

A FAST TIME STEPPING METHOD FOR EVALUATING FRACTIONAL INTEGRALS*

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Abstract. We evaluate the fractional integral $I^\alpha[f](t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau) d\tau$, $0 < \alpha < 1$, at time steps $t = \Delta t, 2\Delta t, \dots, N\Delta t$ by making use of the integral representation of the convolution kernel $t^{\alpha-1} = \frac{1}{\Gamma(1-\alpha)} \int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi$. We construct an efficient Q -point quadrature of this integral representation and use it as a part of a fast time stepping method. The new method has algorithmic complexity $O(NQ)$ and storage requirement $O(Q)$. The number of quadrature nodes Q is independent of N and grows like $O((-\log \epsilon - \log \Delta t)^2)$, where ϵ is the quadrature error tolerance and Δt is the size of the time step. The (possible) singularity of f near $\tau = 0$ is taken into account. This new method is particularly well-suited for long time simulations.

Key words. fractional integrals, fractional differential equations, fast convolution, quadrature of Laplace transform, diffusive representation

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1. Introduction. In recent years models have come from physical applications which involve fractional (noninteger) order integrals and derivatives [2, 6, 18, 24]. Numerical methods for the evaluation of fractional order integrals and the solution of fractional order differential equations can be found in numerous papers (an early work is in [19], and a recent survey can be found in [10]). In the iterative solution of fractional order differential equations, one is led to the repeated evaluation of fractional order integrals, which will be the focus of this paper.

We seek to evaluate the fractional integral of order α ,

$$(1) \quad I^\alpha[f](t) := \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau) d\tau, \quad 0 < \alpha < 1,$$

at time steps $t = \Delta t, 2\Delta t, \dots$ for smooth and nonsmooth f . We have in mind that this is a part of the simulation process of a dynamical model. One may want to simulate this model for very long times, and the final time of simulation may not be fixed a priori.

The principal difficulty in evaluating (1) for long times is that the convolution kernel $t^{\alpha-1}$ decays slowly for large t . Hence, to compute $I^\alpha[f](t)$ the contribution due to $f(\tau)$ for τ far away from t cannot be neglected. This is the reason that systems which contain terms like $I^\alpha[f](t)$ are said to have memory. Hence, a naive discretization of (1),

$$I^\alpha[f](n\Delta t) \approx \sum_{j=0}^n c_{nj} f(j\Delta t)$$

gives rise to an algorithmic complexity which is quadratic in the number of time steps, because the coefficients c_{nj} changes with the time step n , reflecting the fact that $(t-\tau)^{\alpha-1}$ depends on t .

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An additional complication comes from the fact that the input function f may have an integrable end point singularity: in the solution of fractional order differential equations, the input function will be the solution obtained up to the current time step, and it will be a sum of terms of the form

$$(2) \quad \{t^\beta, \beta = j + l\alpha, j, l \in \{0, 1, 2, \dots\}\}.$$

In a classical approach (see [19] and later works) the fractional integral in (1) is approximated as the sum of a discrete convolution and a few correction terms:

$$(3) \quad \frac{1}{\Gamma(\alpha)} \int_0^{n\Delta t} (n\Delta t - \tau)^{\alpha-1} f(\tau) d\tau \approx \Delta t^\alpha \sum_{j=0}^n \omega_{n-j} f(j\Delta t) + \Delta t^\alpha \sum_{j=0}^s w_{nj} f(j\Delta t),$$

$$n = 1, 2, \dots, N.$$

The convolution weights ω_j , $j = 0, \dots, N$, are obtained as the Taylor expansion coefficients of the generating function, taken to the power α , of a linear multistep method for first order ODEs (for example, Euler and backward differentiation formulas). For a fixed N , they can be computed via the fast Fourier transform. The weights of the correction terms w_{nj} , $n = 1, \dots, N$, $j = 1, \dots, s$, are the solution of a generalized Vandermonde linear system, obtained by requiring that s functions with the lowest powers in the set described by (2) satisfy (3) exactly. This system is ill-conditioned, and it must be solved at each time step n (see [9] for further details). Suppose the weights ω_j , $j = 0, \dots, N$, and w_{nj} , $n = 1, \dots, N$, $j = 1, \dots, s$, have been thus obtained. The sum in (3) can be computed for $n = 1, \dots, N$, in $O(N(\log N)^2)$ complexity with $O(N)$ storage, by properly ordering the computations on the triangle $\{(t, \tau) : 0 \leq \tau \leq t \leq T\}$ and using the fast Fourier transform [14].

There are also methods (see, for example, [7]) based on the direct quadrature of (1). In [11] a special meshing of the interval of integration was suggested to improve performance. Other works are in [15, 28].

In another group of works the model containing the fractional integral is reformulated as a system of differential equations by taking advantage of a particular integral representation of the convolution kernel $t^{\alpha-1}$:

$$(4) \quad t^{\alpha-1} = \frac{1}{\Gamma(1-\alpha)} \int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi.$$

This or a similar representation was used for the purpose of analysis in [21, 22, 23, 27] and for the purpose of numerical simulation in [3, 16, 23, 30]. The numerical algorithms suggested by [30] and [3], which are very similar, were used in [18, 29, 30] and analyzed and criticized in [8, 18, 26].

The numerical algorithms formulated in [3, 16, 23, 30] all required a good discretization of (4), i.e., an efficient and accurate quadrature for the function $e^{-\xi t} \xi^{-\alpha}$ on the half-line $[0, \infty)$. The principal difficulty with this problem lies in the fact that $e^{-\xi t} \xi^{-\alpha}$ depends on t , but the quadrature, ideally, should not depend on t . In [16, 23] a quadrature involving logarithmically spaced nodes was proposed. In [30] and other papers that use the method proposed there, generalized Gaussian type quadratures (Gauss–Laguerre for the weight function e^{-x} and Gauss–Jacobi for a weight function containing fractional order end point singularities) were suggested.

We believe the major default of these previous works is that the authors attempted to find a quadrature that is accurate for all $t \in [0, \infty)$ or for all $t \in [0, T_{max}]$, which

is an impossible task, given that the integral does not converge at $t = 0$. This can be clearly seen in the singularity of $t^{\alpha-1}$ at $t = 0$. Hence, in our work, we limit the use of the integral representation in (4) to t which is at least Δt away from 0. We present a quadrature which is efficient and accurate to within a given error tolerance for *all* $t \in [\Delta t, \infty)$.

The idea that an integral representation should only be used for $t \geq \Delta t$ is included in another set of works [17, 20, 25]. But these works use a substantially different integral representation, in fact, a complex contour integral. For the case of the kernel $t^{\alpha-1}$ this representation is

$$(5) \quad t^{\alpha-1} = \Gamma(\alpha) \frac{1}{2\pi i} \int_{\Lambda} e^{\xi t} \xi^{-\alpha} d\xi,$$

where Λ is a contour in the complex plane in the region of analyticity. Those authors were not able to find one unique quadrature set for (5) that is accurate for all $t \in [0, T_{max}]$, so they divided $[0, T_{max}]$ into geometrically growing and overlapping intervals $\bigcup_l [B^{l-1}\Delta t, B^{l+1}\Delta t]$ for some $B > 1$, and a different quadrature (on a different contour) is used for each interval $[B^{l-1}\Delta t, B^{l+1}\Delta t]$. This leads to a complicated time stepping strategy because all quadrature nodes must be advanced at every time step. Clearly, it is also necessary to selectively store and delete the “past” values of f to keep the storage requirement down. However, because the quadrature sets depend on t , if one decides during the course of simulation to continue past T_{max} , additional quadrature sets for further time intervals must be advanced from the beginning. If the values of the input function f for the earlier times were not stored, then they need to be recomputed. The advantage of this approach is that it can be used for a more general class of kernels, but for the particular case of $t^{\alpha-1}$, we believe the method we propose is superior.

