

FAST AND OBLIVIOUS CONVOLUTION QUADRATURE

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Abstract. We give an algorithm to compute N steps of a convolution quadrature approximation to a continuous temporal convolution using only $O(N \log N)$ multiplications and $O(\log N)$ active memory. The method does not require evaluations of the convolution kernel, but instead $O(\log N)$ evaluations of its Laplace transform, which is assumed sectorial. The algorithm can be used for the stable numerical solution with quasi-optimal complexity of linear and nonlinear integral and integro-differential equations of convolution type. In a numerical example we apply it to solve a subdiffusion equation with transparent boundary conditions.

Key words. convolution, numerical integration, Runge-Kutta methods, Volterra integral equation, anomalous diffusion

AMS subject classifications. 65R20

1. Introduction. In this paper we give a fast and memory-saving algorithm for computing the approximation of a continuous convolution (possibly matrix \times vector)

$$\int_0^t f(t-\tau)g(\tau)d\tau, \quad 0 \leq t \leq T, \quad (1.1)$$

by a convolution quadrature with a step size $h > 0$,

$$\sum_{j=0}^n \omega_{n-j}g(jh), \quad n = 1, \dots, N, \quad (1.2)$$

where the convolution quadrature weights ω_n are determined from their generating power series as (see [10, 11, 12])

$$\sum_{n=0}^{\infty} \omega_n \zeta^n = F\left(\frac{\delta(\zeta)}{h}\right). \quad (1.3)$$

Here $F(s)$ is the Laplace transform of the (possibly matrix-valued) convolution kernel $f(t)$, and $\delta(\zeta) = 1 - \zeta$ or $\delta(\zeta) = (1 - \zeta) + \frac{1}{2}(1 - \zeta)^2$ for the methods based on the first or second-order backward difference formula, respectively. We will also consider a similar approximation based on implicit Runge-Kutta formulas such as the Radau IIA methods [13]. Attractive features of such convolution quadratures are that they work well for singular kernels $f(t)$, for kernels with multiple time scales, and in situations where only the Laplace transform $F(s)$ but not the convolution kernel $f(t)$ is known analytically. Perhaps most importantly, they enjoy excellent stability properties when used for the discretization of integral equations or integro-differential equations of convolution type, in a way often strikingly opposed to discretizations with more straightforward quadrature formulas (see references in [12]).

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The direct way to compute (1.2) is to first compute and store the (possibly matrix-valued) weights $\omega_0, \dots, \omega_N$, which can be done accurately with $O(N)$ evaluations of the Laplace transform $F(s)$ [11], and then to compute the discrete convolution. Done naively, this requires $O(N^2)$ multiplications (possibly matrix \times vector) and $O(N)$ active memory for the values $g(jh)$ and for the weights. Using FFT, the number of multiplications can be reduced to $O(N \log N)$, and to $O(N (\log N)^2)$ in the case of integral equations where the values of $g(t)$ are not known beforehand, but where $g(nh)$ is computed only in the n th time step [3]. However, that approach does not reduce the number of F -evaluations and the memory requirements.

Here we give an algorithm, also applicable in the case of linear and nonlinear integral equations, which computes (1.2) in a way that requires

- $O(N \log N)$ multiplications,
- $O(\log N)$ evaluations of the Laplace transform $F(s)$, and
- $O(\log N)$ active memory.

The history $g(jh)$ for $j = 0, \dots, N$ is forgotten in this algorithm, and only logarithmically few linear combinations of the g -values are kept in memory. These are obtained by solving numerically, with step size h , initial value problems of the form $y' = \lambda y + g$ with complex λ . The weights ω_n ($n \leq N$) are not computed explicitly, except the first few, e.g., the first 10 weights.

The algorithm presented here uses ideas of the fast convolution algorithm of [14], which instead of (1.2) makes a different approximation to the continuous convolution. The stability properties of the second-order method of [14] in integro-differential equations such as those of Section 5 are, however, extremely difficult to analyze (cf. also [17]) and remain entirely unclear for higher-order extensions. Here we show how the convolution quadratures (1.2) with all their known favorable properties can be implemented in an equally fast and memory-saving way.

Following the error analysis of [7, 8] we give exponentially convergent error bounds for the contour integral approximations that are employed in this algorithm. They ensure that the constants hidden in the O -symbols of the above work estimates depend only logarithmically on the error tolerance for these contour integral approximations.

We assume a *sectorial* Laplace transform $F(s)$:

$$F(s) \text{ is analytic in a sector } |\arg(s - c)| < \pi - \varphi \text{ with } \varphi < \frac{1}{2}\pi, \text{ and there} \quad (1.4)$$

$$|F(s)| \leq M |s|^{-\nu} \quad \text{for some real } M \text{ and } \nu > 0.$$

The inverse Laplace transform is then given by

$$f(t) = \frac{1}{2\pi i} \int_{\Gamma} e^{t\lambda} F(\lambda) d\lambda, \quad t > 0, \quad (1.5)$$

with Γ a contour in the sector of analyticity, going to infinity with an acute angle to the negative real half-axis and oriented with increasing imaginary part. The function $f(t)$ is analytic in $t > 0$ and satisfies

$$|f(t)| \leq C t^{\nu-1} e^{ct}, \quad t > 0, \quad (1.6)$$

and is therefore locally integrable. (The absolute values on the left-hand sides of the bounds (1.4) and (1.6) are to be interpreted as matrix norms for matrix-valued convolution kernels.)

In Section 2 we review convolution quadrature based on multistep and Runge-Kutta methods. We give a contour integral representation of the convolution quadrature weights whose discretization along hyperbolas or Talbot contours is discussed in

Section 3. The fast and oblivious convolution algorithm is formulated in Section 4. Finally, in Section 5 we give the results of numerical experiments with integral and integro-differential equations originating from regular and anomalous diffusion problems.

