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A family of efficient numerical solvers of time domain boundary integral equations

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Summary
When applicable, boundary integral equation (BIE) methods are an elegant way to transform a differential equation posed on (often unbounded) domain $\Omega \subset \mathbb{R}^n$ to a BIE on the (often bounded) n-1 dimensional boundary $\Gamma = \partial\Omega$. In the frequency domain, this approach has been very successful for the numerical solution of acoustic and electromagnetic scattering problems. In time domain acoustics, numerical methods for boundary integral equations (TDBIE) have until recently received less attention. Nevertheless, good methods do exist and promising results have been achieved in producing efficient and stable numerical solutions. In this talk, we describe a generalization of convolution quadrature, a method that can be used to solve TDBIE numerically. Recently the first author has been involved in proving convergence and stability of high-order Runge-Kutta convolution quadratures and in developing efficient algorithms for their implementation. Here, we extend these results to a family of related methods that are potentially more efficient in situations where high accuracy is not essential, but good (low) dispersion and dissipation properties of the numerical solution are paramount. First numerical experiments with the new method are promising.

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1. Introduction

Consider the wave equation on a possibly unbounded domain $\Omega \subset \mathbb{R}^n$ with boundary $\Gamma = \partial\Omega$:

$$\begin{aligned} \partial_t^2 u(x,t) &= \Delta u(x,t), && (x,t) \in \Omega \times [0,T], \\ u(x,0) &= \partial_t u(x,0) = 0, && x \in \Omega, \\ u(x,t) &= g(x,t), && (x,t) \in \Gamma \times [0,T] \end{aligned} \tag{1}$$

and the family of Helmholtz equations obtained by Laplace transforming (1)

$$\begin{aligned} s^2 \hat{u}(x,s) &= \Delta \hat{u}(x,s), \ (x,s) \in \Omega \times \{z : \mathrm{Re}\, z > 0\}, \\ \hat{u}(x,s) &= \hat{g}(x,s), \ (x,s) \in \Gamma \times \{z : \mathrm{Re}\, z > 0\}, \end{aligned} \tag{2}$$

where $\hat{u}(x,s) = \mathscr{L}u(x,s) = \int_0^\infty e^{-st} u(x,t)dt$ and $\hat{g} = \mathscr{L}g$ denote the Laplace transforms of data g and unknown solution u.

1.1. Boundary integral formulation

From now on, in order to simplify the formulas we will concentrate on the three dimensional case $\Omega \subset \mathbb{R}^3$. A widely accepted method to numerically solve (2), especially at high frequencies, is to represent the solution u as an integral over the boundary of the domain

$$\hat{u}(x,s) = \int_\Gamma \frac{e^{-s|x-y|}}{4\pi|x-y|} \hat{\varphi}(y,s) d\Gamma_y. \tag{3}$$

Since for any choice of $\hat{\varphi}$ such $\hat{u}$ satisfies the homogeneous Helmholtz equation, it suffices to find $\hat{\varphi}$ such that the boundary condition is satisfied.

Taking the inverse Laplace transform of (3) we obtain the boundary integral representation of the time-domain solution

$$u(x,t) = \int_0^t \int_\Gamma \frac{\delta(t-\tau-|x-y|)}{4\pi|x-y|} \varphi(y,\tau) d\Gamma_y d\tau, \tag{4}$$

where $\delta(\cdot)$ is the Dirac delta distribution. The spatial discretization of (4) can be performed in the same multitude of ways as that of the frequency domain counterpart (3), e.g., Galerkin or collocation. For this reason, in this paper we concentrate on the temporal discretization.

2. Convolution quadrature

Convolution quadrature (CQ) has been introduced by Lubich [1, 2] as a quadrature method for convolution

integrals with two very important properties: good stability and exclusive use of the transfer function (while remaining a time domain method) instead of the time-domain kernel. In our application both properties are very welcome, since from early on it has been recognised that numerical discretizations of (4) often become unstable, and since the computation with the analytic function e^{-sr}/r is much easier than with the distributional kernel $\delta(t-r)/r$.

