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Lubich convolution quadratures and their application to problems described by space-time BIEs

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Abstract In the last years several authors have used Lubich convolution quadrature formulas to discretize space-time boundary integral equations representing time dependent problems. These rules have the fundamental property of not using explicitly the expression of the kernel of the integral equation they are applied to, which is instead replaced by that of its Laplace transform, usually given by a simple analytic function.

In this paper, a review of these rules, which includes their main properties, several new remarks and some conjectures, will be presented when they are applied to the heat and wave space-time boundary integral equation formulations. The construction and behavior of the corresponding coefficients are analyzed and tested numerically. When the quadrature is defined by a BDF method, a new approach for the representation of its coefficients is presented.

Keywords Quadrature rules · Discrete convolution · Space-time boundary integral equations · Wave equation · Heat equation

Mathematics Subject Classification (2000) 65D32 · 65M38

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1 Introduction

About twenty years ago Ch. Lubich [8] considered convolution integrals of the following type

$$y(t) := k(t) * \varphi(t) = \int_0^t k(t-\tau)\varphi(\tau)\,\mathrm{d}\tau, \quad t \in [0,T],\ T < \infty \tag{1}$$

and, after having set $t = t_n = nh,\ h = T/N$, for the discretization of $y(t_n)$ defined a new class of quadrature formulas of the form

$$y_n(h) := k(t) *_h \varphi(t) = \sum_{j=0}^{n} \omega_{n-j}(h)\varphi(jh), \qquad n = 0, 1, \ldots, N \tag{2}$$

called "discrete convolution rules".

One of the major and more interesting applications of these rules is the numerical resolution of time-dependent PDE problems via space-time BIE formulations (see [4]), for example of the form:

$$\int_0^t \int_S k(\|x-y\|; t-\tau)\varphi(y,\tau)\,\mathrm{d}S_y\,\mathrm{d}\tau = g(x,t), \qquad x \in S \tag{3}$$

where S is the boundary of the PDE space domain, $k(r;t)$ is the free space PDE fundamental solution, $g(x,t)$ is a given function and $\varphi(y,\tau)$ is the unknown.

A second, but equally significant, application is the evaluation of the potential

$$u(x,t) = \int_0^t \int_S k(\|x-y\|; t-\tau)\varphi(y,\tau)\,\mathrm{d}S_y\,\mathrm{d}\tau \tag{4}$$

at a given point $x \notin S$, once the solution $\varphi(y,\tau)$ of (2) has been determined. This problem is currently under investigation by the authors.

Indeed in the last years several authors have used these time integration rules to solve heat and wave propagation problems (see, for example, [3], [6], [7], [12], [9], [14] and the bibliographies of these papers). We will focus our description to these problems, in particular when the initial conditions are homogeneous and the boundary one is of Dirichlet type. In a forthcoming paper [5] we will use Lubich rules to solve exterior wave problems with non homogeneous initial conditions.

These rules have the fundamental property of not using explicitly the expression of the kernel $k(t-\tau)$, which is instead replaced by that of its Laplace transform, usually given by a simple analytic function. These new formulas do not have any degree of exactness; however, as we will recall in the next section, good convergence properties are guaranteed under certain assumptions on the above Laplace transform and on the function $\varphi(\tau)$. Incidentally, we point out that they are an important example of the more general quadrature formulas more recently described in [13] by the first author.

Thus in Section 2 a review of these rules, which includes some of their main properties and new remarks, will be presented when $k(t-\tau) = k(r; t-\tau)$ is the fundamental solution of the heat and the wave equations. Then, for these kernels, in Section 3 the construction and behavior of the corresponding coefficients ω_{n-j} will be analyzed, pointing out experimentally some new properties. When the convolution quadrature is defined by a BDF method of order $k \leq 6$, a new approach for the construction of its coefficients is presented. In the case of the wave equation, we derive a new analytic

representation for these coefficients, which in some cases turns out to be particularly efficient for their computation. All remarks and conjectures are supported by an intensive numerical testing.

Finally, in Section 4 we apply a Lubich convolution rule to a non smooth problem.

2 Lubich convolution quadratures

In the first part of the development of his theory for the new formulas (see [8]), Lubich assumes that the kernel $k(t)$ is such that its Laplace transform $K(s)$ satisfies the following conditions:

$$K \text{ is analytic in the sector } |\arg(s-c)| < \pi - \phi \text{ with } \phi < \pi/2,\ c \in \mathbb{R}; \tag{5a}$$

$$|K(s)| \le M|s|^{-\mu},\ \mu > 0,\ \text{i.e. } |K(s)| \to 0,\ |s| \to +\infty \text{ in the same sector.} \tag{5b}$$

He calls such a function K "sectorial".

Under these assumptions the Laplace inverse transform certainly exists and is given by the well known Bromwich formula:

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

where for his analysis Lubich takes as Γ a contour in the sector of analyticity, parallel to its boundary and oriented with increasing imaginary part.

In [10] he also shows how to extend his approach to the case $\mu \le 0$.

In the cases of the heat equation $u_t = \triangle u$ and the wave equation $u_{tt} = \triangle u$ we have, respectively:

$$\text{2D heat:}\quad k(t) = k(r;t) = \frac{\mathrm{e}^{-r^2/4t}}{4\pi t}, \quad K(s) = K(r;s) = \frac{1}{2\pi} K_0(r\sqrt{s}), \tag{6a}$$

$$\text{3D heat:}\quad k(t) = k(r;t) = \frac{\mathrm{e}^{-r^2/4t}}{(4\pi t)^{3/2}}, \quad K(s) = K(r;s) = \frac{1}{4\pi r} \mathrm{e}^{-r\sqrt{s}}, \tag{6b}$$

$$\text{2D wave:}\quad k(t) = k(r;t) = \frac{H(t-r)}{2\pi\sqrt{t^2-r^2}},\ K(s) = K(r;s) = \frac{1}{2\pi} K_0(rs), \tag{6c}$$

$$\text{3D wave:}\quad k(t) = k(r;t) = \frac{\delta(t-r)}{4\pi r}, \qquad K(s) = K(r;s) = \frac{1}{4\pi r} \mathrm{e}^{-rs}, \tag{6d}$$

where K_0 denotes the modified Bessel function of the second kind of order 0, $r = \|x-y\|$, and $H(t), \delta(t)$ are the well known Heaviside and Dirac delta functions, respectively. We also recall that $K_0(z) \sim \sqrt{\frac{\pi}{2z}} \mathrm{e}^{-z},\ |z| \to \infty$, and $K_0(z) \sim -\ln z,\ |z| \to 0$ (see [1]) .

Notice that, assuming $r > 0$ fixed, while in the case of the heat equation the Laplace transform $K(s)$ is sectorial, according to the definition given above, with $c > 0, \phi > 0$ arbitrarily small, and $\mu > 0$ as large as one likes, this is not the case for the wave equation. In this latter case, $K(s)$ is analytic in $\mathrm{Re}(s) > \sigma_0 > 0$, for any given σ_0 arbitrarily small, and in this region it satisfies condition (5b) with $\mu = 1/2$ (2D) and $\mu = 0$ (3D). In this latter case, recalling the extension defined in [10] (see also [9]), and assuming $\varphi \in C^m[0,T], m \ge 1$, we ought to interpret integral (1) as follows:

$$\int_0^t k(t-\tau)\varphi(\tau)d\tau = \frac{\mathrm{d}}{\mathrm{d}t} \int_0^t k_1(t-\tau)\varphi(\tau)d\tau \tag{7}$$

where $k(t) = \delta(t-r)$ is the (distributional) derivative of $k_1(t) = H(t-r)$.

Therefore for the wave equation, to express $k(t)$ in terms of $K(s)$ we choose $\Gamma \equiv \sigma + \mathrm{i}\mathbb{R}$ hence use the corresponding Bromwich inversion formula. In the 3D (wave) case we insert in (7) the representation:

$$k_1(t) = \frac{1}{2\pi \mathrm{i}} \int_{\sigma+\mathrm{i}\mathbb{R}} \frac{K(s)}{s} \mathrm{e}^{st} \, \mathrm{d}s. \tag{8}$$

To construct Lubich quadrature formula (2) for our heat and wave kernels, first we replace the kernel k in (1), or k_1 in (7) in the 3D wave case, by its Bromwich representation. In all cases we obtain

$$y(t) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma K(s) \left[\int_0^t \mathrm{e}^{s(t-\tau)} \varphi(\tau) \, \mathrm{d}\tau \right] \mathrm{d}s = \frac{1}{2\pi \mathrm{i}} \int_\Gamma K(s) \; x(t;s) \, \mathrm{d}s, \qquad t > 0. \tag{9}$$

Notice that assuming $\varphi \in C^1[0,T]$, on Γ we have $x(t;s) \sim s^{-1}$, $|s| \to \infty$, for any $t > 0$. Therefore, also in the 3D wave case the integral over Γ exists in the ordinary sense.

Then, denoting by $x(t) = x(t;s)$, we have

$$\frac{\partial x}{\partial t} = \int_0^t s \mathrm{e}^{s(t-\tau)} \varphi(\tau) \, \mathrm{d}\tau + \varphi(t) = s x(t) + \varphi(t).$$

Thus, $x(t)$ is a solution of the following simple first order linear differential equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = s x(t) + \varphi(t) \tag{10}$$

with initial condition

$$x(0) = 0.$$

By considering the values of $y(t)$ at a finite number of equidistant abscissas t_n, the key point now is to replace in (9) the functions $x(t_n;s)$ by an approximation of them, that we obtain by applying to (10) a numerical method having proper stability properties. To this end the integration interval $[0,T]$ is subdivided into N parts of equal length $h = T/N$. If we then apply, for example, a proper linear multistep method (for example a BDF method, $A(\alpha)$-stable with $\alpha > \phi$ (see (5a)) for the heat equation, and A-stable for the wave equation), in general of the form:

$$\alpha_0 x_n + \alpha_1 x_{n-1} + \cdots + \alpha_k x_{n-k} = h[\beta_0(s x_n + \varphi(nh)) + \cdots + \beta_k(s x_{n-k} + \varphi((n-k)h))] \tag{11}$$

where $x_n = x_n(s) \approx x(nh;s)$ and the required initial values are: $x_{-k} = \cdots = x_{-1} = 0$, we define the following approximation of $y(nh)$:

$$y_n(h) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma K(s) x_n(s) \, \mathrm{d}s, \qquad n = 0, 1, \ldots, N. \tag{12}$$

As we shall see in the next section, $x_n(s)$ is an analytic function of s, has one real positive (multiple) pole and behaves like s^{-1} as $|s| \to \infty$. Thus the integral in (12) exists in the usual sense and it can be determined by means of Cauchy integral formula. In Section 3, this straightforward computation, which represents a different route for deriving Lubich's quadrature, will be applied to the 2D wave equation. Notice that this quadrature rule has no degree of exactness, since $x_n(s)$ will never coincide with $x(t_n;s)$.

Lubich's elegant approach (see[8]) to compute integral (12), hence to obtain the quadrature rule (2), although less straightforward than the (more natural) derivation just mentioned, leads however to a simple integral representation on the complex plane for its coefficients $\omega_n(h)$:

$$\omega_n(h) = \frac{1}{2\pi \mathrm{i}} \int_{|z|=\rho} K\left(\frac{\gamma(z)}{h}\right) z^{-(n+1)}\, \mathrm{d}z \tag{13}$$

where

$$\gamma(z) := \frac{\alpha_0 + \alpha_1 z + \cdots + \alpha_k z^k}{\beta_0 + \beta_1 z + \cdots + \beta_k z^k}.$$

and ρ is such that the circle $|z| \leq \rho$ lies in the domain of analyticity of $K(\gamma(z)/h)$.