2. Convolution quadrature. In this section we review briefly convolution quadrature and give a contour integral representation of the convolution quadrature weights on which the fast algorithm of this paper is based.

2.1. Convolution quadrature based on multistep methods. We consider the convolution quadrature (1.2) with weights (1.3). By (1.4) and Cauchy's integral formula we have, with a contour Γ as in (1.5),

$$\sum_{n=0}^{\infty} \omega_n \zeta^n = F\left(\frac{\delta(\zeta)}{h}\right) = \frac{1}{2\pi i} \int_{\Gamma} \left(\frac{\delta(\zeta)}{h} - \lambda\right)^{-1} F(\lambda) d\lambda.$$

Hence, with $e_n(z)$ defined by

$$(\delta(\zeta) - z)^{-1} = \sum_{n=0}^{\infty} e_n(z) \zeta^n, \quad (2.1)$$

we have the integral formula

$$\omega_n = \frac{h}{2\pi i} \int_{\Gamma} e_n(h\lambda) F(\lambda) d\lambda, \quad (2.2)$$

which can be viewed as the discrete analog of (1.5). For the backward Euler discretization $\delta(\zeta) = 1 - \zeta$ we note the explicit formula

$$e_n(z) = (1 - z)^{-n-1}, \quad (2.3)$$

which is of the form $e_n(z) = q(z)r(z)^n$ with $r(z) = \frac{1}{1-z}$ and $q(z) = \frac{1}{1-z}$.

For the second-order BDF method, where $\delta(\zeta) = \sum_{k=1}^p \frac{1}{k}(1 - \zeta)^k$ with $p = 2$, we obtain from a partial fraction decomposition of $(\delta(\zeta) - z)^{-1}$ that

$$e_n(z) = \frac{1}{\sqrt{1+2z}} \left((2 - \sqrt{1+2z})^{-n-1} - (2 + \sqrt{1+2z})^{-n-1} \right), \quad (2.4)$$

which is of the form $e_n(z) = q_1(z)r_1(z)^n + q_2(z)r_2(z)^n$. Connoisseurs of Cardano's formulas find analogous formulas to (2.4) also for the BDF methods of orders 3 and 4.

2.2. Convolution quadrature based on Runge-Kutta methods. We consider an implicit Runge-Kutta method with coefficients a_{ij} , b_j , c_i for $i, j = 1, \dots, m$. We denote the Runge-Kutta matrix by $\mathcal{Q} = (a_{ij})$, the row vector of the weights by $b^T = (b_j)$, and the stability function by

$$r(z) = 1 + zb^T(I - z\mathcal{Q})^{-1}\mathbb{1},$$

where $\mathbb{1} = (1, \dots, 1)^T$. We assume that all eigenvalues of the Runge-Kutta matrix \mathcal{Q} have positive real part and, for simplicity, that the method is A-stable and the row vector of the weights equals the last line of the Runge-Kutta matrix,

$$b_j = a_{mj} \quad \text{for } j = 1, \dots, m,$$

and correspondingly $c_m = 1$. These conditions are in particular satisfied by the Radau IIA family of Runge-Kutta methods [4]. From such a Runge-Kutta method, a convolution quadrature is constructed as follows [13]: Let

$$\Delta(\zeta) = \left(\mathcal{O} + \frac{\zeta}{1-\zeta} \mathbb{1} b^T \right)^{-1} \quad (2.5)$$

and define weight matrices W_n by

$$\sum_{n=0}^{\infty} W_n \zeta^n = F\left(\frac{\Delta(\zeta)}{h}\right). \quad (2.6)$$

Let $\omega_n = (\omega_n^1, \dots, \omega_n^m)$ denote the last row of W_n . Then an approximation to the convolution integral (1.1) at time $t_{n+1} = (n+1)h$ is given by

$$u_{n+1} = \sum_{j=0}^n \sum_{i=1}^m \omega_{n-j}^i g(t_j + c_i h) = \sum_{j=0}^n \omega_{n-j} g_j \quad (2.7)$$

with the column vector $g_j = (g(t_j + c_i h))_{i=1}^m$. For a Runge-Kutta method of classical order p and stage order q , this approximation is known to be convergent of the order $\min(p, q+1+\nu)$ with ν of (1.4).

With the row vector $e_n(z) = (e_n^1(z), \dots, e_n^m(z))$ defined as the last row of the $m \times m$ matrix $E_n(z)$ given by

$$(\Delta(\zeta) - zI_m)^{-1} = \sum_{n=0}^{\infty} E_n(z) \zeta^n, \quad (2.8)$$

we obtain an integral formula like in (2.2),

$$\omega_n = \frac{h}{2\pi i} \int_{\Gamma} e_n(h\lambda) \otimes F(\lambda) d\lambda. \quad (2.9)$$

For $n \geq 0$, $e_n(z)$ is given as

$$e_n(z) = r(z)^n q(z) \quad (2.10)$$

with the row vector $q(z) = b^T(I - z\mathcal{O})^{-1}$; cf. Lemma 2.4 in [13]. We note that

$$y_{n+1}^{(\lambda)} = h \sum_{j=0}^n e_{n-j}(h\lambda) g_j \quad (2.11)$$

is the Runge-Kutta approximation at time t_{n+1} of the linear initial value problem

$$y' = \lambda y + g(t), \quad y(0) = 0. \quad (2.12)$$

The convolution quadrature (2.7) is thus interpreted as

$$u_{n+1} = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) y_{n+1}^{(\lambda)} d\lambda;$$

see Proposition 2.1 in [13].

3. Approximation of the contour integrals. The fast convolution algorithm will be based on discretizing the integrals in (2.2) and (2.9) along suitable complex contours. This approximation is discussed in the present section.