We will formulate one quadrature set that is accurate to a tolerance ϵ for the entire interval $[\Delta t, \infty)$; there is no limitation on T_{max} , so the simulation can continue as long as needed. We show that the number of points in the quadrature set Q is $O((-\log \epsilon - \log \Delta t)^2)$. The complexity of our algorithm is then $O(NQ)$, where N is the number of time steps, and the storage is $O(Q)$. Because Q does not depend on N , the number of time steps does not need to be fixed a priori to achieve linear algorithmic complexity.

In this paper we do not reformulate the fractional integral as a part of the solution of a system of differential equations as is typically done. We simply keep it as an integral and evaluate all needed quantities in integral form, in other words, by numerical quadrature rather than passing via an intermediate ODE method. There are situations where the latter approach may be preferred, such as if a stability analysis of the full numerical algorithm is desired.

The work in this paper is motivated by the approach taken in [12] where a quadrature set is generated for the heat kernel ($\alpha = \frac{1}{2}$) which is valid for $[\Delta t, \infty)$. In this paper we compute quadratures valid for other values of α and give a complete analysis of the quadrature error and a different bound on Q . We show explicitly how these quantities depend on α . In addition, we treat the case of input functions f which may have an end point singularity at $t = 0$.

This paper is organized as follows. In section 2 we describe the overall fast time stepping algorithm. In section 3 we describe the generation of a quadrature for the convolution kernel $t^{\alpha-1}$. In section 4 we discuss the treatment of nonsmooth input functions. Section 5 contains the numerical results and section 6 the conclusions.

2. Fast time stepping. The convolution kernel $t^{\alpha-1}$ is special in that it has the integral representation given in (4). In other words, $t^{\alpha-1}$ is the Laplace transform of $\frac{1}{\Gamma(1-\alpha)}\xi^{-\alpha}$. This and other similar representations were also used in [3, 16, 23, 30] and later works.

We are tempted to take advantage of the representation in (4) in the following way:

$$\begin{aligned} I^\alpha[f](t) &= \frac{1}{\Gamma(\alpha)} \int_0^t \frac{1}{\Gamma(1-\alpha)} \int_0^\infty e^{-\xi(t-\tau)} \xi^{-\alpha} d\xi f(\tau) d\tau \\ &= \frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(1-\alpha)} \int_0^\infty \left(\int_0^t e^{-\xi(t-\tau)} f(\tau) d\tau \right) \xi^{-\alpha} d\xi \\ &= \frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(1-\alpha)} \int_0^\infty g(\xi, t) \xi^{-\alpha} d\xi, \end{aligned}$$

where we have defined the quantity

$$g(\xi, t) := \int_0^t e^{-\xi(t-\tau)} f(\tau) d\tau.$$

A well-known trick in the literature (used for generating nonreflecting boundary conditions [1] and for accelerating convolutions with the heat kernel [13]) involves recognizing that

$$g(\xi, t) = e^{-\xi\Delta t} g(\xi, t - \Delta t) + \Psi(\xi, t, \Delta t),$$

where

$$\Psi(\xi, t, \Delta t) = \int_{t-\Delta t}^t e^{-\xi(t-\tau)} f(\tau) d\tau.$$

In other words, obtaining the value $g(\xi, t)$ from the previous value $g(\xi, t - \Delta t)$ requires only a constant multiplication by the exponential decay term $e^{-\xi\Delta t}$, and the computation of $\Psi(t, \Delta t)$, which is local in time. Alternatively, others [3, 16, 23, 30] have preferred the following differential formulation: $g(\xi, t)$ is the solution of a first order ODE in time,

$$\frac{dg}{dt}(\xi, t) = -\xi g(\xi, t) + f(t), \quad g(\xi, 0) = 0.$$

Again, any ODE method can be used to obtain $g(\xi, t)$, $t = \Delta t, 2\Delta t, \dots$, in an amount of work which is linear in the number of time steps.

The principal difficulty of implementing this approach lies in the discretization of the integral

$$(6) \quad \int_0^\infty g(\xi, t) \xi^{-\alpha} d\xi.$$

We need a set of quadrature nodes ξ_1, \dots, ξ_Q and weights w_1, \dots, w_Q for (6). For the formulation of a straightforward algorithm, it is necessary that the quadrature nodes and weights do not change with time. If they do change, we might be forced to follow a complicated time marching strategy as in [20]. Some other quadrature choices were considered in [8].

Returning to (4), we see that obtaining quadrature nodes and weights which are independent of time means that the approximation

$$\int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi \approx \sum_{j=1}^Q e^{-\xi_j t} \xi_j^{-\alpha} w_j$$

needs to be accurate for all t . Clearly, this is not possible as t goes to 0 since there is a singularity in $t^{\alpha-1}$. In both [12] and [20], the approximation is done only on an interval bounded Δt away from $t = 0$. In this paper we will do the same.

In section 3 we will describe how to obtain a quadrature, whose nodes and weights do not depend on t , such that

$$(7) \quad \left| \int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi - \sum_{j=1}^Q e^{-\xi_j t} \xi_j^{-\alpha} w_j \right| \leq \epsilon \quad \forall t \in [\Delta t, \infty).$$

In the rest of this section, we will describe the overall fast time stepping algorithm, given such a quadrature.

Since (7) is not valid on the interval $[0, \Delta t]$, the convolution in (1) must be broken into two parts. Following the notation of [12], the part where (7) is valid will be called the history part, corresponding to the contribution of $f(\tau)$ on $[0, t - \Delta t]$, which is *historical* with respect to the current time t . The part where (7) is not valid will be called the local part, corresponding to the contribution of $f(\tau)$ on $[t - \Delta t, t]$, which is *local* with respect to the current time t .

We will use the following notation: $I^\alpha[f](t)$ is the sum of two parts

$$I^\alpha[f](t) = H^\alpha[f](t) + L^\alpha[f](t),$$

where the history part is

$$(8) \quad H^\alpha[f](t) := \frac{1}{\Gamma(\alpha)} \int_0^{t-\Delta t} (t-\tau)^{\alpha-1} f(\tau) d\tau$$

and the local part is

$$(9) \quad L^\alpha[f](t) := \frac{1}{\Gamma(\alpha)} \int_{t-\Delta t}^t (t-\tau)^{\alpha-1} f(\tau) d\tau.$$

We will formulate an algorithm based entirely on the discretization of the integrals in (8) and (9). We do not pass via any intermediate algorithms such as linear multistep methods for first order differential equations, as was done in [3, 16, 23, 30], because in this paper we are not concerned with the formulation of a full numerical algorithm for a larger mathematical model in which the fractional integral is one component. In that case, the choice of how to compute the various quantities in our method will be influenced by the desired accuracy and stability properties of the full algorithm.

