtain

$$\begin{aligned} |J_\lambda| &\leq \frac{1}{2} \log \frac{16}{1-\lambda} \left(1 + \sqrt{\frac{2}{7}}(1-\lambda)\right) \overset{(13)}{\leq} \frac{1}{2} \log\left(16\sqrt{q}\right) \left(1 + 16\sqrt{\frac{1}{7q}}\right) \\ &\leq 10 + 2\log q. \end{aligned}$$

Hence, we get

$$\frac{\pi}{|J_\lambda|}\rho \geq \frac{\pi}{3C_0}\frac{\min\left\{M^{-1/2}, m^{-1}\right\}}{10+2\log q}.$$

■

Corollary 13 *Let the assumptions of Theorem 12 be satisfied and let τ and R be as in Theorem 12. Then, the choice of the number of quadrature points according to*

$$N_Q > \tau^{-1}\left(c+\log\left(\frac{1}{\varepsilon}\right)+2R+(p+2)\log M\right) \tag{22}$$

with $c \geq \log\left(2+20\alpha\frac{C_1^p C_2}{\pi}\right)$ implies an accuracy ε in the approximation (6) *of the divided difference in* (4)*, i.e.,*

$$|\omega_N(0)|\left\|\delta_N(f)-\tilde{\delta}_N(f)\right\|_V \leq \varepsilon.$$

Proof. Since $N_Q \geq \tau^{-1}\log 2$, the denominator in (21) can be estimated from below by $\mathrm{e}^{N_Q\tau}/2$ and we estimate the term $(10+2\log q)$ in (21), generously, by $10M$ (cf. Remark 9). In view of (21) we obtain

$$|\omega_N(0)|\left\|\delta_N(f)-\tilde{\delta}_N(f)\right\|_V \leq 20\alpha\frac{C_1^p C_2}{\pi}\mathrm{e}^{2R+(p+2)\log M-N_Q\tau} \overset{(22)}{\leq} \varepsilon.$$

■

We finally present a version of Theorem 12, where we assume that the mesh is graded at most quadratically, i.e.,

$$\max_{1\leq i\leq N} x_i \leq m^2. \tag{23}$$

In this case, we may choose $M := m^2$. In many applications we also have $N \leq m$ (generalizations to $M \leq Cm^2$ and $N \leq C'm$ are straightforward). This case is considered in the following Corollary.

Corollary 14 *Let $N \leq m$ and assume that (23) is satisfied. Let the assumptions of Theorem 12 be satisfied. Let λ, k be the functions of $q = M/m$ as in (12) and let $f \in \mathcal{A}(\sigma, p, \alpha)$ for some $\sigma < -1$. Then the choice of quadrature points according to*

$$N_Q > m\log(m+1)\left(c_2+c_1\log\left(\frac{1}{\varepsilon}\right)+c_3\log m\right)$$

with some constants

$$c_1 := \frac{30C_0}{\pi\log 2}, \quad c_2 := cc_1, \quad c_3 \geq 4c_1$$

leads to

$$|\omega_N(0)|\left\|\delta_N(f)-\tilde{\delta}_N(f)\right\|_V \leq \varepsilon.$$

Proof. The result follows from Corollary 13 by using the assumptions on N, m, and N_Q in combination with

$$\tau^{-1} = \frac{3C_0}{\pi}\left(10 + 2\log q\right)\max\left(M^{1/2}, m\right) = \frac{3C_0}{\pi}\left(10 + 2\log m\right)m \leq \frac{30C_0}{\pi\log 2} m\log\left(m+1\right).$$

■

The following remark shows that the use of the simple parametrization

$$\gamma_S(\theta) = M(1 - \mathrm{e}^{\mathrm{i}\theta}), \qquad \theta \in [0, 2\pi) =: J_S \tag{24}$$

leads to a much more critical dependence of the number of quadrature points on a large condition number $q = M/m$.

Remark 15 (Convergence with simple parametrization) *As an illustration, we consider the function* $f(z) := \mathrm{e}^{-z}(1+z)^p$ *for some* $p \in \mathbb{N}_0$ *(cf. (1)). Let* γ_S *be chosen as in (24). The condition on the width* ρ_S *of the complex strip* $\mathcal{C}_S := \{\gamma_S(z) : z \in \mathfrak{s}_{\rho_S}(J_S)\}$ *which ensures that* $\mathcal{C}_S$ *stays properly (distance at least* $m/2$*) away from the poles* $(x_i)_i$ *of the integrand is given by*

$$0 < \rho_S \leq \log\frac{q}{q - 1/2}, \quad \textit{where, again, } q = M/m. \tag{25}$$

Note that the quadrature error estimate is given (cf. Theorem 11) for the simple parametrization by

$$\omega_N(0)\left|\delta_N(f) - \delta_N^S(f)\right| \leq \frac{4\pi}{\mathrm{e}^{N_Q\rho_S} - 1}\sup_{\sigma\in\mathfrak{s}_{\rho_S}(J_S)}\left\|g(\sigma)\right\|_V \tag{26}$$

for the approximated divided difference

$$\delta_N^S(f) := \frac{1}{\mathrm{i}\,N_Q}\sum_{\ell=0}^{N_Q-1}\frac{f\circ\gamma_S(t_\ell)}{\omega_N(\gamma_S(t_\ell))}\gamma_S'(t_\ell)$$

and the integrand

$$g_S(\theta) := \frac{1}{2\pi\,\mathrm{i}}\frac{\omega_N(0)\, f\circ\gamma_S(\theta)}{\omega_N(\gamma_S(\theta))}\gamma_S'(\theta) \qquad \forall\theta\in J_S. \tag{27}$$

The estimate $|\gamma_S'(\theta)| \leq M$ *is obvious. Some elementary calculus show that*

$$\sup_{z\in\mathcal{C}_S}|f(z)| \leq (3M)^p + m^p\exp(m)$$

holds. The factors in (27) related to ω_N *satisfy*

$$\sup_{\sigma\in\mathcal{C}_S}\left|\frac{\omega_N(0)}{\omega_N(\sigma)}\right| = \left|\frac{\omega_N(0)}{\prod_{i=1}^N(x_i - \xi_S)}\right| = \frac{1}{\prod_{i=1}^N(1 - \xi_S/x_i)} = \prod_{i=1}^N\left(1 + \frac{\xi_S}{x_i - \xi_S}\right)$$

with $\xi_S := M\left(1-\exp\left(-\rho_S\right)\right)$ *so that (25) implies* $|x_i - \xi_S| > m/2$. *Thus*

$$\sup_{\sigma\in\mathcal{C}_S}\left|\frac{\omega_N(0)}{\omega_N(\sigma)}\right| \leq \exp\sum_{i=1}^{N}\left(\frac{\xi_S}{x_i-\xi_S}\right) \leq \exp(2N).$$

The combination with (26) leads to

$$\omega_N(0)\left|\delta_N(f)-\delta_N^S(f)\right| \leq 2M\frac{\left((3M)^p+m^p\,\mathrm{e}^m\right)\mathrm{e}^{2N}}{\left(1+\frac{1}{2q-1}\right)^{N_Q}-1}. \tag{28}$$

We see that the numerator in (28) is significantly larger compared to the term $\exp(2R)$ *in (21). This explains why the convergence with the simple parametrization is much slower than for our more sophisticated contour and we refer to Section 5 for numerical experiments.*

4 Estimates of Jacobi Elliptic Functions

In this section, we will prove Theorem 10. For this we have to analyze the behavior of the Jacobi elliptic function in a neighborhood of the interval J_λ.

In order to estimate the distance from our integration contour to the boundary of the region $C_{M,\rho}$ (cf. (8)), we have to estimate the derivatives of γ_M and, in turn, the derivatives of z and u (cf. (15)). Let $\mathbb{S}_1 := \{z\in\mathbb{C} \mid |z|=1\}$.

