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Modified Gauss-Laguerre exponential fitting based formulae

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Abstract Modified Gauss-Laguerre exponentially fitted quadrature rules are introduced for the computation of integrals of oscillatory functions over the whole positive semiaxis. Their weights and nodes depend on the frequency of oscillation in the integrand, thus increasing the accuracy of classical Gauss-Laguerre formulae. The asymptotic order is discussed, and an algorithm for determining weights and nodes for a general number N of nodes is provided, resulting an improvement of the existing quadrature formulae. Numerical illustrations are also presented.

Keywords quadrature formulae on infinite intervals · exponential fitting · Gauss-Laguerre formulae · Filon method

1 Introduction

We consider the numerical computation of the following integral

$$I = \int_0^\infty e^{-x} f(x)dx, \tag{1.1}$$

when the integrand $f(x)$ is an oscillatory function of the form

$$f(x) = f_1(x)\cos(\omega x) + f_2(x)\sin(\omega x). \tag{1.2}$$

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The functions $f_1(x)$ and $f_2(x)$ are assumed smooth enough to be well approximated by polynomials.

The accurate computation of integrals of oscillatory functions over unbounded intervals is needed in numerous applications in various branches of physics, engineering, and economics, as for instance in wave absorption and quantum mechanics; see, e.g., [1,4,21,23–25,40]. The numerical evaluation of such integrals has been analyzed by several authors with the aim of obtaining quadrature rules whose error decreases with the frequency ω of oscillation as $O(\omega^{-\alpha})$ when $\omega \to \infty$, for a positive α. The main contributions in this area have been made in the papers [3,10,36] and references therein.

By rewriting the sine and cosine functions as combinations of exponential functions, the integral (1.1) can be recasted as the sum of two integrals of the form

$$I = \int_0^{\infty} F_1(x) e^{i\omega x} dx + \int_0^{\infty} F_2(x) e^{-i\omega x} dx \tag{1.3}$$

where

$$F_1(x) = \frac{e^{-x}}{2} \left(f_1(x) - i f_2(x) \right),$$

and

$$F_2(x) = \frac{e^{-x}}{2} \left(f_1(x) + i f_2(x) \right).$$

Then steepest descent methods [36] or complex Gaussian quadrature rules [3] can be applied to the integral of the form (1.3), by showing optimal asymptotic order $O(\omega^{-2n-1})$, when using $2n$ frequency dependent quadrature points in the complex plane: n points for each of the two integrals in (1.3). However such methods are not well behaved for small values of the frequency, as the nodes are unbounded in the limit for $\omega \to 0$.

An alternative well estabilished procedure for the construction of approximate formulae tuned on highly oscillatory problems is given by the exponential fitting (EF) technique [30,38]. The EF technique consists in determining a numerical method with frequency-dependent coefficients, by imposing that the method is exact on a linear combination of oscillatory functions (i.e. functions of the form (1.2)). In the case of highly oscillating problems, classical methods require the usage of a small integration step, in order to accurately track the high frequency oscillations, while EF methods can use larger steps of integration with respect to classical methods maintaining an high accuracy. The EF approach has been applied to several kinds of problems such as interpolation, numerical differentiation and integration [27,29], numerical solution of ordinary differential equations [12–17,19,20,28,39,42], partial differential equations [18] and integral equations [5–8]. As regards quadrature problems on finite integration domains, the EF Simpson rule has been derived in [27], the more general EF Newton-Cotes rules have been constructed in [32,34,35], while the EF gauss-Legendre rules have been analyzed in [29,33,37,41].