2.1. Linear multistep based CQ

The convolution quadrature of (4) can be obtained by substituting an approximation of the kernel e^{-sr}/r into (3) and taking the inverse Laplace transform. To explain this procedure in detail, let $h>0$ be the time-step and let us introduce the following approximation

$$\frac{e^{-s\cdot r}}{4\pi r} \approx \frac{e^{-\delta(e^{-sh})/h\cdot r}}{4\pi r} = \sum_{j=0}^{\infty} \omega_j^h(r) e^{-sh\cdot j}, \qquad (5)$$

where

$$\delta(\zeta) = \sum_{j=1}^{p} \frac{1}{j}(1-\zeta)^j, \quad p=1,\dots,6. \qquad (6)$$

Note that $\delta(e^{-sh}) = sh + s^{p+1}O(h^{p+1})$, hence (5) is indeed an approximation of the kernel function. Substituting this approximation into (3) and taking the inverse Laplace transform we obtain a convolution quadrature of (4):

$$u^h(x,t) = \sum_{j=0}^{\lfloor t\rfloor} \int_\Gamma \omega_j^h(|x-y|)\varphi(y,t-t_j)d\Gamma_y, \qquad (7)$$

where $t_j = jh$ and we have implicitly assumed the extension $\varphi(x,t)\equiv 0$ for $t\le 0$. The following points are important to have in mind:

(i) The functions $\delta(\zeta)$ are the generating functions of the BDF class of linear multistep methods. Only the first two, i.e., with $p=1,2$, are A-stable as implied by Dahlquist's order barrier.

(ii) Discretization (7) is stable if and only if the underlying linear multistep method is A-stable.

Thus, at least with this construction of the quadrature we are restricted to orders 1 and 2.

2.2. Runge-Kutta based CQ

With A-stable Runge-Kutta methods, higher order, stable discretizations can be obtained. For details we refer the reader to [3] for properties of Runge-Kutta methods and to [4, 5] for Runge-Kutta convolution quadrature. Here, we give enough detail to be able to follow the contributions of the present work.

Using the Butcher tableau notation

$$A=(a_{ij})_{i,j=1}^m, \quad b=(b_1,\dots,b_m)^T,$$
$$c=(c_1,\dots,c_m)^T, \quad \mathbb{1}=(1,\dots,1)^T.$$

the frequency domain kernel is approximated as

$$\frac{e^{-s\cdot r}}{4\pi r} \approx b^T A^{-1} \frac{e^{-\Delta(e^{-sh})/h\cdot r}}{4\pi r}\cdot e^{sh(c-1)}$$
$$= b^T A^{-1} \sum_{j=0}^{\infty} W_j^h(r) e^{-sh\cdot j}\cdot e^{sh(c-1)}, \qquad (8)$$

where $e^c := (e^{c_1},\dots,e^{c_m})^T$. Notice that $W_j^h(r)\in\mathbb{R}^{m\times m}$. Performing the same procedure as in the previous section we obtain the Runge-Kutta based convolution quadrature of (4):

$$u^h(x,t) = b^T A^{-1}$$
$$\cdot \sum_{j=0}^{\lfloor t\rfloor} \int_\Gamma W_j^h(|x-y|)\,[\varphi(y,t-t_{j\ell})]_{\ell=1}^m\, d\Gamma_y, \qquad (9)$$

where $t_{j\ell} = t_j + c_\ell h = (j+c_\ell)h$; notice that $[\varphi(y,t-t_{j\ell})]_{\ell=1}^m$ is a vector in $\mathbb{R}^m$.

2.3. Dissipation and dispersion

The convergence, as $h\to 0$ of the above two schemes, has been investigated in [2] and [4, 5] respectively. For practical use of the methods it is of utmost importance to investigate the pre-asymptotic regime of convergence, i.e., we are interested in understanding how small h has to be chosen with respect to the smallest detail (highest frequency content) in the data g. This question has been analysed in [7]; here we give a different approach to this analysis which very naturally follows from the above derivation of CQ.