The time stepping for $H^\alpha[f](t)$ is a slightly modified version of what appeared in the beginning of this section to take into account the fact that we are staying Δt away from the singularity in the convolution kernel. Let us define the intermediate quantity $h(\xi, t, \Delta t)$:

$$(10) \quad h(\xi, t, \Delta t) := \int_0^{t-\Delta t} e^{-\xi(t-\tau)} f(\tau) d\tau.$$

The quantity $h(\xi_j, t, \Delta t)$ will be updated via the formula

$$(11) \quad h(\xi_j, t, \Delta t) = e^{-\xi_j \Delta t} h(\xi_j, t - \Delta t, \Delta t) + \Phi(\xi_j, t, \Delta t),$$

where

$$(12) \quad \Phi(\xi_j, t, \Delta t) = \int_{t-2\Delta t}^{t-\Delta t} e^{-\xi_j(t-\tau)} f(\tau) d\tau.$$

Because of the approximation in (7) we are free to approximate $H^\alpha[f](t)$ by

$$(13) \quad H^\alpha[f](t) \approx \frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(1-\alpha)} \sum_{j=1}^Q h(\xi_j, t, \Delta t) \xi_j^{-\alpha} w_j.$$

The formulas (9), (11), (12), and (13) form the basis of the time stepping algorithm.

In section 4 we will discuss the computations of the local part in (9) and the update quantity $\Phi(t, \Delta t)$ for the history part in (12), taking into account the possible end point singularity of f . As we will see, both of these computations will be $O(1)$ with respect to the number of time steps.

The overall complexity for the algorithm is $O(NQ)$, where N is the number of time steps and Q is the number of quadrature nodes in (7). The storage is $O(Q)$. In the next section we describe a quadrature satisfying (7) with $Q = O((-\log \epsilon - \log \Delta t)^2)$. We emphasize that Q does not depend on N (or equivalently, T_{max}). This is advantageous when Δt is determined by the accuracy requirements of the simulation. The number of time steps N can be taken as large as desired, and the algorithmic complexity will stay linear.

3. Quadrature of the integral representation. In this section we construct a quadrature of the integral

$$(14) \quad \frac{1}{\Gamma(1-\alpha)} \int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi,$$

which is accurate for all $t \in [\Delta t, \infty)$.

First we remove the integrable singularity $\xi^{-\alpha}$ via the change of variables,

$$(15) \quad \gamma = \frac{1}{1-\alpha}, \quad \eta = \xi^{\frac{1}{\gamma}},$$

to obtain

$$(16) \quad \frac{1}{\Gamma(1-\alpha)} \int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi = \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \int_0^\infty e^{-\eta^\gamma t} d\eta.$$

The constant $\frac{1}{\Gamma(1-\alpha)(1-\alpha)}$ is bounded between 1 and 1.13 when $0 < \alpha < 1$. In each of the plots in Figure 1 we show the behavior of $e^{-\eta^\gamma t}$ for several values of t . Each plot is for a particular value of α . The decay of the integrand is fast when γ or t is large, and it is slow when γ or t is small.

Next we reduce the domain of integration to a finite interval by using the following estimate:

$$\frac{1}{\Gamma(1-\alpha)(1-\alpha)} \int_L^\infty e^{-\eta^\gamma t} d\eta \leq \frac{e^{-tL^\gamma}}{t^{\frac{1}{\gamma}}} \leq \frac{e^{-\Delta t L^\gamma}}{\Delta t^{\frac{1}{\gamma}}} \quad \forall t \in [\Delta t, \infty).$$

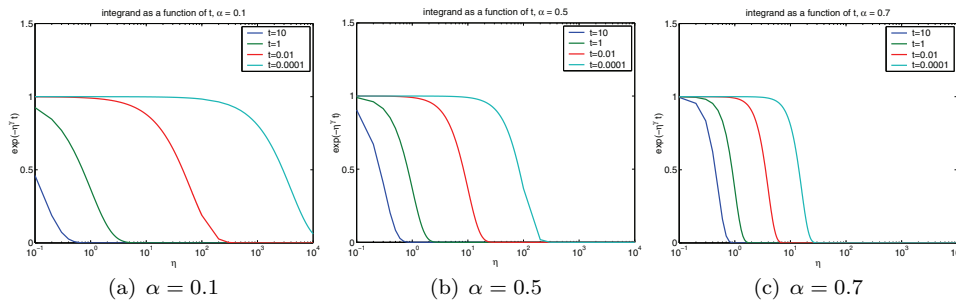


FIG. 1. The behavior of $e^{-\eta^\gamma} t$ for several values of α and t . The decay of the integrand is fast when γ or t is large, and it is slow when γ or t is small. γ and α are related by $\gamma = \frac{1}{1-\alpha}$.

Thus, if we choose $\eta_{max} \geq L(\Delta t, \epsilon, \alpha)$ where

$$L(\Delta t, \epsilon, \alpha) = \left(\frac{\log\left(\frac{\epsilon}{3} \Delta t^{1-\alpha}\right)}{-\Delta t} \right)^{1-\alpha} = \left(\frac{1}{\Delta t} \right)^{1-\alpha} \left(-\log \frac{\epsilon}{3} - (1-\alpha) \log \Delta t \right)^{1-\alpha},$$

we can ensure that

$$\left| \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \int_{\eta_{max}(\Delta t, \epsilon, \alpha)}^\infty e^{-\eta^\gamma} t \, d\eta \right| \leq \frac{\epsilon}{3} \quad \forall t \in [\Delta t, \infty).$$

Since t varies from Δt to ∞ , we need to construct a single quadrature which accurately approximates the integral for this one-parameter family of integrands. Over a generic interval $[a, b]$, the integrand $e^{-\eta^\gamma} t$ varies from almost identically 1 to almost identically 0. A quadrature must approximate accurately this range of behavior.

It is not difficult to see that the region of the most rapid change in the integrand $e^{-\eta^\gamma} t$ occurs at the inflection point $\eta_{inflec} = \left(\frac{\gamma-1}{\gamma t}\right)^{\frac{1}{\gamma}} = \left(\frac{\alpha}{t}\right)^{1-\alpha}$. The inflection points, and hence the regions of the most rapid change, cluster toward $\eta = 0$ as t increases. A quadrature of (16) must capture this clustering near 0. To this end we follow the development in [12] and cover $[0, L(\Delta t, \epsilon, \alpha)]$ by dyadic intervals (in the variable η):

$$\bigcup_{j=j_{min}}^{j_{max}} [a_j := 2^j, b_j := 2^{j+1}] = [a_{j_{min}} = 2^{j_{min}}, b_{j_{max}} = 2^{j_{max}+1}],$$

where a_j and b_j are the end points of the j th dyadic interval. The quadrature we develop will be the union of quadrature sets on each of these intervals $\{[a_j, b_j], j = j_{min}, \dots, j_{max}\}$.

In the following lemma we state the number of dyadic intervals needed to cover $[0, L(\Delta t, \epsilon, \alpha)]$ accurately.