We recall that for the k-step BDF method, $k = 1, \ldots, 6$, we have $\gamma(z) = \sum_{i=1}^{k} \frac{1}{i}(1-z)^i$, with $\alpha_0 = \sum_{i=1}^{k} \frac{1}{i} > 0$. Moreover, these methods are $A(\alpha)$-stable, with $\alpha = 90^\circ, 90^\circ, 86^\circ, 73^\circ, 51^\circ, 17^\circ$, for $k = 1, \ldots, 6$, respectively. In particular, the first two are A-stable.

By introducing the polar coordinate $z = \rho \mathrm{e}^{\mathrm{i}\varphi}$ we have the following integral representation for the coefficients of formula (2):

$$\omega_n(h) = \frac{\rho^{-n}}{2\pi} \int_0^{2\pi} K\left(\frac{\gamma(\rho \mathrm{e}^{\mathrm{i}\varphi})}{h}\right) \mathrm{e}^{-\mathrm{i}n\varphi}\, \mathrm{d}\varphi. \tag{14}$$

This integral can be efficiently computed by using the trapezoidal rule, that is,

$$\omega_n(h) \approx \frac{\rho^{-n}}{L} \sum_{l=0}^{L-1} K\left(\frac{\gamma(\rho \mathrm{e}^{\mathrm{i}l\frac{2\pi}{L}})}{h}\right) \mathrm{e}^{-\mathrm{i}nl\frac{2\pi}{L}}, \qquad n = 0, \ldots, N \tag{15}$$

where the interval $(0, 2\pi)$ has been partitioned into L subintervals of equal length. All the $\omega_n(h)$ can be computed simultaneously by the FFT with $O(N \log N)$ flops.

Assuming that K is computed with a relative accuracy bounded by ε, Lubich has shown that the choice

$$L = 2N, \quad \rho^N = \sqrt{\varepsilon}$$

in (15) leads to an approximation of ω_n with relative error of size $\sqrt{\varepsilon}$. See however the remark made by Schanz and Antes in [14].

The (approximate) numerical approach defined by (15) is quite general, although it requires the use of the complex arithmetic. Moreover, using the double precision arithmetic, with the above choices of L and ρ, according to Lubich's result the coefficients ω_n are computed with a relative accuracy of order $1E-7$. Till very recently it was the only one available. For the 3D wave equation, in [6] the authors have obtained a 3-term recurrence relation for the coefficients generated by the BDF method of order 2. For this same equation, in the next section we will derive recurrence relations for the computation of the coefficients of the quadratures defined by all BDF methods of order $p \leq 6$. These require only the use of the real arithmetic. Taking advantage of our new approach for the construction of Lubich's rules, for the 2D wave equation we will also obtain a new analytic expression for the coefficients of the rules generated by the BDF methods. Unfortunately, for $k \geq 2$ this representation shows a computational severe drawback.

Several convergence results have been proved by Lubich (see [8], [9]). Here we recall the major ones.

Theorem 1 *Assuming that the Laplace transform $K(s)$ satisfies conditions (5a), (5b) and that the chosen k-step multistep method, of order $p = k$, is $A(\alpha)$-stable with $\alpha > \phi$, we have*

$$|y_n(h) - y(nh)| \le Ct_n^{\mu-1}\{h|\varphi(0)| + \cdots + h^{p-1}|\varphi^{(p-2)}(0)| \\ +h^p[|\varphi^{(p-1)}(0)| + t_n \max_{0\le\tau\le t_n} |\varphi^{(p)}(\tau)|]\}$$

where the constant C does not depend on $h \in (0, h_0]$, $0 < t_n = nh \le T$ and $\varphi(\tau) \in C^p[0, T]$, T being fixed.

Notice that if $\varphi(0) = \varphi^{(1)}(0) = \cdots = \varphi^{(p-2)}(0) = 0$, then the quadrature error is $O(h^p)$. Otherwise, to have the maximum convergence order p, Lubich in [8] has suggested to modify the quadrature rule as follows:

$$\bar{y}_n(h) := y_n(h) + \sum_{j=0}^{p-2} w_{nj}(h)\varphi(jh) \tag{16}$$

where the new coefficients $w_{nj}(h)$ are determined by requiring to the rule to integrate exactly all polynomials of degree $p - 2$. For this new formula we have the bound

$$|\bar{y}_n(h) - y(nh)| \le Ct_n^{\mu-1}h^p, \qquad n \ge 1.$$

These convergence results apply in particular to the time integral arising from the heat equation space-time BIE formulation, for any given $r > 0$, when a k-step BDF method, with $k = 1, \ldots, 6$, is used. Unfortunately they do not apply to the wave equation. Lubich has however proved the following alternative results, which holds for this latter equation when $r \ge \epsilon_0 > 0$, ϵ_0 being fixed.

Theorem 2 *Let $K(s)$, $\mathrm{Re}(s) > \sigma_0 > 0$, be analytic and bounded as in (5b) with $\mu \ge 0$. Let the k-step multistep method, of order $p \ge 1$, be A-stable and, when $\mu > 0$, such that its $\gamma(z)$ has no zeros on the unit circle, with the exception of $z = 1$. Then:*

(i) Let $m \ge p + 2 + \mu$. For a smooth function $\varphi(\tau)$ on $[0, T]$ with $\varphi(0) = \cdots = \varphi^{(m-1)}(0) = 0$, we have for $t_n \in [0, T]$

$$|y_n(h) - y(nh)| \le Ch^p \int_0^{t_n} |\varphi^{(m)}(\tau)|d\tau.$$

(ii) For $\varphi(\tau) = \tau^q$ (extended by 0 to negative τ) with real $q > \mu$, we have

$$|y_n(h) - y(nh)| \le Ch^\alpha$$

with $\alpha = \min(\frac{(q+\mu)p}{p+1}, q + 1, p)$.

These error bounds are valid for $0 < h \le h_0$, where h_0 depends only on σ and the discretization method. The constants C depend on σ_0, T, h_0 and the method, and in (ii) also on q.

Notice that in particular, in the wave equation case (2D and 3D) these convergence estimates apply to the BDF methods of order $p = 1, 2$.

In [11] Lubich and Ostermann have also constructed convolution quadratures associated with parabolic problems, obtained by using implicit m-stage Runge-Kutta methods, which, when applied to the differential equation $x' = f(t,x)$ takes the form

$$x_{n+1} = x_n + h\sum_{j=1}^{m} b_j f(t_n + c_j h, X_{nj})$$
$$X_{ni} = x_n + h\sum_{j=1}^{m} a_{ij} f(t_n + c_j h, X_{nj}),\ i = 1,\dots,m$$

having proper stability properties. These new rules take the form

$$y_{n+1}(h) = h\sum_{j=0}^{n}\sum_{\nu=1}^{m} \omega_{n-j,\nu}(h)\varphi(jh + c_\nu h). \tag{17}$$

In particular they considered the 2- and 3-stage Radau IIA methods, which are A-stable. The integral representation they have obtained for the corresponding convolution quadrature coefficients is similar to (13). For these rules they have also derived convergence results. The optimal rate of convergence holds only in any finite interval bounded away from $t = 0$. To have it also near 0, one has to add to (17) a correction term similar to that introduced in (16).

Finally we recall that Lubich has used his discrete convolution rules to solve also problems other than PDE: for example computation of integrals and solution of 1D integral equations (see [8], [9]).

3 Construction and behavior of the BDF quadrature coefficients

As stated in the previous section, Lubich convolution quadrature is obtained by replacing in (9), after having set $t = t_n$, the function $x(t_n; s)$ by $x_n(s)$ (see (12)). Therefore, following the statement we made immediately after (12), here we examine the behavior of $x_n(s)$ when this is obtained by applying a BDF method to equation (10).

To this end we remark preliminarily that $x(t_n; s) = \mathrm{e}^{st} X(t_n; s)$, where $X(t_n; s)$ is analytic. In the $3D$ wave case, on $\Gamma = \sigma + \mathrm{i}\mathbb{R}$, the function $X(t_n; s)$ decays at "infinity" as $|s|^{-1}$. As we shall show next, its approximant $x_n(s)$ turns out to be analytic, having a (multiple) positive real pole and no longer the exponential factor (it will be rational in s), and decays as s^{-1} for $|s| \to \infty$. This is obtained by applying the chosen numerical method to the initial value problem (10) defining $x(t) = x(t; s)$, which gives $x_n(s) \approx x(t_n; s)$.

In the case of a k-step BDF method, whose order is $p = k$ and that in the following we will denote by $BDFk$, we have:

$$\sum_{i=0}^{k} \alpha_i x_{n-i} = h(sx_n + \varphi_n), \quad n = 0, 1, \dots, \qquad x_{-1} = \cdots = x_{-k} = 0 \tag{18}$$

where $\alpha_0 > 0$ and we have set $\varphi_n = \varphi(t_n)$. Thus it is not difficult to obtain an analytic expression for $x_n(s)$. This has the form:

$$x_n(s) = -\frac{h\alpha_1^n \varphi_0}{(hs - \alpha_0)^{n+1}} - \sum_{\ell=1}^{n-1} \frac{h}{(hs - \alpha_0)^{n+1-\ell}} \sum_{i=0}^{\ell} c_i^{(\ell)} \varphi_i - \frac{h\varphi_n}{hs - \alpha_0} \tag{19}$$

where $c_i^{(\ell)} = c_i^{(\ell)}(\alpha_1, \ldots, \alpha_k)$. This expression can be reformulated as follows:

$$x_n(s) = -\frac{hq_{n-1}(hs)}{(hs-\alpha_0)^{n+1}}\varphi_0 - \frac{hq_{n-2}(hs)}{(hs-\alpha_0)^n}\varphi_1 - \cdots - \frac{hq_0(hs)}{(hs-\alpha_0)^2}\varphi_{n-1} - \frac{h\varphi_n}{hs-\alpha_0} \quad (20)$$

where $q_{\ell-1}(\xi)$ is a polynomial of degree at most $\ell-1$, whose coefficients depend only upon the α_i's, but that for notational convenience we write in the form:

$$q_{\ell-1}(\xi) = \sum_{i=0}^{\ell-1} c_{n-\ell}^{(n-\ell+i)}(\xi-\alpha_0)^i, \qquad \ell = 1, \ldots, n \quad (21)$$

although $c_{n-\ell+i}^{(n-\ell)}$ does not depend upon n.

