A Kernel-Independent Sum-of-Exponentials Method

Zixuan Gao*1, Jiuyang Liang†1,2, and Zhenli Xu‡1,2

1School of Mathematical Sciences, Shanghai Jiao Tong University, Shanghai 200240, P. R. China
2Institute of Natural Sciences and MOE-LSC, Shanghai Jiao Tong University, Shanghai, 200240, P. R. China

Abstract

We propose an accurate algorithm for a novel sum-of-exponentials (SOE) approximation of kernel functions, and develop a fast algorithm for convolution quadrature based on the SOE, which allows an order $N$ calculation for $N$ time steps of approximating a continuous temporal convolution integral. The SOE method is constructed by a combination of the de la Vallée-Poussin sums for a semi-analytical exponential expansion of a general kernel, and a model reduction technique for the minimization of the number of exponentials under given error tolerance. We employ the SOE expansion for the finite part of the splitting convolution kernel such that the convolution integral can be solved as a system of ordinary differential equations due to the exponential kernels. The significant features of our algorithm are that the SOE method is efficient and accurate, and works for general kernels with controllable upperbound of positive exponents. We provide numerical analysis for both the new SOE method and the SOE-based convolution quadrature. Numerical results on different kernels, the convolution integral and integral equations demonstrate attractive performance of both accuracy and efficiency of the proposed method.

Key words. Sum-of-exponentials, radial basis kernel, model reduction, convolution quadrature, integral equations

AMS subject classifications. 65R20; 41A30; 42A38

1 Introduction

In this paper, we describe a new numerical algorithm for the construction of sum-of-exponentials (SOE) approximation for a given scalar smooth function $f(x)$ of the form

$$\max_{x \in I} \left| f(x) - \sum_j m_j e^{-s_j x} \right| < \varepsilon,$$

(1.1)

where $I$ is a finite interval which could be an arbitrary subset of $\mathbb{R}^+$, $\varepsilon$ is an error tolerance, and $m_j$ and $s_j$ are parameters representing the weight and exponent of the $j$th exponential, respectively. In Eq. (1.1), both $m_j$ and $s_j$ could be complex, while the real part of $s_j$ is assumed to be non-negative to avoid the explosion at infinity.

Over the past decades, SOE methods has attracted attention in many applications of scientific computing [1, 2, 3, 4, 5], as an SOE approximation enables a recurrence scheme to compute the spatial discrete convolution, and thus dramatically reduces the cost. In some engineering areas, like acoustic and electromagnetic simulations, SOE methods are also involved as an useful tool in constructing discrete complex image representation, which plays...
an important role in developing fast multipole method (FMM) for 3D Helmholtz Green’s function at low frequencies in layered media [6], by applying the Sommerfeld identity [7, 8]. Employing the SOE for constructing fast algorithm for the calculation of pair interaction is also explored in some recent works [9, 10].

How well the SOE with applications to these areas depends on three key factors: the convergence rate of the SOE with the increasing number of exponentials, the robustness especially for kernels with near-singular and moderate oscillating nature, and the range of the maximum (in the sense of module) exponent of the SOE, i.e., $\max_j |s_j|$ in Eq.(1.1). The design of such an SOE approximation for some additional constraints is strongly nonlinear and highly nontrivial, and has been an extensively studied subject [11, 12, 13, 14, 15, 16, 17, 18, 19, 20]. One less studied but important problem is the last issue, i.e., the approximation with small exponents. In fact, a large maximum exponent may take serious effect on both the accuracy and efficiency, as it has a large derivative and the roundoff error where the former will lead to a stiff problem [21, 22] and the latter will increase with the rise of exponent. This problem will be further explained in the Section 3 and Section 4 of this paper, taking examples of convolution quadrature and solving integral equations. Besides, theoretical discussions on the convergence rate are also difficult to be established in some SOE methods based on adaptive partition.

Motivated by above observations, we propose a novel kernel-independent and high-accurate SOE method by a combination of the de la Vallée-Poussin (VP) sum [18] and the model reduction (MR) [25, 26] technique. In the so-called VPMR approach, an accurate SOE approximation is first constructed by employing the VP sum via a variable substitution,

$$x = -n_c \log \left( \frac{1 + \cos r}{2} \right), \quad r \in [0, \pi], \quad (1.2)$$

where the parameters of the exponentials are expressed analytically. The variable substitution introduces a parameter $n_c$ which allows to tune the maximal exponent of the exponentials. Subsequently, the MR technique is used to further reduce the number of exponentials within the given error tolerance based on an observation that

$$\mathcal{L} \left[ \sum_j m_j e^{-s_j x} \right] = \sum_j \frac{m_j}{z + s_j} = c(zI - A)^{-1}b, \quad (1.3)$$

where $\mathcal{L}$ denotes the Laplace transform, $A$ is a diagonal matrix, $b$ and $c$ are column and row vectors, respectively. The right hand of Eq.(1.3) shares the same form of the transfer function of a linear dynamical system, thus the so-called balanced truncation method [25] can be used for the MR, achieving an optimized SOE approximation. The universal error estimation and complexity analysis are both furnished. The error estimation validates that Eq.(1.2) will preserve the smoothness of the resulting function at the origin, and guarantees the global convergence rate. The comparison of accuracy and convergence rate between VPMR and several theoretical methods, including contour integral methods [18] on Gaussian kernel and the classical Prony’s method [19] on four frequently-used kernels which have complicated forms, near-singular properties, or oscillations, show promising efficiency of our method.

The SOEs of the form Eq.(1.1) occur commonly in computational mathematics and computational physics. For instance, [27] describes a scheme for accelerating the convolution quadrature,

$$y(t) = f * g = \int_0^t f(t - \tau)g(\tau)d\tau, \quad (1.4)$$

where $f(\tau)$ is the kernel function, which may have singularity at the origin, and $g(\tau)$ is a smooth function, based on a technique of the Laplace inverse transform of the kernel function such that

$$y(t) = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) \int_0^t e^{\lambda(t-\tau)} g(\tau)d\tau d\lambda. \quad (1.5)$$

The scheme requires the construction of quadratures of $\lambda$ for which the inverse Laplace transform is well approximated, and the resulting convolution integral associated with $\tau$
satisfies a combination of ODEs with form \( u' = \lambda u + g(t) \) with \( u(0) = 0 \) and can be integrated by the RK method. A stable and efficient discretization of the interval \( \Gamma \) requires an \( O(1/h) \) cutoff of both the upper/lower bound of \( \Gamma \) with \( h \) the step size of the RK method. This \( O(1/h) \) cutoff will lead to a stiff problem such that the convergence rate is \( O(h^{\min(p,q+1)}) \) with \( p \) the order and \( q \) the stage order. We describe in detail the construction of efficient quadratures for the discretization of Eq.\((1.4)\) in Section \( 3 \) of this paper, by first replacing the inverse Laplace transform of \( f(t-\tau) \) to the corresponding SOE produced via the VPMR method. Second, for the case of \( f(t-\tau) \) having no singularity, we follow the general procedure of the RK method to evaluate \( y(t) \) recursively; for the case of \( f(t-\tau) \) having singularity at the origin, the singularity part of the convolution integral is extracted and is approximated by combination of the local expansion of \( f(t-\tau) \) and the local interpolation of \( g(\tau) \), and then the RK to the smooth part can be applied. Rigorous error bound is established by following the work of Lubich et al. \([22,28]\), showing \( O(h^p) \) rate of the RK which the stage order is no longer involved.

SOEs also have obvious applications to the discretization of integral equations. In particular, for a given kernel function \( f \) convoluting with an unknown (except the initial point) function, given integral equations of the forms either

\[
(1-\varpi)g(t) + H(t) = \int_0^t f(t - \tau)g(\tau)d\tau \tag{1.6}
\]

with \( H(\tau) \) a given source, \( \varpi \) a real parameter, or the so-called nonlinear Volterra equation

\[
u(t) = a(t) + \int_0^t f(t - \tau)g(\tau,u(\tau))d\tau \tag{1.7}
\]

with \( a(\tau) \) an inhomogeneous known function, the discretization \([27]\) based on the inverse Laplace transform of \( f(t-\tau) \) proceeds by choosing appropriate integral contour such that the convolution part of Eq.\((1.6)\) and Eq.\((1.7)\) are approximated by

\[
\sum_{j=0}^{n} W_{n-j}g_j, \tag{1.8}
\]

with \( t = nh, W \) the weight matrices, and \( g_j \) the numerical value of \( g \) at \( \tau = jh \). Also, the RK method is used for recursively solving the resulting linear/nonlinear equation, and a large \( O(1/h) \) cutoff of the contour will reduce the performance especially for a small step size. In Section \( 4 \), our schemes are developed to construct the discretization of these integral equations by using the SOE of \( f(t-\tau) \) produced by the VPMR method. These schemes provide an efficient means of avoiding stiff problem when solving integral equations, where the convergence rate of the RK is \( O(h^p) \) and the stage order is not involved, as compared with many inverse Laplace-based works \([22,27,28]\). The error estimation of our schemes are non-trivial thanks to the introduced technique of removing singularity, and are rigorously provided.

The remainder of the paper is organized as follows. In Section \( 2 \), we introduce the VPMR method to find an efficient and accurate SOE approximation, and establish both an universal error estimation and a detailed complexity analysis. Comparison results between the VPMR and some existing SOE works on different kernels are also provided. In Section \( 3 \), we describe numerical algorithms with numerical analysis of errors, which are based on SOE and RK method, for temporal convolutions. In Section \( 4 \), we extend our SOE to construct an algorithm for fast solving two kinds of integral equations including the linear convolution equation and the nonlinear Volterra integral equation. Conclusions are given in Section \( 6 \).

2 Sum-of-exponentials Method

In this section, we introduce a kernel-independent SOE method based on the VP sums and the MR for constructing a VPMR algorithm for the SOE approximation. This VPMR
algorithm was originally proposed to design a sum-of-Gaussians approximation which the minimum bandwidth is controllable for all of the non-oscillatory kernel thus speeds up the evaluation of resulting kernel summation problem [29]. This paper extends the VPMR idea to obtain the SOE approximation by first using a different variable change which has better continuity and then applying the MR to the resulting SOE. A new rigorous error estimate for more general cases is also provided in this section.

2.1 The VPMR algorithm

Throughout this work, the kernel function \( f(x) \) is defined on the positive axis \( x \geq 0 \), and has a finite limit at \( x \to \infty \). We introduce a variable change

\[
x = -n_c \log \left( \frac{1 + \cos r}{2} \right), \quad r \in [0, \pi],
\]

(2.1)

such that \( K(r) = f(x) \) is smooth on \([0, \pi]\), and \( n_c \) is a positive number which is used to control the upper bound of the positive exponents. The variable change is a one-to-one map and an even and periodic prolongation of \( K(r) \) can be employed such that the kernel function \( K(r) \) is defined on the whole axis \((-\infty, \infty)\) with \( 2\pi \) period. The kernel can then be represented by the VP-sum [29, 23] approximation, \( K(r) \approx V_n[K(r)] \), where,

\[
V_n[K(r)] = \frac{2}{n\pi} \sum_{\ell=0}^{2n-1} \sum_{j=0}^{\ell} \alpha_j \cos(jr) \int_0^\pi K(\tau) \cos(j\tau) d\tau,
\]

(2.2)

with \( \alpha_j = 1 \) for \( j \geq 1 \) and \( \alpha_0 = 1/2 \). It is noted that generally the VP sums can be expressed as the means of the partial sums \( S_i, i = 0, \cdots, 2n-1, \) of the Fourier series of the kernel function, \( V_k[K(r)] = \sum_{i=0}^{2n-1} S_i/(k + 1) \), for which \( k = 0 \) corresponds to the partial Fourier sums, and \( k = 2n - 1 \) corresponds to the Fejér sums. Here Eq.(2.2) corresponds to the \( k = n \) case.

Substituting the inverse transform \( r = \arccos \left( 2e^{-x/n_c} - 1 \right) \) to Eq.(2.2), one obtains the following approximation of kernel function,

\[
f(x) \approx \frac{1}{\pi} \int_0^\pi K(\tau) d\tau + \sum_{j=1}^{2n-1} A_j T_j(2e^{-x/n_c} - 1),
\]

(2.3)

where \( T_j(x) = \cos(j \arccos x) \) is the Chebyshov polynomial of degree \( j \), and

\[
A_j = \max \left\{ \frac{2}{\pi} \left( \frac{4n - 2j}{n\pi} \right) \right\} \int_0^\pi K(\tau) \cos(j\tau) d\tau
\]

(2.4)

is the coefficient.

By employing the expansion form of Chebyshov polynomials, one can obtain an SOE expansion

\[
f(x) \approx \sum_{j=0}^{2n-1} w_j e^{-jx/n_c},
\]

(2.5)

where the expansion coefficient \( w_j \) is given by,

\[
w_j = \begin{cases}
2a_0 + \sum_{\ell=1}^{n} (-1)^\ell f_{n/2n-\ell} a_\ell + \sum_{\ell=1}^{n} (-1)^n+\ell f_{n/2n-\ell} a_{n+\ell}, & \text{for } j = 0 \\
2^{2j} \sum_{\ell=1}^{n} (-1)^{j-j} f_{(\ell+j)/2n-\ell} (\ell+j)(\ell-j) a_\ell + \sum_{\ell=1}^{n} c_{n/2n-\ell} f_{n/2n-\ell} a_{n+\ell}, & \text{for } 1 \leq j \leq n \\
\sum_{\ell=j-n}^{n} c_{n/2n-\ell} f_{n/2n-\ell} a_{n+\ell}, & \text{for } j > n
\end{cases}
\]

(2.6)
and
\[ e_n^{(\ell)} = (-1)^{n+\ell-j} \left(1 - \frac{\ell}{n}\right) \frac{(n+\ell)}{n+\ell+j} \frac{(n+\ell+j)}{n+\ell-j} 2^{2j}. \tag{2.7} \]

Note that the maximal positive exponent in the exponentials is \((2n-1)/n_c\), thus \(n_c\) determines the upper bound of the positive exponents. It asymptotically becomes constant if one sets \(n_c \propto n\). The controllability of the upper bound is very important because an SOE with large exponent leads to a stiff system when we use them to construct a fast algorithm for the temporal convolution.