LEMMA 1 (bound on the number of dyadic intervals). *Define*

$$j_{min} := \left\lceil \frac{\log\left(\Gamma(1-\alpha)(1-\alpha)\frac{\epsilon}{3}\right)}{\log 2} \right\rceil$$

and

$$j_{max} := \left\lceil \frac{\log L(\Delta t, \epsilon, \alpha)}{\log 2} \right\rceil - 1;$$

then

$$(22) \quad \left| \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \left(\int_0^\infty e^{-\eta^\gamma t} d\eta - \int_{a_{j_{min}}=2^{j_{min}}}^{b_{j_{max}}=2^{j_{max}+1}} e^{-\eta^\gamma t} d\eta \right) \right| \leq \frac{2}{3} \epsilon, \quad t \in [\Delta t, \infty).$$

Proof. Equation (20) ensures that

$$\left| \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \int_0^{a_{j_{min}}=2^{j_{min}}} e^{-\eta^\gamma t} d\eta \right| \leq \frac{\epsilon}{3}, \quad t \in [0, \infty),$$

and (21) ensures that $b_{j_{max}} = 2^{j_{max}+1} \geq L(\Delta t, \epsilon, \alpha)$ and hence (18) will be satisfied. \square

Next we will construct a quadrature set

$$\{\eta_j\} = \{\eta_j^1, \dots, \eta_j^{Q_j}\}, \quad \{v_j\} = \{v_j^1, \dots, v_j^{Q_j}\}$$

for each interval of integration $[a_j = 2^j, b_j = 2^{j+1}]$ with error tolerance $\frac{\epsilon}{3} \frac{(b_j - a_j)}{b_{j_{max}}}$. Once the interval of integration is made finite, there is no problem with $t \leq \Delta t$. We consider all $t \in [0, \infty)$ in the following lemma to take advantage of the scaling property described below.

Due to the fortuitous choice of dyadic intervals we show now that the quadrature set for $[a_j, b_j]$ can be obtained by a simple scaling of the quadrature set for a reference interval, for example, $[a_0 = 1, b_0 = 2]$. This is the subject of the next lemma.

LEMMA 2 (scaling property of quadrature sets on dyadic intervals). *Suppose*

$$\{\eta_0\} = \{\eta_0^1, \dots, \eta_0^{Q_0}\}, \quad \{v_0\} = \{v_0^1, \dots, v_0^{Q_0}\}$$

is the Q_0 -point quadrature set for the interval $[1, 2]$, with tolerance $\frac{\epsilon}{3} \frac{1}{b_{max}}$, i.e.,

$$(23) \quad \left| \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \left(\int_1^2 e^{-\eta^\gamma t} d\eta - \sum_{i=1}^{Q_0} e^{-(\eta_0^i)^\gamma t} v_0^i \right) \right| \leq \frac{\epsilon}{3} \frac{1}{b_{j_{max}}} \quad \forall t \in [0, \infty);$$

then by defining

$$(24) \quad Q_j = Q_0, \quad \eta_j^i = a_j \eta_0^i, \quad v_j^i = a_j v_0^i,$$

the error bound

$$(25) \quad \left| \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \left(\int_{a_j}^{b_j} e^{-\eta^\gamma t} d\eta - \sum_{i=1}^{Q_j} e^{-(\eta_j^i)^\gamma t} v_j^i \right) \right| \leq \frac{\epsilon}{3} \frac{(b_j - a_j)}{b_{j_{max}}} \quad \forall t \in [0, \infty)$$

is satisfied for all j .

Proof. Using the fact that $b_j - a_j = a_j$, we obtain

$$\begin{aligned} \int_{a_j}^{b_j} e^{-\eta^\gamma t} d\eta - \sum_{i=1}^{Q_j} e^{-(\eta_j^i)^\gamma t} v_j^i &= \int_1^2 a_j e^{-(a_j \eta)^\gamma t} d\eta - \sum_{i=1}^{Q_0} e^{-(a_j \eta_0^i)^\gamma t} a_j v_0^i \\ &= a_j \left(\int_1^2 e^{-\eta^\gamma ((a_j)^\gamma t)} d\eta - \sum_{i=1}^{Q_0} e^{-(\eta_0^i)^\gamma ((a_j)^\gamma t)} v_0^i \right), \end{aligned}$$

and hence

$$\max_{t \in [0, \infty)} \left| \int_{a_j}^{b_j} e^{-\eta^\gamma t} d\eta - \sum_{i=1}^{Q_j} e^{-(\eta_j^i)^\gamma t} v_j^i \right| = a_j \max_{t \in [0, \infty)} \left| \int_1^2 e^{-\eta^\gamma t} d\eta - \sum_{i=1}^{Q_0} e^{-(\eta_0^i)^\gamma t} v_0^i \right|.$$

The position t where the maximum occurs is simply scaled by $(a_j)^\gamma$ when going from $[a_j, b_j]$ to $[1, 2]$. Clearly, with the choice in (24), (25) is satisfied for all j if (23) is satisfied for the reference interval $[1, 2]$. \square

Now we tackle the only remaining problem: finding a quadrature for the reference interval $\eta \in [1, 2]$ satisfying (23). Because we want a fast converging quadrature, we turn to the Gauss–Legendre quadrature for smooth integrands. To obtain an asymptotic bound on Q_0 we use the following theorem due to Davis and Rabinowitz [5].

DEFINITION 1. We denote by L_ρ , $\rho > 1$, the ellipse in the complex plane whose foci are at $z = \pm 1$, whose major axis is the line segment $[-A(\rho), A(\rho)]$ lying along the x -axis, and whose minor axis is the segment $[-B(\rho), B(\rho)]$ lying along the y -axis, where

$$A(\rho) = \frac{1}{2}(\rho + \rho^{-1}), \quad B(\rho) := \frac{1}{2}(\rho - \rho^{-1}).$$

This ellipse collapses to the line segment $[-1, 1]$ on the x -axis when $\rho = 1$ and becomes a circle of diameter ρ when $\rho \rightarrow \infty$.

The formulation of the following theorem was taken from [4].

THEOREM 1. Let g be analytic on $[-1, 1]$ and be continuable analytically so as to be single valued and regular in the ellipse L_ρ defined above. Let $\{x_1, \dots, x_Q\}$ and $\{w_1, \dots, w_Q\}$ be the nodes and weights, respectively, of the Q -point Gauss–Legendre quadrature on the interval $[-1, 1]$; then given $\delta > 0$, there exists $N(\delta)$ such that if $Q \geq N(\delta)$, the following is satisfied:

$$\left| \int_{-1}^1 g(x) dx - \sum_{i=1}^Q g(x^i) w^i \right| \leq 2K(\rho) M(\rho) \frac{(1 - \frac{\delta}{\rho})^{-Q}}{\rho^{2Q}},$$

where $K(\rho) := \frac{l(L_\rho)}{\pi(\rho - \rho^{-1})}$, $l(L_\rho)$ is the length of L_ρ , and $M(\rho) := \max_{z \in L_\rho} |g(z)|$.

Thus, the asymptotic convergence of the Gauss–Legendre quadrature is $O(\rho^{-2Q})$ if we can bound $M(\rho)$, which is a maximum taken over a region in the complex plane.

We now proceed to find a ρ for which we can bound $M(\rho)$ by 1.

LEMMA 3 (convergence of the Gauss–Legendre quadrature on reference interval).