To derive formulas (20), (21) and (23) below, first we solve (18) for x_n:

$$x_n = \frac{1}{hs-\alpha_0}\left(\sum_{i=1}^{k}\alpha_i x_{n-i} - h\varphi_n\right), \quad n = 0, 1, \ldots, \qquad x_{-1} = \cdots = x_{-k} = 0. \quad (22)$$

From this we immediately obtain an explicit representation of x_0:

$$x_0 = -\frac{h}{hs-\alpha_0}\varphi_0.$$

Then, using this formula for x_0 and (22) for $n = 1$, we obtain the formula for x_1:

$$x_1 = \frac{1}{hs-\alpha_0}(\alpha_1 x_0 - h\varphi_1) = -\frac{\alpha_1 h}{(hs-\alpha_0)^2}\varphi_0 - \frac{h}{hs-\alpha_0}\varphi_1.$$

Using these expressions for x_0, x_1 and (22) for $n = 2$, we obtain the formula for x_2 (here we suppose that $k > 1$; for $k = 1$ formulas are very simple):

$$\begin{aligned} x_2 &= \frac{1}{hs-\alpha_0}(\alpha_1 x_1 + \alpha_2 x_0 - h\varphi_2) \\ &= \frac{1}{hs-\alpha_0}\left(-\frac{\alpha_1^2 h}{(hs-\alpha_0)^2}\varphi_0 - \frac{\alpha_1 h}{hs-\alpha_0}\varphi_1 - \frac{\alpha_2 h}{hs-\alpha_0}\varphi_0 - h\varphi_2\right) \\ &= -\frac{h(\alpha_1^2 + \alpha_2(hs-\alpha_0))}{(hs-\alpha_0)^3}\varphi_0 - \frac{\alpha_1 h}{(hs-\alpha_0)^2}\varphi_1 - \frac{h}{hs-\alpha_0}\varphi_2. \end{aligned}$$

Continuing in this way, in the case of the $BDFk$ method, $k = 1, 2, \ldots, 6$, we obtain the formula for x_i, $i = 0, 1, \ldots, k$. Finally, using the mathematical induction principle, a straightforward calculation gives representations (20) and (21) with

$$c_{n-j}^{(n-j+\ell)} = \sum_{i=1}^{k}\alpha_i c_{n-j+i}^{(n-j+\ell+1)}, \qquad \ell = 0, 1, \ldots, n;\ j = 1, 2, \ldots, n, \quad (23)$$

where k is the order of the BDF method.

To obtain this latter representation, for notational convenience we introduce the following zero coefficients:

$$\begin{aligned} &c_n^{(n+j)} = 0, \quad j = 1, \ldots, n \\ &c_i^{(j)} = 0, \quad j = \max\{1, i+1-k\}, \ldots, i-1;\ i = 2, \ldots, n+k-1 \\ &c_{n+j}^{(n+j+\ell)} = 0, \quad j = 1, \ldots, k-1;\ \ell = 0, 1, \ldots, n. \end{aligned} \quad (24)$$

Moreover, we set $c_n^{(n)} = 1$. Notice that it is a simple task to check that $c_{n-j}^{(n-j)} = \alpha_1^j$ for all $j = 1, \ldots, n$.

Then, we construct the coefficients according to the following tableau:

$$
\begin{array}{cccc|cccccc}
 & & & & c_0^{(0)} & c_0^{(1)} & c_0^{(2)} & c_0^{(3)} & \cdots & c_0^{(n)} \\
 & & & & c_1^{(1)} & c_1^{(2)} & c_1^{(3)} & c_1^{(4)} & \cdots & c_1^{(n+1)} \\
 & & & c_2^{(1)} & c_2^{(2)} & c_2^{(3)} & c_2^{(4)} & c_2^{(5)} & \cdots & c_2^{(n+2)} \\
 & & c_3^{(1)} & c_3^{(2)} & c_3^{(3)} & c_3^{(4)} & c_3^{(5)} & c_3^{(6)} & \cdots & c_3^{(n+3)} \\
 & & & & \vdots & & & & & \\
c_k^{(1)} & \cdots & c_k^{(k-2)} & c_k^{(k-1)} & c_k^{(k)} & c_k^{(k+1)} & c_k^{(k+2)} & c_k^{(k+3)} & \cdots & c_k^{(n+k)} \\
c_{k+1}^{(2)} & \cdots & c_{k+1}^{(k-1)} & c_{k+1}^{(k)} & c_{k+1}^{(k+1)} & c_{k+1}^{(k+2)} & c_{k+1}^{(k+3)} & c_{k+1}^{(k+4)} & \cdots & c_{k+1}^{(n+k+1)} \\
\vdots & & & & & & & & & \\
c_n^{(n-k+1)} & \cdots & c_n^{(n-2)} & c_n^{(n-1)} & c_n^{(n)} = 1 & c_n^{(n+1)} = 0 & \cdots & & & c_n^{(2n)} = 0 \\
\hline
c_{n+1}^{(n-k+2)} & \cdots & & c_{n+1}^{(n)} & c_{n+1}^{(n+1)} & \cdots & & & & \\
\vdots & & & & & & & & & \\
c_{n+k-1}^{(n)} & \cdots & & & c_{n+k-1}^{(n+k-1)} & \cdots & & & &
\end{array}
$$

Notice that the zero coefficients (24) are those positioned on the left hand side of the vertical line and below the horizontal line in the previous scheme. According to formulas (23), to calculate the coefficient $c_i^{(j)}$ we start from the position of the scheme which is immediately below this coefficient, move down and to the left hand side along the diagonal, multiplying the first k elements respectively by α_i, $i = 1, \ldots, k$, and sum these k products.

By inserting expansion (20) into (12), a straightforward calculation, requiring the application of Cauchy integral formula to each singular term, then leads to the sum (2), hence to a representation of its coefficients.

In particular, for $k = 1$ we have:

$$c_{n-j}^{(n-i)} = \delta_{ij}\alpha_1^j$$

where δ_{ij} is the Kronecker's delta symbol.

For $k = 2$ we have:

$$
\begin{aligned}
&c_{n-j}^{(n-j)} = \alpha_1^j, \quad j = 0, 1, \ldots, n; \\
&c_{n-j}^{(n-j+\ell)} = 0 \quad \text{for } \ell > [j/2]; \\
&c_{n-j}^{(n-j+\ell)} = \alpha_1 c_{n-j+1}^{(n-j+\ell+1)} + \alpha_2 c_{n-j+2}^{(n-j+\ell+1)} \quad \text{for } \ell = 1, \ldots, [j/2].
\end{aligned}
$$

We recall that the coefficients α_i for $BDF1$ and $BDF2$ are:
$BDF1$ $\alpha_0 = 1$, $\alpha_1 = -1$;
$BDF2$ $\alpha_0 = 3/2$, $\alpha_1 = -2$, $\alpha_2 = 1/2$;

Remark 1 Using the recurrence relation (23) for the coefficients $c_{n-\ell}^{(n-\ell+i)}$, it is not difficult to derive corresponding recurrence relations for the polynomials $q_{\ell-1}(\xi)$. In

particular, in the case of the $BDF2$ method, we have the following recurrence relation:

$$q_{\ell-1}(\xi) = -2q_{\ell-2}(\xi) + \frac{1}{2}\left(\xi - \frac{3}{2}\right) q_{\ell-3}(\xi), \quad \ell \geq 3,$$
$$q_0(\xi) = -2, \quad q_1(\xi) = 4 + \frac{1}{2}\left(\xi - \frac{3}{2}\right),$$

where the degree of the polynomial $q_{\ell-1}(\xi)$, $\ell \geq 2$ is $[\ell/2]$. In general, for the $BDFk$ method one obtains a $k+1$-term recurrence relation.

Since the quadrature rule (2) can be obtained from (12) replacing $x_n(s)$ by its analytic representation (20), we obtain

$$\omega_0(h) = -\frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{hK(s)}{hs - \alpha_0}\, \mathrm{d}s$$

and

$$\omega_\ell(h) = -\frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{hK(s)q_{\ell-1}(hs)}{(hs-\alpha_0)^{\ell+1}}\, \mathrm{d}s = -\frac{h^{-\ell}}{2\pi \mathrm{i}} \int_\Gamma \frac{K(s)q_{\ell-1}(hs)}{(s-\alpha_0/h)^{\ell+1}}\, \mathrm{d}s, \quad \ell = 1, \ldots, n.$$

Now, we apply Cauchy integral formula to calculate each ω_ℓ, $\ell = 0, 1, \ldots, n$. For $\ell = 0$, we have

$$\omega_0(h) = -\frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{hK(s)}{hs - \alpha_0}\, \mathrm{d}s = -\frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{K(s)}{s - \alpha_0/h}\, \mathrm{d}s = K(\alpha_0/h). \tag{25}$$

while for $\ell = 1, \ldots, n$

$$\omega_\ell(h) = \frac{1}{\ell! h^\ell} \lim_{s \to \alpha_0/h} \frac{\mathrm{d}^\ell}{\mathrm{d}s^\ell}(K(s)q_{\ell-1}(hs)).$$

Since

$$q_{\ell-1}^{(\ell)}(\alpha_0) = 0, \quad q_{\ell-1}^{(i)}(\alpha_0) = h^i i!\, c_{n-\ell}^{(n-\ell+i)}, \;\; \ell = 1, \ldots, n; \;\; i = 0, 1, \ldots, \ell-1,$$

applying the Leibnitz's formula for the ℓ-th derivative of a product we obtain

$$\begin{aligned}
\omega_\ell(h) &= \frac{1}{h^\ell \ell!} \sum_{i=0}^{\ell} \frac{\ell!}{i!(\ell-i)!} K^{(i)}(\alpha_0/h) q_{\ell-1}^{(\ell-i)}(\alpha_0) \\
&= \frac{1}{h^\ell} \sum_{i=1}^{\ell} \frac{h^{\ell-i}}{i!(\ell-i)!} K^{(i)}(\alpha_0/h)(\ell-i)! c_{n-\ell}^{(n-\ell+\ell-i)} \\
&= \sum_{i=1}^{\ell} \frac{1}{h^i i!} K^{(i)}(\alpha_0/h) c_{n-\ell}^{(n-i)}, \quad \ell = 1, \ldots, n.
\end{aligned} \tag{26}$$

where we recall that the values of the coefficients $c_{n-\ell}^{(n-i)}$ do not depend upon n.

Thus the following main statement holds.

Theorem 3 *For the coefficients of the quadrature rule (2) the following two alternative representations hold:*

$$\omega_0(h) = K(\alpha_0/h), \quad \omega_\ell(h) = \sum_{i=1}^{\ell} \frac{1}{h^i i!} K^{(i)}(\alpha_0/h) c_{n-\ell}^{(n-i)}, \quad \ell = 1, \dots, n \tag{27}$$

$$\omega_\ell(h) = \frac{1}{\ell!} \frac{\partial^\ell K\left(\frac{\gamma(z)}{h}\right)}{\partial z^\ell}\bigg|_{z=0}, \quad \ell \geq 0 \tag{28}$$

where the latter has been obtained by Lubich in [8].

Remark 2 Recalling that $\omega_\ell(h) = \omega_\ell(h; r)$, from Theorem 3 the following properties follow:

$$\omega_\ell(h; r) = \omega_\ell\left(1; \frac{r}{\sqrt{h}}\right), \text{ for } K \text{ defined by (6a)},$$
$$\omega_\ell(h; r) = \frac{1}{\sqrt{h}}\omega_\ell\left(1; \frac{r}{\sqrt{h}}\right), \text{ for } K \text{ defined by (6b)},$$
$$\omega_\ell(h; r) = \omega_\ell\left(1; \frac{r}{h}\right), \text{ for } K \text{ defined by (6c)},$$
$$\omega_\ell(h; r) = \frac{1}{h}\omega_\ell\left(1; \frac{r}{h}\right), \text{ for } K \text{ defined by (6d)}.$$

Although the representations given in Theorem 3 hold for any (BDF) Lubich convolution quadrature, in the case of the wave equation kernel they can be simplified significantly.