In the case of infinite integration domain, the EF Gauss-Laguerre quadrature rules were introduced in [10,11], and they have the same optimal asymptotic order of methods in [3,36], also maintaining a good accuracy for small values of ω, as they naturally tend to the corresponding classical Gauss-Laguerre formulae for $\omega \to 0$. On the other hand the determination of nodes and weights of EF formulae involves the numerical solution of nonlinear systems of equations of dimension $2N$, where N is the number of quadrature nodes. Such systems can be affected by ill-conditioning as N and/or ω increase, and the choice of the initial approximation for Newton's iterative method is a quite delicate task, in order to guarantee the convergence of the iterative process, as discussed in [10,11]. As a matter of fact in the paper [10], in order to determine the formulae up to $N = 6$, an appropriate choice of the initial approximation for Newton's iterative process has been provided.

It is the purpose of this work to develop new modified Gauss-Laguerre EF based formulae, which share the property of optimal behaviour for both small and large ω values with the standard EF rules, while reducing the computation of the nodes to the solution of a single nonlinear equation, independently of the number N of quadrature nodes, and also reducing the ill conditioning issues related to the standard EF procedure as N and ω increase.

The paper is organized as follows. In Section 2 we recall the classical Gauss-Laguerre quadrature rules, while in Section 3 we describe the construction of the modified EF Gauss-Laguerre rules, whose asymptotic order is analyzed in Section 4. In Section 5 we describe an algorithm for the computation of the nodes, numerical illustrations are presented in Section 6, and conclusions are reported in Section 7. The paper also contains the Appendix A where the properties of the $\eta_m(Z)$ functions, frequently used in the paper, are recalled and the Appendix B with a Mathematica code for the computation of the function whose zeros are the nodes of the new quadrature rule.

2 Classical Gauss-Laguerre quadrature rules

The classical Gauss-Laguerre quadrature rule [22] for the numerical computation of the integral (1.1) is of the form

$$I \simeq \sum_{k=1}^{N} w_k f(x_k), \tag{2.1}$$

where the weights and the nodes are obtained by imposing that the rule is exact on the functions

$$x^{n-1}, \ n = 1, 2, ..., 2N.$$

By defining the functional

$$\mathcal{L}[f(x), \mathbf{a}] = \int_0^\infty e^{-x} f(x) dx - \sum_{k=1}^{N} w_k f(x_k),$$

where $\mathbf{a}$ is a vector with $2N$ components which collects the weights and the nodes, namely $\mathbf{a} = [w_1, w_2, ..., w_N, x_1, x_2, ..., x_N]$, the desired values of the components of $\mathbf{a}$ are obtained by imposing the condition

$$\mathcal{L}[x^{n-1}, \mathbf{a}] = 0, \;\; n = 1, 2, ..., 2N.$$

Such conditions lead to the nonlinear system

$$\sum_{k=1}^{N} w_k x_k^{n-1} = m_{n-1}, \quad n = 1, \ldots, 2N, \tag{2.2}$$

where

$$m_n = \int_0^\infty e^{-x} x^n dx = n! \tag{2.3}$$

Alternatively, the nodes x_k can be computed as the roots of the $N-th$ orthogonal polynomial with respect to the weigth function e^{-x}, i.e. the Gauss-Laguerre polynomial, which we denote as:

$$p_N(x) = \sum_{n=0}^{N} c_n x^n, \tag{2.4}$$

whose coefficients can be computed by setting $c_N = 1$ and solving the linear system

$$\begin{pmatrix} m_0 & m_1 & \cdots & m_{N-1} \\ m_1 & m_2 & \cdots & m_N \\ \vdots & \vdots & \ddots & \vdots \\ m_{N-1} & m_N & \cdots & m_{2N-2} \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_{N-1} \end{pmatrix} = - \begin{pmatrix} m_N \\ m_{N+1} \\ \vdots \\ m_{2N-1} \end{pmatrix}, \tag{2.5}$$

in the unknowns $c_0, ..., c_{N-1}$. In order to avoid high order of magnitude in the values of the Laguerre polynomial (2.4), the polynomial is generally normalized by considering

$$L_N(x) = P_N(x)/c_0, \tag{2.6}$$

in such a way that the coefficient of the highest term is $\frac{(-1)^N}{N!}$. The weights are

$$w_n = \int_0^\infty e^{-x} l_n(x) = \frac{x_n}{(N+1)^2 \left[p_{N+1}(x_n)\right]^2},$$

where $l_n(x)$ is the $n-th$ Lagrange polynomial with respect to the nodes $x_0, ..., x_N$.