Define

$$(26) \quad \rho_{max}(\gamma) := \sqrt{\frac{17w^2 + 1 + 4\sqrt{18w^4 + 2w^2}}{w^2 + 1}}, \quad \text{where } w := \tan \frac{\pi}{2\gamma},$$

and let

$$\{\eta_0\} = \{\eta_0^1, \dots, \eta_0^{Q_0}\}, \quad \{v_0\} = \{v_0^1, \dots, v_0^{Q_0}\}$$

be the Q_0 -point Gauss–Legendre quadrature scaled on $[1, 2]$; then

$$(27) \quad E(Q_0, t, \alpha) := \left| \left(\int_1^2 e^{-\eta^\gamma t} d\eta - \sum_{i=1}^{Q_0} e^{-(\eta_0^i)^\gamma t} v_0^i \right) \right| \leq K(\rho_{max}) \frac{(1 - \frac{\delta}{\rho_{max}})^{-Q_0}}{(\rho_{max})^{2Q_0}} \quad \forall t \in [0, \infty).$$

Thus, the asymptotic behavior of $E(Q_0, t, \alpha)$ is

$$(28) \quad E(Q_0, t, \alpha) = O\left((\rho_{max}(\gamma))^{-2Q_0}\right) \quad \forall t \in [0, \infty).$$

The limiting values of ρ_{max} are

$$(29) \quad \lim_{\alpha \rightarrow 0^+, \gamma \rightarrow 1^+} \rho_{max}(\gamma) = 3 + 2\sqrt{2} \approx 5.828427124 \quad \text{and} \quad \lim_{\alpha \rightarrow 1^-, \gamma \rightarrow \infty} \rho_{max}(\gamma) = 1.$$

To first order,

$$\lim_{\alpha \rightarrow 1^-, \gamma \rightarrow \infty} \rho_{max}(\gamma) \approx 1 + \frac{\sqrt{2} \pi}{\gamma} = 1 + \sqrt{2} \pi (1 - \alpha).$$

Proof. We scale our integrand onto the standard Gauss–Legendre quadrature interval $[-1, 1]$:

$$(30) \quad \tilde{g}(\eta, t, \gamma) := e^{-\eta^\gamma t} = g\left(x = 2\left(\eta - \frac{3}{2}\right)\right), \quad \eta \in [1, 2],$$

where the shifted and scaled function defined on $[-1, 1]$ is

$$(31) \quad g(x) := \tilde{g}\left(\frac{1}{2}x + \frac{3}{2}, t, \gamma\right), \quad x \in [-1, 1].$$

Clearly,

$$\begin{aligned} \int_1^2 \tilde{g}(\eta, t, \gamma) d\eta - \sum_{i=1}^Q \left[\tilde{g}\left(\left(\frac{1}{2}x^i + \frac{3}{2}\right), t, \gamma\right) \left(\frac{1}{2}w^i\right) \right] \\ = \frac{1}{2} \left(\int_{-1}^1 g(x) dx - \sum_{i=1}^Q g(x^i)w^i \right), \end{aligned}$$

where the scaled Gauss–Legendre quadrature set on $[1, 2]$ is

$$\eta^i = \frac{1}{2}x^i + \frac{3}{2}, \quad v^i = \frac{1}{2}w^i, \quad i = 1, \dots, Q.$$

It is easy to see that the error on $[1, 2]$ is half the error on $[-1, 1]$:

$$\left| \int_1^2 \tilde{g}(\eta, t, \gamma) d\eta - \sum_{i=1}^Q \tilde{g}(\eta^i, t, \gamma) v^i \right| = \frac{1}{2} \left| \int_{-1}^1 g(x) dx - \sum_{i=1}^Q g(x^i)w^i \right|.$$

We now focus on bounding $M(\rho)$ for g :

$$M(\rho) = \max_{z \in L_\rho} |g(z)| = \max_{z \in L_\rho} \left| \tilde{g}\left(\frac{1}{2}z + \frac{3}{2}, t, \gamma\right) \right| = \max_{\tilde{z} \in \{\frac{1}{2}L_\rho + \frac{3}{2}\}} |\tilde{g}(\tilde{z}, t, \gamma)|.$$

Looking at the set

$$\tilde{L}_\rho := \left\{ \frac{1}{2}L_\rho + \frac{3}{2} \right\},$$

we see it remains an ellipse, now centered at $(\frac{3}{2}, 0)$, whose major axis is the line segment $[-\tilde{A}(\rho) + \frac{3}{2}, \tilde{A}(\rho) + \frac{3}{2}]$ lying along the x -axis and whose minor axis is the segment $[\frac{3}{2} - i\tilde{B}(\rho), \frac{3}{2} + i\tilde{B}(\rho)]$, where

$$\tilde{A}(\rho) = \frac{1}{4}(\rho + \rho^{-1}), \quad \tilde{B}(\rho) := \frac{1}{4}(\rho - \rho^{-1}).$$

We keep \tilde{L}_ρ in the right half-plane, away from the singularity of $\log z$ at $z = 0$, meaning

$$\tilde{A}(\rho) < \frac{3}{2} \implies \rho < 3 + 2\sqrt{2}.$$

We now make an estimate for

$$M(\rho) = \max_{\tilde{z} \in \tilde{L}_\rho} \left| e^{-\tilde{z}^\gamma t} \right| = \max_{\tilde{z} \in \tilde{L}_\rho} \left| e^{-|\tilde{z}|^\gamma e^{i\gamma \arg \tilde{z}} t} \right| = \max_{\tilde{z} \in \tilde{L}_\rho} e^{-|\tilde{z}|^\gamma \cos(\gamma \arg \tilde{z}) t}.$$

We choose to bound $M(\rho)$ by

$$(32) \quad M(\rho) \leq 1 \quad \forall t \in [0, \infty),$$

which will be satisfied if

$$(33) \quad \cos(\gamma \arg \tilde{z}) \geq 0 \iff -\frac{\pi}{2} \leq \gamma \arg \tilde{z} \leq \frac{\pi}{2} \iff -\frac{\pi}{2\gamma} \leq \arg \tilde{z} \leq \frac{\pi}{2\gamma},$$

where we put the branch cut for \arg on the negative real axis. We use the standard parametrization of \tilde{L}_ρ :

$$\tilde{L}_\rho = \left\{ \tilde{z} = \left(\frac{3}{2} + \tilde{A}(\rho) \cos \theta, \tilde{B}(\rho) \sin \theta \right), \theta \in [0, 2\pi] \right\}.$$

The angle of a point on \tilde{L}_ρ is given by

$$\arg \tilde{z} = \arctan \left(\frac{\tilde{B}(\rho) \sin \theta}{\frac{3}{2} + \tilde{A}(\rho) \cos \theta} \right) = \arctan \left(\frac{(\rho^2 - 1) \sin \theta}{6\rho + (1 + \rho^2) \cos \theta} \right),$$

with the maximum absolute angle

$$\max_{\tilde{z} \in \tilde{L}_\rho} |\arg \tilde{z}| = \arctan \left(\frac{\rho^2 - 1}{\sqrt{(34 - \rho^2)\rho^2 - 1}} \right)$$

occurring at two positions satisfying

$$\cos \theta = -\frac{\rho^2 + 1}{6\rho}$$

in the left half of the ellipse. The condition in (33) will be satisfied if we choose ρ such that

$$\arctan \left(\frac{\rho^2 - 1}{\sqrt{(34 - \rho^2)\rho^2 - 1}} \right) \leq \frac{\pi}{2\gamma},$$

which after some algebra becomes

$$1 \leq \rho \leq \rho_{max}(\gamma) \leq 3 + 2\sqrt{2},$$

where $\rho_{max}(\gamma)$ is defined by (26). The limiting values of $\rho_{max}(\gamma)$ for $\gamma = 1$ and $\gamma = \infty$ are easily obtained from the definition. \square

Given the asymptotic bound on the quadrature error in (28) we obtain the following bound on Q_0 .