One can employ the MR to reduce the number of exponentials to achieve a nearly optimal SOE approximation. We introduce the balanced truncation method in the model order reductions [30, 25] for the purpose. Namely, we find an appropriate \(P\)-term exponentials to approximate Eq. (2.5)
\[ \sum_{j=0}^{2n-1} w_j e^{-jx/n_c} \approx \sum_{\ell=1}^{P} m_{\ell} e^{-s_{\ell}x}, \tag{2.8} \]
with \(P < 2n - 1\), such that the error is with a given tolerance. Based on extensive numerical experiments, we have found that the maximum positive exponent remains \(\max|s_{\ell}| \approx (2n - 1)/n_c\) after the MR. The first step of the MR procedure is to apply the Laplace transform on the SOE expansion (excluding \(j = 0\)), which results in a sum-of-poles representation and one can simply express it as a transfer function of a linear dynamical system,
\[ \mathcal{L} \left[ \sum_{j=1}^{2n-1} w_j e^{-jx/n_c} \right] = \sum_{j=1}^{2n-1} \frac{w_j}{z + j/n_c} = c(zI - A)^{-1}b, \tag{2.9} \]
where \(A\) is a \((2n-1) \times (2n-1)\) diagonal matrix, \(b\) and \(c\) are column and row vectors of dimension \((2n-1)\), respectively. The key for the MR is to obtain the Hankel singular values by solving two Lyapunov equations,
\[ AP + PA^* + bb^* = 0, \quad A^*Q + QA + c^*c = 0. \tag{2.10} \]
The \(i\)-th Hankel singular value is defined as \(\sigma_i = \sqrt{\lambda_i(PQ)}\), where \(\lambda_i(PQ)\) is the \(i\)-th eigenvalue of the product of matrices \(P\) and \(Q\).

The next step of the MR is to find a balancing transformation matrix \(X\) via the square root method [30, 25]. Under this transformation and by defining matrices \(\tilde{A} = XAX^{-1}\), \(\tilde{b} = Xb\), \(\tilde{c} = cX^{-1}\), the solutions \(P\) and \(Q\) to the two Lyapunov equations,
\[ \tilde{A}P + P\tilde{A}^* + \tilde{b}\tilde{b}^* = 0, \quad \tilde{A}^*Q + Q\tilde{A} + \tilde{c}\tilde{c} = 0, \tag{2.11} \]
become equal and diagonal [30],
\[ P = Q = \text{diag}(\sigma_1, \ldots, \sigma_n). \tag{2.12} \]
The reduced \((P-1)\)-order model is then obtained by simply taking the \((P-1) \times (P-1), (P-1)\times 1\) and \(1 \times (P-1)\) leading blocks of \(A\), \(b\) and \(\tilde{c}\), respectively. Then the corresponding transfer function \(\tilde{c}(zI - \tilde{A})^{-1}\tilde{b}\) satisfies [26, 31]
\[ \sigma_{P-1} \leq \sup_{z \in \mathbb{C}} \left| \tilde{c}(zI - \tilde{A})^{-1}\tilde{b} - c(zI - A)^{-1}b \right| \leq 2(\sigma_P + \sigma_{P+1} + \cdots + \sigma_n). \tag{2.13} \]
Note that the transformation matrix \(X\) can be obtained via other balancing methods, such as the stochastic balancing and the positive real balancing which yields solution to appropriate Lyapunov and/or Riccati equations equal and diagonal [30, 32]. Detailed procedures of the MR approach we use are summarized in Table 1.

**Remark 2.1.** Since the VPMR approach requires high-precision matrix manipulation, we employ the Multiple Precision Toolbox [33] in order to implement the algorithm. These packages are used in both steps of the VP-sum and the model-reduction procedures. The computer code of the VPMR approach is released as open source, which is available at https://github.com/ZXGao97.
Algorithm 1 Model Reduction of Eq. (2.8) based on balancing transformation

Input: \(\{w_i\}_{i=0}^{2n-1}, n_c\) and the tolerance error \(\varepsilon\).

Output: \(\{m_l\}_{l=0}^{P-1}\) and \(\{s_l\}_{l=0}^{P-1}\).

1. Form a diagonal matrix \(A = -\text{diag}(1/n_c, 2/n_c, \cdots, (2n - 1)/n_c)\), a column vector \(B = (\sqrt{|w_1|}, \sqrt{|w_2|}, \cdots, \sqrt{|w_{2n-1}|})^T\), and a row vector \(C = (\text{sgn}(w_1)\sqrt{|w_1|}, \text{sgn}(w_2)\sqrt{|w_2|}, \cdots, \text{sgn}(w_{2n-1})\sqrt{|w_{2n-1}|})\).
2. Solve the Lyapunov equations \(AP + PA^T = -BB^T\) and \(AQ + QA^T = -C^TC\).
3. Compute the Cholesky factor \(S\) and \(L\) of the solutions of the Lyapunov equations \(P\) and \(Q\), respectively, such that \(P = SS^T\) and \(Q = LL^T\) hold.
4. Compute the singular value decomposition of \(S^TL\) such that \(S^TL = U\Sigma V^T\), where \(\Sigma = \text{diag}(\sigma_1, \sigma_2, \cdots, \sigma_{2n-1})\) with \(\sigma_i\) the so-called Hankel singular value.
5. Compute the transform matrix \(\tilde{T} = SU\Sigma^{-\frac{1}{2}}\).
6. Form a matrix \(\tilde{A} = \tilde{T}^{-1}AT\), a column vector \(\tilde{B} = \tilde{T}^{-1}B\), and a row vector \(\tilde{C} = C\tilde{T}\).
7. Find \(P\) such that \(2\sum_{i=1}^{2n-1}\sigma_i \leq \varepsilon\).
8. Form a matrix \(\tilde{A}\) which denotes from the first \((P-1)\times(P-1)\) block of \(\tilde{A}\), a column vector \(\tilde{B}\) which denotes from the first \((P-1)\) rows of \(\tilde{B}\), and a row vector \(\tilde{C}\) which denotes from the first \((P-1)\) columns of \(\tilde{C}\).
9. Compute the eigenvalue decomposition \(\tilde{A} = \Lambda X \Lambda^{-1}\). Set \(s_l = \Lambda_{ll}, l = 1, 2, \cdots, P - 1\) and \(s_0 = 0\).
10. Compute \(\mathcal{B} = X^{-1}\tilde{B}, \mathcal{C} = \tilde{C}X\). Let \(m_0 = w_0\) and \(m_l = \mathcal{B}_l\mathcal{C}_l\) with \(l = 1, 2, \cdots, P - 1\).
11. return \(\{m_l\}_{l=0}^{P-1}\) and \(\{s_l\}_{l=0}^{P-1}\).

Remark 2.2. If the smooth function \(f(x)\) has a limit at infinity, our method works on the whole positive-axis, thus the interval could be an arbitrary subset of \(\mathbb{R}\). If the limit does not exist, the above VPMR method has low accuracy because of the discontinuity of the transformed function \(K(r)\). This reason will be further explained in section 2.3. In order to achieve higher accuracy, one could truncate \(f(x)\) at a required point, then connect a fast decreasing function (for example, the Gaussian function) behind the cutoff point such that a new function \(f^{*}(x)\) to localize the kernel function. The higher-order differentiable properties of \(f^{*}(x)\) can be kept.

Remark 2.3. After the VP approach, the exponents \(-j/n_c\) and the weights \(w_j\) given in the left hand of Eq. (2.8) are real, whereas the MR approach does not guarantee that the exponents \(-s_l\) and the weights \(m_l\) given in the right hand of Eq. (2.8) are real. In most cases, \(-s_l\) and \(m_l\) are complex whereas the MR approach guarantees that the real parts of \(s_l\) are positive for all \(l\) [25]. An interesting theorem [34] is that \(s_l\) are real and \(m_l\) are positive when \(w_j\) are positive. It seems to be more useful for other integral discretization-based SOE approximations whose weights are all positive [11]. However, the limitation of such integral-based method is the difficulty in extending to general kernels.

2.2 Computation details and complexity analysis of the VPMR algorithm

In this subsection, we perform some analysis to the complexity of the VPMR method.

First, we consider the VP-sum procedure. The coefficients \(a_j\) in Eq. (2.4) are evaluated using either the adaptive Gauss-Legendre integral quadrature [35] (function “quadgk” in MATLAB) or the 2D dilation quadrature (degenerate into 1D case) [36], with average
number of quadratures $\tilde{N}$. The adaptive Gauss-Legendre quadrature is efficient for kernel with non-oscillation or low frequency oscillation, whereas may not work for high frequency oscillating integral. The 2D dilation quadrature is more appropriate for integrating near-singular and oscillating kernels with high precision and efficiency. The construction of the coefficients $w_j$ using Eq.\((\ref{eq:2.6})\) requires expensive combinatorial number, but can be done via simple combinatorial recursions

$$
\left(\frac{n + \ell + j}{n + \ell - j}\right) = \frac{(2j + 1)(n + \ell + j)}{(n + \ell - j)(n + \ell - j - 1)}.
$$

(2.14)

The complexity of $w_j$ is thus $\sim O(2n^2)$. The total complexity of the procedure of the VP-sum is $O(2n\tilde{N} + 2n^2)$.

Second, we study the MR procedure based on square root factorization as given in Algorithm 1. Because $A$ is a $(2n - 1) \times (2n - 1)$ diagonal matrix, $b$ and $c$ are column and row vectors of dimension $(2n - 1)$, the two Lyapunov equations can be solved directly via $\sim O((2n - 1)^2)$ operations due to the productions of $bb^*$ and $c^*c$. To obtain the Hankel singular value, we compute the Cholesky factor $S$ and $L$ of the solutions of the Lyapunov equations $P$ and $Q$ (both $P$ and $Q$ are symmetric positive definite), respectively, and then compute the singular value decomposition (SVD) of $S^T L$. The efficiently implemented Cholesky factorization requires $(2n - 1)^3/6 + O((2n - 1)^2)$ operations \cite{37}. The SVD factorization and the matrix-matrix products in the Step 4-6 of Algorithm 1 need $O((2n - 1)^3)$ operations. In the Step 7-10 of Algorithm 1, we construct a low-rank approximation of the whole system by truncating the Hankel singular value at $k$-th. Similar analysis can be applied that the complexity for Step 7-10 yields $O(k^3)$.

Overall, the total computational complexity of the VPMR method is given by $O(2n\tilde{N} + 2n^2 + (2n - 1)^3/6 + (2n - 1)^2 + (2n - 1)^3 + k^3)$. The leading part is contributed from the SVD factorization appeared in Step 4 of the Algorithm 1. We note that $n \approx 1000$ is generally accurate enough for the VPMR method in most cases, thus the complexity is relatively not very big though $O((2n)^3)$ operations are needed. Furthermore, some approaches can be used for improving the efficiency like the randomized singular value decomposition (RSVD) method \cite{38,39} which reduce the computational cost of SVD from $O(n^3)$ to $O(kn^2 + k^2n)$.

### 2.3 Error estimate of the VPMR algorithm

In this subsection, we discuss the convergence rate of the VPMR method with respect to the number of terms $n$ to approximate the kernel function $f(x)$. Because the errors of the VP-sum and the MR approach can be treated separately, we only need to do the error estimate of approximating $K(r)$ using the VP-sum $V_n[K(r)]$ in Eq.\((\ref{eq:2.2})\), due to the estimate of the MR approach has been given in Eq.\((\ref{eq:2.13})\).

An observation is that the $2\pi$-periodic function $K(r)$ is smooth on $(0, \pi)$ and $(-\pi, 0)$ whereas may not become $C^\infty$ at $r \in \{-\pi, 0, \pi\}$, i.e., $K(r)$ is piecewise smooth at its definitional domain. This is because that we make an even and periodic prolongation of $K(r)$ such that $K(r)$ is defined on the whole axis $(-\infty, \infty)$ instead of $[0, \pi]$. Approximation properties of the VP-sum in the uniform metric are considered for certain classes of continuous and smooth functions in many papers \cite{40,41,42,43,44,45}. However, local approximation properties of the VP-sum for piecewise smooth functions have been little studied. From recent work \cite{29}, the results are summarized as the following theorem.

**Theorem 2.1.** If $K(r)$ defined by the variable change Eq.\((\ref{eq:2.1})\) is not differentiable at $r = 0$, its VP-sum $V_n[K(r)]$ still converges to $K(r)$ uniformly on $\mathbb{R}$, whereas the rate of convergence at $r = 0$ is much slower than that at any other point, that

$$
V_n[K(0)] - K(0) = -\frac{\ln 2}{\pi r}K'(r)|_{r=0} + o(n^{-1}), \quad V_n[K(r)] - K(r) = o(n^{-1}) \text{ for } r \neq 0.
$$

(2.15)

Furthermore, suppose that $K(r)$ is twice-differentiable on $[0, \pi]$ with $K'(r)|_{r=0} = 0$ and
are twofold. First, for

\begin{align}
V_n[K(0)] - K(0) &= O(n^{-2}), \\
V_n[K(r)] - K(r) &= o(n^{-2}) \text{ for } r \neq 0.
\end{align}

(2.16)

In fact, one can simply check that the function \( K(r) \) defined by the variable change Eq. (2.1) is naturally satisfies \( K'(r)\big|_{r=0} = 0 \). This result means that our VP-sum approximation has at least two order convergence rate for independent kernels.

Furthermore, the limitations of above error estimate Theorem 2.1 are twofold. First, for the kernel with higher order continuity conditions, the VP-sum may have higher convergence rate (for example, exponential decay when \( K(r) \) becomes even function and vanishes at \( r = \pi \)) but not provided. Second, if \( K(r) \) itself is a piecewise smooth function (for example, when \( f(x) \) is required to be localized as in Remark 2.2), Theorem 2.1 is not valid. For these concerns, we try to derive a more general relationship between \( K(r) \) and its VP-sum as follows. To prove this relationship, we need to use the following lemma.

**Lemma 2.1.** The following inequalities hold for \( n \geq 1 \)

\[
\int_{-\pi}^{\pi} n^\eta \left| \sum_{\ell=n}^{2n-1} \sum_{j=\ell+1}^{\infty} \frac{\sin \left( j\tau - \frac{\eta \pi}{2} \right)}{j^{\eta+1}} \right| d\tau \leq \begin{cases} 
\frac{16(n+2)^2}{(1 + \frac{n}{\pi})^n}, & \eta \geq 1, \\
32 \ln \left( 1 + \frac{n}{n+1} \right) + 58, & \eta = 0.
\end{cases}
\]

(2.17)

The proof of Lemma 2.1 is an extension of Lemma 2.3 from Ref. [48] and Statement 2 from Ref. [47], we omit it.

**Theorem 2.2.** (The error bound of the VP sum) Denote \( W^{n,m}(\Omega) \) the Sobolev spaces which satisfies

\[
W^{n,m}(\Omega) = \{ u \in L^n(\Omega) \mid \tilde{\partial}^\alpha u \in L^n(\Omega), |\alpha| \leq \eta \},
\]

(2.18)

where \( \tilde{\partial} \) indicates the generalized derivatives operation. Let \( F = \{ T_j, j = 0, \ldots, P \} \) becomes a finite division of the interval \([-\pi, \pi] \) which satisfies

\[
-\pi = T_0 < T_1 < \cdots < T_P = \pi
\]

(2.19)

such that the \( 2\pi \)-periodic function \( K(r) \in W^{n,\infty}([-\pi, \pi]) \) can be converted into a function from \( C^\infty([T_i, T_{i+1})) \) by redefining it at the endpoints on each closed interval \([T_i, T_{i+1}] \). Then the following estimate of the remainder term of the VP-sum holds:

\[
|V_n[K(r)] - K(r)| \leq \begin{cases} 
\frac{16(\eta + 2)^2 M_{\eta+1}}{\pi n(n+1)\eta}, & \text{for } \eta \geq 1, \\
\frac{M_{\eta+1}}{\eta}(58 + 32 \ln 2), & \text{for } \eta = 0,
\end{cases}
\]

(2.20)

where \( M_{\eta+1} = \max_r \{|K^{(\eta+1)}(r)|\} \).