3 Construction of the modified EF Gauss-Laguerre rules

The EF Gauss-Laguerre quadrature rule has been obtained in [10] by imposing that the formula is exact on the functions

$$x^{n-1}e^{\pm\mu x},\ n = 1, 2, ..., N,$$

i.e. by imposing

$$\mathcal{L}[x^{n-1}e^{\pm\mu x}, \mathbf{a}] = 0,\ n = 1, 2, ..., N, \tag{3.1}$$

where $\mu = i\omega$. The following Theorem provides a different form for the nonlinear system derived in [10] in the weights and nodes. This new formulation will be useful for the definition of the modified EF Gauss-Laguerre rules.

Theorem 1 *The weights and the nodes of the EF Gauss-Laguerre quadrature rule are solution of the nonlinear system*

$$\left\{ \sum_{k=1}^{N} w_k x_k^{n-1} \frac{\eta_{\lfloor \frac{n-2}{2} \rfloor}(x_k^2 Z)}{\eta_{\lfloor \frac{n-2}{2} \rfloor}(0)} = M_{n-1}(Z), \qquad n = 1, \ldots, 2N, \right. \tag{3.2}$$

where

$$M_n(Z) = \frac{n!}{(1-Z)^{\lceil \frac{n+1}{2} \rceil}} \tag{3.3}$$

$Z = \mu^2 = -\omega^2$ and the set of functions $\eta_m(Z)$, $m = -1, 0, 1, 2, \ldots$, defined in [26], are recalled in the Appendix A.

Proof From Theorem 2.1 in [10], by dividing the first set of N equations by $\eta_{n-2}(0) = \frac{2^{n-2}(n-2)!}{(2n-3)!}$, and the second set of N equations by $\eta_{n-1}(0) = \frac{2^{n-1}(n-1)!}{(2n-1)!}$, we obtain

$$\left\{ \begin{array}{l} \displaystyle\sum_{k=1}^{N} w_k x_k^{2n-2} \frac{\eta_{n-2}(x_k^2 Z)}{\eta_{n-2}(0)} = M_{2n-2}(Z), \quad n = 1, \ldots, N \\ \displaystyle\sum_{k=1}^{N} w_k x_k^{2n-1} \frac{\eta_{n-1}(x_k^2 Z)}{\eta_{n-1}(0)} = M_{2n-1}(Z), \quad n = 1, \ldots, N \end{array} \right. , \tag{3.4}$$

from which the thesis follows.

In the paper [10] an algorithm for the computation of weights and nodes as solutions of the nonlinear system (3.4) has been developed. Such algorithm is based on an iteration procedure, whose first stage consists in a convenient split of this system of $2N$ equations into two subsystems of N equations each. In the iteration procedure the first subsystem is used as a linear system for the weights w_k, while the second as a nonlinear system for the nodes x_k, which is treated by means of Newton's method. However the choice of a suitable initial approximation for the iterative procedure is not trivial, and an adequate choice has been furnished in [10] for $\omega \in [0, 50]$ and a number of nodes $N \leq 6$. Our first aim is to formulate modified EF Gauss-Laguerre formulae which do not require the solution of a nonlinear system, such that they can be derived for higher values of N.