In order to give an idea of the behavior of the width of the region $\mathcal{C}_{M,\rho}$, we point out the following special values of γ_M and γ_M' (cf. [1, Sec. 16.5])

$$\begin{aligned}
\gamma_M\left(-K+\frac{\mathrm{i}}{2}K'\right) &= 0, & \gamma_M'\left(-K+\frac{\mathrm{i}}{2}K'\right) &= O(m)\\
\gamma_M\left(0+\frac{\mathrm{i}}{2}K'\right) &= m+\mathrm{i}m\sqrt{2q-1}, & \gamma_M'\left(-K+\frac{\mathrm{i}}{2}K'\right) &= O(\sqrt{Mm})\\
\gamma_M\left(K+\frac{\mathrm{i}}{2}K'\right) &= 2M, & \gamma_M'\left(-K+\frac{\mathrm{i}}{2}K'\right) &= O(M)
\end{aligned}$$

The above formulae indicate that the derivative of our parametrization gets smaller as our contour becomes closer to the imaginary axis. This property is essential in order to avoid that the boundary of the region $C_{M,\rho}$ enters "too" much the left half plane (where the integrand is allowed to grow exponentially) or getting too close to the poles in $\mathcal{I}$ (cf. Remark 5) as can be seen from the mean value theorem

$$\gamma_M(\sigma+\rho\zeta) = \gamma_M(\sigma)+\rho\gamma_M'(\xi),$$

for some ξ in between σ and $\sigma+\rho\zeta$.

In the rest of this section we will derive sharp estimates for γ_M' and the width of $C_{M,\rho}$ which are explicit with respect to ρ and all the parameters involved in the approximation formula (6). We have chosen the constants in the estimates such that the expressions become as simple as possible (cf. Remark 9) and, hence, avoided to optimize them.

Remark 16 *For all $\sigma \in J_\lambda$ we have $|\operatorname{sn}(\sigma)| = \lambda^{-1/4}$. Hence*

$$\eta_\sigma := \lambda^{1/4} \operatorname{sn} \sigma \quad \textit{satisfies} \quad |\eta_\sigma| = 1. \tag{29}$$

Proof. We write $\sigma = a + \frac{\mathrm{i}}{2} K'(\lambda)$ for $a := tK(\lambda)$ and all $t \in (-1, 3)$. Hence,

$$\operatorname{sn}(\sigma) = \operatorname{sn}\left(a + \frac{\mathrm{i}}{2} K'(\lambda)\right) \overset{[1,\ 16.5.4,\ 16.17.1]}{=} \frac{\left(1 + \lambda^{1/2}\right) \operatorname{sn} a + \mathrm{i} \operatorname{cn} a \operatorname{dn} a}{\lambda^{1/4}\left(1 + \lambda^{1/2} \operatorname{sn}^2 a\right)}.$$

We have

$$|\operatorname{sn}(\sigma)| \overset{[1,\ 16.9.1]}{=} \frac{\sqrt{\left(1+\lambda^{1/2}\right)^2 \operatorname{sn}^2 a + \left(1 - \operatorname{sn}^2 a\right)\left(1 - \lambda \operatorname{sn}^2 a\right)}}{\lambda^{1/4}\left(1 + \lambda^{1/2} \operatorname{sn}^2 a\right)} = \frac{\sqrt{2\lambda^{1/2} \operatorname{sn}^2 a + 1 + \lambda \operatorname{sn}^4 a}}{\lambda^{1/4}\left(1 + \lambda^{1/2} \operatorname{sn}^2 a\right)}$$

$$= \frac{1 + \lambda^{1/2} \operatorname{sn}^2 a}{\lambda^{1/4}\left(1 + \lambda^{1/2} \operatorname{sn}^2 a\right)} = \lambda^{-1/4}.$$

■

Lemma 17 *Let $\sigma \in J_\lambda$ and η_ρ be as in (29). For any $0 \le \rho \le \pi/6$ and $\zeta \in \mathbb{S}_1$ it holds*

$$\operatorname{sn}(\sigma + \rho\zeta) = \lambda^{-1/4} \eta_\sigma (1 - \varepsilon), \tag{30}$$

where $\varepsilon = \varepsilon_\lambda(\rho\zeta, \sigma)$ satisfies for all $0 \le \rho \le \pi/6$ and $\zeta \in \mathbb{S}_1$

$$|\varepsilon_\lambda(\rho\zeta, \sigma)| \le 6\left(\rho + \left|\lambda^{1/2} - \eta_\sigma^2\right|\right)\rho. \tag{31}$$

Proof. The addition formula [1, 16.17.1] gives us

$$\operatorname{sn}(\sigma + \rho\zeta) = \operatorname{sn}(\sigma)\left(1 - \varepsilon_\lambda(\rho\zeta, \sigma)\right)$$

where

$$\varepsilon_\lambda(y, \sigma) = \frac{1 - \operatorname{cn} y \operatorname{dn} y - \lambda^{1/2} \eta_\sigma^2 \operatorname{sn}^2 y - \eta_\sigma^{-1} \operatorname{sn} y \sqrt{\left(\lambda^{1/2} - \eta_\sigma^2\right)\left(1 - \lambda^{1/2} \eta_\sigma^2\right)}}{1 - \lambda^{1/2} \eta_\sigma^2 \operatorname{sn}^2 y}. \tag{32}$$

The term $\varepsilon_\lambda(y, \sigma)$ can be estimated in the considered range of ρ by using [27, Theorem 1]:

$$|\operatorname{sn}(\rho\zeta)| \le \tan\rho, \qquad |\operatorname{cn}(\rho\zeta)| \le \frac{1}{\cos\rho}, \qquad |\operatorname{dn}(\rho\zeta)| \le \frac{1}{\cos\rho}.$$

Since

$$1 - \operatorname{cn}(\rho\zeta) \operatorname{dn}(\rho\zeta) = \operatorname{sn}^2(\rho\zeta) \frac{(1 + \lambda) - \lambda \operatorname{sn}^2(\rho\zeta)}{1 + \sqrt{\left(1 - \operatorname{sn}^2(\rho\zeta)\right)\left(1 - \lambda \operatorname{sn}^2(\rho\zeta)\right)}},$$

we obtain for any $0 \leq \rho \leq \pi/6$

$$\left|1-\operatorname{cn}(\rho\zeta)\operatorname{dn}(\rho\zeta)\right| \leq \tan^2\rho \frac{2}{1+\sqrt{\left(1-\tan^2\rho\right)\left(1-\lambda\tan^2\rho\right)}} \leq \frac{2\tan^2\rho}{2-\tan^2\rho}.$$

The other term in the numerator of (32) can be estimated by

$$\left|\lambda^{1/2}\eta_\sigma^2\operatorname{sn}^2\rho\zeta\right| + \left|\eta_\sigma^{-1}\operatorname{sn}\rho\zeta\sqrt{\left(\lambda^{1/2}-\eta_\sigma^2\right)\left(1-\lambda^{1/2}\eta_\sigma^2\right)}\right| \leq \tan^2\rho + \tan\rho\sqrt{\left|\lambda^{1/2}-\eta_\sigma^2\right|\left|1-\lambda^{1/2}\eta_\sigma^2\right|}.$$