**Proof.** Recalling the definition of \( n \)-th VP-sum Eq.(2.2) with \( n \geq 1 \), the approximate error is given by

\[
V_n[K(r)] - K(r) = -\frac{1}{n\pi} \sum_{\ell=n}^{2n-1} \sum_{j=\ell+1}^{\infty} \cos(jr) \int_{-\pi}^{\pi} K(\tau) \cos(j\tau) d\tau.
\]

(2.21)

Using the division \( F \) defined on \([-\pi, \pi] \), we rewrite the integral in the right term of Eq.(2.21) as the sum of the integrals over the integral domain formed by \( F \).

\[
\int_{-\pi}^{\pi} K(\tau) \cos(j\tau) d\tau = \sum_{i=1}^{P} \int_{T_{i-1}}^{T_i} K(\tau) \cos(j\tau) d\tau.
\]

(2.22)
After $\eta + 1$ times integrating by parts, we rewrite the integration at each subintegral in the form

$$
\int_{T_{i-1}}^{T_i} K(\tau) \cos(j\tau) d\tau = \sum_{k=0}^{\eta} \frac{K^{(k)}(T_i) \sin\left(\frac{jT_i - k\pi}{2}\right) - K^{(k)}(T_{i-1}) \sin\left(\frac{jT_{i-1} - k\pi}{2}\right)}{j^{k+1}}
$$

$$
+ \int_{T_{i-1}}^{T_i} K^{(\eta+1)}(\tau) \frac{\sin\left(\frac{j\tau - \eta\pi}{2}\right)}{j^{\eta+1}} d\tau,
$$

(2.23)

where the subscripts $-$ and $+$ indicate the left sided limit and the right sided limit, respectively. Substituting the expressions Eq.(2.23) and Eq.(2.22) into the remainder term Eq.(2.21) and recalling $K(r)$ is a $2\pi$-periodic function, therefore,

$$
V_n[K(r)] - K(r) = - \frac{1}{n\pi} \sum_{\ell = n}^{2n-1} \sum_{j = \ell + 1}^{\infty} \cos(jr) \sum_{i=1}^{P} \sum_{k=0}^{\eta} \left[ \frac{K^{(k)}(T_i) \sin\left(\frac{jT_i - k\pi}{2}\right)}{j^{k+1}} \right]
$$

$$
- \frac{K^{(\eta+1)}(T_{i-1}) \sin\left(\frac{jT_{i-1} - k\pi}{2}\right)}{j^{\eta+1}}
$$

$$
- \frac{1}{n\pi} \sum_{\ell = n}^{2n-1} \sum_{j = \ell + 1}^{\infty} \cos(jr) \sum_{i=1}^{P} \int_{T_{i-1}}^{T_i} K^{(\eta+1)}(\tau) \frac{\sin\left(\frac{j\tau - \eta\pi}{2}\right)}{j^{\eta+1}} d\tau.
$$

(2.24)

Note that the first term in Eq.(2.24) vanishes because $K(r) \in W^{\eta, \infty}([-\pi, \pi])$ such that the left-hand limits and right-hand limits of $\{K^{(k)}(r), k = 0, 1, \cdots, \eta\}$ at the endpoint in the division $\eta$ are equal. Taking Lemma 2.1 into Eq.(2.24), for $\eta \geq 1$, we obtain

$$
|V_n[K(r)] - K(r)| = \left| \frac{1}{n\pi} \sum_{\ell = n}^{2n-1} \sum_{j = \ell + 1}^{\infty} \cos(jr) \sum_{i=1}^{P} \int_{T_{i-1}}^{T_i} K^{(\eta+1)}(\tau) \frac{\sin\left(\frac{j\tau - \eta\pi}{2}\right)}{j^{\eta+1}} d\tau \right|
$$

$$
\leq \frac{M_{\eta+1}}{\eta\eta+1} \int_{-\pi}^{\pi} \left| \frac{n^9}{\ell + \infty} \sum_{\ell = n}^{2n-1} \sum_{j = \ell + 1}^{\infty} \frac{\sin\left(\frac{j\tau - \eta\pi}{2}\right)}{j^{\eta+1}} \right| d\tau
$$

(2.25)

$$
\leq \frac{16(\eta + 2)^2 M_{\eta+1}}{\pi n(n+1)^9}.
$$

Similarly,

$$
|V_n[K(r)] - K(r)| \leq \frac{M_1}{n \pi} \left[ 32 \ln \left( 1 + \frac{n}{n+1} \right) + 58 \right]
$$

(2.26)

$$
\leq \frac{M_1}{n \pi} (32 \ln 2 + 58)
$$

when $\eta = 0$.

Theorem 2.2 states that if $K(r)$ is a smooth function except the origin, and is $\eta$ times continuously differentiable at $r = 0$, and $K^{(\eta+1)}(r)$ bounded, then the VP-sum of $K(r)$ has at least $(\eta + 1)$-order convergence rate. For example, the Gaussian kernel $f(x) = e^{-x^2/45}$ is an even function that the corresponding $K(r)$ is infinitely differentiable such that the VP-sum of the Gaussian kernel has spectral convergence. For general cases, assuming that the approximate interval we interested in is $[0, \bar{\delta}]$ and a fast decreasing function may connect after $\bar{\delta}$ to localize the kernel function as in Remark 2.2, then the following convergence rate of the VP-sum of the new function $f^*(x)$ at $[0, \bar{\delta}]$ holds
Theorem 2.3. Assume that $f^*(x)$ is a smooth function defined on the positive axis except the connecting point $x = \bar{x}$, and fast decrease at $x \to \infty$. After the variable change and the even and periodic prolongation, if $f^*(x)$ has bounded derivatives at $x = \bar{x}$ until $\eta$-th order, then the convergence rate of the VP-sum of the resulting function $K(r)$ is at least $O(n^{−\eta−1})$.

By Ref. [49], Theorem 2.3 can be derived by the following theorem, which is a frequently-used formula in obtaining higher derivatives.

Theorem 2.4. (Faà di Bruno’s Formula) If $f$ and $\Phi$ are functions with a sufficient number of derivatives, then

$$
\frac{d^m}{dr^m} f(\Phi(r)) = \sum \frac{m!}{b_1!b_2!\cdots b_m!} f^{(k)}(\Phi(r)) \left( \frac{\Phi'(r)}{1!} \right)^{b_1} \left( \frac{\Phi''(r)}{2!} \right)^{b_2} \cdots \left( \frac{\Phi^{(m)}(r)}{m!} \right)^{b_m}
$$

(2.27)

where the sum is over all different solutions in nonnegative integers $b_1, \ldots, b_m$ of $b_1 + 2b_2 + \cdots + mb_m = m$, and $k := b_1 + \cdots + b_m$.

Now back to the proof of Theorem 2.3.

Proof of Theorem 2.3. Recalling the variable change given in Eq. (2.1), the corresponding $\Phi(r)$ reads

$$
\Phi(r) = -n_c \log \left( \frac{1 + \cos r}{2} \right), \quad r \in [0, \pi].
$$

(2.28)

It is observed that $\Phi(r)$ is an even function such that $\Phi^{(k)}(r)$ vanishes and $\Phi^{(k)}(r) \sim O(r)$ as $r \to 0$ when $k$ is an odd number. When $k$ is an even number, it can be checked that $K^{(k)}_-(0) = K^{(k)}_+(0) = \delta^{(k)} f(\Phi(0))$. Above all, $K(r)$ is infinitely differentiable at the origin, i.e., $K(r) \in W^\infty[-\pi, \pi]$ due to the localization at $\Phi^{(k)}(r) = \bar{x}$. After the use of Theorem 2.2, we finish the proof.

2.4 SOE approximations of frequently-used kernels

2.4.1 The Gaussian kernel

We investigate the performance of the VPMR approach for the SOE approximations of the Gaussian kernel which is frequently required in many applications [18, 50]. The inverse Laplace transform representation of the Gaussian kernel $e^{-x^2/4\delta}$ is,

$$
e^{-z^2} = \frac{1}{2\pi i} \int_{\Gamma} e^z \sqrt{\frac{\pi}{z}} e^{-\frac{z^2}{4\delta}} dz,
$$

(2.29)

where $\Gamma$ can be any contour in the complex plane that starts from $-\infty$ in the third quadrant, goes around 0 and returns back to $-\infty$ in the second quadrant. There are mainly three kinds of contours, including the parabolic, the hyperbolic and the modified Talbot contours [51, 52]. All these contours have certain parameters that need to be optimized in order to achieve optimal convergence rate [53, 54, 55]. Alternatively, one can obtain an SOE approximation of Gaussian kernel by the best rational approximation using the residue theorem and Cauchy’s theorem [52].

We perform the comparison on SOE approximations of the Gaussian kernel using our VPMR method given in Section 2 and other existing work discussed above. We take $\delta = 1$. The maximum error

$$
E_\infty = \max_{x \in [0,100]} \left| e^{-\frac{x^2}{4\delta}} - \sum_j m_j e^{-s_j x} \right|
$$

(2.30)

is used to measure the performance, where 100000 monitoring points are randomly sampled from $[10^{-5}, 10^2]$ to estimate the maximum. For the comparison, the results of contour integrals and the best rational approximations are taken from Jiang [18], where the methods are fully optimized and the contours are discretized via the midpoint rule. And the MR is
used to reduce the number of exponentials. For the VPMR, the parameter \( n_c \) is set to \( \lceil n/4 \rceil \), thus the maximum exponent is about 8. The results are displayed in Figure 1. The results demonstrate that the VPMR has advantages in both convergence rate and accuracy. For all five methods, an error level of \( 10^{-13} \) can be achieved with the reduced number \( P \) of exponentials in the SOE approximation not bigger than 20. It was measured \cite{18} that the convergence rate is about \( O(6.3^{-n}) \) of all three contours, and \( O(7.5^{-n}) \) for the best rational approximation. The VPMR achieves a convergence rate of about \( O(9.0^{-n}) \).

2.4.2 SOE approximations of other important kernels

We study the performance of the SOE to approximate the exact kernels with the increase of \( P \). Four different kernels, the Matérn kernel, the power function, the Ewald splitting kernel, and the Helmholtz kernel, are used to test the algorithm. Unlike the Gaussian kernel, some of these kernels have complicated forms thus are difficult to obtain SOE via theoretical approach. We perform the comparison on SOE approximations using the classical Prony’s method \cite{19} which requires only the value of kernel at discrete points. We use the Prony Toolbox \cite{56} which is a software tool in MATLAB in order to perform the Prony analysis.

The first one is the Matérn kernel \cite{57, 58, 59, 60}, often used as a covariance function in modeling Gaussian processes and machine learning. The Matérn kernel of order \( \nu > 0 \) is defined as

\[
 f(x) = \frac{(\sqrt{2\nu}|x|)^\nu}{2^{\nu-1} \Gamma(\nu)} K_\nu(\sqrt{2\nu}|x|),
\]

where \( \nu \) is the smoothness parameter, \( K_\nu \) is the modified Bessel function of the second kind of order \( \nu \) and \( \Gamma \) is the Gamma function. The definition Eq.(2.31) satisfies that \( f(0) = 1 \) for any \( \nu \) and \( f(x) \) has high-order differentiability at the origin when \( \nu \) is larger. In this example, we employ VPMR method to perform the comparison on SOE approximations of the Matérn kernel with different smoothness \( \nu \) and \( \delta = 0 \). Numerical results are given in Figure 2 (a), which demonstrate that the convergence rate of the SOE becomes higher for better smoothness. The efficiency of the resulting SOE produced by the VPMR is very attractive and it needs less than 40 terms for all \( \nu \) to achieve \( 10^{-9} \) maximum error, whereas the convergence rate of the Prony method is slow and only \( 10^{-3} \) for all \( \nu \) can be achieved.

Secondly, we consider the weak-singular power function with \( f(x) = x^{\alpha-1} \), which is frequently required in computational physics \cite{3, 11}. The power function has the following
Figure 2: Maximum errors of the SOE approximations of different kernels, on comparison of the VPMR with the Prony, (a) the Matérn kernel, (b) the power function kernel, (c) the Ewald splitting kernel, and (d) Helmholtz kernel, as functions of the number of exponentials.

inverse Laplace transform expression [12],

\[ x^{\alpha-1} = \frac{1}{\Gamma(1 - \alpha)} \int_{-\infty}^{\infty} e^{-e^{t}x+(1-\alpha)t} dt. \]  

A suitable quadrature rule to Eq. (2.32) yields an explicit discretization to obtain a sum of exponentials. Although constructing the SOE approximation from integral representation can achieve a given accuracy, the uncontrollable increase of exponent values limits the practical use (as the convergence conditions require a tolerable exponent value, see Ref. [22] and Theorem 3.1 in this paper). The results on SOE approximation of the power function using the VPMR method are given in Figure 2 (b), for three different values of \( \alpha \). The value of \( \delta \) is set to 0.05 and the maximal exponent is set to about 5. Its needs 600 terms for all \( \alpha \) to achieve \( 10^{-8} \) maximum error. This convergence is fast considering that the SOE based on the inverse Laplace transform requires the maximal exponent to be about \( 10^3 \) to achieve the same level of accuracy. Furthermore, comparing with the results conducted by the Prony method, the convergence rate of the VPMR method is much more fast.

When \( \alpha = 0 \), the singular power function with expression \( 1/x \) is referred as the Green’s function of 3D Poisson’s equation with free boundary condition, which is frequently used in fast electrostatic sums. In practice, it is not straightforward to evaluate the electrostatic interaction because \( 1/x \) has properties of both short range and long range. The Ewald method solves this problem by dividing the Coulomb potential into near and far parts [61],

\[ \frac{1}{x} = \frac{\text{erfc} (\Lambda x)}{x} + \frac{\text{erf} (\Lambda x)}{x}, \]  

where the parameter \( \Lambda \) describes the inverse of cutoff radius and balances the proportion of computational cost between these two parts. The near part is often truncated at a suitable
cutoff radius and computed as an explicit sum of pairwise interactions. Here we study the SOE for the far part Ewald kernel $\text{erf}(\Lambda x)/x$, which is often studied in Fourier space [62], for different values of $\Lambda$. Figure 2 (c) shows the errors of the SOE approximation as a function of $P$ for different $\Lambda$. We observe that the VPMR needs 400 terms for all $\Lambda$ to achieve $10^{-9}$ maximum error, whereas the Prony has about $10^{-3}$ maximum error with the same number of terms which has six orders of magnitude lower than the VPMR.