From (5) it is clear that the continuous wave number s is replaced by a discrete approximation $\delta(e^{-sh})/h$. Comparing the two is often called the dissipation and dispersion analysis [7]. For the highest order A-stable BDF method, i.e., $p=2$, we easily obtain

$$\frac{1}{h}\delta(e^{-sh}) = \frac{1}{h}(1-e^{-sh}) + \frac{1}{2h}(1-e^{-sh})^2$$
$$= s - \frac{1}{3}s^3h^2 + \frac{1}{4}s^4h^3 + O(h^4). \qquad (10)$$

Therefore if $s=\mathrm{i}\omega$ with $\omega\in\mathbb{R}$ and $|\omega|\gg 1$, i.e., high oscillations are involved, we have to choose $h\ll 3|\omega|^{-3/2}$ in order to obtain good accuracy. This is clearly wasteful if we compare it with the usual sampling condition $h\propto|\omega|^{-1}$.

Similar analysis for Runge-Kutta methods is possible and from [5, Lemma 4] we obtain that, with $r=1$ in (8),

$$\text{error in (8)} = s^{p+1}O(h^p), \qquad (11)$$

where p is the classical order of the Runge-Kutta method; it is important to recall that unlike for linear multistep methods, we have no restriction on order p here. One class of Runge-Kutta methods is particularly suited to our problems: the m-stage Radau IIA

methods [3], which have classical order $p = 2m-1$ and stage order $q = m$. For example the 3-stage Radau IIA method has (classical) order 5 and has an excellent constant hidden in the order notation of (11):

$$\text{error in (8) for 3-stage Radau IIA} = C_{\text{IIA}_3} \cdot s^6 h^5 + s^6 O(h^6),\ C_{\text{IIA}_3} \approx \frac{1}{1300}. \qquad (12)$$

3. A family of modified CQ

3.1. Motivation

Even though the Radau IIA based convolution quadratures have proved to be extremely efficient in solving wave propagation problems, see [6], two points can be raised:

(i) Since the kernel $W_j(r) : \mathbb{R}_{>0} \to \mathbb{R}^{m\times m}$ is matrix valued, it seems necessary to compute m^2 integral operators at each time-step. Could this be reduced to m?

(ii) In space we rarely use high order method for boundary integral equations. Is the high order in time really necessary?

A partial answer to the first point has been given in [6], where via the use of discrete Fourier transforms (DFT) an algorithm that needs to construct only m integral operators per time-step has been described. Nevertheless, at least for the first few time-steps one would like to avoid the use of DFT. The second point motivates another question which may contain an answer to the first problem:

- Can we, by sacrificing convergence orders, modify a Runge-Kutta method to obtain a single stage method more efficient at moderate accuracies?

3.2. A family of modified RK CQ and its properties

A possible answer to this question is the subject of the present paper. Our solution consists of defining a family of modified Runge-Kutta convolution quadratures:

$$\frac{e^{-s\cdot r}}{4\pi r} \approx b^T A^{-1} \frac{e^{-\Delta(e^{-sh})/h\cdot r}}{4\pi r} I(e^{-sh}) = \sum_{j=0}^{\infty} w_j^h(r) e^{-sh\cdot j}, \qquad (13)$$

with the function $I(\zeta)$ satisfying the following properties.

Assumption 3.1. *Given a vector $c \in \mathbb{R}^{m\times 1}$, let the function $I(\zeta) : \mathbb{C} \to \mathbb{C}^{m\times 1}$ satisfy:*

(i) $I(\zeta)$ is analytic for $|\zeta| \le 1$ and given by

$$I(\zeta) = \sum_{j=0}^{\infty} I_j \zeta^j, \qquad I_j \in \mathbb{R}^{m\times 1}.$$

(ii) $I(e^{-z}) = e^{-z(c-1)} + O(z^{p_1})$, for $z \to 0$.