3.1. Quadrature on Talbot contours and hyperbolas. The fast algorithm approximates the quadrature weights ω_n by linear combinations of the exponential approximations $e_n(h\lambda)$, locally on a sequence of fast-growing time intervals $nh \in I_\ell$:

$$I_\ell = [B^{\ell-1}h, 2B^\ell h), \quad (3.1)$$

where the base $B > 1$ is an integer. For example, $B = 10$ was found a good choice in our numerical experiments. The approximation on I_ℓ results from applying the trapezoidal rule to a parametrization of the contour integral for the convolution quadrature weights,

$$\omega_n = \frac{h}{2\pi i} \int_{\Gamma_\ell} e_n(h\lambda) \otimes F(\lambda) d\lambda \approx h \sum_{k=-K}^K w_k^{(\ell)} e_n(h\lambda_k^{(\ell)}) \otimes F(\lambda_k^{(\ell)}), \quad nh \in I_\ell, \quad (3.2)$$

with an appropriately chosen complex contour Γ_ℓ . The number of quadrature points on Γ_ℓ , $2K + 1$, is chosen independent of ℓ . It is much smaller than what would be required for a uniform approximation of the contour integral on the whole interval $[0, T]$. Only a few of the first convolution quadrature weights, ω_n for $n \leq N_0$ (e.g., $N_0 = 10$), are approximated differently, using the trapezoidal rule discretization of the integral over a circle as discussed in [11, 13]:

$$\omega_n = \text{last row of } \frac{1}{2\pi i} \int_{|\zeta|=\rho} \zeta^{-n-1} F\left(\frac{\Delta(\zeta)}{h}\right) d\zeta, \quad n \leq N_0. \quad (3.3)$$

The numerical integration in (2.2) or (2.9) is done by applying the trapezoidal rule with equidistant steps to a parameterization of a hyperbola [8] or a Talbot contour [18, 16]. The Talbot contour is given by

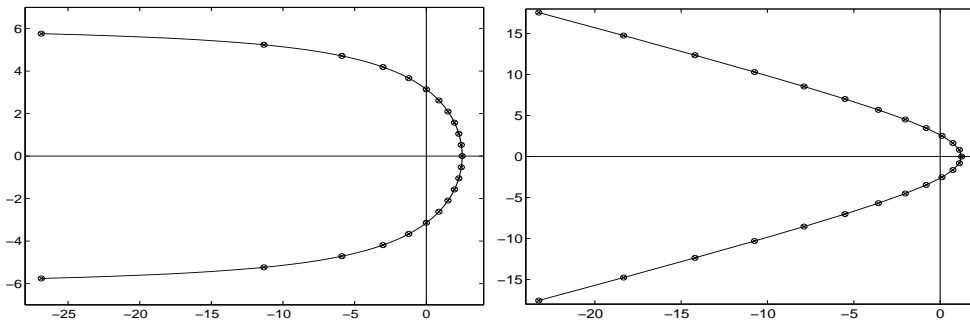


FIG. 3.1. Talbot contour (left) and hyperbola (right).

$$(-\pi, \pi) \rightarrow \Gamma : \theta \mapsto \gamma(\theta) = \sigma + \mu(\theta \cot(\theta) + i\nu\theta) \quad (3.4)$$

where the parameters μ , ν and σ are such that the singularities of $F(s)$ lie to the left of the contour and that the singularities of $e_n(hs)$ lie to the right of the contour. See left part of Figure 3.1 for $\sigma = 0$. The parameter μ will depend on ℓ via the right

end-point of I_ℓ , which yields a Talbot contour Γ_ℓ depending on the approximation interval I_ℓ . The weights and quadrature points in (3.2) are given by (omitting ℓ in the notation)

$$w_k = -\frac{i}{2(K+1)} \gamma'(\theta_k), \quad \lambda_k = \gamma(\theta_k) \quad \text{with} \quad \theta_k = \frac{k\pi}{K+1}.$$

Alternatively, the hyperbola is given by

$$\mathbb{R} \rightarrow \Gamma : \theta \mapsto \gamma(\theta) = \mu(1 - \sin(\alpha + i\theta)) \quad (3.5)$$

where the parameters μ and α are such that the singularities of $F(s)$ lie to the left of the contour. See the right part of Figure 3.1 for $\alpha = \pi/2 - 1/2$. The weights and quadrature points in (3.2) are given by (omitting ℓ in the notation)

$$w_k = \frac{i\tau}{2\pi} \gamma'(\theta_k), \quad \lambda_k = \gamma(\theta_k) \quad \text{with} \quad \theta_k = k\tau,$$

where τ is a step length parameter.

3.2. Numerical experiments. In view of the examples of Section 5 we present here numerical experiments with

$$f(t) = \frac{1}{\sqrt{\pi t}}, \quad \text{for which} \quad F(s) = s^{-1/2}.$$

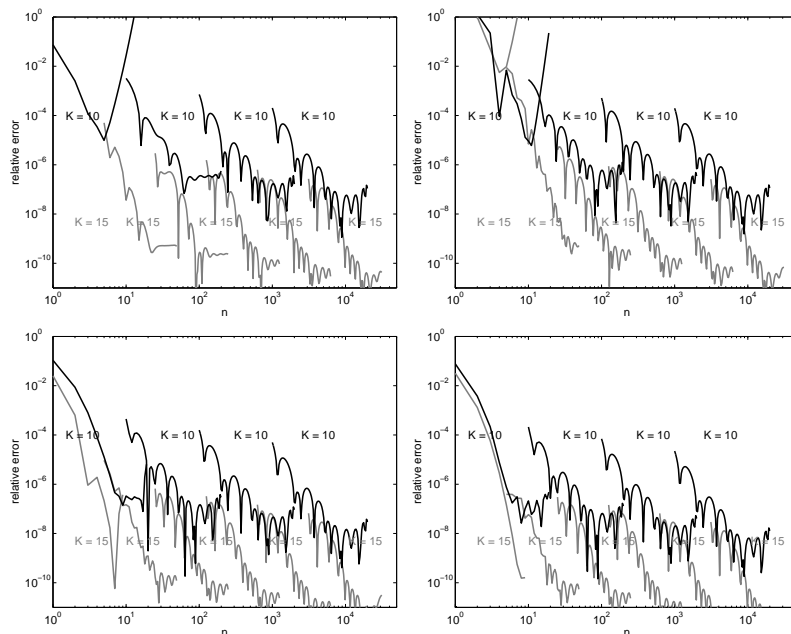


FIG. 3.2. Talbot quadrature errors versus time for $K = 15$, $B = 5$ and $K = 10$, $B = 10$ for different Integrators. (Implicit Euler, BDF(2), RadauIIA(3) and RadauIIA(5) in clockwise order starting from the upper left corner)