Note that

$$1-\lambda^{1/2}\eta_\sigma^2 = 1-\lambda+\lambda^{1/2}(\lambda^{1/2}-\eta_\sigma^2)$$

and we use $\sqrt{a+b} \leq \sqrt{a}+\sqrt{b}$ for non-negative a, b in order to estimate

$$\left|\sqrt{\left(\lambda^{1/2}-\eta_\sigma^2\right)\left(1-\lambda^{1/2}\eta_\sigma^2\right)}\right| \leq 2\sqrt{1-\lambda^{1/2}}\sqrt{\left|\lambda^{1/2}-\eta_\sigma^2\right|} + \left|\lambda^{1/2}-\eta_\sigma^2\right| \leq 3\left|\lambda^{1/2}-\eta_\sigma^2\right|,$$

so that we obtain for $0 \leq \rho \leq \pi/6$

$$\left|\lambda^{1/2}\eta_\sigma^2\operatorname{sn}^2\rho\zeta\right| + \left|\eta_\sigma^{-1}\left(\operatorname{sn}\rho\zeta\right)\sqrt{\left(\lambda^{1/2}-\eta_\sigma^2\right)\left(1-\lambda^{1/2}\eta_\sigma^2\right)}\right| \leq \tan\rho\left(\tan\rho+3\left|\lambda^{1/2}-\eta_\sigma^2\right|\right).$$

The denominator of (32) for $0 \leq \rho \leq \pi/6$ can be estimated by

$$\frac{1}{\left|1-\lambda^{1/2}\operatorname{sn}^2\rho\zeta\right|} \leq \frac{1}{1-\tan^2\rho} \leq \frac{3}{2}.$$

The combination of these estimates leads to

$$\left|\varepsilon_\lambda(\rho\zeta,\sigma)\right| \leq \frac{3}{2}\left(\frac{11}{5}\tan^2\rho + 3\left|\lambda^{1/2}-\eta_\sigma^2\right|\tan\rho\right).$$

We employ $\tan\rho \leq 2\frac{\sqrt{3}}{\pi}\rho$ for all $0 \leq \rho \leq \pi/6$ (cf. (13)) to obtain

$$\left|\varepsilon_\lambda(\rho\zeta,\sigma)\right| \leq 6\left(\rho+\left|\lambda^{1/2}-\eta_\sigma^2\right|\rho\right)\rho.$$

■

Lemma 18 *The contour $\gamma_M(\sigma)$ (cf. Definition 7) is a parametrization of the circle $\mathcal{C}_M$ with radius M about M and can be written in the form*

$$\gamma_M(\sigma) = M\left(1+\frac{1-k^{1/2}\overline{\eta_\sigma}}{1-k^{1/2}\eta_\sigma}\eta_\sigma\right) \tag{33}$$

with η_σ as in (29) and k as in (12). For the derivatives we get

$$\left|\gamma_M'(\sigma)\right| \leq 16\lambda^{1/4}M\frac{\sqrt{2q-1}}{q-1}\frac{\left|\lambda^{1/4}+\eta_\sigma\right|}{\left|\lambda^{1/4}-\eta_\sigma\right|}. \tag{34}$$

Proof. We introduce the short hands

$$u = \operatorname{sn}\sigma = \lambda^{-1/4}\eta_\sigma, \qquad \lambda = k^2, \qquad \nu = \sqrt{2q-1}, \qquad x = k^{1/2}\operatorname{Re}\eta_\sigma, \qquad y = k^{1/2}\operatorname{Im}\eta_\sigma. \tag{35}$$

Then, the definition of $z(u)$ (cf. (15)) leads to

$$\begin{aligned} z(u) - M &= \frac{M}{(q-1)}\frac{\nu - q + (\nu+q)k^{1/2}\eta_\sigma}{1-k^{1/2}\eta_\sigma} \\ &= \frac{M(q+\nu)}{q-1}\frac{x-k+\mathrm{i}\,y}{1-x-\mathrm{i}\,y} = \frac{M}{\sqrt{k}}\frac{x-k+\mathrm{i}\,y}{1-x-\mathrm{i}\,y} = M\eta_\sigma\frac{1-k^{1/2}\overline{\eta_\sigma}}{1-k^{1/2}\eta_\sigma}. \end{aligned}$$

From

$$\left|\frac{x-k+\mathrm{i}\,y}{1-x-\mathrm{i}\,y}\right| = \sqrt{\frac{(x-k)^2+y^2}{(1-x)^2+y^2}} = \sqrt{k}$$

we conclude that $|z(u) - M| = M$, i.e., $\gamma_M(\sigma)$ is a parametrization of $\mathcal{C}_M$.

For the derivative $\gamma_M'(\sigma)$ we obtain

$$\gamma_M'(\sigma) \overset{[1,\ 16.16.1]}{=} M\frac{\sqrt{2q-1}}{q-1}\frac{2\lambda^{1/2}\operatorname{cn}(\sigma)\operatorname{dn}(\sigma)}{\left(\lambda^{1/2}\operatorname{sn}(\sigma)-1\right)^2} = M\frac{\sqrt{2q-1}}{q-1}\frac{2\lambda^{1/2}\sqrt{\left(1-\lambda^{-1/2}\eta_\sigma^2\right)\left(1-\lambda^{1/2}\eta_\sigma^2\right)}}{\left(\lambda^{1/4}\eta_\sigma-1\right)^2}.$$

In order to prove estimate (34) we need Lemma 19 below. ■

Next, we will estimate the derivative γ_M' in a neighborhood of J_λ.

Lemma 19 *For $\sigma \in J_\lambda$ it holds*

$$|\gamma_M'(\sigma+\rho\zeta)| = \gamma_M'(\sigma) + \rho\mathfrak{R},$$

for all $\rho \leq \frac{\left|\lambda^{1/2}-\eta_\sigma^2\right|^{1/2}}{40}$ and all $\zeta \in \mathbb{S}_1$, where

$$|\mathfrak{R}| \leq 184\frac{\sqrt{2q-1}}{q-1}\frac{M}{\left|\lambda^{1/4}-\eta_\sigma\right|^2}.$$

Proof. Let $\sigma \in J_\lambda$. The first derivative of γ_M can be written in the form

$$\gamma_M'(\sigma+\rho\zeta) \overset{[1,\ 16.16.1]}{=} M\frac{\sqrt{2q-1}}{q-1}\frac{2\lambda^{1/2}\operatorname{cn}(\sigma+\rho\zeta)\operatorname{dn}(\sigma+\rho\zeta)}{\left(\lambda^{1/2}\operatorname{sn}(\sigma+\rho\zeta)-1\right)^2}.$$

We use (30) and write

$$x := x(\varepsilon) := \operatorname{sn}(\sigma+\rho\zeta) = \eta_\sigma\frac{1-\varepsilon}{\lambda^{1/4}},$$

so that

$$\gamma_M'(\sigma+\rho\zeta) \overset{[1,\ 16.16.1]}{=} C_{M,q}\,g(x),$$

where $C_{M,q} := 2M\lambda^{1/2}\frac{\sqrt{2q-1}}{q-1}$ and

$$g(x) := g_1(x)\, g_2(x) \quad \text{and} \quad g_1(x) := \sqrt{(1-x^2)(1-\lambda x^2)} \quad \text{and} \quad g_2(x) := \left(1-\lambda^{1/2}x\right)^{-2}.$$

We obtain for $0 \leq \rho \leq \frac{\left|\lambda^{1/2}-\eta_\sigma^2\right|^{1/2}}{40}$ the estimate

$$|\varepsilon| \leq 6\left(\rho + \left|\lambda^{1/2}-\eta_\sigma^2\right|\right)\rho \leq \frac{1}{4}\left|\lambda^{1/2}-\eta_\sigma^2\right| \quad \text{and} \quad |\varepsilon| \leq 1/2. \tag{36}$$