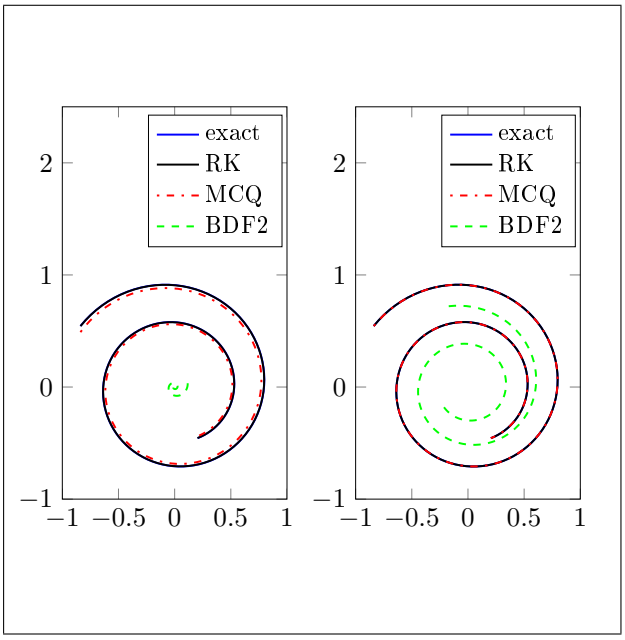

Figure 1. For $s = 10\mathrm{i}$ and $r \in [1, 2]$, we plot e^{-sr}/r and its BDF2 (5), 3-stage Radau IIA (8), and the BDF6 modification of the latter. In the left plot $h = 0.1$ and in the right $h = 0.05$.

From these assumptions we conclude, that $w_j^h(r) : \mathbb{R}_{>0} \to \mathbb{R}$ and that, for $r = 1$,

$$\text{error in (13)} = s^{p_1} O(h^{p_1}) + s^{p+1} O(h^p); \qquad (14)$$

see the proof of Theorem 3.2 below. The estimate (14) shows that the additional error is controlled under the sampling condition $|sh| \ll 1$, implying that the modification has not destroyed the good qualitative properties of the Runge-Kutta approximation. Here are some possible choices of $I(\zeta)$:

(i) $I(\zeta) = c + (1-c)\zeta$, this choice giving $p_1 = 2$.

(ii) $I_{\text{BDF}p}(\zeta) = e^{\delta_p(\zeta)(c-1)}$, where $\delta_p(\zeta)$ is the generating function of the pth order BDF method; this choice gives $p_1 = p+1$. Notice that here we are *not* restricted by A-stability therefore orders until $p_1 = 6+1 = 7$ are admissible.

In Figure 1 we compare the dispersion and dissipation properties of the highest order multistep CQ, the 3-stage Radau IIA CQ, and the highest order modified CQ of the latter Radau method. In these plots dissipation can be seen by incorrect scaling of the spiral and dispersion by incorrect phase of the start and the end of the spiral. With both values of h in Figure 1, there is no difference to the naked eye between the exact curve and Runge-Kutta approximation, for the smaller h this becomes true also for the modified approximation, whereas the BDF2 approximation is very poor with both choices of h.

3.3. Convergence theory

We state the convergence theory in a more general setting. For this we assume that a transfer function $K(s)$ is given which satisfies

$$K(s) \text{ is analytic and } |K(s)| \le C(\sigma)\frac{|s|^\mu}{(\mathrm{Re}\, s)^\nu}, \quad (15)$$

for $\mathrm{Re}\, s > \sigma > 0$. We are then interested in computing the convolution

$$\begin{aligned} u(t) &= \int_0^t k(t-\tau)g(\tau)d\tau \\ &= \mathscr{L}^{-1}\left[K(s)\mathscr{L}g(s)\right](t). \end{aligned}$$

In [5] it has been shown that the Runge-Kutta convolution quadrature of the above integral converges at the rate $\mathrm{O}(h^p + h^{q+1-\mu+\nu})$, where p is the classical order of the Runge-Kutta method, q is the stage order, and the Runge-Kutta method has to satisfy certain assumptions including A-stability. We state next the extension of this result to the above described modified scheme.

Theorem 3.2. *Let an A-stable Runge-Kutta method of order p and stage order q be given by its Butcher tableau and let it satisfy Assumption 2 in [5]. Further let $K(s)$ satisfy (15), g be sufficiently smooth and compatible, and $I(\zeta)$ satisfy Assumption 3.1. Then for sufficiently small $h > 0$ and $t \in [0, T]$,*

$$\begin{aligned} |u^h(t) - u(t)| = \mathrm{O}(h^{p_1 - \max(\mu-\nu, 0)} \\ + h^{q+1-\mu+\nu} + h^p), \end{aligned}$$

where

$$u^h(t) := \sum_{j=0}^{\lfloor t \rfloor} w_j^h g(t - t_j),$$

and

$$b^T A^{-1} K(\Delta(\zeta)/h) I(\zeta) = \sum_{j=0}^{\infty} w_j^h \zeta^j.$$

The constants hidden in the O*-notation, depend on T, g, $I(\zeta)$, and the choice of the Runge-Kutta method, but not on h.*