LEMMA 4 (asymptotic bound on Q_0 for the reference interval). *The number of Gauss–Legendre quadrature nodes required on the reference interval $[1, 2]$ to satisfy the error bound in (23) has the following asymptotic bound:*

$$(34) \quad \begin{aligned} Q_0 &= O\left(\frac{-\log \epsilon + j_{max} + 1}{2 \log(\rho_{max}(\gamma))}\right) = O\left(\frac{-\log \epsilon + \log(L(\Delta t, \epsilon, \alpha))}{2 \log(\rho_{max}(\gamma))}\right) \\ &= O\left(\frac{-\log \epsilon - \log \Delta t + \log(-\log \epsilon - \log \Delta t)}{2 \log(\rho_{max}(\gamma))}\right). \end{aligned}$$

Proof. Given that the error of the Q_0 -point quadrature is asymptotically $(\rho_{max})^{-2Q}$ from Lemma 3, equation (28), we equate $(\rho_{max})^{-2Q}$ with the right-hand side of (23) to obtain the first equality in (34); then we replace j_{max} by its definition in (21). \square

In Algorithm 1 we describe the procedure outlined in the previous lemmas for generating a unique quadrature for

$$\frac{1}{\Gamma(1 - \alpha)} \int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi,$$

valid $\forall t \in [\Delta t, \infty)$.

We now prove the following theorem concerning our proposed quadrature.

THEOREM 2. *The quadrature in (35) in Algorithm 1 satisfies the error bound*

$$\left| \frac{1}{\Gamma(1 - \alpha)} \int_0^\infty e^{-\xi t} \xi^{-\alpha} d\xi - \frac{1}{\Gamma(1 - \alpha)(1 - \alpha)} \sum_{k=1}^Q e^{-(\eta^k)^\gamma t} v^k \right| \leq \epsilon \quad \forall t \in [\Delta t, \infty),$$

with the number of quadrature nodes Q satisfying the asymptotic bound

$$Q = O\left(\frac{(-\log \epsilon - \log \Delta t)^2}{2 \log(\rho_{max}(\gamma))}\right).$$

Proof. In Lemma 1 (equation (22)), we have shown

$$\left| \frac{1}{\Gamma(1 - \alpha)(1 - \alpha)} \left(\int_0^\infty e^{-\eta^\gamma t} d\eta - \int_{a_{j_{min}}=2^{j_{min}}}^{b_{j_{max}}=2^{j_{max}+1}} e^{-\eta^\gamma t} d\eta \right) \right| \leq \frac{2}{3} \epsilon \quad \forall t \in [\Delta t, \infty).$$

In Lemma 2 (equation (25)), we have shown

$$\left| \frac{1}{\Gamma(1 - \alpha)(1 - \alpha)} \left(\int_{a_j}^{b_j} e^{-\eta^\gamma t} d\eta - \sum_{i=1}^{Q_j} e^{-(\eta_j^i)^\gamma t} v_j^i \right) \right| \leq \frac{\epsilon}{3} \frac{(b_j - a_j)}{b_{j_{max}}} \quad \forall t \in [0, \infty)$$

ALGORITHM 1. Generation of a quadrature for $\frac{1}{\Gamma(1-\alpha)} \int_0^\infty e^{-\xi} t \xi^{-\alpha} d\xi$ valid $\forall t \in [\Delta t, \infty)$.

1. Choose quadrature tolerance ϵ . Set

$$j_{min} = \left\lfloor \frac{\log(\Gamma(1-\alpha)(1-\alpha)\frac{\epsilon}{3})}{\log 2} \right\rfloor, \quad j_{max} = \left\lceil \frac{\log L(\Delta t, \epsilon, \alpha)}{\log 2} \right\rceil - 1,$$

where

$$L(\Delta t, \epsilon, \alpha) = \left(\frac{\log(\frac{\epsilon}{3} \Delta t^{1-\alpha})}{-\Delta t} \right)^{1-\alpha}.$$

2. Generate lowest order Q -point Gauss-Legendre quadrature on $\eta \in [1, 2]$,

$$\text{nodes: } \{\eta_0^1, \dots, \eta_0^Q\}, \text{ weights: } \{v_0^1, \dots, v_0^Q\},$$

satisfying

$$\left| \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \left(\int_1^2 e^{-\eta^\gamma} t d\eta - \sum_{i=1}^Q e^{-(\eta_i^0)^\gamma} t v_0^i \right) \right| \leq \frac{\epsilon}{3} \frac{1}{2^{j_{max}+1}} \quad \forall t \in [0, \infty),$$

where $\gamma = \frac{1}{1-\alpha}$, by iteratively increasing Q and sweeping over $t \in [0, \infty)$. We note that numerically, it is necessary to check only the range of $t \in [t_{min}, t_{max}]$ for which $e^{-\eta^\gamma} t$ is not almost identically 0 or 1 on $\eta \in [1, 2]$. A good choice is

$$t_{min} = -\log(1-\epsilon) 2^{-\gamma}, \quad t_{max} = -\log \epsilon.$$

3. The complete $Q = ((j_{max} - j_{min} + 1)Q_0)$ -point quadrature is

$$\frac{1}{\Gamma(1-\alpha)} \int_0^\infty e^{-\xi} t \xi^{-\alpha} d\xi \approx \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \sum_{k=1}^Q e^{-(\eta^k)^\gamma} t v^k,$$

where

(35)

$$\text{nodes: } \{\eta^k\} = \bigcup_{j=j_{min}}^{j_{max}} \{2^j \eta_0^1, \dots, 2^j \eta_0^Q\}, \text{ weights: } \{v^k\} = \bigcup_{j=j_{min}}^{j_{max}} \{2^j v_0^1, \dots, 2^j v_0^Q\}.$$

for all $j = j_{min}, \dots, j_{max}$. Summing over j we obtain

$$\left| \frac{1}{\Gamma(1-\alpha)(1-\alpha)} \left(\int_{a_{j_{min}}}^{b_{j_{max}}} e^{-\eta^\gamma} t d\eta - \sum_{i=1}^Q e^{-(\eta^i)^\gamma} t v^i \right) \right| \leq \frac{\epsilon}{3} \quad \forall t \in [0, \infty),$$

and the error bound is proved. The asymptotic bound on $Q = (j_{max} - j_{min} + 1)Q_0$ is obtained by noting that

$$\begin{aligned} j_{min} &= O(-\log \epsilon), \\ j_{max} + 1 &= O(\log L(\Delta t, \epsilon, \alpha)) \\ &= O(-\log \Delta t + \log(-\log \epsilon - \log \Delta t)), \end{aligned}$$

and the asymptotic bound on Q_0 is given in Lemma 4, equation (34). \square

In Figure 2 we show the quadrature error $E(Q_0, t, \alpha)$, associated with the reference interval $[1, 2]$, defined in (27). In Figure 2(a) we plot $E(Q_0, t, \alpha)$ as a function of t , given a fixed $Q_0 = 6$ and various values of α . In Figure 2(b) the numerically computed