The error is calculated with respect to a reference solution, obtained for a discretization of the contour integral with a large number of integration points. For the

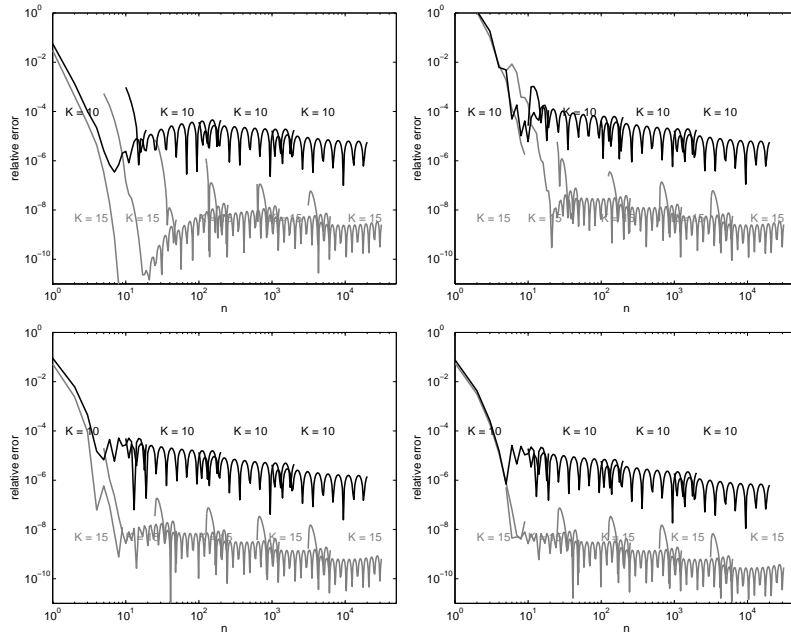


FIG. 3.3. Hyperbola quadrature errors versus time for $K = 15$, $B = 5$ and $K = 10$, $B = 10$ for different Integrators. (Implicit Euler, BDF(2), RadauIIA(3) and RadauIIA(5) in clockwise order starting from the upper left corner)

Radau IIA methods of order 3 and 5, where the ω_n are row vectors of dimension 2 and 3, respectively, we plot the error of the last entry.

Using the Tabot contours, the following choices of parameters were found to give good results. A relative accuracy of about 10^{-3} on the interval I_ℓ for $\ell \geq 2$ with right end-point T_ℓ is obtained with $B = 10$, $K = 10$, $\mu = 8/T_\ell$, $\nu = 0.6$. For a relative approximation error of 10^{-6} , take $B = 5$, $K = 15$, and the other parameters as before, cf. Fig. 3.2. For $n > 20$ there is no substantial difference between the different Runge-Kutta methods. Since the approximations to the first few convolution quadrature weights are poor, they will not be used in the algorithm.

Using the hyperbola contours, a relative accuracy of about 10^{-4} on the interval I_ℓ for $\ell \geq 2$ with right end-point T_ℓ is obtained with $B = 10$, $K = 10$, $\alpha = 1$, $\mu = 3.6/T_\ell$ and $\tau = 0.64$. For a relative approximation error of $3 \cdot 10^{-8}$, we take $B = 5$, $K = 15$, $\alpha = 1$, cf. Fig. 3.3. For $n > 20$ there is again no essential difference between the different Runge-Kutta methods.

Fig. 3.4 shows the relative errors on the interval $[10, 20000]$ (similar for any interval $[a, 2000a]$ with $a > 10$) for the RadauIIA(3) method with $K = 10, 20, 40, 80, 160, 320, 640$. For the implicit Euler, the BDF(2) and the RadauIIA(5) method these error plots look similar. This behavior of the errors clearly demonstrates the advantage of using local approximations. With $B = 10$, we need three approximation intervals to cover the interval $[10, 20000]$, so that for a work of $3 \cdot K$ with $K = 10$ we obtain better accuracy than with $K = 640$ over the whole interval.

In this example the maximum quadrature errors using the hyperbolas are smaller than those for the Talbot contours. Moreover, the hyperbolas allow to choose larger intervals. On the other hand, the Talbot contours turned out to be less sensitive to

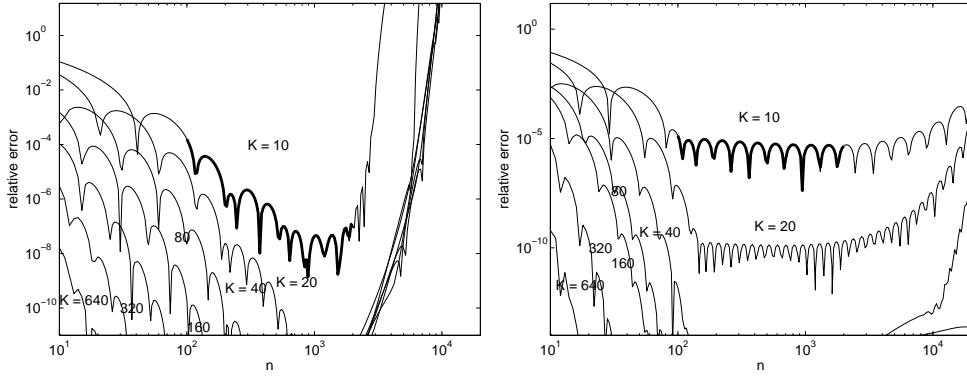


FIG. 3.4. Talbot (left) and hyperbola (right) quadrature error versus n for the RadauIIA(3) method with $K = 10, 20, 40, 80, 160, 320, 640$. The bold parts of the error curve correspond to the lower left parts of Figs. 3.2 and 3.3. Note the different scaling of the y axis.

the choice of parameters and the Laplace transform functions than the hyperbolas.