Proof. The proof can be done using the same line of reasoning as in [5], here we just give the main steps. The following auxiliary result is needed: There exists $c_0 > 0$ such that for $|sh| < c_0$

$$b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) = \mathrm{O}(h^{-\mu+\nu} + s^\mu),$$

which can be shown using the techniques of [5, Lemma 4]. Combining this estimate with [5, Lemma 4] gives, for $|sh| < c_0$,

$$\begin{aligned} b^T A^{-1} K\left(\frac{\Delta(e^{-sh})}{h}\right) I(e^{-sh}) = K(s) \\ + s^{p_1}\,\mathrm{O}(h^{p_1-\mu+\nu}) + s^{p_1+\mu}\,\mathrm{O}(h^{p_1}) \\ + s^{\mu+1+p}\,\mathrm{O}(h^p) + s^{q+1}\,\mathrm{O}(h^{q+1-\mu+\nu}). \end{aligned}$$

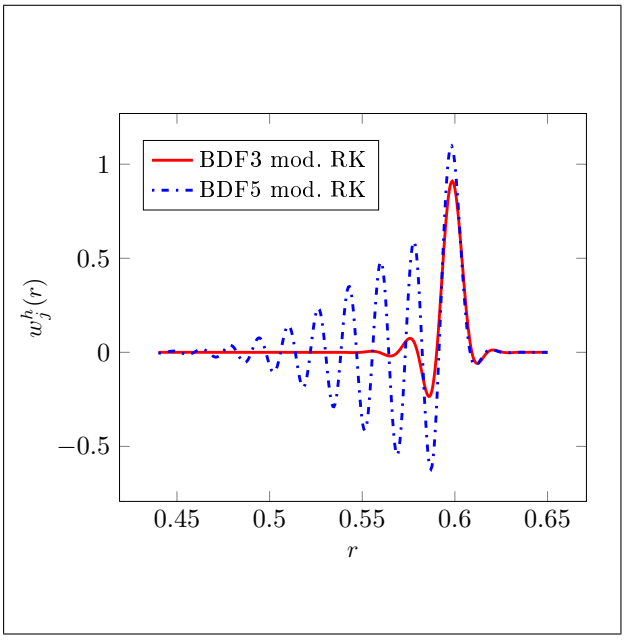

Figure 2. The weights $w_j^h(r)$ with $j = 120$, $h = 5\times10^{-3}$, of the BDF3 and BDF5 modifications of the 3-stage Radau IIA method.

Taking the inverse Laplace transform of the error expression and bounding the two cases $|sh| < c_0$ and $|sh| > c_0$ separately as in [5, Theorem 3], gives the required result. □

Remark 3.3. *By* sufficiently smooth and compatible, *we mean that $g(t)$ is sufficiently many times continuously differentiable and that sufficiently many derivatives of g vanish at $t = 0$.*

Remark 3.4. *The Laplace domain single layer operator $V(s) : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$, see (3),*

$$V(s)\hat{\varphi}(x) := \int_\Gamma \frac{e^{-s|x-y|}}{4\pi|x-y|}\hat{\varphi}(y)d\Gamma_y,$$

satisfies (15) with $\mu = \nu = 1$ [8]. Therefore we expect orders of convergence $\mathrm{O}(h^{q+1} + h^{p_1})$. In particular for the 3-stage Radua IIA method, which has stage order $q = 3$ and modified method based on BDF of order $p \ge 3$, we expect the convergence order to be 4. A lower order BDF formula would reduce the convergence order.

3.4. Implementation

A detailed description of algorithms for implementation of standard convolution quadratures is given in [6] and [7]. The same algorithms are applicable to the modified version. These algorithms all make use of the fast Fourier transform, do not involve explicit evaluations of the kernel functions $\omega_j^h(r)$, $W_j^h(r)$, or in our case $w_j^h(r)$, but only of the Laplace domain approximations (5), (8), and (13) respectively.