Finally, we test the performance of the VPMR for the Helmholtz kernel which has a strong oscillation. The kernel is the Green’s function of the Helmholtz equation. In 2D and 3D, they are given by,

$$f_{2D}(x) = \frac{i}{4} H_0^{(1)}(kx), \quad f_{3D}(x) = \frac{e^{ikx}}{4\pi x},$$ \hspace{1cm} (2.34)

where $H_0^{(1)}$ is the zeroth order Hankel function of the first kind. The Helmholtz equation with high wave number is notoriously difficult to solve numerically, since the larger the value of $k$, the stronger the oscillation of the Helmholtz kernel. An efficient SOE approximation for Helmholtz kernel is also difficult due to this issue. We study the performance of the VPMR approach for the SOE approximations of 2D and 3D Helmholtz kernels on domain $[\delta, 10]$ with $\delta \ll 1$. The results are given in Figure 2 (d) with parameters $k = 50$ (a large wave number) and $\delta = 0.05$. One can observe that 1000 exponentials achieve the error levels of $10^{-9}$ and $10^{-10}$ for 2D and 3D cases, respectively, whereas the Prony achieves the lower levels of $10^{-5}$ for both cases. Note that the 2D/3D Helmholtz kernel yields the well known Sommerfeld integral representation

$$f_{2D}(r) = \frac{1}{4\pi} \int_{-\infty}^{\infty} e^{-\sqrt{\lambda^2 - k^2} |r|} e^{i \lambda r_z} d\lambda$$ \hspace{1cm} (2.35)

and

$$f_{3D}(r) = i \int_0^\infty \frac{\rho^2}{k_z} J_0(k \rho r_z) e^{ikz |r|} dk \rho,$$ \hspace{1cm} (2.36)

where $r = (r_x, r_y)$ for 2D, $r = (r_\rho, r_\theta, r_z)$ for 3D, $k_z = \sqrt{k^2 - k_\rho^2}$, and $J_0$ is the zeroth order Bessel function of the first kind. The Sommerfeld integrals Eq.(2.35) and Eq.(2.36) play a central role in scattering theory. Numerical calculation of the Sommerfeld integrations requires contour deformation to avoid the square root singularity in the integrand and additional approaches to deal with the probable highly oscillatory integrand. The SOE approximation provided by the VPMR method may furnish an useful tool to design fast algorithm for wide applications in electromagnetic scattering field, which will be explored in our future work.

3 The Application of SOE on Convolution Quadrature

One of important applications of the SOE is to quickly approximate convolution quadrature. In this section, we consider the approximation of convolution quadrature between a given kernel $f(t)$ and smooth function $g(t)$ as follows,

$$y(t) = f \ast g = \int_0^t f(t - \tau) g(\tau) d\tau.$$ \hspace{1cm} (3.1)

The convolution quadrature approximation has attracted wide interest due to its broad applications in scientific computing such as integro-partial differential equations [63, 64], fractional differential equations [65, 66, 67, 68, 69], and nonlinear Volterra equations [70, 71, 72, 73]. The temporal convolution quadrature is often evaluated based on a technique of the Laplace inverse transform and Runge-Kutta (RK) time stepping, proposed by Lubich [74, 75]. As introduced in the introduction part, with the Laplace transform $F(s)$ of the kernel function, the convolution integral can be written as,

$$y(t) = \frac{1}{2\pi i} \int_{\Gamma} F(\lambda) \int_0^t e^{\lambda(t-\tau)} g(\tau) d\tau d\lambda.$$ \hspace{1cm} (3.2)
Let \( u(t) = \int_0^t e^{\lambda(t-\tau)} g(\tau) d\tau \), which satisfies ODE \( u' = \lambda u + g(t) \) with \( u(0) = 0 \) and can be integrated by the RK method. The contour integral on \( \Gamma \) can be calculated by employing a numerical quadrature. This method is essentially an interpolation method which uses the linear combination of the interpolation points of function \( g(t) \) for approximating the convolution. The attractive features of convolution quadratures include that they work well for kernels of singular, multiple time scales, and highly oscillatory with given the Laplace transform of the kernel function \([76]\). Schädl et al. \([27]\) developed an improved algorithm with \( O(N \log N) \) multiplications and \( O(\log N) \) active memory for \( N \) time steps. López-Fernández and Sauter \([77]\) introduced a generalized convolution quadrature allowing for variable time steps. These improved algorithms make the Lubich’s method more adaptable and less storage space. However, it was pointed out that this type of algorithms is restricted to sectorial convolution kernels and thus not applicable to wave equations \([77]\). Additionally, it requires the analytical Laplace transform of the kernel function, which can be difficult for some functions such as the Matérn kernel often used in machine learning and statistics \([78]\).

One has to approximate the kernel by rational polynomials to obtain the Laplace transform, leading to a difficulty of error estimates.

Lubich’s method is equivalent to approximate the kernel function by using the Laplace transform where the discrete points on the contour line are the exponents. A different idea for convolution quadratures can be the use of the SOE approximation to the kernel function and the RK step for each exponential is then performed. The advantages of this idea are twofold:

(i) An alternative and more efficient SOE method is introduced other than the Laplace transform for better approximation of some kernels. Here the “better” means that the maximal exponent of the exponents can be tuned to an \( O(1) \) constant instead of \( O(1/h) \) in the Laplace transform-based methods with \( h \) the step size of RK. The convergence order of the error bound with respect to \( h \) is thus consistent with the order of RK method whereas the stage order of RK is not involved.

(ii) One can perform model reduction techniques to reduce the number of exponentials such that the computational cost can be saved.

### 3.1 Fast convolution

We then consider the evaluation of the convolution \( y(t) \) given in Eq.(3.1). One first assumes that \( f(\tau) \) has no singularity, then an SOE expansion of the kernel by the VPMR reads,

\[
\begin{align*}
\tilde{f}(\tau) & \approx f_{es}(\tau) = \sum_{\ell=1}^{P} m_{\ell} e^{-s_{\ell} \tau}, \quad \tau \in [0, t] \\
\text{with } m_{\ell}, s_{\ell} & \in \mathbb{C} \quad \text{and the real part } \Re(s_{\ell}) \geq 0, \text{ which holds } \|f(\tau) - f_{es}(\tau)\|_{\infty} < \varepsilon \text{ for a prescribed accuracy } 0 < \varepsilon \ll 1.
\end{align*}
\]

The SOE expansion leads to an approximate representation of \( y(t) \) by the summation of \( P \) exponential integrals

\[
y(t) \approx \int_0^t f_{es}(t-\tau) g(\tau) d\tau = \sum_{\ell=1}^{P} m_{\ell} Y_{\ell}(t),
\]

with

\[
Y_{\ell}(t) = \int_0^t e^{-s_{\ell}(t-\tau)} g(\tau) d\tau.
\]

Each term of the above summation can be viewed as the solution at \( \tau = t \) of the following ODE,

\[
Y'_{\ell}(\tau) = -s_{\ell} Y_{\ell}(\tau) + g(\tau) \text{ with } Y(0) = 0.
\]

Eq.(3.6) can be efficiently computed via the RK method with step size \( h \) (i.e., \( t = Nh \)) to obtain a high-accurate solution within \( O(N) \) operations.
To be specific, we employ implicit $S$-stage RK method of the form

$$Y_{t}^{n+1} = Y_{t}^{n} + h \sum_{i=1}^{S} b_i K_i,$$

(3.7)

where

$$K_i = -s_i \left( Y_{t}^{n} + h \sum_{j=1}^{S} a_{ij} K_j \right) + g(t_n + c_i h), \quad i = 1, 2, \ldots, S,$$

(3.8)

with $a_{ij}$, $b_i$ and $c_i$ being coefficients, and $Y_t^n$ being the discretization of $Y_t(nh)$. We suppose that a RK method of order $p$ and stage order $q$ is employed (follow the definitions of Ref. [22]), namely, the local truncation error is $O(h^{p+1})$ and each internal stage error is $O(h^{q+1})$. Let us denote $A = (a_{ij})_{S \times S}$, $\beta = (b_1, \cdots, b_S)$ and $\zeta = (c_1, \cdots, c_S)$. They are usually arranged in a mnemonic device which is known as the Butcher tableau. The stability function of the RK method Eq.(3.7) is defined as

$$r(z) = 1 + z \beta^T (I - z A)^{-1} E = \frac{\det(I - z A + z E \beta^T)}{\det(I - z A)}.$$

(3.9)

where $E$ is the column vector of ones and $z = -s_i h$. We choose suitable implicit RK such that $b_j = a_{Sj}$ for $j = 1, \cdots, S$, $c_q = 1$, and all eigenvalues of $A$ have positive real parts. This implies that the method is L-stable, i.e.,

$$|r(z)| \leq 1$$

for $\Re(z) \leq 0$ and $r(\infty) = 0$. (3.10)

This stability condition is important considering that ODE (3.6) may become stiff when the positive exponent is large.

Substituting Eq.(3.7) into Eq.(3.6), one can express the solution of the ODE as,

$$Y_{t}^{n+1} = \sum_{j=0}^{n} v_{n-j}(z_{t}) g_{j} = r(z_{t})Y_{t}^{n} + h \psi_{t} g_{n},$$

(3.11)

where $\psi_{t} = \beta^T (I - z_{t} A)^{-1}$, $z_{t} = -s_i h$, and $v_{n}(z)$ and $g_{j}$ are defined by,

$$v_{n}(z) = r(z)^n \beta^T (I - z A)^{-1}, \quad g_{j} = (g(t_{j} + c_{1} h), \cdots, g(t_{j} + c_{S} h))^T.$$  

(3.12)

Then, the convolution integral Eq.(3.1) at time $t$ is approximated by,

$$y(t) \approx \sum_{\ell=1}^{P} m_{\ell} \left[ r(z_{t}) Y_{\ell}^{N-1} + h \psi_{\ell} g_{N-1} \right],$$

(3.13)

with $Y_{\ell}^{N-1}$ being recursively solved using Eq.(3.11). Since $\psi_{\ell}$ and $g_{N-1}$ are row and column vectors of dimension $q$, the complexity of each time step is $O(P)$.

When the kernel $f(\tau)$ has a singularity (or near singular) at the origin, one shall remove the singularity by splitting the integral into two parts. For a given $t_0 \ll 1$ and $T = t - t_0$, the convolution integral is written as,

$$y(t) = \int_{0}^{t_0} f(\tau) g(t - \tau) d\tau + \int_{0}^{T} f(t - \tau) g(\tau) d\tau := I_1 + I_2.$$ 

(3.14)

Note that $I_2$ has no singularity any more, thus it can be computed using the aforementioned way. To evaluate $I_1$ over interval $[0, t_0]$, one first approximates $g(\tau)$ with polynomial interpolation, and $f(\tau)$ can be expanded by its generalized Taylor series

$$f(\tau) = a_{0} \tau^{-\alpha} + a_{1} \tau + a_{2} \tau^2 + ...$$

(3.15)

where $a_{0} \tau^{-\alpha}$ is the leading order asymptotic of the kernel, and may become weak singular with $0 \leq \alpha < 1$. For weak singular or nearly singular kernels, it is important to have
some a priori asymptotic analysis around the singularity point. With such techniques, the
contribution is simplified to a polynomial-polynomial convolution. Take $t_0 = O(h)$ and let
$G(\tau)$ be the interpolation polynomial of $g(\tau)$. One has,

$$I_1 \approx \int_0^{t_0} \left[ a_0 \tau^{-\alpha} + a_1 \tau + a_2 \tau^2 + \cdots \right] G(t - \tau) d\tau,$$

(3.16)

which can be evaluated explicitly.

We summarize the method in Algorithm 2. Note that except steps 5, 6, 9 and 10, all
of the other steps are precomputed. Moreover, the singular part $I_1$ does not depend on $t$
and is computed only once in the calculation. Thus, the overall computation cost for the
convolution integral is $O(NP)$ where $N$ is the number of time steps.

**Remark 3.1.** One important reason for traditional numerical methods having lower conver-
gence order for weakly singular kernels is that the kernels can not be expanded as standard
Taylor’s series about the singularities. In order to approximate a kernel near its singularity,
the generalized Taylor series Eq.(3.15) [79, 80, 81, 82] is introduced in this paper. We do not
review the literature here, and one can refer to these papers for obtaining the detailed form
of Eq.(3.15). In some recent works, this technique is also introduced to generate fractional
order degenerate kernel methods [83, 84], Taylor-collocation methods [85], and approaches
for computing series solution [86] for solving equation-based problems.

---

### Algorithm 2

**Convolution quadrature based on the SOE**

**Input:** Time $t$, quadrature kernel $f(\tau)$ and $g(\tau)$

**Output:** Convolution quadrature $y(t)$ given in Eq.(3.1)

1. Choose a suitable step size $h$ and the butcher table of the RK method
2. Precompute the explicit expression of $v_n(z)$ given in Eq.(3.12)
3. if $f$ does not have singularity at $0$ then
   4. Construct an SOE expansion of $f$ on $[0, t]$
   5. Compute $\{g_j\}_{j=0}^N$
   6. Evaluate $y(t)$ according to Eq.(3.13)
4. else
   7. Split $y$ into the sum of local integral $I_1$ and convolution $I_2$ for a specified $t_0$
   8. Explicitly approximate $I_1$ by Eq.(3.16)
   9. Employ steps 4-6 to evaluate $I_2$, then sum up $I_1$ and $I_2$
11. end if

---

### 3.2 Error estimate

We present the error analysis of the fast convolution algorithm. We assume that the kernel
$f(\tau)$ has singularity at the origin. The solution $y_h(t)$ to approximate the decomposition in
Eq.(3.14) is given by,

$$y_h(t) = I_1^h + I_2^h,$$

(3.17)

where $I_1^h$ and $I_2^h$ are numerical approximations of $I_1$ and $I_2$.

Consider the estimate of $I_1^h$. Suppose that $g(t - \tau) \in C^\gamma([0, t_0])$ with $\gamma$ being an integer
and $G(t - \tau)$ is a $L$-order interpolation approximation of $g(t - \tau)$ with $L \leq \gamma$. By standard
numerical analysis, the interpolation error is,

$$|G(t - \tau) - g(t - \tau)| \leq C_0 \|g^{(L)}\|_{\infty} h^L, \forall \tau \in [0, t_0].$$

(3.18)

If we truncate the generalized Taylor series Eq.(3.15) at $M$-th order such that $f(\tau) \approx f_M(\tau)$,
satisfies we firstly consider the following four lemmas. The proof of these lemmas can be found in Lemma 3.2. Consider that the RK method is applied to Lemma 3.4.

\[ z(t) = y(t) + \int_0^t f(s)ds \]

\[ |I_1 - I_1^h| = \left| \int_0^t (f(t) - f_M(t)) g(t) d\tau + \int_0^t f_M(t)(g(t) - G(t)) d\tau \right| \]

\[ \leq \int_0^t |f(t) - f_M(t)| |g(t)| d\tau + \int_0^t |f_M(t)| |g(t) - G(t)| d\tau \]

\[ \leq C_1 t_0^{M+1} \int_0^t |g(t)| d\tau + C_0 \|g\|_\infty h^L \int_0^t |f_M(t)| d\tau \]

\[ \leq C_1 (n_0h)^{M+1} |g|_{L^1} + C_0 C_{f_M, t_0} \|g\|_\infty h^L \]

where \( C_{f_M, t_0} = \frac{t_0^{n_0}}{0} \|f_M(t)\| d\tau \) is bounded because the convolution Eq.(3.1) is well defined, and \( C_0 \) and \( C_1 \) are constants.