3.1 $2D$ wave equation

In the case of the $2D$ wave equation, where

$$K(s) = \frac{1}{2\pi} K_0(rs),$$

K_0 being the modified Bessel function of the second kind of order 0, we use representation (27). Since

$$\frac{\mathrm{d}^i}{\mathrm{d}s^i} K(s) = \frac{r^i}{2\pi} \frac{\mathrm{d}^i}{\mathrm{d}z^i} K_0(z)\big|_{z=rs},$$

in order to apply formula (26), we need to calculate the i-th derivative of $K_0(z)$, $i \in \mathbb{N}$.

Lemma 1 *The i-th derivative of $K_0(z)$, $i \in \mathbb{N}$, is given as follows*

$$\frac{\mathrm{d}^i}{\mathrm{d}z^i} K_0(z) = \begin{cases} \frac{1}{2^{i-1}} \left[\sum_{j=0}^{i/2-1} \binom{i}{j} K_{i-2j}(z) + \frac{1}{2}\binom{i}{i/2} K_0(z) \right], & i - \textit{even}, \\ -\frac{1}{2^{i-1}} \sum_{j=0}^{(i-1)/2} \binom{i}{j} K_{i-2j}(z), & i - \textit{odd} \end{cases} \tag{29}$$

where $K_m(z)$ denotes the m-th order modified Bessel function of the second kind.

Proof Representation (29) follows from relation (9.6.29) in [1]. □

Setting $x = \alpha_0 r/h$ and defining

$$D_i(x) = \begin{cases} \displaystyle\sum_{j=0}^{i/2-1} \frac{K_{i-2j}(x)}{j!(i-j)!} + \frac{1}{2}\frac{K_0(x)}{[(i/2)!]^2}, & i - \text{even}, \\ \displaystyle -\sum_{j=0}^{(i-1)/2} \frac{K_{i-2j}(x)}{j!(i-j)!}, & i - \text{odd} \end{cases} \tag{30}$$

we have

$$K_0^{(i)}(x) = 2^{1-i} i! D_i(x).$$

This expression leads to the following representation for the coefficients ω_ℓ.

Theorem 4 *For the quadrature coefficients associated with the BDFk methods, $k = 1, \dots 6$, the following representation holds:*

$$\begin{aligned} \omega_0(h) &= \frac{1}{2\pi} K_0(x) > 0, \\ \omega_\ell(h) &= \frac{1}{\pi} \sum_{i=1}^{\ell} \left(\frac{x}{2\alpha_0}\right)^i c_{n-\ell}^{(n-i)} D_i(x), \qquad \ell \geq 1. \end{aligned} \tag{31}$$

where we have set $x = \alpha_0 r/h$ and the coefficient $c_{n-\ell}^{(n-i)}$ does not depend on n.

Notice that this new representation gives us the exact behavior of the coefficients ω_ℓ when $x \to 0$ (see the second part of Remark 3). In particular one obtains the following behaviors:

$$\begin{aligned} \omega_0(h) &\sim -\ln x \\ |\omega_\ell(h)| &\leq C_\ell, \qquad \ell \geq 1. \end{aligned}$$

The above expression (31) can be slightly simplified in the case of the $BDF1$ method.

Corollary 1 *For the BDF1 method we have:*

$$\begin{aligned} \omega_0(h) &= \frac{1}{2\pi} K_0(x) > 0, \\ \omega_\ell(h) &= \frac{(-1)^\ell}{\pi} \left(\frac{x}{2}\right)^\ell D_\ell(x) > 0, \qquad \ell \geq 1, \end{aligned}$$

where $D_\ell(x)$ is defined in (30) and $x = \frac{r}{h}$.

In the case of the $BDF2$ method, for the coefficients of (31) we have

$$c_{n-\ell}^{(n-\ell+m)} = (-1)^\ell \, 2^{\ell-3m} \binom{\ell-m}{m}, \quad m = 0, \dots, \lfloor n/2 \rfloor; \ \ell = 2m, \dots, n$$

all others being equal to zero. Therefore, from expression (31) we obtain the following representation.

Corollary 2 *For the BDF2 method we have:*

$$\omega_0(h) = \frac{1}{2\pi} K_0\left(x\right) > 0,$$
$$\omega_\ell(h) = \frac{(-1)^\ell}{\pi} \sum_{i=\lceil \ell/2 \rceil}^{\ell} \left(\frac{2}{3}\right)^i \frac{1}{4^{\ell-i}} \frac{i!\; x^i D_i(x)}{(\ell-i)!(2i-\ell)!}, \qquad \ell \geq 1, \tag{32}$$

where $D_\ell(x)$ is defined in (30) and $x = \frac{3}{2}\frac{r}{h}$.

Remark 3 For the $BDF1$ method, the expressions given in Corollary 1 allow to compute the ω coefficients with full accuracy, since they are given by a sum of positive terms. Unfortunately, for the $BDFk,\ k \geq 2$, methods, representations (31) and (32) give rise to a severe numerical cancelation phenomenon when the value of ℓ is moderate/large, especially when x is small. The reason for this lies in the behavior of the K Bessel functions when $x \to 0$ (see below). This phenomenon disappears as soon as x takes larger values. More, for x sufficiently large, several terms of the sums (30), (32) can be even neglected, thus reducing significantly the computational cost.

In particular, in the case of $BDF2$, using the double precision arithmetic, for $x = \frac{3r}{2h} = 10^{-1}$ the value of ω_{32} has been computed with 12 exact decimal digits, ω_{40} with 8 decimal digits. For ω_{64} we had 7 decimal digits only for $x \geq 90$. The references values have been obtained by using an extended precision arithmetic.

Nevertheless, there might be applications where one has to compute only single convolution integrals on $(0,t)$, with x not small. For example, after having solved equation (3), when one has to compute the associated potential (4) at a given point not too close to the boundary S. In this case it may be convenient to split the interval in two parts: $(0,t_0),(t_0,t),\ t_0 < t$, and apply Lubich's rule, with a very few nodes, only on the smaller subinterval (t_0,t). By adopting this approach, the use of the above exact representations of the ω-coefficients, which in this case would not suffer from cancellation, could give some advantages. This type of application is currently under investigation.

We recall (see [1]) that for $m \geq 0$ fixed, when x is large we have

$$K_m(x) \sim \sqrt{\frac{\pi}{2x}} \mathrm{e}^{-x},$$

while for $x \to 0$

$$K_0(x) \sim -\ln x,$$
$$K_m(x) \sim 2^{m-1}(m-1)!\; x^{-m},\ m \geq 1.$$

Thus in the latter case

$$x^m K_m(x) \sim 2^{m-1}(m-1)!.$$

3.2 $3D$ wave equation

In this case we prefer to use the representation (28), i.e.,

$$\omega_n(h) = \frac{1}{n!} \left. \frac{\partial^n K\left(\frac{\gamma(z)}{h}; r\right)}{\partial z^n} \right|_{z=0}. \tag{33}$$

This leads to a recurrence relation for the computation of the $\omega_n = \omega_n(h;r)$. Indeed, for the Laplace transform given by (6d), having defined

$$v_n := \frac{\partial^n}{\partial z^n} \mathrm{e}^{-\frac{r}{h}\gamma(z)}\Big|_{z=0}$$

we obtain

$$\begin{cases} v_0 = \mathrm{e}^{-\frac{r}{h}\gamma(0)}, \\ v_{m+1} = -\dfrac{r}{h}\displaystyle\sum_{\ell=0}^{m} \binom{m}{\ell} v_\ell \gamma^{(m+1-\ell)}(0), \quad m = 0, 1, \ldots, n-1. \end{cases}$$

Thus, setting

$$u_m = \frac{v_m}{m!} \mathrm{e}^{\frac{r}{h}\gamma(0)},$$

we have

$$\begin{cases} u_0 = 1, \\ u_{m+1} = -\dfrac{r}{h}\dfrac{1}{m+1}\displaystyle\sum_{\ell=0}^{m} u_\ell \frac{\gamma^{(m+1-\ell)}(0)}{(m-\ell)!}, \quad m = 0, 1, \ldots, n-1 \end{cases}$$

and

$$\omega_n = \frac{\mathrm{e}^{-\frac{r}{h}\gamma(0)}}{4\pi r} u_n.$$

Notice however that in the case of a $BDFk$ method $\gamma(z)$ is a polynomial of degree k and we have $\gamma^{(m+1-\ell)}(0) = 0$ whenever $m+1-\ell > k$. Thus the previous representation of u_{m+1} takes the simplified form:

$$u_{m+1} = -\frac{r}{h}\frac{1}{m+1}\sum_{\ell=m_k}^{m} u_\ell \frac{\gamma^{(m+1-\ell)}(0)}{(m-\ell)!}, \qquad m = 0, 1, \ldots, n-1 \tag{34}$$

where $m_k = \max\{0, m+1-k\}$. This means that u_{m+1} ought to contain the factor $(r/h)^{\lfloor m/k \rfloor + 1}$, that is,

$$u_{m+1} = \left(\frac{r}{h}\right)^{\lfloor m/k \rfloor + 1} \bar{u}_{m+1}, \qquad m \geq 0.$$

Thus, for any fixed h and $n \geq k+1$ we have $\omega_n(h;r) \to 0$ as $r \to 0$. In particular, only $\omega_0(h;r)$ has a singularity (of order 1) at $r = 0$; the following ones are all smooth.

In the case of the $BDF1$ method, recalling that $\gamma(0) = 1$, $\gamma^{(1)}(0) = -1$ and $\gamma^{(m)}(0) = 0$ for $m \geq 2$, we have

$$u_0 = 1, \quad u_{m+1} = \frac{1}{(m+1)!}\left(\frac{r}{h}\right)^{m+1}, \ m \geq 0,$$

hence,

$$\omega_n = \frac{\mathrm{e}^{-r/h}}{4\pi r n!}\left(\frac{r}{h}\right)^n > 0.$$

For the $BDF2$ method, for which $\gamma(0) = 3/2$, $\gamma^{(1)}(0) = -2$, $\gamma^{(2)}(0) = 1$, and $\gamma^{(m)}(0) = 0$, for $m \geq 3$, we obtain

$$\begin{cases} u_0 = 1, \\ u_1 = -\dfrac{r}{h}\gamma^{(1)}(0), \\ u_{m+1} = -\dfrac{r}{h}\dfrac{1}{m+1}\left[\gamma^{(1)}(0)u_m + \gamma^{(2)}(0)u_{m-1}\right], \ m \geq 1. \end{cases}$$

In this case for the new functions

$$q_m := m!\left(\frac{2h}{r}\right)^{m/2} u_m$$

the following recurrence relationship holds:

$$\begin{cases} q_0 = 1, \\ q_1 = 2\sqrt{\dfrac{r}{2h}}, \\ q_{m+1} = 2\sqrt{\dfrac{2r}{h}}q_m - 2mq_{m-1}, \ m \geq 1. \end{cases}$$

As already noticed by Hackbusch et al. (see [6]), setting $x = \sqrt{2r/h}$ this is the well known 3-term recurrence relation defining the Hermite orthogonal polynomials $H_m(x)$. Therefore when we use the $BDF2$ method we have

$$\omega_0 = \frac{1}{4\pi r}\exp\left(-\frac{3r}{2h}\right), \quad \omega_n = \frac{1}{4\pi r n!}\exp\left(-\frac{3r}{2h}\right)\left(\frac{r}{2h}\right)^{n/2} H_n\left(\sqrt{\frac{2r}{h}}\right).$$

This representation has been used in [6] to compute the ω_n.