$$\max_{t \in [0, \infty)} E(Q_0, t, \alpha)$$

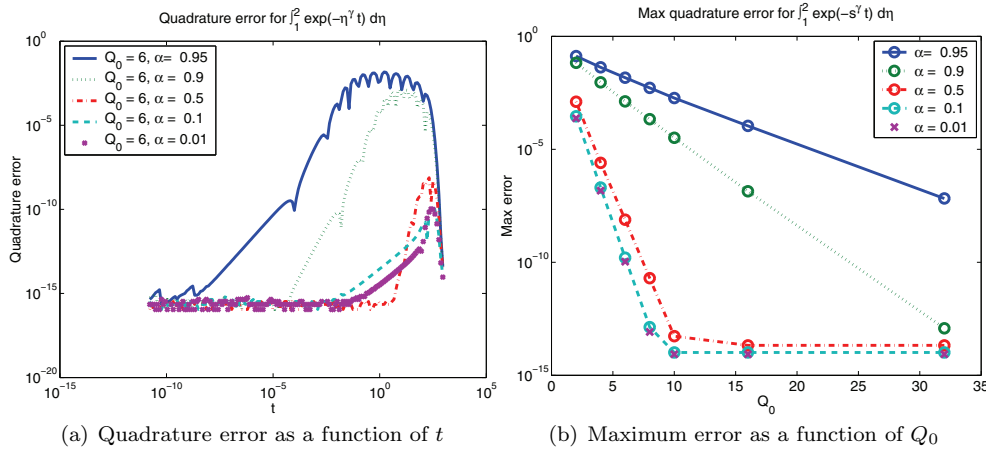


FIG. 2. Quadrature error for various values of $\gamma = \frac{1}{1-\alpha}$ on the reference interval $[1, 2]$.

is plotted against Q_0 for various values of α . We see that on a given interval, a larger α gives rise to a higher quadrature error and a slower convergence.

The slopes of the lines in Figure 2(b) can be used to approximate $\rho_{max}(\gamma)$ via

$$E(Q_0, t, \alpha) \approx C(\rho_{max}(\gamma))^{-2Q_0}.$$

In Table 3.1 we show the two point fit for $\rho_{max}(\gamma)$ at various Q_0 for different values of α , and compare them to the analytically obtained $\rho_{max}(\gamma)$ in (26). We see that (28) with the analytically derived value of $\rho_{max}(\gamma)$ is an extremely good description of the actual convergence of the quadrature. (The values of 1.0 at the bottom right corner of the table are just an indication that machine precision has been reached.)

In Figure 3 we show the total number of quadrature points to reach tolerance $\epsilon = 10^{-6}$ for various values of Δt at three different α values (see Figure 3(a)–(c)). In Figure 3(d) we show the analytically predicted value

$$Q_{predict} = (j_{max} - j_{min} + 1)(Q_0)_{predict},$$

TABLE 3.1
Quadrature convergence is well described by analytically obtained error bound in (28).

α	0.95	0.9	0.5	0.1	0.01
Analytically obtained $\rho_{max}(\gamma)$					
	1.2462	1.5360	4.2361	5.7608	5.8277
Numerically computed $\rho_{max}(\gamma)$					
Q_0					
4	1.3325	1.6485	4.7496	6.1415	6.3162
6	1.3002	1.6255	4.2453	5.9843	6.1017
8	1.2972	1.5725	4.4344	5.8508	5.9832
10	1.2951	1.6035	4.3851	1.9106	1.7662
16	1.2669	1.5753	1.0807	1.0000	1.0000
32	1.2602	1.5467	1.0000	1.0000	1.0000

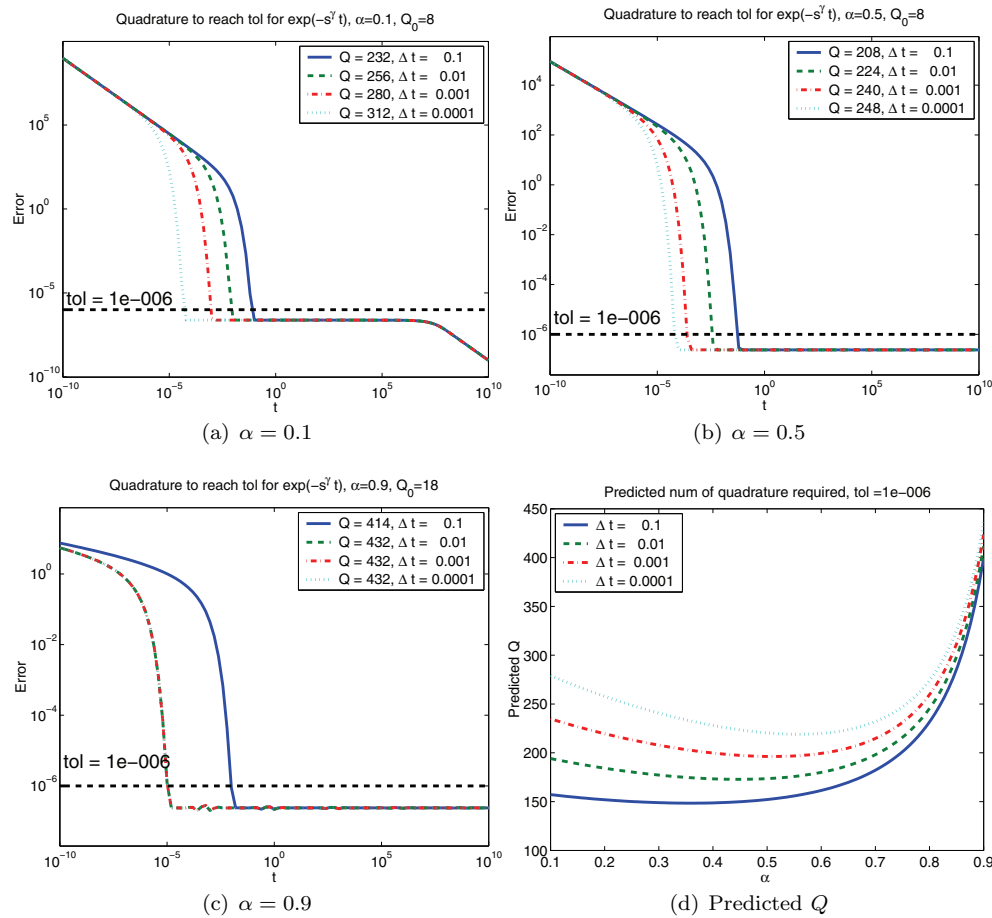


FIG. 3. Predicted Q to reach tolerance and actual Q to reach tolerance.

where $(Q_0)_{predict}$ is the smallest positive integer satisfying

$$(\rho_{max}(\gamma))^{-2(Q_0)_{predict}} = \frac{\epsilon}{3} \frac{1}{b_{j_{max}}}.$$

We see that despite some slight underestimates of Q at the low range of α or Δt , the values given by the curves in Figure 3(d) have very good predictive value. The wide spread of Q at different Δt values for smaller values of α and the tightness of the spread for larger values of α are consistent with the numerical results in Figure 3(a)–(c). We can also see that at smaller values of Δt , α values close to 0 and 1 both give higher required Q than an α in the middle of the interval $[0, 1]$.

4. Treatment of nonsmooth input functions. In the solution of fractional order differential equations, the input function f will be a sum of powers of t of the form

$$(36) \quad \{t^\beta, \beta = j + l\alpha, j, l \in \{0, 1, 2, \dots\}\}.$$

Clearly, f has a singularity (in its derivatives) at $t = 0$, which must be treated by special quadrature.

There are three integrals which must be computed. At time step n , we need to evaluate the update integral $\Phi(\xi_j, n\Delta t, \Delta t)$, given in (12), to obtain each spectral component $h(\xi_j, n\Delta t, \Delta t)$ of the historical part. We also need to compute the local part $L^\alpha[f](n\Delta t)$, defined in (9). In addition, there is the initial computation of $h(\xi_j, n_0\Delta t, \Delta t)$. We now address the computation of each of these integrals.