For the functions g_2, g_2' we need some auxiliary estimates. The modulus of x can be estimated by

$$\frac{1}{2\lambda^{1/4}} \leq |x| \leq \frac{3}{2\lambda^{1/4}}. \tag{37}$$

Then,

$$\begin{aligned}\left|1-\lambda^{1/2}x\right| &= \left|1-\lambda^{1/4}\eta_\sigma(1-\varepsilon)\right| = \left|1-\lambda^{1/4}\eta_\sigma + \lambda^{1/4}\eta_\sigma\varepsilon\right| \\ &\geq \left|1-\lambda^{1/4}\eta_\sigma\right| - \lambda^{1/4}|\varepsilon| \geq \left|1-\lambda^{1/4}\eta_\sigma\right| - \lambda^{1/4}\frac{1}{4}\left|\lambda^{1/2}-\eta_\sigma^2\right|.\end{aligned}$$

Note that $\left|1-\lambda^{1/4}\eta_\sigma\right| = \left|\lambda^{1/4}-\eta_\sigma\right|$ so that

$$\left|1-\lambda^{1/2}x\right| \geq \left|\lambda^{1/4}-\eta_\sigma\right|\left(1-\frac{1}{4}\left|\lambda^{1/4}+\eta_\sigma\right|\right) \geq \frac{1}{2}\left|\lambda^{1/4}-\eta_\sigma\right|. \tag{38}$$

Thus,

$$|g_2(x)| \leq \frac{4}{\left|\lambda^{1/4}-\eta_\sigma\right|^2} \quad \text{and} \quad |g_2'(x)| \leq \frac{2}{\left|1-\lambda^{1/2}x\right|^3} \leq \frac{16}{\left|\lambda^{1/4}-\eta_\sigma\right|^3}. \tag{39}$$

The estimate of the first derivative of g_1 is more involved. Explicit calculation leads to

$$g_1'(x) = -x\left(\sqrt{\frac{1-\lambda x^2}{1-x^2}} + \lambda\sqrt{\frac{1-x^2}{1-\lambda x^2}}\right). \tag{40}$$

Similarly as for (38) we get

$$\left|1+\lambda^{1/2}x\right| \geq \frac{1}{2}\left|\lambda^{1/4}+\eta_\sigma\right| \tag{41}$$

so that the combination of (38) and (41) yields

$$\left|1-\lambda x^2\right| \geq \frac{1}{4}\left|\lambda^{1/2}-\eta_\sigma^2\right|. \tag{42}$$

For the lower estimate of $\left|1-x^2\right|$ we argue as follows. It holds

$$\begin{aligned}\left|1-x^2\right| &= \left|1-\eta_\sigma^2\frac{(1-\varepsilon)^2}{\lambda^{1/2}}\right| = \lambda^{-1/2}\left|\lambda^{1/2}-\eta_\sigma^2(1-\varepsilon)^2\right| \\ &\geq \lambda^{-1/2}\left(\left|\lambda^{1/2}-\eta_\sigma^2\right| - |\varepsilon(2-\varepsilon)|\right).\end{aligned} \tag{43}$$

Since $0 \leq \rho \leq \frac{\left|\lambda^{1/2}-\eta_\sigma^2\right|^{1/2}}{40}$ and $\left|\lambda^{1/2}-\eta_\sigma^2\right| \leq \sqrt{2}\left|\lambda^{1/2}-\eta_\sigma^2\right|^{1/2}$, we get from (36) the estimates

$$|\varepsilon| \leq \frac{1}{4}\left|\lambda^{1/2}-\eta_\sigma^2\right| \qquad \text{and} \qquad |\varepsilon(2-\varepsilon)| \leq \frac{1}{2}\left|\lambda^{1/2}-\eta_\sigma^2\right| \tag{44}$$

so that

$$\left|1-x^2\right| \geq \frac{\left|\lambda^{1/2}-\eta_\sigma^2\right|}{2\lambda^{1/2}}. \tag{45}$$

The estimates of $\left|1-\lambda x^2\right|$ and $\left|1-x^2\right|$ from above follow from

$$\begin{aligned}\left|1-\lambda^{1/2}x\right| &\leq \left|1-\lambda^{1/4}\eta_\sigma\right| + \lambda^{1/4}|\varepsilon| \leq \left|1-\lambda^{1/4}\eta_\sigma\right| + \lambda^{1/4}\frac{1}{4}\left|\lambda^{1/2}-\eta_\sigma^2\right| \\ &\leq \left|\lambda^{1/4}-\eta_\sigma\right|\left(1+\lambda^{1/4}\frac{1}{4}\left|\lambda^{1/4}+\eta_\sigma\right|\right) \leq \frac{3}{2}\left|\lambda^{1/4}-\eta_\sigma\right|.\end{aligned}$$

Replacing η_σ by $-\eta_\sigma$ leads to

$$\left|1+\lambda^{1/2}x\right| \leq \frac{3}{2}\left|\lambda^{1/4}+\eta_\sigma\right|$$

and, in turn,

$$\left|1-\lambda x^2\right| \leq \frac{9}{4}\left|\lambda^{1/2}-\eta_\sigma^2\right|. \tag{46}$$

To estimate $\left|1-x^2\right|$ from above we argue as in (43), (44) to obtain

$$\left|1-x^2\right| \leq \frac{3}{2\lambda^{1/2}}\left|\lambda^{1/2}-\eta_\sigma^2\right|. \tag{47}$$

The combination of (37), (40), (42), (45), (46), and (47) results in

$$\left|g_1'(x)\right| \leq 7.$$

It remains to estimate $g_1(x)$. We use (46) and (47) to obtain

$$|g_1(x)| \leq \sqrt{\left|1-x^2\right|\left|1-\lambda x^2\right|} \leq 2\frac{\left|\lambda^{1/2}-\eta_\sigma^2\right|}{\lambda^{1/4}}. \tag{48}$$

In total, we have proved

$$\gamma_M'(\sigma+\rho\zeta) = \gamma_M'(\sigma) + \rho\mathfrak{R}, \tag{49}$$

where

$$\begin{aligned}|\mathfrak{R}| &\leq \max_{\substack{0\leq\mu\leq\rho \\ |\zeta|=1}} \left|\gamma_M''(\sigma+\mu\zeta)\right| \leq C_{M,q} \max_{\substack{|\varepsilon|\leq\frac{1}{4}\left|\lambda^{1/2}-\eta_\sigma^2\right| \\ x=\eta_\sigma\frac{1-\varepsilon}{\lambda^{1/4}}}} \left|g_1'(x)\,g_2(x)+g_1(x)\,g_2'(x)\right| \\ &\leq 184\lambda^{1/4}M\frac{\sqrt{2q-1}}{q-1}\frac{1}{\left|\lambda^{1/4}-\eta_\sigma\right|^2}.\end{aligned} \tag{50}$$

■

Proof of estimate (34).