The BDF methods of order $k \geq 3$ are not A-stable, and according to Lubich's theory they should not be used to solve the wave equation. However, as it will be pointed out at the end of this section, the corresponding rules could nevertheless be used in practice. Thus we derive similar recursion relationships for the computation of their ω_n. This because for these rules, the approach (15) produces severe numerical cancelation, in particular for $k = 5, 6$.

For the $BDF3$ method, where $\gamma(0) = 11/6$, $\gamma^{(1)}(0) = -3$, $\gamma^{(2)}(0) = 3$, $\gamma^{(3)}(0) = -2$, and $\gamma^{(m)}(0) = 0$ for $m \geq 4$, we have

$$\begin{cases} u_0 = 1, \\ u_1 = 3\dfrac{r}{h}, \\ u_2 = -\dfrac{r}{h}\dfrac{3}{2}\left(u_0 - u_1\right), \\ u_{m+1} = \dfrac{r}{h}\dfrac{1}{m+1}\left(u_{m-2} - 3u_{m-1} + 3u_m\right), \ m \geq 2. \end{cases}$$

For the $BDF4$ method, where $\gamma(0) = 25/12$, $\gamma^{(1)}(0) = -4$, $\gamma^{(2)}(0) = 6$, $\gamma^{(3)}(0) = -8$, $\gamma^{(4)}(0) = 6$, $\gamma^{(m)}(0) = 0$ for $m \geq 5$, we have

$$\begin{cases} u_0 = 1, \\ u_1 = 4\dfrac{r}{h}, \\ u_2 = -\dfrac{r}{h}\left(3u_0 - u_1\right), \\ u_3 = \dfrac{r}{h}\dfrac{2}{3}\left(2u_0 - 3u_1 + 2u_2\right), \\ u_{m+1} = -\dfrac{r}{h}\dfrac{1}{m+1}\left(u_{m-3} - 4u_{m-2} + 6u_{m-1} - 4u_m\right), \ m \geq 3. \end{cases}$$

For the $BDF5$ method, where $\gamma(0) = 137/60$, $\gamma^{(1)}(0) = -5$, $\gamma^{(2)}(0) = 10$, $\gamma^{(3)}(0) = -20$, $\gamma^{(4)}(0) = 30$, $\gamma^{(5)}(0) = -24$ $\gamma^{(m)}(0) = 0$ for $m \geq 6$, we have

$$\begin{cases} u_0 = 1, \\ u_1 = 5\dfrac{r}{h}, \\ u_2 = -\dfrac{r}{h}\dfrac{5}{2}\left(2u_0 - u_1\right), \\ u_3 = \dfrac{r}{h}\dfrac{5}{3}\left(2u_0 - 2u_1 + u_2\right), \\ u_4 = -\dfrac{r}{h}\dfrac{5}{4}\left(u_0 - 2u_1 + 2u_2 - u_3\right), \\ u_{m+1} = \dfrac{r}{h}\dfrac{1}{m+1}\left(u_{m-4} - 5u_{m-3} + 10u_{m-2} - 10u_{m-1} + 5u_m\right), \ m \geq 4. \end{cases}$$

Finally, for the $BDF6$ method, where $\gamma(0) = 147/60$, $\gamma^{(1)}(0) = -6$, $\gamma^{(2)}(0) = 15$, $\gamma^{(3)}(0) = -40$, $\gamma^{(4)}(0) = 90$, $\gamma^{(5)}(0) = -144$, $\gamma^{(6)}(0) = 120$, $\gamma^{(m)}(0) = 0$ for $m \geq 7$, we have

$$\begin{cases} u_0 = 1, \\ u_1 = 6\dfrac{r}{h}, \\ u_2 = -\dfrac{r}{h}\dfrac{3}{2}\left(5u_0 - 2u_1\right), \\ u_3 = \dfrac{r}{h}\dfrac{1}{3}\left(20u_0 - 15u_1 + 6u_2\right), \\ u_4 = -\dfrac{r}{h}\dfrac{1}{4}\left(15u_0 - 20u_1 + 15u_2 - 6u_3\right), \\ u_5 = \dfrac{r}{h}\dfrac{1}{4}\left(6u_0 - 15u_1 + 20u_2 - 15u_1 + 6u_0\right), \\ u_{m+1} = -\dfrac{r}{h}\dfrac{1}{m+1}\left(u_{m-5} - 6u_{m-4} + 15u_{m-3} - 20u_{m-2} + 15u_{m-1} - 6u_m\right), \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad m \geq 5. \end{cases}$$

Notice that this approach, besides being exact in exact arithmetic, has a computational cost of $O(N)$ flops. Moreover, when the BDF method is not A-stable ($k \geq 3$), in particular for $k \geq 4$, the trapezoidal rule (15) gives rise to very large summands, hence to severe numerical cancelation, which completely destroy even the correct order of magnitude of the computed coefficients. For these reasons in all the testing we have performed for the (wave) 3D case, the coefficients ω_n have been determined using the above recurrence relations, which appear to be stable.

3.3 Coefficient behavior

Taking into account Remark 2, in Figures 1–8 we have plotted the behaviors of some ω coefficients associated with the $BDFk$ methods (of order $p = k$), denoted by $\omega_n(1; d)$, and with the m-stage ($m = 2, 3$) Radau IIA methods of order $p = 3, 5$, denoted by $\omega_{n,\nu}(1; d)$ (see (17)), considered in this paper. We recall that in the case of the latter coefficients (see their representation given in [11]), the same relationships given in Remark 2 apply to $\bar{\omega}_n(h; r) = h\omega_{n,\nu}(h; r)$. In particular we have plotted the behaviors of these coefficients for two fixed values of n ($n = 20, 100$), and letting the variable d vary from 0.01 to 200.

For the $3D$ wave case, in [6] the authors have taken advantage of this behavior of the coefficients of the $BDF2$ method to reduce significantly the computational cost required by the construction of the matrix associated with the Galerkin BEM they have used. As shown in Figures 5–8, also the coefficients $\omega_{n,\nu}$ of the Radau methods show a similar behavior, actually having fewer oscillations and a smaller "support".

To simplify the code programming, all the coefficients have been computed using expression (15), except for the 3D wave case where we have used our recurrence relations.

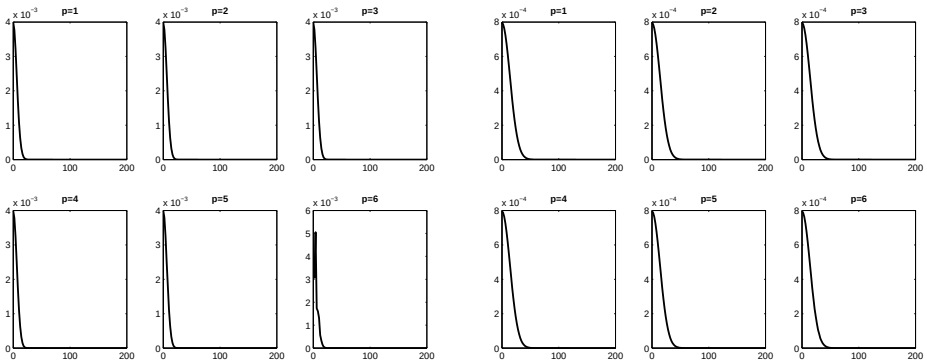

Fig. 1 2D heat, BDF: $\omega_{20}(1;d)$ (left-side) and $\omega_{100}(1;d)$ (right-side), $d = 0.01 : 200$.

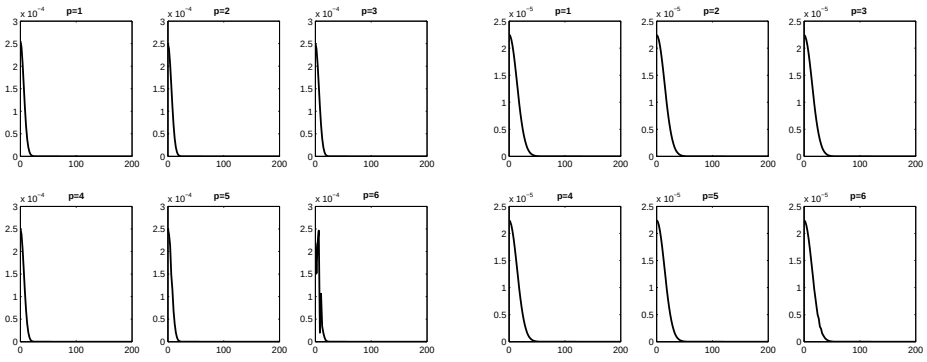

Fig. 2 3D heat, BDF: $\omega_{20}(1;d)$ (left-side) and $\omega_{100}(1;d)$ (right-side), $d = 0.01 : 200$.

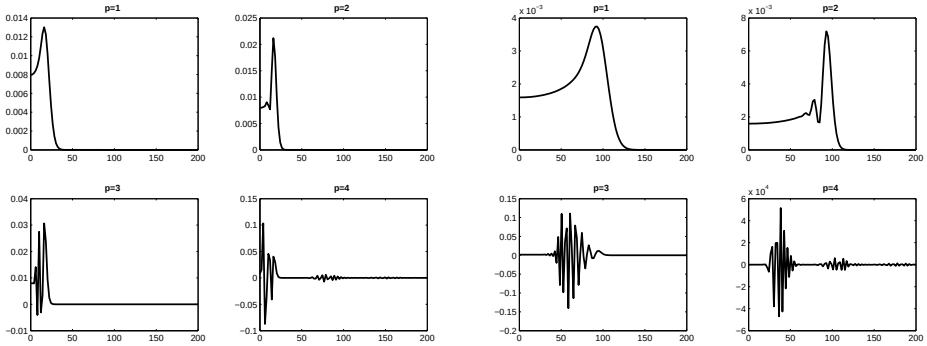

Fig. 3 2D wave, BDF: $\omega_{20}(1;d)$ (left-side) and $\omega_{100}(1;d)$ (right-side), $d = 0.01 : 200$.

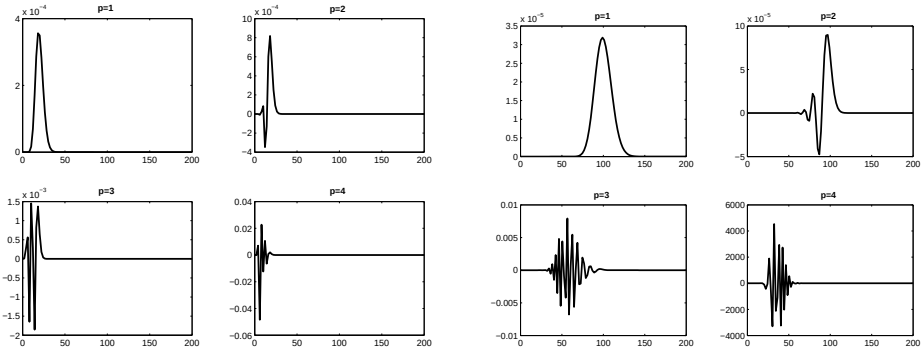

Fig. 4 3D wave, BDF: $\omega_{20}(1;d)$ (left-side) and $\omega_{100}(1;d)$ (right-side), $d = 0.01 : 200$.