The new formulation (3.2) for the nonlinear system in the weights and nodes, is analogous to the formulation (2.2) for the nonlinear system in the classical case (they are exactly the same if we put $Z = 0$ in (3.2)). For this reason, in analogy to the definition (2.4) for the Laguerre polynomial in the classical case, we define the function

$$f_N(x,\omega) = \sum_{n=0}^{N} C_n^N(Z) x^n \frac{\eta_{\lfloor \frac{n-1}{2} \rfloor}(x^2 Z)}{\eta_{\lfloor \frac{n-1}{2} \rfloor}(0)}, \quad Z = -\omega^2, \tag{3.5}$$

where $C_N(Z) \equiv 1$, and $C_0(Z), ..., C_{N-1}(Z)$ are computed as solution of the linear system

$$\begin{pmatrix} M_0(Z) & M_1(Z) & \cdots & M_{N-1}(Z) \\ M_1(Z) & M_2(Z) & \cdots & M_N(Z) \\ \vdots & \vdots & \ddots & \vdots \\ M_{N-1}(Z) & M_N(Z) & \cdots & M_{2N-2}(Z) \end{pmatrix} \begin{pmatrix} C_0^N(Z) \\ C_1^N(Z) \\ \vdots \\ C_{N-1}^N(Z) \end{pmatrix} = - \begin{pmatrix} M_N(Z) \\ M_{N+1}(Z) \\ \vdots \\ M_{2N-1}(Z) \end{pmatrix}. \tag{3.6}$$

As the moments $M_n(Z)$ in (3.3) tend to the classical moments (2.3) as $Z \to 0$, then $\lim_{Z\to 0} C_n^N(Z) = c_n$, where c_n are defined in (2.5), and

$$\lim_{\omega\to 0} f_N(x,\omega) = p_N(x), \forall x \in \mathbb{R},$$

that is the function $f_N(x,\omega)$ tends to the Laguerre polynomial $p_N(x)$ for small values of the frequency.

Definition 1 We define the Modified Exponentially Fitted (MEF) Gauss-Laguerre quadrature rule by

$$I \simeq I_N = \sum_{i=1}^{N} (a_i f_1(x_i) + b_i f_2(x_i)) \tag{3.7}$$

where the functions f_1 and f_2 are given in (1.2), the frequency dependent nodes $x_i = x_i(\omega)$, $i = 1, ..., N$, are defined as the smallest N positive solutions of the nonlinear equation

$$f_N(x,\omega) = 0, \tag{3.8}$$

and $a_i(\omega)$, $b_i(\omega)$ are frequency-dependent weights, computed as

$$a_i(\omega) = \int_0^\infty e^{-x} l_i(x) \cos(\omega x) dx,$$
$$b_i(\omega) = \int_0^\infty e^{-x} l_i(x) \sin(\omega x) dx,$$

where $l_i(x)$ is the $i-th$ Lagrange fundamental polynomial with respect to the abscissae x_i, $i = 1, ..., N$.

As in the case of the classical formulae, the nodes can be determined by solving the normalized equation

$$\frac{f_N(x,\omega)}{C_0^N(Z)} = 0. \tag{3.9}$$

With the aim of analyzing the solvability of the nonlinear equation (3.9), for $\omega > 0$ we define the function

$$\bar{f}_N(x,\omega) = \frac{f_N(\frac{x}{\omega},\omega)}{C_0^N(Z)} = \sum_{n=0}^{N} \bar{C}_n^N(Z) x^n \frac{\eta_{\lfloor \frac{n-1}{2} \rfloor}(-x^2)}{\eta_{\lfloor \frac{n-1}{2} \rfloor}(0)} \tag{3.10}$$

where

$$\bar{C}_n^N(Z) = \frac{C_n^N(Z)}{\omega^n C_0^N(Z)}, \quad Z = -\omega^2. \tag{3.11}$$

Then, for $\omega > 0$, the nodes of MEF Gauss-Laguerre quadrature rule can be computed as

$$x_i = \frac{\bar{x}_i}{\omega}, i = 1, .., N \tag{3.12}$$

where $\bar{x}_i$ are the smallest N positive solutions of

$$\bar{f}_N(x,\omega) = 0. \tag{3.13}$$

We now analyze the solvability of the nonlinear equation (3.13).