Note that $\rho = 0$ implies $\varepsilon = 0$ (in (30)) and, in turn $x = \lambda^{-1/4}\eta_\sigma$. We have

$$\gamma_M'(\sigma) = C_{M,q}\, g\left(\lambda^{-1/4}\eta_\sigma\right).$$

From (48) and (39) we get

$$|\gamma_M'(\sigma)| \le 16\lambda^{1/4} M \frac{\sqrt{2q-1}}{q-1} \frac{\left|\lambda^{1/4}+\eta_\sigma\right|}{\left|\lambda^{1/4}-\eta_\sigma\right|}.$$

■

Corollary 20 *For all* $0 \le \rho \le \frac{q^{-1/4}}{40}$, *it holds*

$$|\gamma_M'(\sigma)| \overset{(13)}{\le} M\frac{\sqrt{2q-1}}{q-1}\left(64\sqrt{q}+736q\rho\right) \qquad \forall\sigma\in\mathfrak{s}_\rho\left(J_\lambda\right).$$

Proof. It is easy to verify (cf. (13)) that the condition on ρ implies

$$\rho \le \frac{\sqrt{\left|\lambda^{1/2}-\eta_\sigma^2\right|}}{40} \qquad \forall\sigma\in J_\lambda \tag{51}$$

and, hence, Lemma 19 is applicable. We employ estimate (34) and Lemma 19 to obtain

$$\begin{aligned}|\gamma_M'(\sigma+\rho\zeta)| &\le M\frac{\sqrt{2q-1}}{q-1}\left(16\lambda^{1/4}\frac{\left|\lambda^{1/4}+1\right|}{\left|\lambda^{1/4}-1\right|}+184\frac{\rho}{\left|\lambda^{1/4}-1\right|^2}\right)\\ &\overset{(13)}{\le} M\frac{\sqrt{2q-1}}{q-1}\left(64\sqrt{q}+736q\rho\right).\end{aligned}$$

■

Corollary 21 *Let* $0 \le \rho \le \frac{q^{-1/4}}{40}$. *Then, the distance of the boundary of the region* $\mathcal{C}_{M,\rho}$ *to the contour* $\mathcal{C}_M$ *can be estimated by*

$$|\gamma_M(\sigma+\rho\zeta)-\gamma_M(\sigma)| \le 92M\frac{\sqrt{2q-1}}{q-1}\rho\left(\frac{\left|\lambda^{1/2}-\eta_\sigma^2\right|+\rho}{\left|\lambda^{1/4}-\eta_\sigma\right|^2}\right) \qquad \forall\sigma\in J_\lambda \quad \textit{and} \quad \zeta\in\mathbb{S}_1. \tag{52}$$

Proof. Again, the condition on ρ implies (51) and Lemma 19 is applicable. We have

$$\begin{aligned}|\gamma_M(\sigma+\rho\zeta)-\gamma_M(\sigma)| &\overset{(49)}{\le} \rho\left|\gamma_M'(\sigma)\right|+\frac{\rho^2}{2}|\mathfrak{R}|\\ &\overset{(34),(50)}{\le} 92M\frac{\sqrt{2q-1}}{q-1}\rho\left(\frac{\left|\lambda^{1/2}-\eta_\sigma^2\right|+\rho}{\left|\lambda^{1/4}-\eta_\sigma\right|^2}\right).\end{aligned}$$

■

In the following the width of $\mathcal{C}_{M,\rho}$ will be estimated in terms of $z\in\mathcal{C}_M$.

Corollary 22 *Let* $0 \leq \rho \leq \frac{q^{-1/4}}{40}$. *For any* $z = M(1+\theta)$, $\theta \in \mathbb{S}_1$, *the width of* $\mathcal{C}_{M,\rho}$ *is bounded by*

$$\operatorname{dist}(z, \partial C_{M,\rho}) \leq 261 \frac{M\rho}{q-1} \left(q\left|1+\theta\right| + 1 + \left(q^{3/2} \left|1+\theta\right|^2 + q^{1/2} \right) \rho \right). \tag{53}$$

Proof. From (33) we conclude that any point on $\mathcal{C}_M$ can be written as $z = M(1+\theta)$ for $\theta \in \mathbb{S}_1$ and corresponds to

$$\eta_\sigma = \frac{\theta + k^{1/2}}{1 + k^{1/2}\theta}. \tag{54}$$

We combine (52) and (54) to bound the width of $\mathcal{C}_{M,\rho}$ for any $z = M(1+\theta)$ by

$$\operatorname{dist}(z, \partial C_{M,\rho}) \leq 92M \frac{\sqrt{2q-1}}{q-1} \rho \left(\frac{\left|2k^{1/2} + (k+1)\theta\right|}{1-k} + \frac{\left|1 + k^{1/2}\theta\right|^2 \rho}{(1-k)^2} \right).$$

For the first term in the bracket, we get with ν as in (35)

$$\frac{\left|2k^{1/2} + k\theta + \theta\right|}{1-k} = \frac{\left|q(1+\theta) - 1\right|}{\nu} \leq \frac{q\left|1+\theta\right| + 1}{\nu}$$

and for the second one

$$\frac{\left|1 + k^{1/2}\theta\right|^2 \rho}{(1-k)^2} = \frac{\left|q(1+\theta) + \nu - \theta\right|^2 \rho}{4\nu^2} \leq \left(q^2 \left|1+\theta\right|^2 + (\nu+1)^2 \right) \frac{\rho}{2\nu^2}.$$

This leads to

$$\operatorname{dist}(z, \partial C_{M,\rho}) \leq 92M \frac{1}{q-1} \rho \left(q\left|1+\theta\right| + 1 + \left(q^{3/2} \left|1+\theta\right|^2 + \sqrt{2} q^{1/2} \right) 2\rho \right).$$

■

The following theorem estimates how far the contour $\gamma_M(\sigma + \mathrm{i}\,\rho)$ enters the left half plane. The title of the Theorem is motivated by the shape of the outer contour, as depicted in Figure 1.

Theorem 23 (Kidney Distance) *Let* $c_0 \in (0,1)$, m, M, *and* q *be as in (3). For any* $\rho \leq (3C_0)^{-1} \min\left\{M^{-1/2}, m^{-1}\right\}$ *with* $C_0 = \frac{370}{c_0}$, *it holds for* μ *as in (10)*

$$\mu(M, \rho) \geq -1.$$

Proof. For $\theta \in \mathbb{S}_1$, we define $x_\theta := 1 + \operatorname{Re}\theta$ and $y_\theta := \operatorname{Im}\theta$ and note that $M(x_\theta + \mathrm{i}\,y_\theta) \in \mathcal{C}_M$, $x_\theta \in [0,2]$ and $y_\theta \in [-1,1]$. The right-hand side in (53) defines a function $d_{\lambda,M,q,\rho}(\theta)$ and we write short $d(\theta)$ if there is no confusion. It holds

$$\mu(M, \rho) \geq \min_{\theta \in \mathbb{S}_1} \left\{ M x_\theta - d(\theta) \right\} \tag{55}$$

and we will estimate the right-hand side in (55) from below. The relation $(x_\theta - 1)^2 + y_\theta^2 = 1$ implies $|1+\theta|^2 = x_\theta^2 + y_\theta^2 = 2x_\theta$ and we obtain the estimate

$$d(\theta) \le C_0 M \rho \left(\sqrt{x_\theta} + q^{-1} + \left(q^{1/2} x_\theta + q^{-1/2} \right) \rho \right) \quad \text{with} \quad C_0 := \frac{370}{c_0}. \tag{56}$$

For $0 \le x_\theta \le 1/M$ and $0 \le \rho \le \frac{M^{-1/2}}{3C_0}$ we get

$$3\rho\sqrt{x_\theta} \le \frac{1}{C_0 M}.$$

For $1/M \le x_\theta \le 2$ and, again, $0 \le \rho \le \frac{M^{-1/2}}{3C_0}$ it holds

$$3\rho\sqrt{x_\theta} \le 3\rho\frac{x_\theta}{\sqrt{x_\theta}} \le 3\rho\sqrt{M}x_\theta \le \frac{x_\theta}{C_0}$$

so that for all x_θ and $0 \le \rho \le \frac{M^{-1/2}}{3C_0}$ we have shown

$$\rho\sqrt{x_\theta} \le \frac{1}{3C_0}\left(x_\theta + \frac{1}{M} \right).$$

For the second term in the right-hand side in (56) we get for $0 \le \rho \le \frac{1}{3mC_0}$ the estimate

$$\frac{\rho}{q} \le \frac{1}{3C_0 M} \le \frac{1}{3C_0}\left(x_\theta + \frac{1}{M} \right).$$

The last bracket of the right-hand side in (56) can be estimated for $0 \le \rho \le \frac{M^{-1/2}}{3C_0}$ by

$$\begin{aligned} \left(q^{1/2} x_\theta + q^{-1/2} \right) \rho^2 &\le \frac{1}{(3C_0)^2} \left(\frac{1}{\sqrt{mM}} x_\theta + \sqrt{\frac{m}{M}} \frac{1}{M} \right) \\ &\overset{(3a)}{\le} \frac{1}{(3C_0)^2} \left(x_\theta + \frac{1}{M} \right) \le \frac{1}{3C_0}\left(x_\theta + \frac{1}{M} \right). \end{aligned}$$

In total we have proved that the function $d(\theta)$ can be estimated by

$$d(\theta) \le M x_\theta + 1.$$

Thus,

$$\mu_{M,\rho} \ge \min_{\theta \in \mathbb{S}_1} \{ M x_\theta - d(\theta) \} \ge -1.$$

■

The following Theorem estimates how far the contour $\gamma_M(\sigma - i\rho)$ moves towards the interval $\mathcal{I} = [m, M]$ containing the poles of our integrand in (4). The title of the theorem is again motivated by the shape of this contour, see Figure 1.