A closely related, but rarely discussed method in the literature is to pre-compute a certain numerical

representation of the functions $w_j^h(r)$ and work directly with this. From the definition of the weights (13) and the Cauchy integral formula we have

$$w_j^h(r) = \frac{b^T A^{-1}}{2\pi \mathrm{i}} \oint_C \frac{e^{-\Delta(\zeta)/h\cdot r}}{4\pi r} I(\zeta)\zeta^{-j-1} d\zeta,$$

where the integration contour C can be chosen as a circle in the complex plane centred at the origin. This integral can be very efficiently and accurately computed using the trapezoid rule accelerated by FFT [1, 7]. Since the kernel is only needed in the interval $r \in [0, \mathrm{diam}(\Gamma)]$, a precomputation of $w_j^h(r)$, $j = 0, 1, \ldots, N$ can be stored as, e.g., piecewise polynomial functions.

The shapes of function $w_j^h(r)$, with $j = 120$ and $h = 5 \times 10^{-3}$ are plotted in Figure 2 in the range of r for which the functions significantly differ from zero. Two types of modified weights are shown: BDF3 and BDF5 modified 3-stage Radau IIA method. Note that both functions have a peak near $r \approx jh = 0.6$, but that the BDF5 modification also has a long oscillatory tail, the latter is a negative property with regards to the efficient implementation; see the following remark.

Remark 3.5. *To construct a completely discrete system the operators with kernels $w_j^h(|x-y|)$ need to be discretized. When using, e.g., Galerkin discretization in space, matrices of the type*

$$A_{ij}^n = \int_\Gamma \int_\Gamma w_n^h(|x-y|)\varphi_i(y)\varphi_j(x) d\Gamma_y d\Gamma_x$$

need to be constructed, where $\varphi_j(\cdot)$ are the usual piecewise polynomial functions. Because of the shape of the kernels, see Figure 2, these matrices are considerably sparse. The sparsity can even be increased with the use of higher-order Runge-Kutta methods and lower order modifications.

4. Numerical experiments

4.1. Illustrative experiment

To illustrate the results of Theorem 3.2, we compute the convolution integral

$$\begin{aligned} u(t) &= \int_0^t k(t-\tau) g(\tau) d\tau \\ &= \mathscr{L}^{-1}\{K(s)\mathscr{L}g(s)\}(t) \end{aligned} \tag{16}$$

on the interval $t \in [0, T]$. We consider the two examples:

1. $K(s) = \frac{1}{s} - \frac{e^{-2s}}{s}$, i.e., (15) holds with $\mu = -1$ and $\nu = 0$, $g(t) = e^{-0.2t}\sin^8 t$, $T = 1$.
2. $K(s) = se^{-s}$, i.e., (15) holds with $\mu = 1$ and any $\nu \in \mathbb{R}$, $g(t) = e^{-0.5t}\sin^7 t$, $T = 2$.

Table I. Convergence of the modified 3-stage Radau IIA based convolution quadrature of (16).

	example 1.		example 2.	
N	error	rate	error	rate
4	$2.7e-3$	0	$1.8e-1$	0
8	$5.8e-4$	2.3	$2.5e-2$	2.9
16	$1.3e-4$	2.2	$4.8e-3$	2.4
32	$3.1e-5$	2.1	$1.1e-3$	2.1
64	$7.5e-6$	2.0	$2.6e-4$	2.1
128	$1.8e-6$	2.0	$6.4e-5$	2.0

In both examples we choose $I(\zeta) = c + (1-c)\zeta$, i.e., $p_1 = 2$. The exact solution for both examples can be obtained by inverse Laplace transform, e.g., for the second example the exact solution is $u(t) = g'(t-1)$. The error is computed as

$$\text{error} = \sqrt{h\sum_{j=0}^{N}(u^h(t_j) - u(t_j))^2},$$

with $t_j = jh$ and $h = T/N$. The results are displayed in Table I and are consistent with Theorem 3.2.