For the exponential convolution part \( I_2^h \), the kernel function \( f(t - \tau) \) is approximated by its SOE expansion \( f_{es}(t - \tau) \) on \([0, T]\) with the error tolerance \( \varepsilon \), then the error reads,

\[ |I_2 - I_2^h| = \left| \int_0^T (f(t) - f_{es}(t)) g(t) d\tau + \sum_{t=1}^P m_t E_{RK}^t(t) \right| \]

\[ \leq \varepsilon \|g\|_{L^1} + P \max h \|E_{RK}^\max(t)\| \]

where \( E_{RK}^t \) is the error introduced by employing the RK method to solve the \( t \)-th ODE Eq.(3.6), \( m_\max = \max \|[m_t]\|_{t=1}^P \) and \( E_{RK}^\max(t) = \max \{ |E_{RK}^t| \}_{t=1}^P \). To estimate \( E_{RK}^\max(t) \), we firstly consider the following four lemmas. The proof of these lemmas can be found in [28, 22].

Lemma 3.1. When the RK method is applied to \( y' = \lambda y + g \), the stability function \( r(z) \) satisfies

\[ r(z) - e^z = O(z^{p+1}) \]

for \( z \to 0 \).

Lemma 3.2. Consider that the RK method is applied to \( y' = \lambda y + g \) with \( h \) the step size and \( r(z) \) the stability function where \( z = \lambda h \). We define

\[ f^{(k)}_n(z) = \sum_{\nu=0}^n r(z)^{-\nu} \nu^k, \]

then the following upper bound

\[ |z r(z^n f^{(k)}_n(z))| \leq C(n + |z|^{-1})^{k} e^{R(z)n} \]

holds.

Lemma 3.3. For the RK method with order \( p \), the following estimate

\[ \beta^T (I - zA)^{-1} (kA\xi^{k-1} - \xi^k) = O(z^{p-k}) \quad \text{as} \quad z \to 0 \]

(3.24) holds for \( k = 1, 2, \ldots, p \) where \( \xi^k = (c_1^k, c_2^k, \ldots, c_q^k) \) and the definitions of \( \beta, I, \) and \( A \) follow Section 3.1.

Lemma 3.4. The error at time \( t_n = nh \) of the RK method with \( h \) the step size applied to \( y' = \lambda y + t^l/l! \), \( y(0) = 0 \), \( t \in [0, T] \), is given by

\[ e_n = \lambda^{-l-1} (r(h\lambda)^n - e^{nh\lambda}) - \sum_{k=q+1}^p h^n \sum_{\nu=1}^{n-1} r^{(k)}_{n-1-\nu}(h\lambda) \lambda^{k-\nu-1} \sum_{\kappa=0}^{l-k} \frac{(\lambda h\lambda)^{\kappa}}{\kappa!} \]

\[ = \lambda^{-l-1} (r(h\lambda)^n - e^{nh\lambda}) - \tilde{e}_n \]

(3.25)
with \( r(z) \) the stability function,
\[
r_n^{(k)}(z) = r(z)^n z^T (I - zA)^{-1} \delta^{(k)}, \tag{3.26}
\]
and
\[
\delta^{(k)} = A \xi^{k-1} - \xi^k / k \tag{3.27}
\]
where \( p \) and \( q \) are the order and the stage order of the RK method, respectively. The definitions of \( \beta, I, A, \) and \( \xi^k \) follow Lemma 3.3.

We have the following theorem to estimate \( E_{\text{RK}}^{\max}(t) \).

**Theorem 3.1.** Suppose a \( S \)-stage implicit \( L \)-stable RK method. Let \( p \) be the approximate order of the RK, and \( q \leq p-1 \) be the stage order satisfies condition Eq.(3.10). Let \( h \) be the time step. If \( g(\tau) \in C^{(\gamma)}([0, t - t_0], \gamma \geq p \) and max \( |s_\ell h| \leq 1 \), then the error \( E_{\text{RK}}^{\max}(t) \) is bounded by
\[
|E_{\text{RK}}^{\max}(t)| \leq C h^p \left( \sum_{\ell=0}^{p-1} \|g^{(\ell)}(0)\|_\infty + \max_{0 \leq \tau \leq t - t_0} \|g^{(p)}(\tau)\|_\infty \right), \tag{3.28}
\]
where \( C \) is a constant.

**Proof.** For this proof, \( C \) will denote a generic constant that is allowed to depend on \( T \). We first consider the numerical error of which the RK method is applied to \( y' = -s_\ell g + h^t / h! \), \( y(0) = 0 \), where we recall \( s_\ell \) the exponent of the \( \ell \)-th exponential of the SOE constructed by the VPMR method. From Lemma 3.1, for \( nh \leq T \), we have
\[
|r(-h s_\ell)^n - e^{-n h s_\ell}| = \left| (r(-h s_\ell) - e^{-h s_\ell}) \sum_{\nu=0}^{n-1} r(-h s_\ell)^{n-1-\nu} e^{-\nu h s_\ell} \right| \leq C h^p, \tag{3.29}
\]
where the boundness of the stability function \( |r(-h s_\ell)^{(n-1-\nu)}| \) and \( |e^{-\nu h s_\ell}| \) are employed. By Lemma 3.4, with \( \lambda = -s_\ell \), the error \( e_n \) can be split into two parts as in Eq.(3.25), where the first part has an estimate by applying Eq.(3.29) directly:
\[
|(-s_\ell)^{-1-\nu} (r(-h s_\ell)^n - e^{-n h s_\ell})| \leq |s_\ell|^{p-l-1} h^p = O(h^p). \tag{3.30}
\]
Eq.(3.30) takes the advantage of the VPMR method that max \( s_\ell \) is restricted as \( O(1) \), thus \( |s_\ell|^{p-l-1} \) is \( O(1) \).

Next, recalling the definition of \( f_n^{(k)}(z) \) given in Lemma 3.2 and the expression of the second part \( \tilde{e}_n \), we have
\[
\tilde{e}_n = \sum_{k=q+1}^{p} h^k \sum_{\nu=1}^{n-1} r_n^{(k)}(-s_\ell h)^n (-s_\ell h)^{a_{-\ell}} \sum_{\nu=0}^{l-k} \frac{\lambda s_\ell h)^{\nu}}{\kappa!}
\]
\[
= h^{l+1} \sum_{k=q+1}^{p} \sum_{\nu=1}^{n-1} r(-s_\ell h)^{n-1-\nu} \beta^T (I + s_\ell h A)^{-1} \delta^{(k)} (-s_\ell h)^{k-1-\ell} \sum_{\nu=0}^{l-k} \frac{(-s_\ell h)^{\nu}}{\kappa!}
\]
\[
= h^{l+1} \sum_{k=q+1}^{p} \beta^T (I + s_\ell h A)^{-1} \delta^{(k)} (-s_\ell h)^{k-1-\ell} \sum_{\nu=0}^{l-k} \frac{(-s_\ell h)^{\nu}}{\kappa!} (-s_\ell h)^{a_{-\ell}} f_n^{(k)}(-s_\ell h). \tag{3.31}
\]

By substituting Lemmas 3.2 and 3.3 into Eq.(3.31), we obtain
\[
|\tilde{e}_n| \leq C h^{l+1} \sum_{k=q+1}^{p} |s_\ell h|^{p-\nu} \left| \sum_{\nu=0}^{l-k} \frac{(-s_\ell h)^{\nu}}{\kappa!} \right| (n + |s_\ell h|^{-1})^\nu e^{\Re(-s_\ell h)n} \tag{3.32}
\]
\[
\leq C h^p |s_\ell|^{p-l-1} (1 + n|s_\ell h|)^{l-g-1}
\]
\[
\leq C h^p |s_\ell|^{p-q-2} = O(h^p) \tag{3.32}
\]
where the last inequality because $|s_t/h| \leq 1$ and $\max |s_t|$ is $O(1)$.

From Eqs.(3.30) and (3.32), we obtain $e_n = O(h^p)$. The error bound for general smooth functions $g$ then follows with the Peano kernel argument of [22]. Since $g(\tau) \in C^{(\gamma)}([0, T])$ with $\gamma \geq p$, we may treat each of the terms in the Taylor expansion of $g$ separately:

$$g(T) = \sum_{l=0}^{p-1} \frac{T^l}{l!} g^{(l)}(0) + \int_0^T \frac{\tau^{p-1}}{(p-1)!} g^{(p)}(T - \tau) d\tau. \quad (3.33)$$

From [22], it is proved that the error of the RK method applied to the equation with inhomogeneity $g^{(l)}(0)T^l/l!$ is given by $e_n g^{(l)}(0)$. By Eq.(3.33), the error bound Eq.(3.28) could be obtained by estimating each term in the Taylor expansion of $g$ separately.

Combining Eqs.(3.19), (3.20) and (3.28), we find that the error satisfies $|y(t) - y_h(t)| = O \left( h^d + \varepsilon \right)$ for $d = \min \{ M + 1, L, p \}$.

**Remark 3.2.** Differently, the Laplace transform-based methods have a common error bound $O \left( \min \{ p, q+1 \} \right)$ in which the stage order $q$ is also involved. This $O(h^{q+1})$ comes from the contour integral over the segment $|\Im(\lambda)| \leq 1/h$ of the Laplace transform with $\lambda$ the integration path (see the proofs of Theorem 4.1 in [28] and Lemma 5.1 in [22] for examples). Our convolution method takes advantage of the SOE constructed by the VPMR method, namely the maximal exponent which is independent of the step size $h$, can easily guarantee $|s_t/h| \leq 1$. In fact, the proof of Theorem 3.1 is similar to the proof of Lemma 5.1 in [22], sharing the same $O(h^p)$ convergence rate. This elimination of $O(h^{q+1})$ term will improve the convergence rate when $p > q + 1$, as the Lobatto IIIC method (with $p = 4$ and $q = 2$) which is used in the numerical tests of this paper. In other words, our method avoids solving stiff problem via the RK.

**Remark 3.3.** In Section 3.1, we propose the $t_0 = O(h)$ condition to guarantee the $O(h^{M+1} + h^L)$ decay of the error bound of approximation Eq.(3.16). In practice, considering the error estimate in Eq.(3.19), the choice of $t_0$ has a broader rule that $t_0^{M+1} \sim \varepsilon$ and $\int_{t_0}^T |f_M(\tau)| d\tau = O(1)$ which will not affect the overall accuracy and independent of $h$. In other words, choosing $t_0$ independent of $h$ has an additional advantage that one SOE can be used for different $h$. This rule for the choice of $t_0$ can also be used for the algorithms developed in Section 4.

### 3.3 Numerical Examples

We present numerical results to illustrate the performance of the SOE approximation method developed in this paper. We test the performance of the SOE to approximate the exact kernels $f(x)$ with the increase of $P$. To assess the accuracy, we compute the maximum error $E_\infty$ of the resulted SOE approximation $f_{\text{es}}(x) = \sum_{j=1}^P m_j e^{-s_j x}$ with $P$. It can be viewed as an approximation of the continuous $L^\infty$ norm defined by,

$$E_\infty = \max \left\{ |f_{\text{es}}(x_i) - f(x_i)|, i = 1, \ldots, M \right\}, \quad (3.34)$$

where $\{x_i, i = 1, \ldots, M\}$ are monitoring points randomly distributed from $(-\delta, 10]$ with $\delta \ll 1$ and we take $M = 10000$. Second, the application and behavior of the fast convolution quadrature algorithm are illustrated from some examples in which the Lobatto IIIC [87] is employed as the RK method, i.e., with $S = 3, p = 4$ and $q = 2$. The error and convergence order are used to measure the accuracy of the algorithm. The SOE for all different kernels are done with manually tuned parameters, which is optimized to obtain the required accuracy at a near-minimal number of exponentials. All the calculations in this section are performed with Matlab code on an Intel TM core of clock rate 2.50 GHz with 24 GB of memory.

In Eq.(3.4), we take a Gaussian kernel $f(\tau) = e^{-\tau^2/4}$, $g(\tau) = \sin \tau$, and calculate the temporal convolution,

$$y(t) = \int_0^t e^{-\frac{(t-\tau)^2}{4}} \sin \tau d\tau. \quad (3.35)$$

The reference “exact” solution is obtained via adaptive Gauss-Kronrod quadrature with $10^{-14}$ absolute accuracy. Table 1 displays the results of $y$ at time $t = 1, 4$ and 10 for different
time steps. The SOE approximation parameters take $\varepsilon = 8.1e - 14$, $n_c/(2n - 1) = 1/8$ and the reduced number of exponentials is $P = 20$. A fourth order convergence in $h$ is clearly shown, in agreement with the convergence order of the RK. It is also found that the error does not accumulate with the increase of $t$. Figure 3 presents the CPU time as function of $t$, and the linear scaling with respect to $t$ is illustrated.

Table 1: Absolute errors and convergence rates to calculate convolution Eq.(3.35) for different $t$

| Step size $h$ | $t = 1$ | Order | $t = 4$ | Order | $t = 10$ | Order |
|--------------|---------|--------|---------|--------|----------|--------|
| 0.25         | 4.49e - 6 | -      | 3.31e - 6 | -      | 3.53e - 6 | -      |
| 0.1          | 1.19e - 7 | 3.93   | 1.03e - 7 | 3.62   | 1.06e - 7 | 3.70   |
| 0.05         | 7.46e - 9 | 3.95   | 6.79e - 9 | 3.71   | 6.90e - 9 | 3.77   |
| 0.025        | 4.68e - 10 | 3.96  | 4.36e - 10 | 3.77  | 4.41e - 10 | 3.82  |
| 0.01         | 1.20e - 11 | 3.97   | 1.14e - 11 | 3.82  | 1.15e - 11 | 3.86  |
| 0.005        | 7.21e - 13 | 3.98   | 6.96e - 13 | 3.85  | 7.10e - 13 | 3.88  |

Figure 3: CPU time as function of $t$ for different time steps $h = 0.05$ (red square), 0.01 (green circle) and 0.005 (blue triangle). The solid lines are linear fitting of these data.