We note here that any error incurred in evaluating $L^\alpha[f](n\Delta t)$ is a one time error since this quantity is not used for future evaluations. Any error incurred in evaluating $\Phi(\xi_j, n\Delta t, \Delta t)$ and hence $h(\xi_j, n\Delta t, \Delta t)$ does not grow because looking at (11) we see that at each time step $h(\xi_j, t, \Delta t)$ is damped by the quantity $e^{-\xi_j \Delta t} \leq 1$. This means that any error in evaluating $\Phi(\xi_j, n\Delta t, \Delta t)$ or $h(\xi_j, n\Delta t, \Delta t)$ is damped to an extent indicated by the magnitude of $\xi_j \Delta t$. When the quadrature node is large, error is damped rapidly, and when it is close to 0, the error is damped slowly (but it never grows).

4.1. Initial computation of $h(\xi_j, n_0\Delta t, \Delta t)$. We need to initialize the values of the spectral components of the historical part. Suppose we want an accuracy of order p . Let

$$(37) \quad \mathbb{P} = \{\beta_i = j + l\alpha, j, l \in \{0, 1, 2, \dots\} : \beta_i < p\},$$

and $n_0 = |\mathbb{P}|$ be the cardinality of \mathbb{P} . At the initial time step n_0 , we need to compute

$$(38) \quad h(\xi, n_0\Delta t, \Delta t) = \int_0^{n_0\Delta t - \Delta t} e^{-\xi(n_0\Delta t - \tau)} f(\tau) d\tau$$

while noting that f , being of the form in (36), is singular at $\tau = 0$. We project f onto the n_0 -dimensional subspace spanned by the n_0 lowest powers of τ ,

$$(39) \quad f(\tau) = \sum_{i=1}^{n_0} a_i \tau^{\beta_i}, \beta_i \in \mathbb{P},$$

by solving the standard interpolant linear system.

Analytical integration of each term gives the formula

$$(40) \quad \int_0^{t-\Delta t} e^{-\xi(t-\tau)} \tau^\beta d\tau = \frac{(t-\Delta t)^\beta \left(\beta e^{-\xi t} (-\xi(t-\Delta t))^{-\beta} (\Gamma(\beta, -\xi(t-\Delta t)) - \Gamma(\beta)) + e^{-\xi \Delta t} \right)}{\xi}.$$

Because we did not find a reliable code which evaluates the incomplete gamma function for negative arguments, we evaluated the integral in (40) numerically by high order Gauss-Jacobi quadrature with the weight function τ^β .

4.2. Computation of update integral $\Phi(\xi_j, n\Delta t, \Delta t)$. Once the initial values of $h(\xi_j, n_0\Delta t, \Delta t)$ have been computed, we must march forward in time. At each

time step $n > n_0$, we need to compute the update integral in (12), which is of the form

$$(41) \quad \Phi(\xi_j, n\Delta t, \Delta t) = \int_{n\Delta t - 2\Delta t}^{n\Delta t - \Delta t} e^{-\xi_j(n\Delta t - \tau)} f(\tau) d\tau.$$

For $n < n_{smooth}$, we fit f to the sum of powers in (39). For $n \geq n_{smooth}$, meaning f is now sufficiently smooth in the interval of integration, we fit $f(\tau)$ to a polynomial:

$$(42) \quad f(n\Delta t - \tau) = \sum_{i=0}^{p-1} a_i (n\Delta t - \tau)^i.$$

For both, the resulting terms are integrated numerically (by high order Gauss–Jacobi quadrature for nonsmooth and by high order Gauss–Legendre quadrature for smooth) for the reason described in section 4.1. In numerical tests, we have chosen n_{smooth} to be 10.

4.3. Computation of local part $L^\alpha[f](n\Delta t)$. Finally, we come to the computation of the local part in the time domain:

$$(43) \quad L^\alpha[f](n\Delta t) := \frac{1}{\Gamma(\alpha)} \int_{n\Delta t - \Delta t}^{n\Delta t} (n\Delta t - \tau)^{\alpha-1} f(\tau) d\tau.$$

Again, we fit f to the sum of powers in (39) for $n < n_{smooth}$ and to a polynomial for $n \geq n_{smooth}$.

For $n < n_{smooth}$, the resulting terms are

$$\int_{t-\Delta t}^t (t-\tau)^{\alpha-1} \tau^\beta d\tau = \frac{t^{\alpha+\beta} \Gamma(\alpha) \Gamma(\beta+1)}{\Gamma(\alpha+\beta+1)} - \frac{t^{\alpha-1} (t-\Delta t)^{\beta+1} \text{hypergeom}([\beta+1, -\alpha+1], [\beta+2], \frac{t-\Delta t}{t})}{\beta+1},$$

which are computed numerically by high order Gauss–Jacobi quadrature with the weight function $(t-\tau)^{\alpha-1}$, due to the lack of a reliable code to evaluate the hypergeometric function.

For $n \geq n_{smooth}$, the resulting terms are

$$\int_{t-\Delta t}^t (t-\tau)^{\alpha-1} (t-\tau)^j d\tau = \frac{\Delta t^{\alpha+j}}{\alpha+j}$$

and are evaluated directly.

5. Numerical results. We show the convergence of the method for $\alpha = 0.7$ at three different orders, where we have interpolated f by using the values $p = 2, 3$, or 4 in (37) and (42). The quadrature error tolerance was set to $\epsilon = 10^{-9}$. The test function is

$$f(\tau) = \frac{\tau}{1+\tau} + \sin 16.3\tau + \tau^\alpha + \tau^{2\alpha} + \tau^{1+\alpha} + \tau^{2+2\alpha},$$

and the fractional integral was evaluated from $t = 0$ to $t = 2$.

In Figure 4, we plot the total error and the errors of the history and the local parts as a function of Δt . These errors are measured in the L^2 norm.

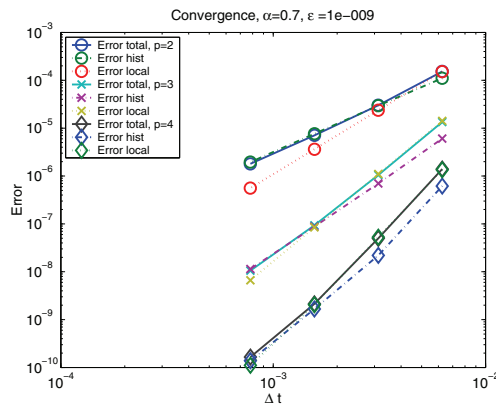


FIG. 4. Convergence of algorithm at three different orders p . Fractional order $\alpha = 0.7$ and quadrature tolerance $\epsilon = 10^{-9}$.

6. Conclusions. We presented a method of evaluating fractional integrals by using an efficient quadrature of the integral representation of the convolution kernel $t^{\alpha-1}$. This quadrature is to be used as part of a fast time stepping method. The new method has algorithmic complexity $O(NQ)$ and storage requirement $O(Q)$, where N is the number of time steps and Q is the number of nodes in the quadrature. We have shown that Q is independent of N and grows as $O((-\log \epsilon - \log \Delta t)^2)$, where ϵ is the quadrature error tolerance and Δt is the size of the time step. The possible end point singularity of the input function is taken into account by this algorithm.

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