4.2. Scattering by a unit sphere

We consider (4) with $\Gamma = \mathbb{S}^2 = \{x \in \mathbb{R}^3\,;\, |x| = 1\}$ and let $\varphi(x,t) = \psi(t)Y_\ell^m(x)$, where Y_ℓ^m is a spherical harmonics [9]. The spherical harmonics Y_ℓ^m are eigenfunctions of the single layer potential for the Helmholtz equation:

$$\int_{\mathbb{S}^2} \frac{e^{-s|x-y|}}{4\pi|x-y|} Y_\ell^m(y) d\Gamma_y = \lambda_\ell(s) Y_\ell^m(x),$$

the expressions for the eigenvalues $\lambda_\ell(s)$ can be found in [9]. Therefore, see also [6] and [10],

$$\begin{aligned} \int_0^t \int_{\mathbb{S}^2} \frac{\delta(t-\tau-|x-y|)}{4\pi|x-y|} \psi(t) Y_\ell^m(y) d\Gamma_y d\tau \\ = g(t) Y_\ell^m(x), \end{aligned}$$

where

$$g(t) = \mathscr{L}^{-1}\{\lambda_\ell(s)\mathscr{L}\psi(s)\}(t).$$

In this section we investigate the computation of $g(t)$ with $\ell = 2$, $\psi(t) = e^{-0.4t}\sin^5(4\pi t)$, and $T = 10$. In Figure 3, we show the convergence of

$$\text{error} = \sqrt{h\sum_{j=0}^{N}(g(t_j) - g^h(t_j))^2}$$

against the number of time steps $N = Th$ on the interval $[0, T]$ for different methods; note that for the 3-stage Runge-Kutta method we plot the error against

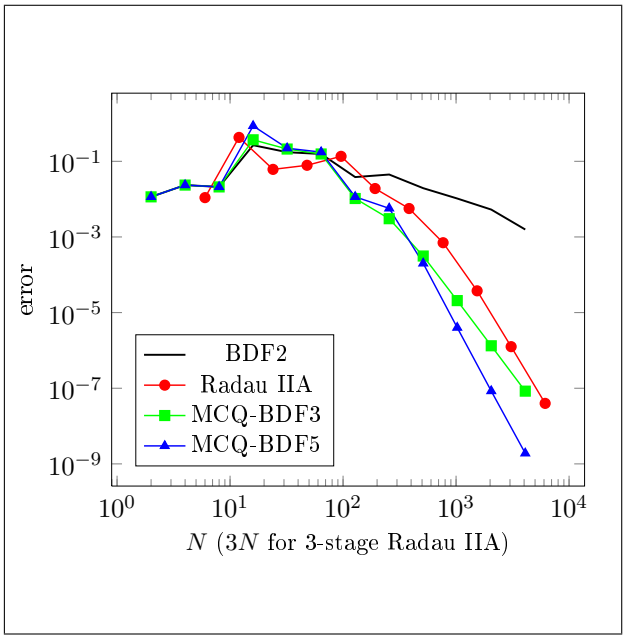

Figure 3. The convergence of the methods BDF2, 3-stage Radau IIA, 3-stage Radau IIA based on modified convolution quadrature with the choice of $I(e^{-sh}) = e^{\delta(e^{-sh})(c-1)}$, $\delta(e^{-sh})$ is the generating function of BDF3 and BDF5, respectively.

$3N$ since at least $3N$ integral operators need to be constructed in this case compared to N for the other methods. The results show that both modifications perform very well: even up to high accuracies they are significantly better than the original Runge-Kutta method and show overwhelmingly better convergence than the BDF2 scheme.

5. CONCLUSIONS

We have described a new class of modified Runge-Kutta convolution quadratures and discussed their potential as time-discretization methods of time-domain boundary integral equations of acoustic scattering. Further, we have proved a convergence theorem for the new method, discussed its qualitative properties, and performed a number of numerical experiments on academic problems. These numerical experiments have shown that the new method has good potential for acoustic scattering problems. This gives us motivation to further investigate this new family of quadratures.

The most important omission in the current work is that we have discussed only the *evaluation* of the time domain integrals (4) and not the *solution* of the integral equation. The difficulty here is both to prove that the time-discretized system has a unique solution and that it is bounded. What gives us hope that this problem can be analysed is that in most applications we only need backward stability. That is, once an approximate density $\varphi^h(x,t)$ is found, often it is itself not of independent interest, but one is rather interested in the solution $u^h(x,t)$ obtained by applying the boundary integral operator to φ^h, see (4). Investigation of these questions will be the subject of future work.

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