Theorem 2 *The nonlinear equation* (3.13)*, where the function* $\bar{f}_N$ *is defined in* (3.10)*, has infinite many simple roots in* $[0,+\infty)$*.*

Proof We first of all observe that, by using the recurrence relation (A.2), such equation can be recasted as

$$p(x,\omega)\cos(x) + q(x,\omega)\sin(x) = 0 \tag{3.14}$$

where $p(x,\omega)$ and $q(x,\omega)$ are polynomials, in the variable x, of degree at most $\lfloor \frac{N-1}{2} \rfloor$ and $\lceil \frac{N-1}{2} \rceil$, respectively, with ω-depending coefficients. Then, by setting

$$g(x,\omega) = -\frac{p(x,\omega)}{q(x,\omega)}, \tag{3.15}$$

we have that, for any $\omega > 0$, there exists an $X > 0$ such that $g(x,\omega)$ is continuous in the interval $(X,+\infty)$, as it is sufficient to chose X as the biggest real zero of the polynomial $q(x,\omega)$. Moreover, as the degree of the polynomial $p(x,\omega)$ is less or equal to the degree of $q(x,\omega)$, we have

$$\lim_{x\to\infty} g(x,\omega) < \infty.$$

Then the equation (3.13), which can finally be written as

$$\tan(x) - g(x,\omega) = 0, \tag{3.16}$$

has infinite many solutions in the interval $(X, +\infty)$. Let $\xi = \xi(\omega)$ be a multiple root of the nonlinear equation (3.16), then we have that the both function and its first derivative vanish in ξ:

$$\tan(\xi) = g(\xi, \omega),$$

and

$$1 + \tan^2(\xi) - g'(\xi, \omega) = 0.$$

By using the expression $\tan^2(\xi) = g^2(\xi, \omega)$ and by computing the derivative of the function $g(x, \omega)$ in (3.15), we then obtain

$$p^2(\xi, \omega) + q^2(\xi, \omega) + p'(\xi, \omega)q(\xi, \omega) - p(\xi, \omega)q'(\xi, \omega) = 0.$$

The thesis follows by observing that the polynomial $p^2(x, \omega) + q^2(x, \omega) + p'(x, \omega)q(x, \omega) - p(x, \omega)q'(x, \omega)$ has a finite number of roots.

4 Asymptotic order

We now study the asymptotic behaviour of the MEF Gauss-Laguerre quadrature rule as the frequency ω increases.

Theorem 3 *The coefficient computed by* (3.6) *satisfy*

$$C_n^N(Z) = \begin{cases} O\left(Z^{-\lceil \frac{N-n}{2} \rceil}\right) & N \text{ even} \\ O\left(Z^{-\lfloor \frac{N-n}{2} \rfloor}\right) & N \text{ odd} \end{cases}, \quad Z \to \infty. \tag{4.1}$$

Proof By Cramer's rule the coefficient $C_n^N(Z)$ can be computed as

$$C_n^N(Z) = \frac{\det(A_n)}{\det(A)},$$

with

$$A = \begin{pmatrix} M_0(Z) & \cdots & M_n(Z) & \cdots & M_{N-1}(Z) \\ M_1(Z) & \cdots & M_{n+1}(Z) & \cdots & M_N(Z) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ M_{N-1}(Z) & \cdots & M_{n+N-1}(Z) & \cdots & M_{2N-2}(Z) \end{pmatrix},$$

$$A_n = \begin{pmatrix} M_0(Z) & \cdots & M_N(Z) & \cdots & M_{N-1}(Z) \\ M_1(Z) & \cdots & M_{N+1}(Z) & \cdots & M_N(Z) \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ M_{N-1}(Z) & \cdots & M_{2N-1}(Z) & \cdots & M_{2N-2}(Z) \end{pmatrix}.$$

As $M_n(Z) = O\left(Z^{-\lceil \frac{n+1}{2} \rceil}\right)$, we have $\det(A) = O\left(Z^{-N\lceil \frac{N}{2} \rceil}\right)$ and $\det(A_n) = O\left(Z^{-(N-1)\lceil \frac{N}{2} \rceil - \lceil \frac{2N-n}{2} \rceil}\right)$, from which the thesis follows.