The next example studies the convolution of the singular power function $f(\tau) = \tau^{\alpha-1}$ with $0 < \alpha < 1$ and a smooth source $g(\tau) = \cos \tau$. The convolution is called the Riemann-Liouville fractional integral \[88\] and is written as,

$$y(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - \tau)^{\alpha-1} \cos \tau d\tau,$$

where $\Gamma(\alpha)$ is the Gamma function. This problem has exact solution,

$$y(t) = \frac{2^{1-\alpha} \sqrt{\pi t^\alpha}}{\alpha \Gamma \left(\frac{3}{2}\right) \Gamma \left(\frac{1+\alpha}{2}\right)} \hat{H} \left(1, \left[\frac{1}{2} (1 + \alpha), 1 + \frac{1}{2} \alpha\right], -\frac{t^2}{4}\right),$$

where $\hat{H}(\{a_i\}_{i=1}^{\delta_1}, \{b_j\}_{j=1}^{\delta_2}, \tau)$ is the generalized hypergeometric function defined as follows,

$$\hat{H}(\{a_i\}_{i=1}^{\delta_1}, \{b_j\}_{j=1}^{\delta_2}, \tau) = \sum_{\ell=0}^{\infty} \frac{\prod_{i=1}^{\delta_1} (a_i)_{\ell}}{\prod_{j=1}^{\delta_2} (b_j)_{\ell}} \left(\frac{\tau^\ell}{\ell!}\right),$$

with $\delta_1$ and $\delta_2$ being two positive integers and $(\cdot)_{\ell} = \Gamma(\cdot + \ell)/\Gamma(\cdot)$ is the Pochhammer symbol. In the SOE approximation, one takes $n_c$ such that $n_c/(2n - 1) = 0.15, 0.2$ and 0.4 for $\alpha = 0.1, 0.5$ and 0.9, respectively. $t_0$ takes 0.05, such that the values of $\int_0^t \tau^{\alpha-1} d\tau$ are
7.411, 0.447, and 0.075 for \( \alpha = 0.1, 0.5 \) and 0.9, respectively. And the number of exponentials keeps \( P = 640 \). The error level of the approximation is \( \sim 10^{-9} \). In Eq. (3.14), the convolution is split into \( I_1 \) and \( I_2 \). We use a four-order scheme in \( I_1 \) and the Lobatto IIIIC method for \( I_2 \). The maximal absolute errors of \( I \) for different \( t \) are presented in Table 2, together with the corresponding convergence rates. Most of the data show approximate fourth-order convergence, in agreement with the theoretical analysis, whereas some disagreements appear due to the possible accumulate of rounding error comes from the SOE or the interpolation, especially for \( \alpha = 0.1 \) which corresponding to more singular nature.

It is noted that the power function as the kernel function requires a large \( P \) to achieve high accuracy and the SOE approaches have been studied in literature [12, 3, 11]. Typically, one shall use hundreds of exponentials to achieve error of 8 \( \sim \) 9 digits, but the maximal exponent is \( \sim 10^3 \) which dramatically decrease the convergence precision of RK. The VPML has slightly less number of exponentials for this level of accuracy, but with controllable upperbound of the positive exponents, thus has better performance. We remark that the convolution quadrature will be improved if one introduces better techniques such as the Ewald splitting (see [62] for recent work and reference therein) and approximates the smooth part by the SOE expansion. This is not the central issue of this work, and we save it for future study.

| \( \alpha \) | Step size \( h \) | \( t = 1 \) | Order | \( t = 4 \) | Order | \( t = 8 \) | Order |
|---|---|---|---|---|---|---|---|
| 0.25 | 4.11e−5 | - | 4.11e−5 | - | 7.97e−5 | - | 4.11e−5 |
| 0.1 | 4.61e−6 | 3.64 | 1.73e−6 | 3.45 | 3.04e−6 | 3.57 | 7.97e−5 |
| 0.0625 | 7.80e−7 | 3.69 | 3.10e−7 | 3.52 | 5.29e−7 | 3.62 | 2.28e−7 |
| 0.05 | 3.32e−7 | 3.71 | 1.35e−7 | 3.55 | 2.28e−7 | 3.64 | 1.58e−7 |
| 0.025 | 2.25e−8 | 3.76 | 9.62e−9 | 3.63 | 1.58e−8 | 3.70 | 3.64 |
| 0.25 | 4.22e−5 | - | 1.02e−5 | - | 2.41e−5 | - | 2.41e−5 |
| 0.1 | 1.40e−6 | 3.72 | 3.95e−7 | 3.55 | 8.26e−7 | 3.68 | 1.39e−7 |
| 0.0625 | 2.31e−7 | 3.76 | 6.85e−8 | 3.61 | 1.39e−7 | 3.72 | 1.39e−7 |
| 0.05 | 9.75e−8 | 3.77 | 2.94e−8 | 3.63 | 5.92e−8 | 3.73 | 5.92e−8 |
| 0.025 | 6.55e−9 | 3.81 | 2.40e−9 | 3.63 | 4.34e−9 | 3.74 | 4.34e−9 |
| 0.25 | 5.54e−6 | - | 1.55e−6 | - | 3.74e−6 | - | 3.74e−6 |
| 0.1 | 1.69e−7 | 3.81 | 4.82e−8 | 3.78 | 1.09e−7 | 3.86 | 1.09e−7 |
| 0.0625 | 2.72e−8 | 3.84 | 7.49e−9 | 3.84 | 1.58e−8 | 3.94 | 1.58e−8 |
| 0.05 | 1.14e−8 | 3.84 | 2.94e−9 | 3.89 | 5.41e−9 | 4.06 | 5.41e−9 |
| 0.025 | 8.88e−10 | 3.80 | 1.96e−10 | 3.90 | 1.47e−9 | 3.41 | 1.47e−9 |

4 Convolution Quadrature Equations

In this section, we extend the SOE-based fast convolution method to solve two kinds of convolution equations, which has strong connection with the solution of many problems in applications [89, 88]. Our method provides both memory-saving and high-efficiency with \( O(N) \) complexity for \( N \) time steps, avoiding solving stiff problems.

4.1 Linear convolution equations

We consider a class of linear convolution equations of the form,

\[
(1 - \omega)g(t) + H(t) = \int_0^t f(t - \tau)g(\tau)d\tau
\]

where \( H(\tau) \) is a given source, \( f(\tau) \) is the kernel function, \( \omega \) is a real parameter, and \( g(\tau) \) is unknown except the initial point \( g(0) = g_0 \). This class of integral equations has been frequently studied, e.g., it can be derived from solving linear parabolic and hyperbolic
evolution equations by the method of lines [77]. When the kernel takes \( f(t - \tau) = (t - \tau)^{-\alpha} \) with parameter \( 0 < \alpha < 1 \), the equation Eq.(4.1) is the so-called Abel integral equation for \( \varpi = 1 \) or the generalized Abel integral equation for \( \varpi \neq 1 \). The equation Eq.(4.1) is the solution of the reduced Abel problem and is essentially equivalent to the theory of generalized differentiation and integration [88, 90].

When the kernel function is not singular, we approximate \( f(t - \tau) \) by its SOE expansion. The discretization of Eq.\([4.1]\) by the RK (as in Eq.(3.13)) at time \( t = Nh \) reads,

\[
(1 - \varpi)g_N + H_N = \sum_{\ell=1}^{P} m_{\ell} \left[ r(z_{\ell})Y_{\ell}^{N-1} + h\psi_{\ell}g_{N-1} \right] 
\]

where \( H_j = H(jh) \), \( \psi_{\ell} \) and \( g_{N-1} \) are defined in Section 3. We define \( g(t_j) \) as the integer stage and \( g(t_j + ch) \) the internal stage when \( 0 < c < 1 \). To reduce unknowns, one can approximate the internal stages by integer stages using the \( m \)-point interpolation,

\[
g(t_j + c_h) = \sum_{\ell=1}^{m} \alpha_{\ell} g(t_{j-\ell+2})
\]

where \( \alpha_{\ell} \) are interpolation weights. A recursive scheme is then formulated by solving a linear equation with one unknown quantity at each time step, and thus the solution can be calculated explicitly.

If the kernel has a singularity at the origin, one employs the aforementioned splitting technique Eq.(3.14) to remove it. Let \( t_0 = n_0h \ll 1 \) with integer \( n_0 \). When \( t < t_0 \), one replaces \( f(t - \tau) \) by the generalized Taylor expansion and \( g(\tau) \) by the local interpolation polynomial, respectively. The convolution equation then degenerates into a simple system of linear equations. When \( t \geq t_0 \), the convolution equation Eq.(4.1) reads,

\[
(1 - \varpi)g(t) + H(t) = \int_{0}^{t_0} f(\tau)g(t - \tau)d\tau + \int_{t_0}^{T} f(t - \tau)g(\tau)d\tau.
\]

Approximating \( f(t - \tau) \) by the SOE on \([0, T]\) and Eq.(4.4) can be solved with exactly the same way as the nonsingular case.

We consider the approximation error for the case of singular kernels. For the singular part in the right hand of Eq.(4.4), \( f(\tau) \) is approximated by \( f_M(\tau) \) with \( \tau^{-\alpha} \) the leading order asymptotic of the kernel, and \( g(t - \tau) \) is approximated as an \( L \)-order interpolation. It is not difficult to prove that the integration of singular integrand within \([0, t_0]\) has error of \( O(h^{M+1} + h^L) \). For the smooth part in the right hand of Eq.(4.4), kernel \( f(t - \tau) \) is approximated by its \( P \)-term SOE expansion \( f_{es}(t - \tau) \) within a prescribed \( \varepsilon \) and the internal stages of \( g(\tau) \) are approximated by an \( m \)-point interpolation at the integer stages (as shown in Eq.\([4.3]\)). With an \( L \)-stable \( S \)-stage RK method with order \( p \) and \( q + 1 \leq p \), one has,

\[
(1 - \varpi)g(t) + H(t) = \sum_{\ell=1}^{P} m_{\ell}e^{-s_{\ell}t_0} \int_{0}^{T} e^{-s_{\ell}(T-\tau)}g(\tau)d\tau + \int_{0}^{T} f_{\varepsilon}(t - \tau)g(\tau)d\tau + \int_{0}^{t_0} f(\tau)g(t - \tau)d\tau
\]

\[
= \sum_{\ell=1}^{P} M_{\ell}Y_{\ell}(T) + \int_{0}^{t_0} f(\tau)g(t - \tau)d\tau + O(\varepsilon),
\]

where \( M_{\ell} = m_{\ell}e^{-s_{\ell}t_0} \), \( f_{\varepsilon} = f - f_{es} \), and \( Y_{\ell}(T) \) is the solution of the ODE, \( Y_{\ell}(\tau) = -s_{\ell}Y_{\ell}(\tau) + g(\tau) \) with \( Y_{\ell}(0) = 0 \). Suppose that \( T = N_T h \). To clearly see the error behavior, by using Eq.(4.2) one rewrites Eq.(4.5) as,

\[
(1 - \varpi)g(t) + H(t) = \sum_{\ell=1}^{P} M_{\ell}Y_{\ell}^{N_T} + \int_{0}^{t_0} f_M(\tau)G(t - \tau)d\tau + O(h^d + \varepsilon),
\]
where $Y^N_{\ell}$ is the numerical discretization of $Y_\ell(T)$ via RK. Note that $c_\ell = 1$ and the stability function $r(z_\ell)$ satisfies $r(z_\ell) = e^{\gamma h_{\ell}} + O(h_{\ell}^{\alpha+1})$ [87] thus it is $O(1)$ for every $\ell$.

Let us write the middle term in Eq. (4.6) as $\int_0^T f_M(\tau)G(t-\tau)d\tau = R(t) + \kappa g(t)$, where the coefficient $\kappa$ of $g(t)$ is obviously $O(h^{1-\alpha})$. The solution of $g(t)$ is given by,

$$ g(t) = \frac{1}{1-\omega - \kappa} \left[ h \sum_{\ell=1}^{P} \sum_{j=0}^{N_T-1} \sum_{s=1}^q M_{\ell} v_{\ell N_T-1-j}^s g_j^s + R(t) - H(t) + O(h^d + \varepsilon) \right] $$

$$ = \frac{1}{1-\omega - \kappa} \left[ h \sum_{j=0}^{N_T-1} \sum_{k=1}^m \xi_{jk} g(t_{j+k+2}) + R(t) - H(t) + O(h^d + \varepsilon) \right], \quad (4.7) $$

where $v_{\ell N_T-1-j}^s$ is the s-th component of $v_{N_T-1-j}(z_\ell)$, $g_j^s = g(t_j + c_s h)$, and

$$ \xi_{jk} = \sum_{\ell=1}^P \sum_{s=1}^q M_{\ell} v_{\ell N_T-1-j}^s \alpha_k^s $$

is an $O(1)$ constant related to the RK method and SOE coefficients. Since the internal point interpolation is $O(h^L)$, the error of $g(t)$ is bounded by

$$ \gamma_N \leq \left| \frac{1}{1-\omega - \kappa} \left[ \sum_{\ell=1}^{N_T} h\Xi_{\ell}(\gamma_{\ell} + O(h^L)) + O(h^d + \varepsilon) \right] \right|, \quad (4.9) $$

where $\gamma_{\ell} = |g(t_\ell) - g|$ and $\Xi_{\ell} = \sum_{j+k+2=\ell} \xi_{jk}$.

Obviously, if $\omega = 1$, the convergence rate for solving $g(t)$ is $O(h^{d-1+\alpha} + \varepsilon h^{\alpha-1})$. Otherwise, if $\omega \neq 1$, the convergence rate is $O(h^d + \varepsilon)$. Note that the error in the initial value will not affect the convergence rate after a period of time.

### 4.2 Nonlinear Volterra integral equations

As another typical problem, we consider the nonlinear Volterra integral equation,

$$ u(t) = a(t) + \int_0^t f(t - \tau) g(\tau, u(\tau)) d\tau, \quad t \geq 0 \quad (4.10) $$

where $g(\tau, u(\tau))$ is a smooth nonlinear function and $a(\tau)$ is an inhomogeneous known function. The unknown $u(\tau)$ is needed to be solved at the uniform time steps with the initial condition $u(0) = u_0$. The nonlinear Volterra integral equation Eq. (4.10) arises in a variety of applications, including continuum mechanics, potential theory, electricity and magnetism [91, 92, 93]. The extension of the RK-based algorithm is less immediate, because the integral approximation uses the internal stages of the RK method.

We use the same setup as before with the kernel singularity at the origin, uniform time step $h$ and parameter $t_0 = n_0 h$ satisfying $0 < t_0 \ll 1$. When $t < t_0$, similar as before, $f(t - \tau)$ and $g(t, u(t))$ are approximated by the generalized Taylor expansion and the local polynomial interpolation, respectively. The numerical solution of $u(t)$ at the interpolating points on $[0, t_0]$ is then solved via Newton’s iteration algorithm. When $t \geq t_0$, $f(t - \tau)$ is approximated by its SOE expansion on $[0, T]$ such that the solution is rewritten as the summation of a known function and the convolution of the exponentials and a nonlinear function. We can introduce an RK-based convolution quadrature under the assumptions of Section 3.1, then follow a recursive process to solve $u(t)$ step by step. The discretization of the nonlinear Volterra equation at time $t = Nh$ reads,

$$ u(t) \approx u_N = a_N + \sum_{\ell=1}^P M_{\ell} \left[ r(z_\ell) Y^N_{\ell} + h\psi_{\ell} g_{N_T-1} \right] + \int_0^t f_M(\tau)G(t-\tau, u(t-\tau)) d\tau. \quad (4.11) $$

23
The values at internal stages \( u(t_j + c_ih) \) with \( 0 < c_i < 1 \) are approximated by interpolation at the integer points, which reduces the cost of solving nonlinear equation.