We remark that the small oscillations appearing in the center of the two graphs $p = 4$ in Fig.3, are due to the numerical cancelation generated by the trapezoidal sum (15). Indeed, if we compute $\omega_{20}(1;d)$ using our exact representation given in (31), they disappear. Thus, apart from these latter oscillations, the curves reported in the figures above represent the exact behavior of the corresponding ω coefficients.

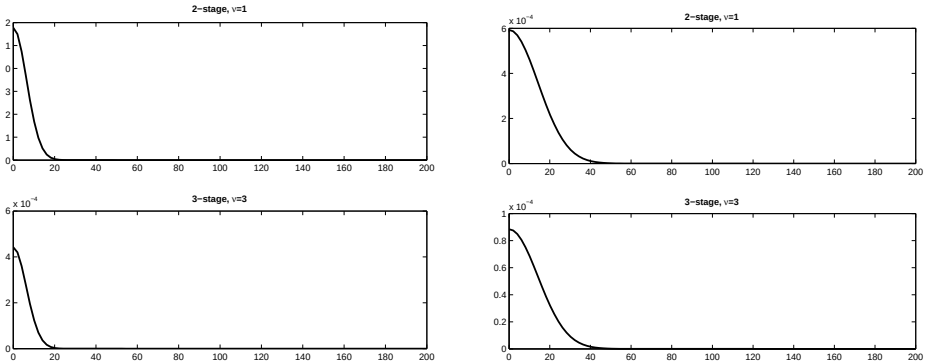

Fig. 5 2D heat, RK: $\omega_{20,\nu}(1;d)$ (left-side) and $\omega_{100,\nu}(1;d)$ (right-side), $d = 0.01 : 200$.

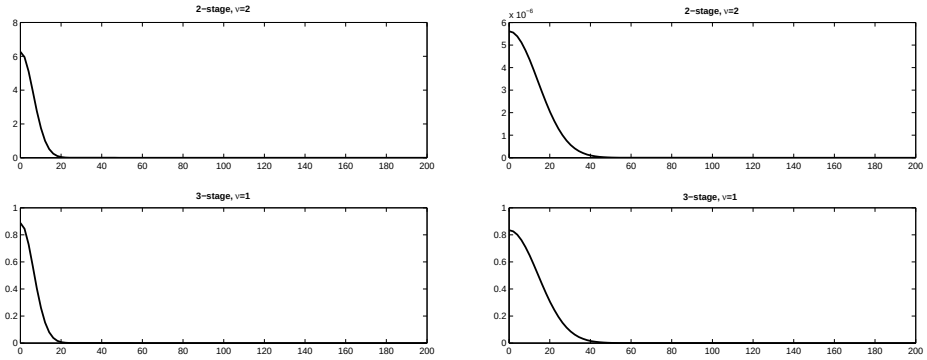

Fig. 6 3D heat, RK: $\omega_{20,\nu}(1;d)$ (left-side) and $\omega_{100,\nu}(1;d)$ (right-side), $d = 0.01 : 200$.

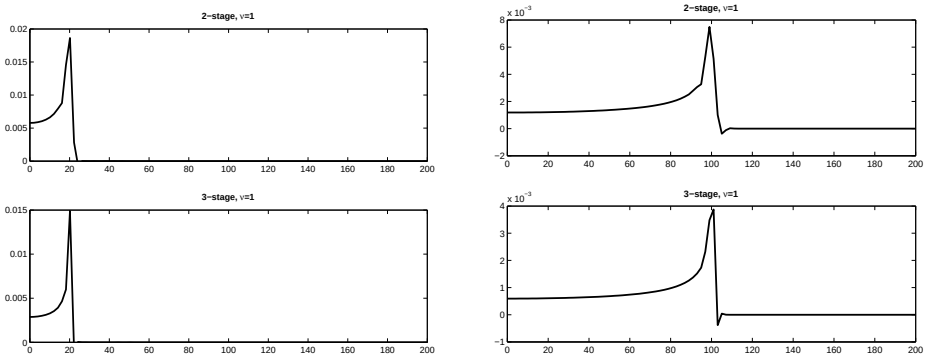

Fig. 7 2D wave, RK: $\omega_{20,\nu}(1;d)$ (left-side) and $\omega_{100,\nu}(1;d)$ (right-side), $d = 0.01 : 200$.

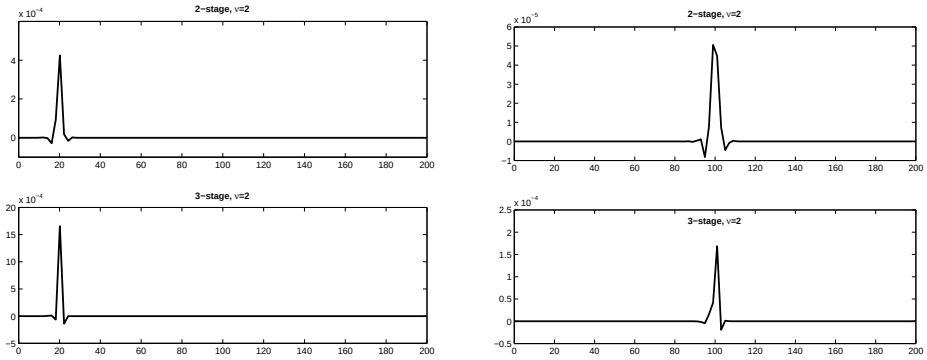

Fig. 8 3D wave, RK: $\omega_{20,\nu}(1;d)$ (left-side) and $\omega_{100,\nu}(1;d)$ (right-side), $d = 0.01 : 200$.

We remark that the (apparent) peaks appearing in Figures 7,8 are due to a scale effect, caused by the large size of the d domain compared to that of the practical support of the $\omega_{n,\nu}$ coefficients. In fact, if we restrict the d-interval, for example to $[10, 30]$ and $[85, 115]$ for $n = 20$ and $n = 100$, respectively, then, as expected, the $\omega_{n,\nu}$ curves are very smooth.

In the following graphs (Figures 9–12), where d is fixed and $n = 0 : 100$, we present the behavior of some of the $\omega_n(1;d)$ coefficients and of the quantities $\omega_n(1;d) = \sum_{\nu=1}^{m} \omega_{n,\nu}(1;d)$, as a function of n, generated, respectively, by the BDF methods of order $p = 1 : 6$ and by the (A-stable) Runge-Kutta Radau IIA of order 3 and 5, in the heat and the wave equation cases (see the dotted curves). In the same graphs, the continuous curves define $k(d;t)$ as a function of t. In the Radau case, the behavior of the single stage coefficients $\omega_{n,\nu}(1;d)$ is very similar to that of their sum (over ν); however it has a smaller hight and their sum defines a better approximation of the kernel k.

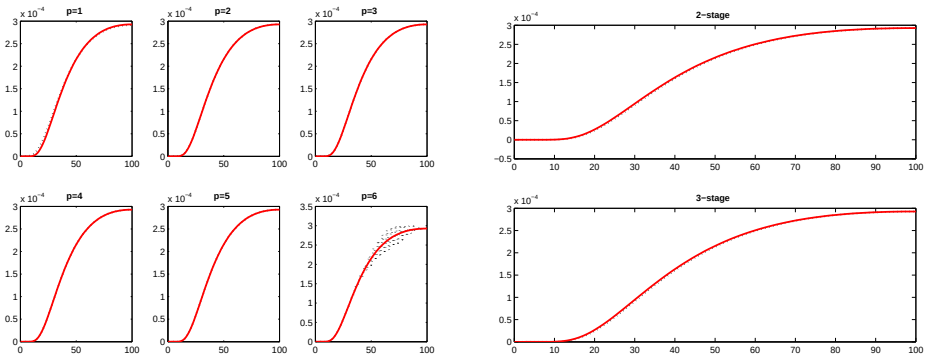

Fig. 9 2D heat: $\omega_n(1;20)$, $n = 0 : 100$, and $k(20;t)$ (BDF left-side, RK right-side).

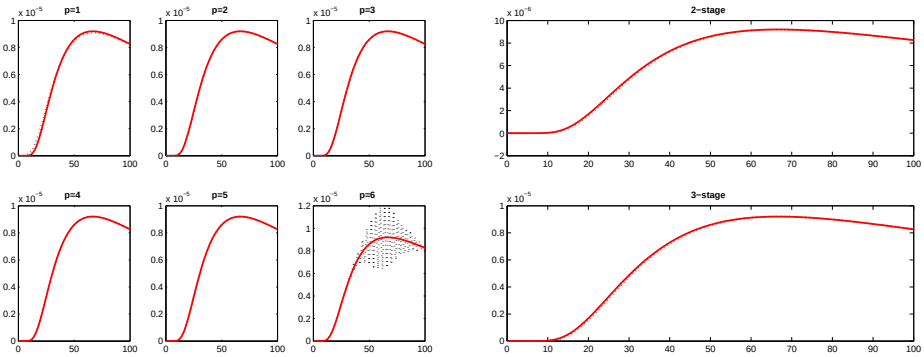

Fig. 10 3D heat: $\omega_n(1;20)$, $n = 0:100$, and $k(20;t)$ (BDF left-side, RK right-side).

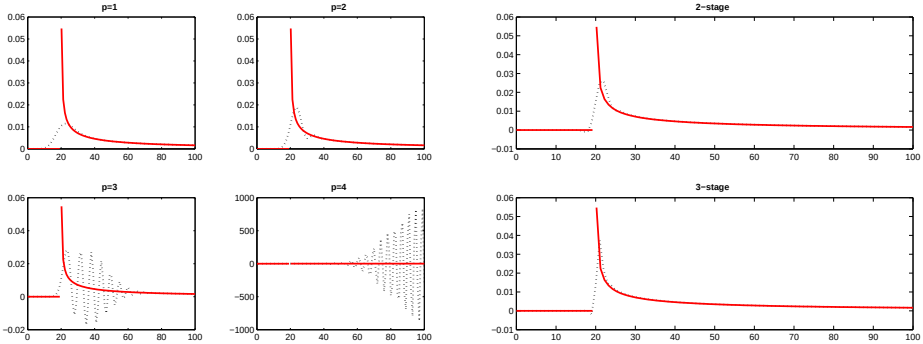

Fig. 11 2D wave: $\omega_n(1;20)$, $n = 0:100$, and $k(20;t)$ (BDF left-side, RK right-side).

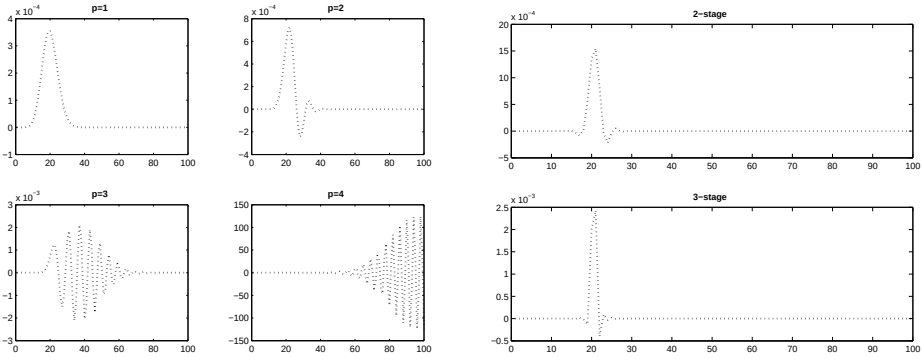

Fig. 12 3D wave: $\omega_n(1;20)$, $n = 0:100$ (BDF left-side, RK right-side).