As a consequence of the previous theorem we have the following

Corollary 1 *For any $a \in \mathbb{R}$,*

$$f_N\left(\frac{a}{\omega},\omega\right) = \begin{cases} O\left(\omega^{-N}\right) & N \text{ even} \\ O\left(\omega^{-N+1}\right) & N \text{ odd} \end{cases}, \quad \omega \to \infty.$$

This allows to prove the followig theorem.

Theorem 4 *The nodes of the MEF Gauss-Laguerre quadrature rule, defined in Definition 1, satisfy*

$$x_i = O\left(\omega^{-1}\right), \qquad i = 1, ...N, \quad \omega \to \infty. \tag{4.2}$$

Proof For any fixed frequency $\omega > 0$, let us consider the polynomial $p_N(x, Z)$ which interpolates the function $f_N(x, \omega)$ in the $N+1$ abscissae $x_0 := 0$ and x_i, $i = 1, ..., N$. As $f_N(x_i, \omega) = 0$, $i = 1, ..., N$ and $f_N(x_0, \omega) = C_0^N(Z)$, with $Z = -\omega^2$. By denoting with $E_N(x, \omega)$ the interpolation error, we have

$$f_N(x,\omega) = p_N(x,\omega) + E_N(x,\omega),$$

with

$$p_N(x,\omega) = (-1)^N C_0^N(Z) \prod_{i=1}^{N} \left(\frac{x}{x_i} - 1\right)$$

Then we have by Corollary 1 that

$$p_N\left(\frac{1}{\omega},\omega\right) = (-1)^N C_0^N(Z) \prod_{i=1}^{N} \left(\frac{1}{\omega x_i} - 1\right) = \begin{cases} O\left(\omega^{-N}\right) & N \text{ even} \\ O\left(\omega^{-N+1}\right) & N \text{ odd} \end{cases}$$

As we have

$$C_0^N(Z) = \begin{cases} O\left(\omega^{-N}\right) & N \text{ even} \\ O\left(\omega^{-N+1}\right) & N \text{ odd} \end{cases},$$

this condition leads to (4.2).

Theorem 5 *The error of the MEF quadrature rule* (3.7) *has the asymptotic decay*

$$|I - I_N| = O(\omega^{-N-1}), \quad \omega \to \infty.$$

Proof By Taylor expansion of the functions $f_1(x)$ and $f_2(x)$ we have

$$f_1(x) = q_{N-1}(x) + R(x)x^N,$$
$$f_1(x) = \bar{q}_{N-1}(x) + \bar{R}(x)x^N,$$

with q_{N-1}, $\bar{q}_{N-1}$ polynomials of degree $\leq N-1$ and $R(x)$, $\bar{R}(x)$ analytic functions. Then the error of the method is

$$I - I_N = \int_0^\infty e^{-x}\left(f_1(x)\cos(\omega x) + f_2(x)\sin(\omega x)\right)dx - \sum_{i=1}^{N}\left(a_i f_1(x_i) + b_i f_2(x_i)\right) =$$
$$= \int_0^\infty e^{-x} R(x) x^N \cos(\omega x) dx - \sum_{i=1}^{N} a_i R(x_i) x_i^N + \int_0^\infty e^{-x} \bar{R}(x) x^N \sin(\omega x) dx - \sum_{i=1}^{N} b_i \bar{R}(x_i) x_i^N.$$