Theorem 24 (Egg Distance) *Let $A \in [m, M]$. For $\rho \le (3C_0)^{-1} \min\{M^{-1/2}, m^{-1}\}$ we have*

$$\operatorname{dist}(A, \mathcal{C}_{M,\rho}) \ge \left(1 - 2M^{-1/2} - \frac{2}{3} m^{-1}\right) A.$$

Proof. We write $A = M\xi$ for $\xi \in [q^{-1}, 1]$. The distance of A to the contour can be bounded from below by

$$\operatorname{dist}(M\xi, \mathcal{C}_{M,\rho}) \ge \min_{\theta \in \mathbb{S}_1} |M(1+\theta) - d(\theta)\theta - M\xi|.$$

With the choice $0 \le \rho \le (3C_0)^{-1} \min\{M^{-1/2}, m^{-1}\}$ we obtain for the distance function and x_θ as in the proof of Theorem 23

$$d(\theta) \le \frac{2}{3}\left(\sqrt{M x_\theta} + 1\right). \tag{57}$$

Note that

$$|M(1+\theta) - d(\theta)\theta - M\xi| \ge M|1+\theta-\xi| - |d(\theta)| \ge M\sqrt{\xi^2 + 2x_\theta(1-\xi)} - \frac{2}{3}\left(\sqrt{M x_\theta} + 1\right).$$

With the aid of the symbolic algebra program MATHEMATICA, we find that the right-hand side takes a minimum as a function of $x_\theta \in [0, 2]$ at

$$x_\theta = \begin{cases} 2 & \text{if } 1 - \frac{1}{\sqrt{18M} - 1} \le \xi \le 1, \\ \frac{\xi^2}{(9M(1-\xi) - 2)(1-\xi)} & \text{if } 0 \le \xi \le 1 - \frac{1}{\sqrt{18M} - 1}. \end{cases}$$

Hence, after some manipulations we get

$$|M(1+\theta) - d(\theta)\theta - M\xi| \ge \begin{cases} M(2-\xi) - 2\sqrt{M} & \text{if } 1 - \frac{1}{\sqrt{18M} - 1} \le \xi \le 1, \\ \left(M - 2\sqrt{M}\right)\xi - \frac{2}{3} & \text{if } 0 \le \xi \le 1 - \frac{1}{\sqrt{18M} - 1}. \end{cases}$$

Since $\xi \ge q^{-1}$ we have $2/3 \le (2/3)\,\xi q$ and the assertion follows. ∎

Corollary 25 *For $\rho \le (3C_0)^{-1} \min\{M^{-1/2}, m^{-1}\}$ we have*

$$\max\{|z| : z \in \mathcal{C}_{M,\rho}\} \le \frac{10}{3} M.$$

Proof. The assertion follows from (57) and $\max\{|z| : z \in \mathcal{C}_M\} = 2M$. ∎

In order to estimate the length of the interval J_λ we need to estimate the complete elliptic integral.

Lemma 26 *The complete elliptic integral K is strictly monotonously increasing in $[0, 1[$ and satisfies the estimate*

$$\frac{\pi}{2} \le K(\lambda) \le \frac{1}{2} \log \frac{16}{1-\lambda}\left(1 + \sqrt{\frac{2}{7}}(1-\lambda)\right) \quad \forall \lambda \in [0, 1[.$$

Proof. The strict monotonicity and the endpoint value at $\lambda = 0$ follow directly from (11a).

From [14, 8.113 (3) (with the substitution $k^2 \leftarrow \lambda$ therein)] we obtain

$$\begin{aligned} K(\lambda) &= \sum_{\ell=0}^{\infty} \left(\frac{(2\ell)!}{(\ell!)^2} \right)^2 \left(\frac{1-\lambda}{16} \right)^{\ell} \left(\log \frac{4}{\sqrt{1-\lambda}} - 2 \sum_{m=1}^{\ell} \frac{1}{(2m-1)\,2m} \right) \\ &= \frac{1}{2} \log \frac{16}{1-\lambda} + \sum_{\ell=1}^{\infty} \left(\frac{(2\ell)!}{\ell!^2} \right)^2 \left(\frac{1-\lambda}{16} \right)^{\ell} \left(\frac{1}{2} \log \frac{16}{1-\lambda} - 2 \sum_{m=1}^{\ell} \frac{1}{(2m-1)\,2m} \right). \end{aligned}$$

By using

$$\sum_{m=1}^{\infty} \frac{1}{(2m-1)\,2m} = \log 2$$

we get

$$|K(\lambda)| \leq \frac{1}{2} \log \frac{16}{1-\lambda} \left(1 + \frac{1-\lambda}{8} \sum_{\ell=1}^{\infty} \left(\frac{(2\ell)!}{\ell!^2} \right)^2 \left(\frac{1-\lambda}{16} \right)^{\ell-1} \right).$$

The infinite sum on the right-hand side is monotonously decreasing for $\lambda \in]0,1]$. Hence, for $\lambda \in \left[\frac{1}{2}, 1\right]$ we have

$$|K(\lambda)| \leq \frac{1}{2} \log \frac{16}{1-\lambda} \left(1 + \frac{1-\lambda}{8} \sum_{\ell=1}^{\infty} \frac{(2\ell)!}{(\ell!)^2} \left(\frac{1}{32} \right)^{\ell-1} \right) \leq \frac{1}{2} \log \frac{16}{1-\lambda} \left(1 + \sqrt{\frac{2}{7}} (1-\lambda) \right). \tag{58}$$

The definition (11a) shows that $K(\lambda)$ is strictly monotonously increasing in $\lambda \in [0,1]$ so that estimate (58) holds for all $\lambda \in [0,1[$. ■

5 Numerical Experiments

As explained in the introduction our main application is the approximation of high order divided differences as they arise when using variable time stepping in the *generalized convolution quadrature* method (GCQ) for approximating convolution operators. The quadrature problem is particularly challenging if the application is related to the *retarded potential boundary integral equations* (RPBIE) for solving the three-dimensional wave and Maxwell equation in exterior domains (see [22]).