By looking at expressions (1) and (2) it seems natural to conjecture that, apart for a normalization constant, we should have

$$\omega_n(h) \approx k(r; nh)$$

in some sense, where r, h are fixed and $nh \geq 0$ is varying. Indeed a property of this type, for the heat equation kernel and the BDF methods, has been proved by Lubich in [8]. In fact, in this specific case we can rewrite Theorem 4.1 in [8] in the following form:

Theorem 5 *Under the assumptions of Theorem 1 and for any given (fixed) $r > 0$ and $T > 0$, in the case of the heat kernel, for $n \geq 1$ we have*

$$|h^{-1}\omega_n(h) - k(r; nh)| \leq C_{T,r} h^p$$

where the constant $C_{T,r}$ does not depend on $h \in (0, \bar{h}]$ and on n, $h \leq nh \leq T$, and p is the order of the chosen BDF method.

Notice that recalling the expressions of the heat kernels and the first two identities in Remark 2, to the left hand side of the above inequality we can give the new form

$$h^{-\ell/2}|\omega_n(1; d) - k(d; n)|$$

where $\ell = 2, 3$ in the $2D, 3D$ cases, respectively. This, and a corresponding remark for the Radau IIA methods, are the main reason for having compared in the previous graphs, and in the conjectures that will follow, the quantity between the absolute values.

Conjectures. In the case of the heat equation, for the BDF methods in each graph we have also reported the (continuous) curve $k(d; t)$, $0 \leq t \leq 100$. Except for the method of order 6, the values of the ω_n's lie on the curve $k(d; t)$. For the Radau IIA rules, $k(d; n)$ is compared with $\sum_{\nu=1}^{m} \omega_{n,\nu}(1; d)$. Although for these latter there are no convergence results like that stated in the previous theorem, the two graphs are surprisingly in a very good agreement. Thus, in the Radau case, it is the sum $\sum_{\nu=1}^{m} \omega_{n,\nu}(1; d)$ that has to be considered as an approximation of the kernel value $k(d; n)$, not the single stage coefficients $\omega_{n,\nu}$, which do not give equally good approximation of the corresponding values $k(d; n + 1 - c_\nu)$.

In the case of the wave equation, the coefficients $\omega_n(1; d)$ generated by the A-stable BDF methods all define a good (smooth) approximation of the Dirac delta function centered at $t = d$. Moreover, since for fixed d the coefficients $\omega_n(1; d)$ appear negligible whenever n is not in a neighborhood of d, of the form $(d - \epsilon_n, d + \delta_n)$, $0 < \epsilon_n, \delta_n < d$, in general many of them can be ignored when computing the corresponding convolution quadrature, thus reducing significantly its computational cost.

In Tables 1, 2 we report the values of the convolution quadrature stability factors

$$F_N(d) = \sum_{n=0}^{N} |\omega_n(1; d)|$$

for the BDF methods, and

$$F_N(d) = \sum_{n=0}^{N-1} \sum_{\nu=1}^{m} |\omega_{n,\nu}(1; d)|$$

Table 1 $F_{200}(d)$, $d = 5, 20, 100$, for the heat equation case.

	2D heat			3D heat		
	$d = 5$	$d = 20$	$d = 100$	$d = 5$	$d = 20$	$d = 100$
p	BDF					
1	$2.33 - 001$	$4.47 - 002$	$3.36 - 008$	$1.28 - 002$	$1.26 - 03$	$6.74 - 10$
2	$2.33 - 001$	$4.47 - 002$	$2.31 - 008$	$1.28 - 002$	$1.26 - 03$	$4.77 - 10$
3	$2.33 - 001$	$4.47 - 002$	$2.28 - 008$	$1.28 - 002$	$1.26 - 03$	$4.71 - 10$
4	$2.33 - 001$	$4.47 - 002$	$2.28 - 008$	$2.28 - 002$	$1.26 - 03$	$4.71 - 10$
5	$2.33 - 001$	$4.47 - 002$	$2.28 - 008$	$1.28 - 002$	$1.26 - 03$	$4.71 - 10$
6	$2.33 - 001$	$4.47 - 002$	$2.28 - 008$	$1.48 - 002$	$1.26 - 03$	$4.71 - 10$
p	RK					
3	$2.32 - 001$	$4.45 - 002$	$2.21 - 008$	$1.28 - 002$	$1.26 - 03$	$4.56 - 10$
5	$2.32 - 001$	$4.45 - 002$	$2.21 - 008$	$1.28 - 002$	$1.26 - 03$	$4.56 - 10$

Table 2 $F_{200}(d)$, $d = 5, 20, 100$, for the wave equation case.

	2D wave			3D wave		
	$d = 5$	$d = 20$	$d = 100$	$d = 5$	$d = 20$	$d = 100$
p	BDF					
1	$6.98 - 001$	$4.77 - 001$	$2.10 - 001$	$1.59 - 002$	$3.98 - 03$	$7.96 - 04$
2	$6.98 - 001$	$4.77 - 001$	$2.10 - 001$	$2.04 - 002$	$5.68 - 03$	$1.31 - 03$
3	$7.03 - 001$	$6.82 - 001$	$7.66 + 001$	$4.45 - 002$	$4.16 - 02$	$3.23 + 00$
4	$2.77 + 000$	$2.65 + 004$	$4.56 + 011$	$7.33 - 001$	$3.57 + 03$	$4.02 + 09$
p	RK					
3	$7.03 - 001$	$4.80 - 001$	$2.12 - 001$	$2.00 - 002$	$4.96 - 03$	$9.87 - 04$
5	$7.04 - 001$	$4.81 - 001$	$2.12 - 001$	$2.32 - 002$	$5.64 - 03$	$1.12 - 03$

for the m-stage Radau IIA methods ($m = 2, 3$), where we have chosen $N = 200$ and $d = 5, 20, 100$.

In the case of the wave equation, the convolution quadratures obtained by using BDF methods of order $p \geq 3$ are all unstable (mildly for $p = 3$, and strongly for $p \geq 4$). In Table 2 we have not reported the values of $F_{200}(d)$ corresponding to the cases $p = 5, 6$ because they increase very rapidly. Vice versa, as expected, Table 1 shows that in the heat case we have stability for all formulas.

Convergence properties of convolution quadratures, associated with Runge-Kutta type methods such as the Radau IIA ones, have been obtained in [11], when these methods are applied to convolution integrals whose kernels have sectorial Laplace transforms. To our knowledge, similar results have not been derived in the non sectorial case, in particular for a convolution integral associated with the wave equation. Nevertheless, since these methods are A-stable, we have applied them to time integrals arising from the 2D and 3D wave equation, of the form:

$$y(t) = \int_0^t k(r; t - \tau)\varphi(\tau)\,\mathrm{d}\tau, \qquad 0 < t \leq 1,$$

with $r > 0$ fixed. In Tables 3,4 we have reported the absolute error estimates $|y_N(h) - y(1)|$, $h = 1/N$, (first part of each column), coupled with the corresponding estimated order of convergence (second part of each column). Due to space reasons, in Tables 5,6 we have reported only the error estimates, since the estimated convergence orders confirm the theoretical ones. The error estimates have been computed by comparing $y_N(h)$ with the exact value $y(1)$ in the case of the 3D wave equation, and with the more accurate approximation $y_{256}(h)$ in all the other cases.

Table 3 2D wave, $\varphi(\tau) = \exp(\tau)\tau^5$, $r = 0.5$.

N	BDF $p=1$		BDF $p=2$		RK $p=3$		RK $p=5$	
4	7.07−02		2.67−02		2.30−03		6.49−06	
		1.39		1.80		3.01		6.04
8	2.70−02		7.69−03		2.86−04		9.87−08	
		1.29		1.78		3.05		5.56
16	1.10−02		2.25−03		3.44−05		2.09−09	
		1.19		1.83		3.03		5.33
32	4.85−03		6.30−04		4.21−06		5.21−11	
		1.11		1.90		3.02		5.18
64	2.25−03		1.69−04		5.20−07		1.43−12	
		1.06		1.95		3.01		5.14
128	1.08−03		4.38−05		6.46−08		4.07−14	

Table 4 3D wave, $\varphi(\tau) = \exp(\tau)\tau^5$, $r = 0.5$.

N	BDF $p=1$		BDF $p=2$		RK $p=3$		RK $p=5$	
4	7.42−02		3.22−02		1.79−03		2.54−05	
		1.16		1.64		2.77		5.42
8	3.32−02		1.03−02		2.62−04		5.92−07	
		1.14		1.72		2.98		5.12
16	1.50−02		3.13−03		3.31−05		1.70−08	
		1.10		1.83		3.00		5.06
32	7.03−03		8.80−04		4.13−06		5.10−10	
		1.06		1.91		3.00		5.03
64	3.38−03		2.34−04		5.15−07		1.56−11	
		1.03		1.95		3.00		5.02
128	1.65−03		6.06−05		6.42−08		4.82−13	
		1.01		1.98		3.00		4.38
256	8.18−04		1.54−05		8.01−09		2.32−14	

Table 5 2D wave, $BDFp$, $\varphi(\tau) = \exp(\tau)\tau^9$, $r = 0.5$.

N	$p=1$	$p=2$	$p=3$	$p=4$	$p=5$	$p=6$
4	5.63−02	1.91−02	9.77−03	6.06−03	4.19−03	3.11−03
8	1.41−02	3.31−03	1.41−03	7.76−04	4.86−04	3.29−04
16	3.72−03	6.76−04	2.43−03	1.09−04	5.23−05	2.45−05
32	1.15−03	1.66−04	4.27−05	1.19−05	3.17−06	8.87−07
64	4.25−04	4.38−05	6.64−06	9.92−07	1.67−02	3.68+13
128	1.78−04	1.16−05	9.32−07	7.29−02	6.28+23	5.20+79

Table 6 3D wave, $BDFp$, $\varphi(\tau) = \exp(\tau)\tau^9$, $r = 0.5$.

N	$p=1$	$p=2$	$p=3$	$p=4$	$p=5$	$p=6$
4	6.50−02	2.62−02	1.46−02	9.54−03	6.83−03	5.19−03
8	2.05−02	5.61−03	2.55−03	1.44−03	9.13−04	6.19−04
16	6.34−03	1.30−03	4.78−04	2.11−04	9.66−05	4.15−05
32	2.20−03	3.38−04	8.49−05	2.23−05	5.45−05	1.04−06
64	8.67−04	9.10−05	1.31−05	1.81−06	3.89−07	8.07−06
128	3.78−04	2.41−05	1.82−06	1.60−07	2.17−03	1.61+01
256	1.76−04	6.22−06	2.40−07	1.22+02	2.73+08	2.74+16

We have performed an intensive testing also for other values of $r > 0$ and for smoother functions $\varphi(\tau)$. All the results we have obtained are very similar to those reported in the above tables. Thus they seem to confirm the expected behavior of all the methods we have considered.