By integration by parts the integrals in the previous expression have asymptotic size $O(\omega^{-N-1})$. The terms in the sum have a factor which is of size $O(\omega^{-N})$, since $x_i = O\left(\omega^{-1}\right)$. It remains to show that $a_i = O\left(\omega^{-1}\right)$ and $b_i = O\left(\omega^{-1}\right)$. We show that $a_i = O\left(\omega^{-1}\right)$, then the same result for b_i can be obtained in a similar way. By repeatedly applying the integration by part rule to the integral defining $a_i(\omega)$, we obtain

$$a_i(\omega) = \int_0^\infty e^{-x} l_i(x)\cos(\omega x)dx = \left. \sum_{k=0}^{N-1} (-1)^k l_i^{(k)}(x) F_{k+1}(x) \right|_0^\infty ,$$

where $l_i^{(k)}(x)$ represents the $k-$th derivative of the Lagrange fundamental polynomial $l_i(x)$, and the functions $F_k(x)$, $k \geq 1$ are recursively defined by

$$\begin{aligned} F_1(x) &= \int_0^x e^{-t}\cos(\omega t)dt \\ F_{k+1}(x) &= \int_0^x F_k(t)dt \end{aligned}$$

As $\lim_{x\to\infty} F_k(x) = 0$ we have

$$a_i(\omega) = -\sum_{k=0}^{N-1} (-1)^k l_i^{(k)}(0) F_{k+1}(0).$$

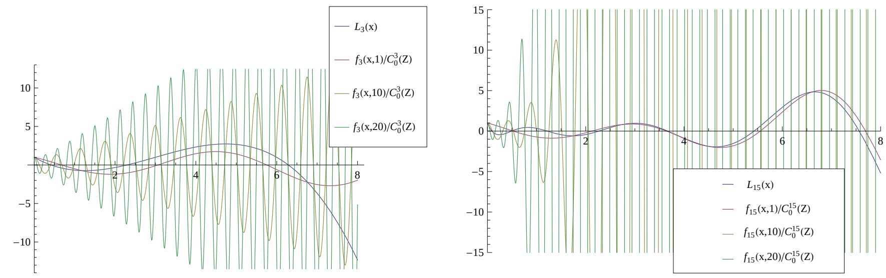
By observing that

$$F_{k+1}(0) = \begin{cases} O\left(\omega^{-k-2}\right) & k \ even \\ O\left(\omega^{-k-1}\right) & k \ odd \end{cases},$$

and $l_i^{(k)}(0) = O\left(\omega^k\right)$, as $x_i = O\left(\omega^{-1}\right)$, we obtain $a_i = O\left(\omega^{-1}\right)$.

5 Determination of nodes

The determination of the nodes of the MEF Gauss-Laguerre quadrature rule (3.7) requires the solution of the nonlinear equation (3.9), or, equivalently, of the equation (3.13). From the numerical point of view the two equations are not equivalent. Infact the function $f_N(x,\omega)$ in equation (3.9) is defined by (3.5), so the computation of its zeros may lead to problems for increasing values of the frequency ω because the η functions in (3.5) oscillate with increasing frequency, and the solutions are more and more one close to the other, resulting an ill-conditioned problem for the computation of (almost) multiple zeros. We report for example in Figure 1, for $N = 3$ and $N = 15$, the plot of the normalized Gauss-Laguerre polynomial (2.6), which corresponds to the first hand side of (3.9) with $\omega = 0$, and the first hand side of (3.9) with different values of ω. We observe as for increasing ω, the function oscillates with higher frequency.



(a) $N = 3$ (b) $N = 15$

Fig. 1: Plot of the normalized Gauss-Laguerre polynomial $L_N(x)$ (2.6) compared with the first hand side of (3.9), with different values of ω.

The function $\bar{f}_N(x,\omega)$ in equation (3.13), defined by (3.10), instead, does not exhibit increasing oscillations as ω increases (see Figure 2). The following theorem estabilishes the asymptotic behaviour of the function $\bar{f}_N(x,\omega)$ in (3.10), as $\omega \to \infty$, which will be useful in order to determine initial approximations for Newton iterative process in solving (3.13).