The application of the GCQ to the wave equation leads to an integral operator-valued integrand $\mathcal{K}$ in (5), i.e., $f \leftarrow \mathcal{K}$, which is a function of the frequency variable $z \in \mathbb{C}$. From, e.g., [22, (3), (9), Proposition 8], it follows that the function

$$f(z) = (1+z)^4 \mathrm{e}^{-z} \tag{59}$$

reflects the characteristic (spectral) properties of the operator valued function $\mathcal{K}$: a) exponential growth to the left half plane, b) polynomial growth to the right, and c) an oscillatory behavior for increasing imaginary part. We will use this function f for our numerical experiments and refer to [21] for the application to the wave equation. Our choice of nodes x_ℓ is also related to the variable time stepping in the GCQ method. If the solution of the retarded potential integral equation (or its derivative) has a singularity, say, at time $t = 0$, then, from the approximation point of view, an *algebraic grading* of the time steps towards the origin can properly resolve the singularity. This consideration is reflected by our choice

$$t_\ell = \left(\frac{\ell}{N}\right)^\alpha, \qquad \Delta_\ell = t_{\ell+1} - t_\ell, \quad \text{for } \ell = 0, 1, \dots$$

with the *grading exponent* α; $\alpha = 1$ corresponds to uniform time steps while $\alpha = 2$ is a typical choice for resolving a qualitative behavior $O\left(t^{1/2}\right)$ of the solution at the origin. The arising divided differences are related to the reciprocal mesh sizes (cf. [22]), more precisely, are given by

$$x_\ell = \frac{1}{\Delta_\ell}, \quad \text{for} \quad \forall \ell = 1, \dots, N, \tag{60}$$

and our goal is to approximate the scaled divided differences

$$\begin{aligned} \omega_N(0)\frac{1}{2\pi \mathrm{i}}[x_1, \dots, x_N]f &= \prod_{\ell=1}^{N}(-x_\ell)\frac{1}{2\pi \mathrm{i}}\int_{\mathcal{C}_M} \frac{f(z)}{\prod_{\ell=1}^{N}(z - x_\ell)}\,dz \\ &= \frac{1}{2\pi \mathrm{i}}\int_{\mathcal{C}_M} \frac{f(z)}{\prod_{\ell=1}^{N}(1 - \frac{z}{x_\ell})}\,dz \end{aligned} \tag{61}$$

by our new contour quadrature. With this notation (61) becomes

$$\frac{1}{2\pi \mathrm{i}}\int_{\mathcal{C}_M} \frac{f(z)}{\prod_{\ell=1}^{N}(1 - \Delta_\ell z)}\,dz. \tag{62}$$

The computation of "exact" solutions for this experiments is not a trivial task and we employed the software MATHEMATICA, which allows to work with arbitrary high precision. Even though, we were not able to compute reliable reference solutions with MATHEMATICA for very high order divided differences for all values of α, in particular for α in between 0.5 and 1.8. In these cases, we have computed a reference solution with our method by using $\max\{3 \cdot 10^5, 2N^2\}$ quadrature points.

Experiment 1: Performance for Quadratic Mesh Grading Relative errors for different values of N_Q and N are provided in Table 1.

The upper half of the table, i.e., $N_Q \in [20, 320]$, shows the fast convergence with respect to N_Q and, in addition, that the convergence starts later for higher order divided differences. We also see that for $N_Q < N$ the accuracy becomes unreliable and the asymptotic convergence is not yet reached.

$\alpha = 2$					
N_Q	$N = 8$	$N = 32$	$N = 128$	$N = 512$	$N = 2048$
20	$\underline{2.1502\text{e} - 1}$	3.5308	1.4086	1.0001	1.0000
40	3.7623e − 3	$\underline{5.9599\text{e} - 2}$	2.0090e − 1	4.4724e − 1	1.0000
80	7.3213e − 9	4.2988e − 5	2.2862e − 3	3.0797e − 1	2.8917e − 1
160	2.5628e − 15	4.2252e − 10	$\underline{9.9688\text{e} - 12}$	1.5785e − 2	7.9961e − 1
320	2.2203e − 16	3.2376e − 15	4.8974e − 15	5.8516e − 11	7.7515e − 2
N	3.4100	3.8665e − 1	1.8754e − 8	$\underline{3.6240\text{e} - 15}$	$\underline{1.0184\text{e} - 14}$
$N\log(N)$	3.3270e − 1	3.5767e − 8	5.0626e − 16	7.2342e − 15	5.5631e − 15
$N(\log(N))^2$	3.7623e − 3	1.7210e − 15	1.7291e − 15	5.2064e − 16	3.7840e − 15
N^2	3.5023e − 6	1.9752e − 15	8.7585e − 16	4.1947e − 15	5.5929e − 14

Table 1: Computation of the integral in (62) for x_ℓ in (60) with grading factor $\alpha = 2$. We have underlined in each column the first number, where $N_Q \geq N$ is satisfied (cf. Corollary 14; note that $m = O(N)$ holds in the considered case). Note that the working precision in our MATLAB implementation is about 10^{-16}.

$\alpha = 1.1$					
N_Q	$N = 8$	$N = 32$	$N = 128$	$N = 512$	$N = 2048$
20	$\underline{4.2110\text{e} - 7}$	1.5008 e −1	8.8498 e −1	4.1609 e −1	1.0000
40	2.2196 e −14	$\underline{1.2963\text{e} - 9}$	9.5680 e −2	9.0889 e −1	4.9303 e −1
80	2.2196 e −14	1.2434 e −14	1.7946 e −9	1.0042 e −1	9.7628 e −1
160	2.2201 e −14	1.4694 e −14	$\underline{4.2353\text{e} - 14}$	8.7141 e −9	1.1488 e −1
320	2.2196 e −14	1.3668 e −14	4.2508 e −14	2.1433 e −14	2.8493 e −8
N	1.7713 e −1	3.7742 e −5	4.0800 e −14	$\underline{2.5120\text{e} - 14}$	$\underline{1.5834\text{e} - 13}$
$N\log(N)$	2.6919 e −11	1.3043 e −14	4.2679 e −14	2.6638 e −14	1.6050 e −13
$N(\log(N))^2$	2.2196 e −14	1.2520 e −14	4.0646 e −14	2.5939 e −14	1.7563 e −13
N^2	2.1403 e −14	1.3372 e −14	4.0956 e −14	1.3455 e −14	1.0146 e −13

Table 2: Computation of the integral in (62) for x_ℓ in (60) with grading factor $\alpha = 1.1$. We have underlined in each column the first number, where $N_Q \geq N$ is satisfied (cf. Corollary 14; note that $m = O(N)$ holds in the considered case). The working precision in our MATLAB implementation is about 10^{-16}. For this value of α, the error is compared to a reference solution which was computed by the same method with $\max\{3 \cdot 10^5, 2N^2\}$ quadrature points.

Remark 27 (Application to GCQ) *For the generalized convolution quadrature method, our new contour quadrature can be efficiently employed to approximate the arising contour integrals. The error analysis in [21] shows that the target accuracy* ε *for the contour quadrature approximation has to depend on the discretization parameter* N *– for the details we refer to.[21, Theorem 11, Corollary 12]. The numerical experiments in [21] show that the choice* $N_Q = N \log N$ *preserves the overall convergence rates of the (theoretical) GCQ with exact integration.*

Experiment 2: Robustness towards Uniform Time Steps We have shown numerically that our new contour quadrature allows to approximate efficiently the integral in (62) for strongly graded meshes. In the following experiment we have applied our method to the case of a very mildly graded mesh (close to uniform time stepping) to study the *robustness* of the quadrature method with respect to the grading factor, i.e., α close to 1.

Table 2 clearly indicates that the performance of our quadrature is robust (becomes even better) as the mesh becomes close to a uniform mesh, i.e., the nodes x_ℓ in (61) cluster around a single point. This property avoids that different quadrature strategies have to be implemented depending on the strength of non-uniformity of the nodal points in the divided differences.

Experiment 3: Comparison with Standard Parametrization of the Circle and Direct Evaluation of Divided Differences Our last example illustrates the dramatic improvement of our new contour quadrature in comparison to the simple parameterization $M(1+\exp(\mathrm{i}\theta))$, $\theta \in [0, 2\pi)$ of the circle $\mathcal{C}_M$ in (62) for the quadratically graded mesh. In Figure 2 we show the results for $\alpha = 2$ and different values of N.