Incidentally we notice that when we have computed the integrals associated with 2D and 3D wave equations, with $r > 0$ fixed, using the BDF methods of order $p = 3 : 6$, for the values of N considered, in Tables 5, 6 all the approximations reported show the optimal rate of convergence p, until N does not exceed an integer $N_0 = N_0(p, r/h)$, which seems to decrease as $p, r/h$ increase. We remark however, that if one is satisfied with a certain (low or moderate) accuracy, than this could be achieved by a high order BDF method taking a step size larger than that required by the A-stable BDF method of order 2. For example, in Table 6 with the BDF method of order 6 we obtain a relative accuracy $1.04E-6$ taking $N = 32$, while the BDF method of order 2 with $N = 256$ only gives the accuracy $6.22E-6$. This is also the case of the application mentioned in Remark 3.

We have also used the Lubich rules given by the BDF methods of order $p = 3 : 6$ to solve the wave equation. In this case errors blow up very soon, and furthermore the starting point of the instability strongly depends on the ratio between the time stepsize and the space discretization element size. But in this case, it would be more appropriate to couple the $BDFk$, $k > 2$, method with a space approximant of local degree $k - 1$. However we have not examined this latter situation.

4 An application to a non smooth problem

We have applied the Lubich/collocation and Lubich/Galerkin BEM to space-time BIE formulations of type (3) for the heat and wave equations, associated with homogeneous

initial values and sufficiently smooth compatible boundary data, satisfying the conditions required by the Lubich convergence results. The convolution rules we have used were those satisfying the properties required by the Lubich theory. All the numerical results we have obtained confirmed the expected rate of convergence.

However, in this final section we apply the $BDF1$ and $BDF2$ Lubich rules to a simple (non smooth) exterior problem for the 2D wave equation. This is:

$$\begin{cases} u_{tt}(\mathbf{x},t) - \Delta u(\mathbf{x},t) = 0, & \mathbf{x} \in \mathbb{R}^2 \setminus \Gamma,\ t \in (0,2] \\ u(\mathbf{x},0) = u_t(\mathbf{x},0) = 0, & \mathbf{x} \in \mathbb{R}^2 \setminus \Gamma \\ u(\mathbf{x},t) = g(\mathbf{x},t), & (\mathbf{x},t) \in \Sigma_T := \Gamma \times (0,2] \end{cases}$$

$\Gamma = \{(x,0), x \in [0,1]\}$, first with the smooth compatible Dirichlet boundary datum

$$g(\mathbf{x},t) = t^4 \tag{35}$$

(see Tables 7, 8), and then with

$$g(\mathbf{x},t) = H[t-kx]f(t-kx), \quad f(z) = \begin{cases} \sin^2(4\pi z), & \text{if } 0 \le z \le 1/8 \\ 1, & \text{if } z \ge 1/8 \end{cases} \tag{36}$$

where $k = \cos(\vartheta)$, with $\vartheta \in (0,\pi)$ given (see Figures 13, 14 and Table 9 below, where $\vartheta = \pi/2, \pi/4$).

In the first case, the $BDFk,\ k = 1,2$ methods have been coupled with the Galerkin (see [9]) and collocation BEM, for simplicity both based on piecewise linear (space) approximants associated with a uniform partition.

In the case of the boundary condition (36), which has been taken from [2], the assumptions required by Theorem 2.2 are not all satisfied, and moreover for the solution $\varphi(\mathbf{x},t)$ we expect square root endpoint singularities for any $t > 0$ when $\vartheta = \pi/2$, and for $t > \sqrt{2}/2$ in the case $\vartheta = \pi/4$. Nevertheless we have solved both problems by coupling Lubich $BDF1$ quadrature first with a Galerkin method and then with a midpoint collocation one, taking piecewise constant (space) approximant associated, in spite of the endpoint singularities, with a partition of the domain Γ into M subintervals of length $1/M$.

The ω coefficients of the $BDF1$ method have been computed using the new representation given in Corollary 1, while those of the $BDF2$ method have been determined using (15). The space integrals have been computed by using a 16-point Gauss-Legendre rule on each subinterval.

Since both BEM methods have essentially given the same accuracy, in Tables 7-9 we have reported some of the results produced by the collocation method. In these tables, next to each error column, we have inserted the estimated orders of convergence, which have been obtained by taking as reference values those given by the parameters $M = 128$ and $N = 256$. The parameter M has been taken sufficiently large, but fixed, because we wanted to test the behavior of the sole $BDFk$ rules.

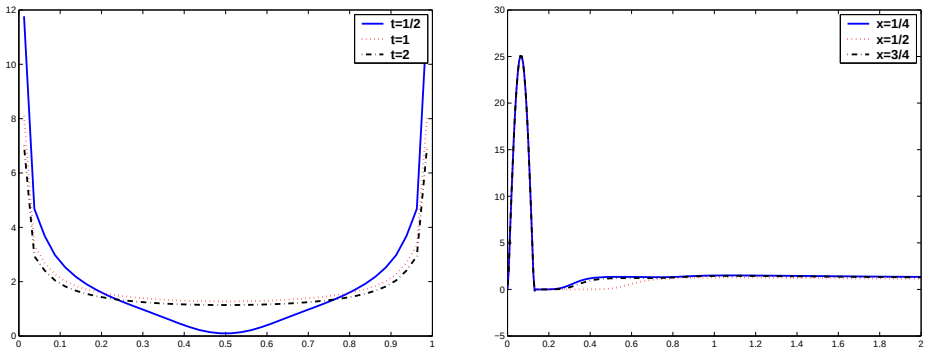

Fig. 13 2D wave eq., collocation method with $BDF1$, $M = 40$ and $N = 320$, and g given by (36) with $\vartheta = \pi/2$; density $\varphi(x,t)$ for $t = 1/2, 1, 2$ by varying x (left-side) and for $x = 1/4, 1/2, 3/4$ by varying t (right-side).

Table 7 2D wave eq. and g given by (35); relative errors at $x = 1/4$ for $t = 1/2, 1, 3/2, 2$ and $M = 128$, by varying N and $p = 1, 2$.

	$p=1$							
N	$(1/4,1/2)$		$(1/4,1)$		$(1/4,3/2)$		$(1/4,2)$	
8	$5.05-01$		$2.74-01$		$1.76-01$		$1.25-01$	
		0.74		0.88		0.92		0.94
16	$3.02-01$		$1.49-01$		$9.29-02$		$6.50-02$	
		0.88		0.94		0.96		0.97
32	$1.65-01$		$7.78-02$		$4.76-02$		$3.31-02$	
		0.95		0.98		0.99		0.99
64	$8.54-02$		$3.95-02$		$2.41-02$		$1.67-02$	
	$p=2$							
N	$(1/4,1/2)$		$(1/4,1)$		$(1/4,3/2)$		$(1/4,2)$	
8	$2.97-01$		$8.54-02$		$3.66-02$		$1.98-02$	
		1.65		1.88		1.93		1.93
16	$9.50-02$		$2.32-02$		$9.59-03$		$5.18-03$	
		1.91		2.02		2.03		1.99
32	$2.52-02$		$5.74-03$		$2.34-03$		$1.31-03$	
		2.17		2.34		2.33		2.07
64	$5.63-03$		$1.13-03$		$4.66-04$		$3.12-04$	

Table 8 2D wave eq. and g given by (35); relative errors at $x = 1/2$ for $t = 1/2, 1, 3/2, 2$ and $M = 128$, by varying N and $p = 1, 2$.

	$p=1$							
N	$(1/2,1/2)$		$(1/2,1)$		$(1/2,3/2)$		$(1/2,2)$	
8	$5.21-01$		$2.89-01$		$1.86-01$		$1.31-01$	
		0.73		0.87		0.92		0.94
16	$3.13-01$		$1.58-01$		$9.82-02$		$6.83-02$	
		0.88		0.94		0.96		0.97
32	$1.71-01$		$8.26-02$		$5.04-02$		$3.48-02$	
		0.95		0.98		0.99		0.99
64	$8.85-02$		$4.20-02$		$2.54-02$		$1.75-02$	
	$p=2$							
N	$(1/2,1/2)$		$(1/2,1)$		$(1/2,3/2)$		$(1/2,2)$	
8	$3.08-01$		$9.01-02$		$3.75-02$		$2.00-02$	
		1.63		1.90		1.96		1.96
16	$9.96-02$		$2.41-02$		$9.67-03$		$5.14-03$	
		1.89		2.04		2.08		2.09
32	$2.69-02$		$5.84-03$		$2.28-03$		$1.21-03$	
		2.14		2.41		2.61		2.59
64	$6.09-03$		$1.13-03$		$3.75-04$		$2.02-04$	

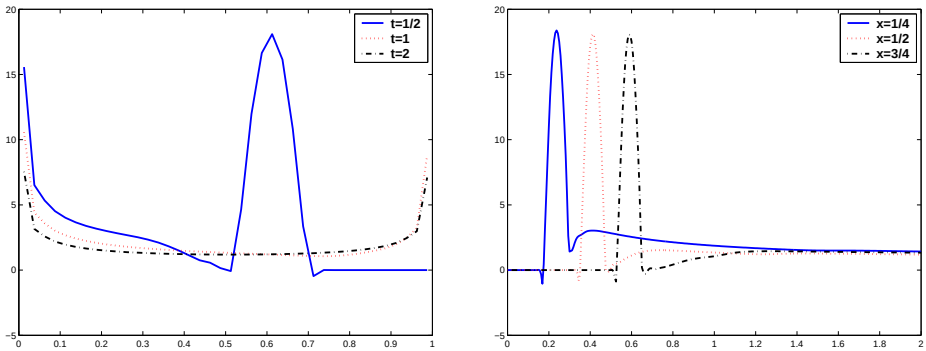

Fig. 14 2D wave eq., collocation method with $BDF1$, $M = 40$ and $N = 320$, and g given by (36) with $\vartheta = \pi/4$; density $\varphi(x,t)$ for $t = 1/2, 1, 2$ by varying x (left-side) and for $x = 1/4, 1/2, 3/4$ by varying t (right-side).

Table 9 2D wave eq., collocation method with $BDF1$, $M = 128$ and by varying N, and g given by (36) with $\vartheta = \pi/2, \pi/4$; relative errors at $x = 1/2, 1/4$ for $t = 1, 3/2, 2$.

	$\vartheta = \pi/2$					
N	$(1/2,1)$		$(1/2,3/2)$		$(1/2,2)$	
8	$2.14-01$		$4.56-02$		$2.86-03$	
		0.98		1.63		0.85
16	$1.08-01$		$1.47-02$		$1.59-03$	
		1.07		1.45		0.45
32	$5.16-02$		$5.40-03$		$1.16-03$	
		1.40		1.24		1.70
64	$1.96-02$		$2.29-03$		$3.60-04$	
	$\vartheta = \pi/4$					
N	$(1/4,1)$		$(1/4,3/2)$		$(1/4,2)$	
8	$7.80-02$		$7.82-03$		$1.32-03$	
		1.81				0.77
16	$2.23-02$		$1.17-02$		$7.76-03$	
		1.48		0.40		1.14
32	$7.98-03$		$8.82-03$		$3.52-03$	
		1.25		0.59		1.67
64	$3.34-03$		$5.88-03$		$1.11-03$	

The results we have obtained in the case of the boundary condition (36), in particular Figure 13, are very similar to those reported in [2], which have been obtained by applying to (3) a full (space-time) Galerkin method, based on an energetic formulation and taking piecewise constant approximations. Thus the Lubich's approach seems to be effective, at least from an engineering point of view, also in cases where the required smoothness conditions are violated.

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