We analyze the convergence rate of the algorithm. The kernel \( f(\tau) \) is approximated by its generalized \( M \)-order Taylor expansion \( f_M(\tau) \) on \([0, t_0]\) and its SOE expansion \( f_{es}(t - \tau) \) with tolerance \( \varepsilon \) on \([0, T]\). \( g(t - \tau, u(t - \tau)) \) is approximated by \( L \)-order interpolation \( G(t - \tau, u(t - \tau)) \) on \([0, t_0]\), and the internal stages of \( g(\tau) \) are approximated by its \( m \)-point interpolation at the integer points on \([0, T]\). The numerical error is to estimate,

\[
|u(t) - u_N| = E_{t_0} + \int_0^T (f(t - \tau) - f_{es}(t - \tau)) g(\tau, u(\tau)) d\tau + \sum_{\ell=1}^P E_{\text{RK}}^\ell(t) \tag{4.12}
\]

where

\[
E_{t_0} = \int_0^{t_0} [f(\tau)g(t - \tau, u(t - \tau)) - f_M(\tau)G(t - \tau, u(t - \tau))] d\tau, \tag{4.13}
\]

and \( E_{\text{RK}}^\ell(t) \) is the error introduced by employing the RK method to solve the ODE. \( E_{t_0} \) has an estimation,

\[
|E_{t_0}| = \left| \int_0^{t_0} (f(\tau) - f_M(\tau))g(t - \tau, u(t - \tau)) + f_M(\tau)(g(t - \tau, u(t - \tau)) - G(t - \tau, u(t - \tau))) d\tau \right| \\
\leq C_0 t_0^{M+1} \left| \int_0^{t_0} g(\tau, u(\tau)) d\tau \right| + C_1 h L \sum_{i=0}^L \|\partial_i^2 \partial^{L-i}_a g(\tau, u(\tau))\|_{\infty} \int_0^{t_0} |f_M(t - \tau)| d\tau \\
\leq C_0 (v_0 h)^{M+1} \|g\|_{L_1} + C_1 C_{f_M, t_0} h^L \sum_{i=0}^L \|\partial_i^2 \partial^{L-i}_a g(\tau, u(\tau))\|_{\infty} \tag{4.14}
\]

where \( C_{f_M, t_0} = \int_0^{t_0} |f_M(t - \tau)| d\tau \) is bounded, and \( C_0 \) and \( C_1 \) are constants. The error estimate of the exponential part reads,

\[
\left| \int_0^T (f(t - \tau) - f_{es}(t - \tau)) g(\tau, u(\tau)) d\tau \right| \leq \varepsilon \|g\|_{L_1}. \tag{4.15}
\]

For \( E_{\text{RK}}^\ell(t) \), we have the following theorem.

**Theorem 4.1.** For nonlinearity \( g(\tau, u(\tau)) \), assume that the following local Lipschitz condition for \( \eta > 0 \),

\[
|g(\tau, v_1) - g(\tau, v_2)| \leq C(\eta) \cdot |v_1 - v_2| \text{ for } |v_1| \leq \eta, |v_2| \leq \eta, 0 < \tau < t. \tag{4.16}
\]

Consider a \( S \)-stage implicit RK method with order \( p \) and stage order \( q \leq p - 1 \), satisfying stable condition Eq.(3.10) and \( \max_i |s_i h| \leq 1 \). If the internal stages are approximated by integer stages using the \( m \)-point \( L \)-order interpolation Eq.(4.3), the error of RK is bounded by

\[
|E_{\text{RK}}^\ell(t)| \leq C_2(\eta) \left[ \max_{j \in \{0, \ldots, N_T\}} |u_j - u(t_j)| + h^p + h^L \right]. \tag{4.17}
\]

**Proof.** Similar to the analysis given in Section 4.1, using the local Lipschitz condition, we
obtain

$$\left| E_{RK}^\ell(t) \right| = \left| hM_\ell \sum_{j=0}^{N_\ell-1} \sum_{s=1}^q \nu_{N_\ell-1-j}^{sf} \sum_{k=1}^m \alpha_k^s g(t_{j-k+2}, u_{t_{j-k+2}}) - g^s_j \right| + O(h^p)$$

$$= \left| hM_\ell \sum_{j=0}^{N_\ell-1} \sum_{s=1}^q \nu_{N_\ell-1-j}^{sf} \sum_{k=1}^m \alpha_k^s [g(t_{j-k+2}, u_{t_{j-k+2}}) - g^0_{j-k+2}] + O(h^p + h^L) \right|$$

$$\leq C(\eta)hM_\ell \sum_{j=0}^{N_\ell-1} \sum_{s=1}^q \nu_{N_\ell-1-j}^{sf} \sum_{k=1}^m \alpha_k^s [u_{j-k+2} - u(t_{j-k+2})] + O(h^p + h^L)$$

$$\leq C_2(\eta) \max_{j \in \{0, \ldots, N_\ell\}} |u_j - u(t_j)| + h^p + h^L$$

(4.18)

where $g^s_j = g(t_j + c_s h, u(t_j + c_s h))$ are the exact value of the stages. Note that the first identity in Eq. (4.18) uses the condition $\max_{\ell} |s_\ell h| \leq 1$ and $s_\ell$ being $O(1)$ for all $\ell$. Otherwise, the $O(h^p)$ term should be replaced by $O(h^{\min(p,q+1)})$.

The error bound of $\left| E_{RK}^\ell(t) \right|$ in Theorem 4.1 contains the maximum error of the solution at the time steps less than the current time. Choosing $t_0$ with the rule in Remark 3.3 can naturally guarantee precision. Combining Eqs. (4.14), (4.15) and (4.17), we obtain the following error bound

$$|u(t) - u_n| = O(h^d + \varepsilon).$$

(4.19)

4.3 Examples

In this subsection, there are four examples, among which the first two are linear integral equations and the third and the fourth are nonlinear integral equations. All the calculations in this section are performed with Matlab code on an Intel TM core of clock rate 2.50 GHz with 24 GB of memory.

4.3.1 Linear convolution equation

The first example is with the Gaussian kernel,

$$g(t) + \frac{\sqrt{\pi}}{2e} f_1(t) + f_2(t) - \cos(t) = \int_t^\infty e^{-\frac{(t-\tau)^2}{4}} g(\tau) d\tau,$$

(4.20)

with

$$f_1(t) = \left[ \text{erf} \left( \frac{1}{2} (t - 2i) \right) + \text{erf} \left( \frac{1}{2} (t + 2i) \right) \right] \cos(t),$$

(4.21)

$$f_2(t) = \left[ -\text{erfi} \left( 1 - \frac{i t}{2} \right) - \text{erfi} \left( 1 + \frac{i t}{2} \right) + 2\text{erf}(1) \right] \sin(t).$$

(4.22)

Here, erf(·) and erfi(·) are the error and imaginary error functions. Eq. (4.20) has exact solution $g(t) = \cos t$. The parameters of RK and interpolation method are the same as the above case. The SOE approximation parameters take $\varepsilon = 8.1e - 14$, $n_c/(2n - 1) = 1/8$ and $P = 20$. A fourth order convergence in step size $h$ is shown, in agreement with the theoretical analysis.

The second example is the generalized Abel equation, which has a singular kernel,

$$3g(t) + H(t) = \int_t^\infty (t - \tau)^{-\alpha} g(\tau) d\tau,$$

(4.23)

where $H(t)$ is obtained with respect to higher accuracy via our algorithm by taking $g(\tau) = \cos \tau$. For the purpose of numerical test, $g(\tau)$ is solved by the our numerical scheme, which
is compared to $\cos \tau$ for the measurement of the error. The SOE approximation parameters take $\varepsilon = 1.4e^{-8}$, $n_c/(2n-1) = 0.2$ and $P = 600$. The $t_0$ is fixed as 0.05. Table 4 displays the error and convergence rate for $\alpha = 0.5$, and again one can observe the errors in agreement with the analysis.

Table 4: Absolute errors and convergences rates for the solution of Eq.(4.23) at different $t$

| Step size $h$ | $t = 2$ | Order | $t = 6$ | Order | $t = 10$ | Order |
|--------------|--------|-------|--------|-------|----------|-------|
| 0.025        | 2.60e-8 | -     | 9.80e-6 | -     | 3.95e-7  | -     |
| 0.01         | 1.13e-8 | 3.74  | 4.25e-8 | 3.74  | 1.71e-7  | 3.74  |
| 0.00625      | 1.47e-9 | 4.14  | 5.20e-9 | 4.24  | 1.97e-8  | 4.33  |
| 0.005        | 5.30e-10| 4.25  | 1.90e-9 | 4.30  | 6.80e-9  | 4.33  |

4.3.2 Nonlinear Volterra integral equation

The third example arises in the analysis of neural networks with post-inhibitory rebound, where the model [94] is given by,

$$u(t) = 1 + \int_0^t (t - \tau)^3 (4 - t + \tau)e^{-t+\tau} \frac{u^4(\tau)}{1 + 2u^2(\tau) + 2u^4(\tau)} d\tau. \tag{4.24}$$

The “exact” solution of Eq.(4.24) at $t = 10$ is $u(10) = 1.25995582337$ [94]. We calculate the absolute error at time $t = 10$ by our algorithm. The interpolation order takes $L = 4$. The SOE parameters are $\varepsilon = 10^{-12}$, $n_c/(2n-1) = 2.25$ and $P = 170$. The error tolerance for the Newton’s method is $10^{-12}$. The accuracy results and CPU time performance (in seconds) are shown in Table 5 for different steps, from which the fourth-order convergence of the algorithm is displayed, in agreement with the theoretical analysis. Due to the number of iterative steps of Newton’s method is different in each time step, the computational time achieves nearly linear scaling with $h$, demonstrating an attractive performance.

Table 5: Absolute errors, convergence rates and CPU time (seconds) for solving the Volterra equation Eq.(4.24)

| Step size $h$ | Error  | Order | CPU time |
|--------------|--------|-------|----------|
| 1           | 2.65e-2 | -     | 1.2e-4   |
| 0.625       | 3.91e-3 | 3.88  | 1.8e-4   |
| 0.5         | 1.44e-3 | 4.02  | 2.7e-4   |
| 0.25        | 4.64e-5 | 4.43  | 4.7e-4   |
| 0.0625      | 2.48e-7 | 4.12  | 1.3e-3   |
| 0.05        | 1.43e-7 | 4.01  | 1.8e-3   |
| 0.01        | 1.90e-10| 4.05  | 7.4e-3   |
The fourth one is with a singular kernel, arising in the theory of superfluidity [93]. The equation is given by,

\[ u(t) = -\int_0^t \frac{(u(\tau) - \sin \tau)^3}{\sqrt{\pi(t - \tau)}} d\tau. \]  

(4.25)

In the calculations, we take \( t_0 = 0.05, \varepsilon = 1.40e - 8, n_c/(2n - 1) = 0.4 \) and \( P = 640 \). The order of interpolation is \( L = 4 \). The “exact” solution is calculated with respect to \( h = 0.0001 \) by our algorithm, with a tolerance of \( 10^{-10} \) in the iteration method. Table 6 displays the errors at \( t = 2, 6 \) and \( 10 \) and the corresponding convergence rates. As expected, a fourth order of convergence is observed, in agreement with theoretical analysis. A few disagreements appear due to the accuracy of the SOE is \( 10^{-10} \) which is dominated in the error when the step size is small.

Table 6: Absolute errors and convergence rates of the Volterra integral equation Eq. (4.25) at different \( t \)

| Step size \( h \) | \( t = 2 \) | Order | \( t = 6 \) | Order | \( t = 10 \) | Order |
|------------------|-----------|-------|-----------|-------|-------------|-------|
| 0.025            | 3.33e - 8 | -     | 1.31e - 7 | -     | 7.39e - 8   | -     |
| 0.0125           | 2.00e - 9 | 4.06  | 8.39e - 9 | 3.97  | 4.14e - 9   | 4.16  |
| 0.01             | 8.78e - 10| 3.97  | 3.63e - 9 | 3.92  | 1.74e - 9   | 4.09  |
| 0.00625          | 1.84e - 10| 3.82  | 6.75e - 10| 3.80  | 1.72e - 10  | 4.37  |

5 Conclusions

We propose an accurate SOE approximation method VPMR for general kernels and develop an accurate and fast algorithm for the temporal convolution, and integral equations with convolution kernels. The SOE is constructed by a combination of the VP sum and the MR method. The VPMR is accurate and efficient with controllable maximal exponents. As applications of the VPMR, the convolution evaluation is computed with \( O(N) \) operations on uniform \( N \) time steps owing to the kernel approximation with exponentials enabling a recurrence formula solved by L-stable RK methods. The kernel singularity can be treated by the splitting of the convolution such that the singular part can be calculated by analytical techniques. The controllable of maximal exponents in the VPMR ensure that the efficiency of proposed algorithm. Our algorithm is friendly for parallelization and favors easy extensions to complicated kernel with the SOE. Numerical results for different kernels show its efficiency, accuracy and universality, demonstrating the attractive features for potential applications in many problems.

Acknowledgment

The authors acknowledge the financial support from the National Natural Science Foundation of China (grant Nos. 12071288 and 21773165), Science and Technology Commission of Shanghai Municipality (grant Nos. 20JC1414100 and 21JC1403700), Strategic Priority Research Program of Chinese Academy of Sciences (grant No. XDA25010403), and the support from the HPC center of Shanghai Jiao Tong University.

Declarations

Conflict of interest

The authors declare that they have no conflict of interest.
Data Availability Statement

The data that support the findings of this study are available from the corresponding author upon reasonable request.

References

[1] G. Beylkin, C. Kurcz, L. Monzón, Fast convolution with the free space Helmholtz Green’s function, Journal of Computational Physics 228 (8) (2009) 2770–2791.

[2] H. Cheng, L. Greengard, V. Rokhlin, A fast adaptive multipole algorithm in three dimensions, Journal of Computational Physics 155 (2) (1999) 468–498.

[3] L. Greengard, S. Jiang, Y. Zhang, The anisotropic truncated kernel method for convolution with free-space Green’s functions, SIAM Journal on Scientific Computing 40 (6) (2018) A3733–A3754.

[4] S. Jiang, L. Greengard, Efficient representation of nonreflecting boundary conditions for the time-dependent Schrödinger equation in two dimensions, Communications on Pure and Applied Mathematics 61 (2) (2008) 261–288.

[5] C. Lubich, A. Schädlle, Fast convolution for nonreflecting boundary conditions, SIAM Journal on Scientific Computing 24 (1) (2002) 161–182.