3.3. Theoretical error bounds of the contour integral approximations.

For the case of the hyperbola, we obtain in the same way as in Theorem 3 of [7] the following error bound which shows exponential convergence.

THEOREM 3.1. *There are positive constants C, d, c_0, \dots, c_4 , and c such that at $t = nh \leq T$ the quadrature error in (3.2) for a hyperbola (3.5) is bounded by*

$$\|E(\tau, K, h, n)\| \leq C h t^{\nu-1} (\mu t)^{1-\nu} \left(\frac{e^{c_0 \mu t}}{e^{2\pi d/\tau} - 1} + e^{(c_1 - c_2 \cosh(K\tau))\mu t} + e^{c_3 \mu t} \left(1 + \frac{c_4 \cosh(K\tau)\mu t}{n/2} \right)^{-n/2} \right),$$

if $n \geq c\mu t$ and $\mu t \geq 1$. Here ν is the exponent of (1.4).

Given an error tolerance ε , the first term in the error bound becomes $O(\varepsilon h t^{\nu-1})$ if τ is chosen so small that $c_0 \mu t - 2\pi d/\tau \leq \log \varepsilon$, which requires an asymptotic proportionality $\frac{1}{\tau} \sim \log \frac{1}{\varepsilon} + \mu t$. For μ chosen such that $\frac{a_1}{B} \log \frac{1}{\varepsilon} \leq \mu t \leq a_1 \log \frac{1}{\varepsilon}$ with an arbitrary positive constant a_1 and with $B > 1$, we obtain that the second term is $O(\varepsilon h t^{\nu-1})$ if $c_1 - c_2 \cosh(K\tau) \leq -B/a_1$, i.e., with $\cosh(K\tau) = a_2$ for a sufficiently large constant a_2 . With the above choice of τ , this yields $K \sim \log \frac{1}{\varepsilon}$. The third term then becomes smaller than $\varepsilon h t^{\nu-1}$ for $n \geq c \log \frac{1}{\varepsilon}$ with a sufficiently large constant c . In summary, this gives the following bound for the required number of quadrature points on the hyperbola.

THEOREM 3.2. *In (3.2), a quadrature error bounded in norm by $\varepsilon h t^{\nu-1}$ for $nh \in I_\ell$ is obtained with $K = O(\log \frac{1}{\varepsilon})$. This holds for $n \geq c \log \frac{1}{\varepsilon}$ (with some constant $c > 0$), with K independent of ℓ and of n and h with $nh \leq T$.*

The approximation is, however, poor for the first few n , as we have seen in the numerical experiments.

We refer to [9] for an optimized strategy to choose the parameters μ, τ, K , which takes also perturbations in the evaluations of the Laplace transform into account.

We expect that a similar result to Theorem 3.2 holds also for the Talbot contours, if the Laplace transform has an analytic continuation beyond the negative real axis from above and below, as is the case for the fractional powers considered above.

4. The fast and oblivious algorithm. We now describe the convolution algorithm, concentrating on Runge-Kutta based convolution quadrature. The algorithm differs slightly depending on whether we want to compute a convolution or to solve an integral or integro-differential equation of convolution type.

4.1. The algorithm for computing convolutions. The algorithm presented here uses the organisation scheme of the fast convolution algorithm described in a step by step manner in [14]. A pseudo-code for the algorithm developed in [14] can be found in [5].

For fixed integer $n \leq N$ and a given base B we split the discrete convolution (1.2) or (2.7) into L sums, where L is the smallest integer such that $n < 2B^L$:

$$u_{n+1} = \sum_{j=0}^n \omega_{n-j} g_j = u_{n+1}^{(0)} + \cdots + u_{n+1}^{(L)}$$

$$\text{with } u_{n+1}^{(0)} = \omega_0 g_n \text{ and } u_{n+1}^{(\ell)} = \sum_{j=b_\ell}^{b_{\ell-1}-1} \omega_{n-j} g_j$$

for suitable $n = b_0 > b_1 > \cdots > b_{L-1} > b_L = 0$. In view of the approximation intervals (3.1), the splitting is done in such a way that for fixed ℓ in each sum from b_ℓ to $b_{\ell-1} - 1$, we have $n - j \in [B^{\ell-1}, 2B^\ell - 2]$. The $b_\ell = \mathbf{b}(\ell)$, $\ell = 1, \dots, L - 1$ are determined recursively by the following pseudo-code.

```

L = 1; q = 0;
for n = 1 to N do
  if 2*B^L == n+1 then L = L+1; endif
  k = 1;
  while mod(n+1, B^k) == 0 & k < L
    q(k) = q(k)+1; k = k+1;
  endwhile
  for k = 1 to L-1 do b(k) = q(k)*B^k; endfor
endfor

```

Note that for growing n , b_ℓ is augmented by B^ℓ every B^ℓ steps. On inserting the integral representation (2.9) of the Runge-Kutta quadrature weights and the relation (2.10), i.e., $e_{n-j}(h\lambda) = r(h\lambda)^{n-j} q(h\lambda)$, we obtain

$$u_{n+1}^{(\ell)} = \sum_{j=b_\ell}^{b_{\ell-1}-1} \omega_{n-j} g_j = \sum_{j=b_\ell}^{b_{\ell-1}-1} \frac{h}{2\pi i} \int_{\Gamma_\ell} e_{n-j}(h\lambda) \otimes F(\lambda) d\lambda g_j \quad (4.1)$$

$$= \frac{1}{2\pi i} \int_{\Gamma_\ell} r(h\lambda)^{n-(b_{\ell-1}-1)} F(\lambda) y^{(\ell)}(h\lambda) d\lambda$$

with

$$y^{(\ell)}(h\lambda) = h \sum_{j=b_\ell}^{b_{\ell-1}-1} e^{(b_{\ell-1}-1)-j}(h\lambda) g_j.$$