The evaluation of Newton table for computing the high order divided differences in our experiment leads, in the case $\alpha = 2$, to huge errors for $N \geq 64$ and even `NaN` approximations for $N \geq 256$. Although rounding errors can be improved by reordering the nodal points in a suitable way, see [18] and references therein, they still grow almost exponentially in the number of points N. Furthermore, in applications where the nodes are generated adaptively, the multiplicity of a node can change in each step and clustering of nodes often arise. In these cases the reordering problem becomes more expensive and delicate. To illustrate the raising cost, we consider a sequence of $3N$ points of the form

$$[a, b, c, a, b, c, a, b, c, \dots].$$

The computation of the corresponding divided differences for these nodal points by employing Newton's table has a complexity of $O(N^3)$ due to re-ordering while our approach leads to a complexity of $O\left(N^2\right)$ up to logarithmic terms. Apart from the complexity, additional errors are introduced if one has to distinguished between those points which are considered to be equal and those which are not.

Finally, in order to show more clearly the dependence on the ratio q we provide also the results of the following experiment. For fixed $N = 200$, we

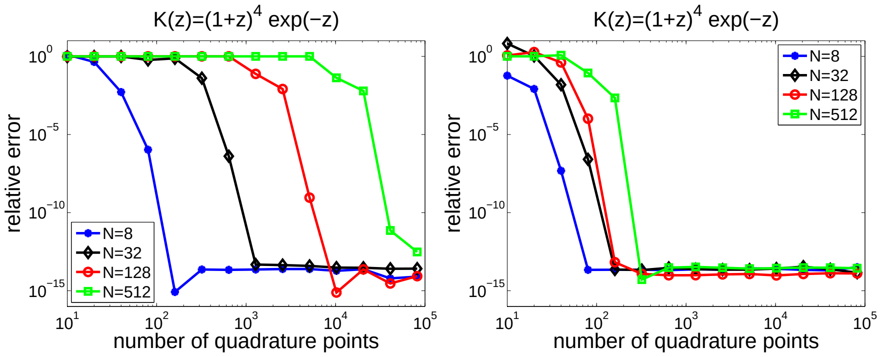

Figure 2: Convergence rates for different values of N. *Left:* With the simple parametrization of $\mathcal{C}_M$ given by $M\,(1+\exp(i\theta))$, $\theta \in [0, 2\pi)$. *Right:* With the parametrization in Definition 7.

consider the grading exponents

$$\alpha = 1.001, 1.8, 2.3, 2.7, 3.1.$$

This values of α lead to the (rounded) ratios $q = \frac{M}{m}$ shown in the legends of Figure 3.

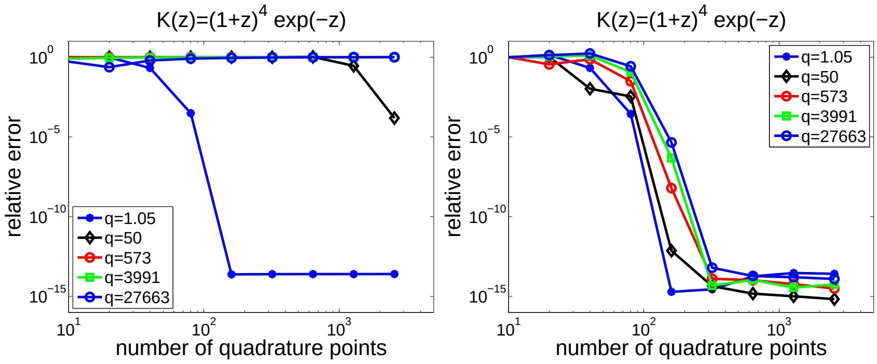

Figure 3: Convergence rates for different values of q. *Left:* With the simple parametrization of $\mathcal{C}_M$ given by $M\,(1+\exp(\mathrm{i}\theta))$, $\theta \in [0, 2\pi)$. *Right:* With the parametrization in Definition 7.

References

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

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

[3] L. Banjai and S. Sauter. Rapid solution of the wave equation in unbounded domains. *SIAM Journal on Numerical Analysis*, 47:227–249, 2008.

[4] L. Banjai and M. Schanz. Wave Propagation Problems treated with Convolution Quadrature and BEM. In *In Fast Boundary Element Methods in Engineering and Industrial Applications*, Edited by U. Langer, M. Schanz, O. Steinbach, W.L. Wendland. Vol. 63, Lecture Notes in Applied and Computational Mechanics, pages 145–187, Chap. 5. Springer, Heidelberg, 2012.

[5] F. Bornemann. Accuracy and stability of computing high-order derivatives of analytic functions by Cauchy integrals. *Found. Comput. Math.*, 11(1):1–63, 2011. DOI:10.1007/s10208-010-9075-z.

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

[7] P. J. Davis. On the numerical integration of periodic analytic functions. In *On numerical approximation. Proceedings of a Symposium, Madison, April 21-23, 1958*, Edited by R. E. Langer. Publication no. 1 of the Mathematics

Research Center, U.S. Army, the University of Wisconsin, pages 45–59. The University of Wisconsin Press, Madison, 1959.

[8] C. de Boor. Divided differences. *Surv. Approx. Theory*, 1:46–69 (electronic), 2005.

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

[10] T. A. Driscoll. Algorithm 843: Improvements to the Schwarz–Christoffel toolbox for matlab. *ACM Trans. Math. Software*, 31:239–251, 2005.

[11] Ö. Eğecioğlu, E. Gallopoulos, and Ç. K. Koç. Fast computation of divided differences and parallel Hermite interpolation. *J. Complexity*, 5(4):417–437, 1989.

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

[13] G. Frobenius. Über die Entwicklung analytischer Functionen in Reihen, die nach gegebenen Functionen fortschreiten. *J. Reine Angew. Math.*, 73:1–30, 1871.

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

[15] W. Hackbusch, W. Kress, and S. Sauter. Sparse convolution quadrature for time domain boundary integral formulations of the wave equation by cutoff and panel-clustering. In M. Schanz and O. Steinbach, editors, *Boundary Element Analysis*, pages 113–134. Springer, 2007.

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

[17] C. Hermite. Formule d'interpolation de Lagrange. *J. Reine Angew. Math.*, 84:70–79, 1878.

[18] N. J. Higham. *Accuracy and stability of numerical algorithms.* Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1996.

[19] N. J. Higham. The numerical stability of barycentric Lagrange interpolation. *IMA J. Numer. Anal.*, 24(4):547–556, 2004. DOI:10.1093/imanum/24.4.547.

[20] R. Kress. Zur numerischen Integration periodischer Funktionen nach der Rechteckregel. *Numer. Math.*, 20:87–92, 1972/73.

[21] M. Lopez-Fernandez and S. A. Sauter. Generalized Convolution Quadrature with Variable Time Stepping. Part II: Algorithms and Numerical Results. Technical Report 09-2012, Institut für Mathematik, Univ. Zürich, 2012.

[22] M. Lopez-Fernandez and S. A. Sauter. Generalized Convolution Quadrature with Variable Time Stepping. *IMA J. Numer. Anal.*, 2013. DOI:10.1093/imanum/drs034.

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

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

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

[26] L. Reichel. Newton interpolation at Leja points. *BIT*, 30(2):332–346, 1990. DOI:10.1007/BF02017352.

[27] K. Schiefermayr. Inequalities for the Jacobian Elliptic Functions with Complex Modulus. *J. Math. Inequ.*, 6:91–94, 2012.

[28] A. Smoktunowicz, I. Wróbel, and P. Kosowski. A new efficient algorithm for polynomial interpolation. *Computing*, 79(1):33–52, 2007.

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