[6] B. Wang, D. Chen, B. Zhang, W. Zhang, M. H. Cho, W. Cai, Taylor expansion based fast multipole method for 3-D Helmholtz equations in layered media, Journal of Computational Physics 401 (2020) 109008.

[7] D. Fang, J. Yang, G. Delisle, Discrete image theory for horizontal electric dipoles in a multilayered medium, in: IEE Proceedings H-microwaves, Antennas and Propagation, Vol. 135, IET, 1988, pp. 297–303.

[8] A. Alparslan, M. I. Aksun, K. A. Michalski, Closed-form Green’s functions in planar layered media for all ranges and materials, IEEE Transactions on Microwave Theory and Techniques 58 (3) (2010) 602–613.

[9] M. Spivak, S. K. Veerapaneni, L. Greengard, The fast generalized Gauss transform, SIAM Journal on Scientific Computing 32 (5) (2010) 3092–3107.

[10] Y. Zhang, C. Zhuang, S. Jiang, Fast one-dimensional convolution with general kernels using sum-of-exponential approximation, Communications in Computational Physics 29 (5) (2021) 1570–1582.

[11] G. Beylkin, L. Monzón, On approximation of functions by exponential sums, Applied and Computational Harmonic Analysis 19 (1) (2005) 17 – 48.

[12] G. Beylkin, L. Monzón, Approximation by exponential sums revisited, Applied and Computational Harmonic Analysis 28 (2) (2010) 131–149.

[13] D. Braess, Asymptotics for the approximation of wave functions by exponential sums, Journal of Approximation Theory 83 (1) (1995) 93–103.

[14] D. Braess, W. Hackbusch, Approximation of $1/x$ by exponential sums in $[1, \infty)$, IMA Journal of Numerical Analysis 25 (4) (2005) 685–697.

[15] D. Braess, W. Hackbusch, On the efficient computation of high-dimensional integrals and the approximation by exponential sums, in: Multiscale, nonlinear and adaptive approximation, Springer, 2009, pp. 39–74.

[16] J. W. Evans, W. B. Gragg, R. J. LeVeque, On least squares exponential sum approximation with positive coefficients, Mathematics of Computation 34 (149) (1980) 203–211.
[17] A. A. Gonchar, E. A. Rakhmanov, Equilibrium distributions and degree of rational approximation of analytic functions, Mathematics of the USSR-Sbornik 62 (2) (1989) 305.

[18] S. Jiang, A fast Gauss transform in one dimension using sum-of-exponentials approximations, arXiv: 1909.09825 (2019).

[19] R. Hamming, Numerical Methods for Scientists and Engineers, Courier Corporation, 2012.

[20] W. J. Wiscombe, J. W. Evans, Exponential-sum fitting of radiative transmission functions, Journal of Computational Physics 24 (4) (1977) 416 – 444.

[21] The uselessness of the Fast Gauss Transform for summing Gaussian radial basis function series, Journal of Computational Physics 229 (4) (2010) 1311 – 1326.

[22] C. Lubich, A. Ostermann, Runge-Kutta methods for parabolic equations and convolution quadrature, Mathematics of Computation 60 (201) (1993) 105–131.

[23] R. Albtoush, K. Al-Khaled, Approximation of periodic functions by Vallée Poussin sums, Hokkaido Mathematical Journal 30 (2) (2001) 269–282.

[24] C. J. de La Vallée-Poussin, Leçons sur l’approximation des fonctions d’une variable réelle, Paris, 1919.

[25] B. Moore, Principal component analysis in linear systems: controllability, observability, and model reduction, IEEE Transactions on Automatic Control 26 (1) (1981) 17–32.

[26] P. Benner, S. Gugercin, K. Willcox, A survey of projection-based model reduction methods for parametric dynamical systems, SIAM Review 57 (4) (2015) 483–531.

[27] A. Schädle, M. López-Fernández, C. Lubich, Fast and oblivious convolution quadrature, SIAM Journal on Scientific Computing 28 (2) (2006) 421–438.

[28] L. Banjai, C. Lubich, An error analysis of Runge–Kutta convolution quadrature, BIT Numerical Mathematics 51 (3) (2011) 483–496.

[29] J. Liang, Z. Gao, Z. Xu, A kernel-independent sum-of-Gaussians method by de la Vallee-Poussin sums, Advances in Applied Mathematics and Mechanics 13 (5) (2021) 1126–1141.

[30] A. Antoulas, D. Sorensen, Approximation of large-scale dynamical systems: an overview, International Journal of Applied Mathematics and Computer Science 11 (5) (2001) 1093–1121.

[31] K. Glover, All optimal hankel-norm approximations of linear multivariable systems and their $L_\infty$-error bounds, International Journal of Control 39 (6) (1984) 1115–1193.

[32] R. Ober, Balanced parametrization of classes of linear systems, SIAM Journal on Control and Optimization 29 (6) (1991) 1251–1287.

[33] B. Barrowes, Multiple Precision Toolbox for MATLAB, MATLAB Central File Exchange (Retrieved August 10, 2020).

[34] W. Liu, V. Sreeram, K. L. Teo, Model reduction for state-space symmetric systems, Systems & Control Letters 34 (4) (1998) 209–215.

[35] L. F. Shampine, Vectorized adaptive quadrature in MATLAB, Journal of Computational and Applied Mathematics 211 (2) (2008) 131–140.

[36] D. Occorsio, G. Serafini, Cubature formulae for nearly singular and highly oscillating integrals, Calcolo 55 (1) (2018) 1–33.
[37] A. Krishnamoorthy, D. Menon, Matrix inversion using Cholesky decomposition, in: 2013 signal processing: Algorithms, architectures, arrangements, and applications (SPA), IEEE, 2013, pp. 70–72.

[38] N. Halko, P.-G. Martinsson, J. A. Tropp, Finding structure with randomness: Probabilistic algorithms for constructing approximate matrix decompositions, SIAM Review 53 (2) (2011) 217–288.

[39] V. Rokhlin, A. Szlam, M. Tygert, A randomized algorithm for principal component analysis, SIAM Journal on Matrix Analysis and Applications 31 (3) (2010) 1100–1124.

[40] H. Lebesgue, Sur les intégrales singulières, in: Annales de la Faculté des sciences de Toulouse: Mathématiques, Vol. 1, 1909, pp. 25–117.

[41] A. Zakharov, Bound on deviations of continuous periodic functions from their De La Vallée-Poussin sums, Mathematical Notes of the Academy of Sciences of the USSR 3 (1) (1968) 45–49.

[42] S. B. Stechkin, The approximation of periodic functions by Fejér sums, Trudy Matematicheskogo Instituta imeni VA Steklova 62 (1961) 48–60.

[43] A. V. Efimov, Approximation of periodic functions by de la Vallee-Poussin sums, Izvestiya Rossiiiskoi Akademii Nauk Seriya Matematicheskaya 23 (5) (1959) 737–770.

[44] S. A. Telyakovskii, Approximation of differentiable functions by de la Vallée Poussin’s sums, in: Doklady Akademii Nauk, Vol. 121, Russian Academy of Sciences, 1958, pp. 426–429.

[45] S. Nikolski, Sur certaines méthodes d’approximation au moyen de sommes trigonométriques, Izvestiya Rossiiiskoi Akademii Nauk. Seriya Matematicheskaya 4 (6) (1940) 509–520.

[46] R. P. Boyer, W. M. Y. Goh, Generalized Gibbs phenomenon for Fourier partial sums and de la Vallée-Poussin sums, Journal of Applied Mathematics and Computing 37 (1-2) (2011) 421–442.

[47] M. G. Magomed-Kasumov, Approximation properties of de la Vallée-Poussin means for piecewise smooth functions, Mathematical Notes 100 (1) (2016) 229–244.

[48] I. I. Sharapudinov, Approximation properties of de la Vallée-Poussin means on classes of Sobolev type with variable exponent, Vestn. Dagestan Res. Center Russian Academy of Sciences 45 (2012) 5–13.

[49] H. Huang, S. Marcantognini, N. Young, Chain rules for higher derivatives, The Mathematical Intelligencer 28 (2) (2006) 61–69.

[50] M. Spivak, S. K. Veerapaneni, L. Greengard, The fast generalized Gauss transform, SIAM Journal on Scientific Computing 32 (5) (2010) 3092–3107.

[51] M. López-Fernández, C. Palencia, A. Schädle, A spectral order method for inverting sectorial Laplace transforms, SIAM Journal on Numerical Analysis 44 (3) (2006) 1332–1350.

[52] L. N. Trefethen, J. A. C. Weideman, Talbot quadratures and rational approximations, BIT Numerical Mathematics 46 (3) (2006) 653–670.

[53] A. Talbot, The accurate numerical inversion of Laplace transforms,IMA Journal of Applied Mathematics 23 (1) (1979) 97–120.

[54] J. Weideman, L. Trefethen, Parabolic and hyperbolic contours for computing the bromwich integral, Mathematics of Computation 76 (259) (2007) 1341–1356.
[55] J. Weideman, Improved contour integral methods for parabolic PDEs, IMA Journal of Numerical Analysis 30 (1) (2010) 334–350.

[56] S. Singh, Prony Toolbox, MATLAB Central File Exchange (Retrieved September 6, 2021).

[57] R. Woodard, Interpolation of spatial data: Some theory for kriging, Springer, 1999.

[58] C. K. I. Williams, Gaussian Processes for Machine Learning, MIT Press, 2005.

[59] A. Denzel, J. Kästner, Gaussian process regression for geometry optimization, The Journal of Chemical Physics 148 (9) (2018) 094114.

[60] P. O. Dral, Gaussian process regression for geometry optimization, Journal on Computational Chemistry 40 (26) (2019) 2339–2347.

[61] P. P. Ewald, Die Berechnung optischer und elektrostatischer Gitterpotentiale, Ann. Phys. 369 (3) (1921) 253–287.

[62] S. Jin, L. Li, Z. Xu, Y. Zhao, A random batch Ewald method for particle systems with Coulomb interactions, SIAM Journal on Scientific Computing 43 (4) (2021) B937–B960.

[63] M. Lopez-Marcos, A difference scheme for a nonlinear partial integro-differential equation, SIAM Journal on Numerical Analysis 27 (1) (1990) 20–31.

[64] J. M. Sanz-Serna, A numerical method for a partial integro-differential equation, SIAM Journal on Numerical Analysis 25 (2) (1988) 319–327.

[65] J. Cao, C. Xu, A high order schema for the numerical solution of the fractional ordinary differential equations, Journal of Computational Physics 238 (2013) 154 – 168.

[66] E. Cuesta, C. Palencia, A fractional trapezoidal rule for integro-differential equations of fractional order in Banach spaces, Applied Numerical Mathematics 45 (2-3) (2003) 139–159.

[67] K. Diethelm, N. J. Ford, Analysis of fractional differential equations, Journal of Mathematical Analysis and Applications 265 (2) (2002) 229–248.

[68] L. Banjai, M. López-Fernández, Efficient high order algorithms for fractional integrals and fractional differential equations, Numerische Mathematik 141 (2) (2019) 289–317.

[69] J.-R. Li, A fast time stepping method for evaluating fractional integrals, SIAM Journal on Scientific Computing 31 (6) (2010) 4696–4714.

[70] G.-A. Zakeri, M. Navab, Sinc collocation approximation of non-smooth solution of a nonlinear weakly singular Volterra integral equation, Journal of Computational Physics 229 (18) (2010) 6548 – 6557.

[71] C. Lubich, Fractional linear multistep methods for Abel-Volterra integral equations of the second kind, Mathematics of Computation 45 (172) (1985) 463–469.

[72] R. K. Miller, Volterra integral equations in a Banach space, Funkcial. Ekvac 18 (2) (1975) 163–193.

[73] F. Mohammadi, A wavelet-based computational method for solving stochastic Itô – Volterra integral equations, Journal of Computational Physics 298 (2015) 254 – 265.

[74] C. Lubich, Convolution quadrature and discretized operational calculus. I, Numerische Mathematik 52 (2) (1988) 129–145.

[75] C. Lubich, Convolution quadrature and discretized operational calculus. II, Numerische Mathematik 52 (4) (1988) 413–425.
C. Lubich, Convolution quadrature revisited, BIT Numerical Mathematics 44 (3) (2004) 503–514.

M. López-Fernández, S. Sauter, Generalized convolution quadrature with variable time stepping, IMA Journal of Numerical Analysis 33 (4) (2013) 1156–1175.

W. B. March, B. Xiao, S. Tharakan, C. D. Yu, G. Biros, A kernel-independent FMM in general dimensions, in: SC ’15: Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, 2015, pp. 1–12.

S. Liao, Beyond Perturbation: Introduction to The Homotopy Analysis Method, CRC press, 2003.

J. Trujillo, M. Rivero, B. Bonilla, On a Riemann–Liouville generalized Taylor’s formula, Journal of Mathematical Analysis and Applications 231 (1) (1999) 255–265.

Z. Liu, T. Wang, G. Gao, A local fractional Taylor expansion and its computation for insufficiently smooth functions, East Asian Journal on Applied Mathematics 5 (2) (2015) 176–191.

T. J. Osler, Taylor’s series generalized for fractional derivatives and applications, SIAM Journal on Mathematical Analysis 2 (1) (1971) 37–48.

W. Tongke, F. Meng, Fractional order degenerate kernel methods for Fredholm integral equations of the second kind with endpoint singularities, Mathematica Numerica Sinica 41 (1) (2019) 66.

J. Guo, T. Wang, Fractional Hermite degenerate kernel method for linear Fredholm integral equations involving endpoint weak singularities, Journal of Applied Analysis & Computation 10 (5) (2020) 1918–1936.

E. Zarei, S. Noeiaghdam, Solving generalized Abel’s integral equations of the first and second kinds via Taylor-collocation method, arXiv preprint arXiv:1804.08571 (2018).

F. Toutounian, H. Nasabzadeh, A new method based on generalized Taylor expansion for computing a series solution of the linear systems, Applied Mathematics and Computation 248 (2014) 602–609.

G. Wanner, E. Hairer, Solving Ordinary Differential Equations, Springer Berlin Heidelberg, 1996.

H. M. Srivastava, R. G. Buschman, Theory and Applications of Convolution Integral equations, Springer Science & Business Media, 2013.

C. Corduneanu, Integral Equations and Stability of Feedback Systems, Academic Press, 1973.

J. D. Tamarkin, On integrable solutions of Abel’s integral equation, Annals of Mathematics 31 (2) (1930) 219–229.

M. A. Jaswon, Integral equation methods in potential theory and elastostatics (1977).

S. Jiang, V. Rokhlin, Second kind integral equations for the classical potential theory on open surfaces II, Journal of Computational Physics 195 (1) (2004) 1–16.

N. Levinson, A nonlinear Volterra equation arising in the theory of superfluidity, Journal of Mathematical Analysis and Applications 1 (1) (1960) 1–11.

U. an der Heiden, Analysis of Neural Networks, Vol. 35, Springer Science & Business Media, 2013.