Comparing this formula with (2.11), we see that $y^{(\ell)}(h\lambda)$ is the Runge-Kutta approximation to the solution at $t = b_{\ell-1}h$ of the linear initial-value problem

$$y' = \lambda y + g(t), \quad y(b_\ell h) = 0, \quad (4.2)$$

and hence $y^{(\ell)}(h\lambda)$ is computed as such, by Runge-Kutta time-stepping. The integrals are discretized with the quadrature formula discussed in Section 3:

$$u_n^{(\ell)} \doteq \sum_{k=-K}^K w_k^{(\ell)} r(h\lambda_k^{(\ell)})^{n-b_{\ell-1}+1} F(\lambda_k^{(\ell)}) y^{(\ell)}(h\lambda_k^{(\ell)}). \quad (4.3)$$

In the n th time step, we thus compute $u_{n+1}^{(\ell)}$ and for subsequent use we update the Runge-Kutta solutions to the $(2K+1)L$ initial value problems (4.2) for the integration points $\lambda_k^{(\ell)}$ on the contours Γ_ℓ for $\ell = 1, \dots, L$, doing one time step from t_n to t_{n+1} in each of these differential equations.

This algorithm does not keep the history g_j ($j = 0, \dots, n$) in memory. For each $\ell = 1, \dots, L$ and $k = -K, \dots, K$, it stores the Runge-Kutta approximation to (4.2) at the current time step, the values $w_k^{(\ell)}$, $\lambda_k^{(\ell)}$, $r(h\lambda_k^{(\ell)})$, $F(\lambda_k^{(\ell)})$, $y^{(\ell)}(h\lambda_k^{(\ell)})$, and two auxiliary values of the dimension of y needed for book-keeping purposes (cf. [14, 5]). There are only $(2K+1)L$ evaluations of the Laplace transform $F(s)$. In the case of real functions $f(t)$ and $g(t)$ only the real parts of the above sums are needed, and hence the factor $2K+1$ can be replaced by $K+1$, since the quadrature points lie symmetric with respect to the real axis. We recall $L \leq \log_B N$ and $K = O(\log \frac{1}{\varepsilon})$, where ε is the accuracy requirement in the discretization of the contour integrals.

In view of the poor approximation of the first convolution quadrature weights by the discretization of the contour integral, we evaluate $u_{n+1}^{(\ell)}$ directly for a few of the first ℓ , e.g., for $\ell = 0, 1$ with $B = 10$. For this we need to keep the $n - b_1 + 1 \leq 2B$ values g_{b_1}, \dots, g_n in memory, but none of the earlier history g_j for $j \leq n - 2B$. We also need the few convolution quadrature weights $\omega_0, \dots, \omega_{2B-1}$, which may be computed from (3.3) with $2B$ evaluations of the Laplace transform $F(s)$.

For the convolution quadrature based on the second-order BDF method a similar fast algorithm is obtained by inserting the formula (2.4) for $e_{n-j}(h\lambda)$ in (4.1).

4.2. The algorithm for solving integral equations. The adaptation of the above algorithm to integral equations such as

$$v(t) = a(t) + \int_0^t f(t-\tau) g(\tau, v(\tau)) d\tau, \quad t \geq 0, \quad (4.4)$$

is straightforward for the case of the convolution quadrature based on the implicit Euler method and the second-order BDF method, which use solution approximations only on the grid $t = nh$. The extension of the Runge-Kutta based algorithm is, however, less immediate, because the integral approximation uses the internal stages of the Runge-Kutta method. Consider a Runge-Kutta based convolution quadrature under the assumptions of Section 2.2. With the column vector of internal stages $v_n = (v_{ni})_{i=1}^m$, the discretization of (4.4) reads

$$v_n = a_n + \sum_{j=0}^n W_{n-j} g_j, \quad n \geq 0, \quad (4.5)$$

with $a_n = (a(t_n + c_i h))_{i=1}^m$, with weight matrices W_n defined by (2.6), and with $g_j = (g(t_j + c_i h, v_{ji}))_{i=1}^m$ depending on the stages v_{ji} . The scheme is implicit in v_n . The solution at t_{n+1} is approximated by the last component of the stage vector v_n ,

$$u_{n+1} = v_{nm}.$$

With the proof of [13, Theorem 4.1] we obtain that the error of this approximation over bounded time intervals is bounded by $O(h^\kappa)$ with $\kappa = \min(p, q + 1)$, where p and q are the classical order and stage order, respectively, of the underlying Runge-Kutta method. This estimate holds under the assumption that the solution is sufficiently smooth. It gives orders 3 and 4 for the 2- and 3-stage Radau IIA methods, respectively. The precise approximation order for the 3-stage method (of classical order 5) may become larger under appropriate conditions on the nonlinearity and the convolution kernel, cf. [13, Theorem 4.2].

The weight matrix W_n has the integral representation, cf. (2.9),

$$W_n = \frac{h}{2\pi i} \int_{\Gamma} E_n(h\lambda) \otimes F(\lambda) d\lambda,$$

where the $m \times m$ matrix $E_n(z)$ is defined by (2.8). By Lemma 2.4 of [13], for $n \geq 1$, $E_n(z)$ is the rank-1 matrix given by

$$\begin{aligned} E_n(z) &= r(z)^{n-1} (I - z\mathcal{Q})^{-1} \mathbb{1} b^T (I - z\mathcal{Q})^{-1} \\ &= r(z)^{-1} (I - z\mathcal{Q})^{-1} \mathbb{1} e_n(z). \end{aligned}$$

These relations permit us to proceed for the history term of (4.5) as we did for (2.7). We split the stage vector v_n as

$$v_n = a_n + v_n^{(0)} + \dots + v_n^{(L)} \quad \text{with} \quad v_n^{(\ell)} = \sum_{j=b_\ell}^{b_{\ell-1}-1} W_{n-j} g_j$$

and obtain, like in (4.1),

$$v_n^{(\ell)} = \frac{1}{2\pi i} \int_{\Gamma_\ell} r(h\lambda)^{n-b_{\ell-1}} (I - h\lambda\mathcal{Q})^{-1} \mathbb{1} \otimes F(\lambda) y^{(\ell)}(h\lambda) d\lambda,$$

where $y^{(\ell)}(h\lambda)$ is again the Runge-Kutta approximation at $t = b_{\ell-1}h$ to the initial-value problem (4.2), now for the inhomogeneity values $g_j = (g(t_j + c_i h, v_{ji}))_{i=1}^m$ in place of $g_j = (g(t_j + c_i h))_{i=1}^m$. For $\ell \geq 2$ or 3, we thus approximate $v_n^{(\ell)}$ as

$$v_n^{(\ell)} \doteq \sum_{k=-K}^K w_k^{(\ell)} r(h\lambda_k^{(\ell)})^{n-b_{\ell-1}} (I - h\lambda_k^{(\ell)}\mathcal{Q})^{-1} \mathbb{1} \otimes F(\lambda_k^{(\ell)}) y^{(\ell)}(h\lambda_k^{(\ell)}).$$

The algorithm stores the same values as before. The memory requirements for the algorithm are thus independent of the number of stages m and remain essentially the same as in the pure convolution case.

5. Numerical experiments. We give two examples to illustrate the application and behavior of the fast convolution algorithm.

5.1. A nonlinear Volterra equation. We consider a nonlinear Volterra integral equation with weakly singular kernel from [6],

$$u(t) = - \int_0^t \frac{(u(\tau) - \sin(\tau))^3}{\sqrt{\pi(t-\tau)}} d\tau. \quad (5.1)$$

The convolution quadrature based on the backward Euler method gives the implicit discretization

$$u_n = \sum_{j=0}^n \omega_{n-j} (u_j - \sin(jh))^3,$$

where ω_n is given by (1.3) with $F(s) = s^{-1/2}$ and $\delta(\zeta) = 1 - \zeta$. To solve the nonlinear equation in each time step we use Newton iterations. The history term is computed by the fast algorithm of the previous section.

We consider also the discretizations based on the backward differentiation method of order 2, cf. Section 2.1, and on the 2- and 3-stage RadauIIA implicit Runge-Kutta methods of orders 3 and 5, respectively; see Sections 2.2 and 4.2.

In the numerical experiment we use the base $B = 5$ and the Talbot contours with $K = 15$ and $K = 30$ and the further parameters as in Section 3.2. We choose a tolerance of 10^{-12} in the Newton method. The error is calculated with respect to a reference solution, obtained with $h = 0.001$. Figure 5.1 shows the evolution of the absolute error and the oscillating solution u .

Figure 5.2 shows the errors $u_n - u(t_n)$ versus the step size h at time $t_n = 60$, for $K = 15$ and $K = 30$.

Figure 5.3 plots the cpu time versus the number of integration steps, up to 10^6 time steps. The near-linear growth of the computational work is clearly visible.

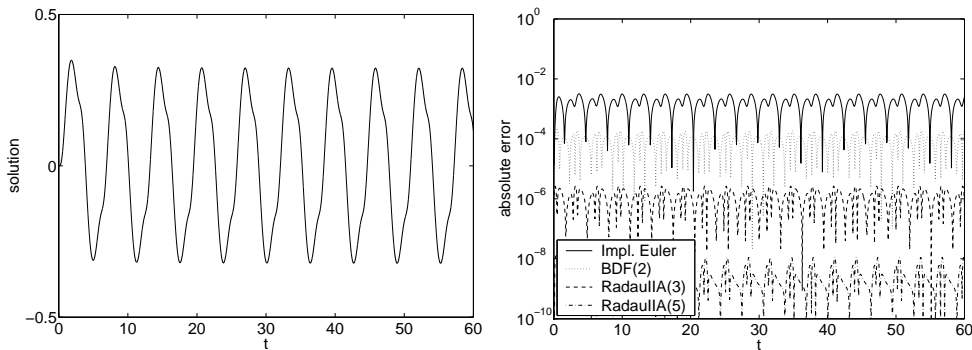


FIG. 5.1. Evolution of the solution over the interval $[0, 60]$ (left) and absolute error for different time integration methods (right) for $h = 0.05$ and $K = 30$.

5.2. Fractional diffusion with transparent boundary conditions. Here we consider a fractional diffusion equation on the real line; see, e.g., [15] for applications of such equations in physics and for numerous references. The equation can be formulated as

$$u(x, t) - u_0(x) = \int_0^t \frac{(t - \tau)^{\alpha-1}}{\Gamma(\alpha)} \partial_{xx} u(x, \tau) d\tau + g(x, t) \quad \text{for } x \in \mathbb{R}, \quad t > 0 \quad (5.2)$$

with the asymptotic condition $u(x, t) \rightarrow 0$ for $x \rightarrow \pm\infty$, for an inhomogeneity g with $g(x, 0) = 0$. To reduce the computation to a finite domain $x \in [-a, a]$ for initial data u_0 and inhomogeneity g with support in $[-a, a]$, we impose transparent boundary conditions at $x = \pm a$, which read

$$u(\pm a, t) = - \int_0^t \frac{(t - \tau)^{\alpha/2-1}}{\Gamma(\alpha/2)} \partial_\nu u(\pm a, \tau) d\tau, \quad (5.3)$$

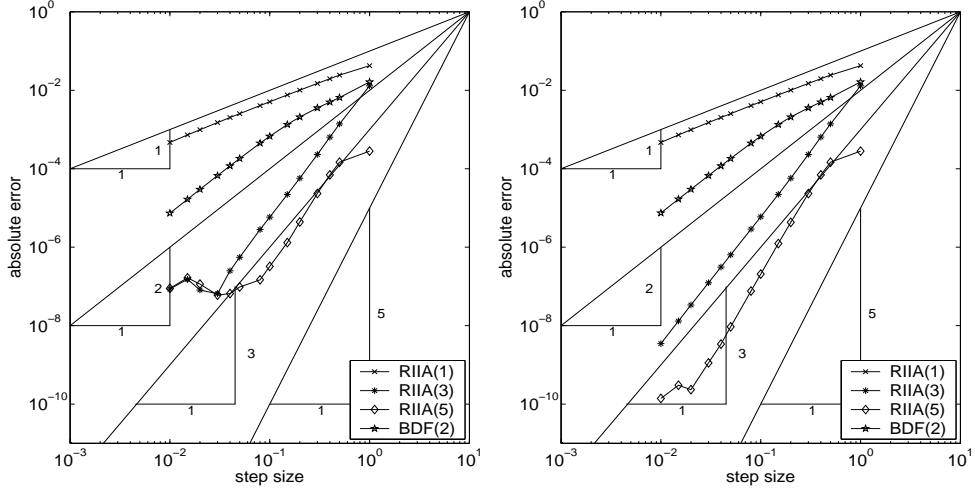


FIG. 5.2. Absolute error vs. step size h , for different integration methods, with $K = 15$ (left) and $K = 30$ (right).

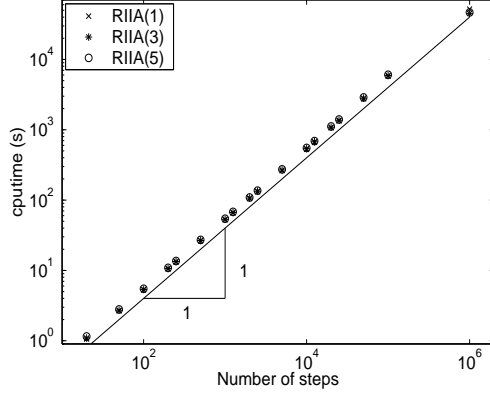


FIG. 5.3. Cpu time in seconds versus the number of integration steps.

with the outward derivative $\partial_\nu = \pm \partial_x$ at $x = \pm a$. These boundary conditions are derived with Laplace transform techniques in the same way as for the wave or the Schrödinger equation; see, e.g., [2]. Space discretisation of (5.2) is done using second order finite differences and a central finite difference to approximate the normal derivative. With the notation

$$\delta_{xx}u_l^n = \frac{1}{\Delta x^2}(u_{l-1}^n - 2u_l^n + u_{l+1}^n), \quad \delta_\nu u_{\pm(M-1)}^n = \frac{1}{2\Delta x}(u_{\pm M}^n - u_{\pm(M-2)}^n)$$

for $a = M\Delta x$, the discrete equation approximating (5.2) is

$$\begin{aligned} u_l^n - u_l^0 &= \sum_{j=0}^n \omega_{n-j}^{(\alpha)} \delta_{xx}u_l^j + g_l^n \quad \text{for } l = -(M-1), \dots, M-1; n > 0, \\ u_{\pm(M-1)}^n &= -\sum_{j=0}^n \omega_{n-j}^{(\alpha/2)} \delta_\nu u_{\pm(M-1)}^j, \end{aligned} \tag{5.4}$$

where the weights $\omega_n^{(\beta)}$ are the convolution quadrature weights for the kernel $f(t) = t^{\beta-1}/\Gamma(\beta)$ with Laplace transform $F(s) = s^{-\beta}$.

In the numerical example we set $a = 5$ and $M = 450$. We consider the problem with $\alpha = 2/3$ and no inhomogeneity, i.e., $g \equiv 0$. The initial value is $u(x,0) = \exp(-x^2)$. Figure 5.4 shows the errors at $t = 2$ in dependence on the step size for the Radau IIA methods of orders 1, 3, 5, obtained with $B = 5$ and $K = 15$ in the fast convolution algorithm. The reference solution is obtained with the Radau IIA method of order 5, with $h = 0.0002$ and $K = 40$. We observe an order reduction for the higher-order methods, which is due to the temporal non-smoothness of the solution at $t = 0$; cf. [1, Sect. 8]. Nevertheless, the higher-order methods give much better accuracy.

The work diagram looks almost identical to Figure 5.3, showing practically linear dependence of the computational work on the number of time steps. The required memory is less than 200 entries per spatial grid point for up to $N \leq 10^4$ steps, and less than 300 entries per grid point for $N \leq 10^6$ steps. These numbers are halved if we run the algorithm with $B = 10$, $K = 10$ instead of $B = 5$, $K = 15$, as is sufficient for less stringent accuracy requirements ($\sim 10^{-3}$).

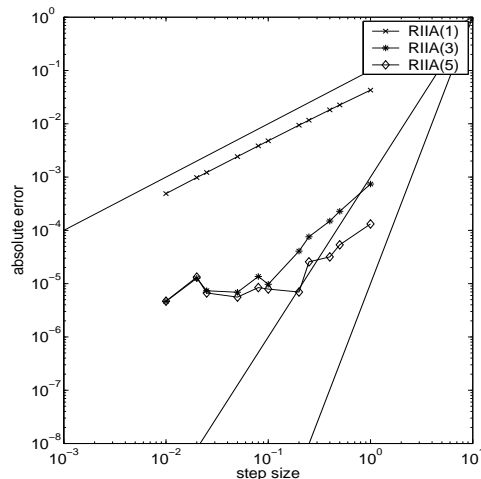


FIG. 5.4. Absolute error vs. time step, for different integration methods, with $K = 15$.

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