Theorem 6 *Let us define*

$$\bar{f}_N(x) := \sum_{n=0}^{\lfloor \frac{N}{2} \rfloor} (-1)^n \frac{D_{2n}^N}{D_0^N} x^{2n} \frac{\eta_{n-1}(-x^2)}{\eta_{n-1}(0)}, \tag{5.1}$$

where $D_N^N = 1$, $D_n^N = (-1)^{\alpha_n} d_n^N$, $n = 0, ..., N-1$ *with*

$$\alpha_n = \begin{cases} \left\lceil \frac{N-n}{2} \right\rceil & N \text{ even} \\ \left\lfloor \frac{N-n}{2} \right\rfloor & N \text{ odd} \end{cases}$$

and $d = [d_0^N, ..., d_{N-1}^N]^T$ *is the solution of*

$$Ad = b \tag{5.2}$$

with

$$a_{ij} = \begin{cases} 0 & i \text{ and } j \text{ even} \\ (i+j-2)! & \text{otherwise} \end{cases}, b_i = \begin{cases} 0 & N \text{ odd and } i \text{ even} \\ -(N+i-1)! & \text{otherwise} \end{cases},$$

$i, j = 1, ..., N$. *Then the function defined in* (3.10) *satisfies*

$$\lim_{\omega \to \infty} \bar{f}_N(x, Z) = \bar{f}_N(x), \tag{5.3}$$

where $Z = -\omega^2$.

Proof Let us define $\delta_n^N(Z) = \frac{C_n^N(Z)}{(-Z)^{-\alpha_n}}$. Then the system (3.6) can be written as

$$A(Z)\delta(Z) = b(Z), \tag{5.4}$$

with $\delta(Z) = [\delta_0^N(Z), ..., \delta_{N-1}^N(Z)]^T$, $a_{ij}(Z) = M_{i+j}(Z) \cdot (-Z)^{\alpha_i+\beta_j}$, $b(Z) = -M_{i+N}(Z) \cdot (-Z)^{\beta_i}$,

$$\beta_i = \begin{cases} \left\lceil \frac{N+i+1}{2} \right\rceil & N \ even \\ \left\lfloor \frac{N+i+1}{2} \right\rfloor & N \ odd \end{cases}.$$

Then the system (5.4), when $\omega \to \infty$, tends to (5.2), and then we have

$$\lim_{\omega\to\infty} \delta_n^N(Z) = d_n^N$$

and then

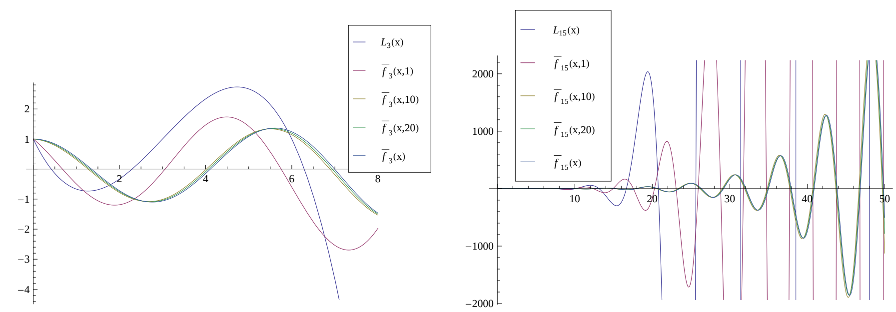
$$\lim_{\omega\to\infty} \frac{C_n^N(Z)}{Z^{-\alpha_n}} = D_n^N,$$

which we know to be finite by (4.1). Then it follows that

$$\lim_{\omega\to\infty} \bar{C}_n^N(Z) = \begin{cases} (-1)^{\frac{n}{2}} \frac{D_n^N}{D_0^N} & n \ even \\ 0 & n \ odd \end{cases}.$$

from which the thesis follows.

Figure 2 shows the plots, for $N = 3$ and $N = 15$, of the normalized Gauss-Laguerre polynomial (2.6) compared with the function (3.10) with different values of ω and the limit function (5.1). We note as, differently from Figure 1, the functions (3.10) do not increase their frequency of oscillation as ω increases and instead they approach to the limit function (5.1).



(a) $N = 3$ (b) $N = 15$

Fig. 2: Plot of the normalized Gauss-Laguerre polynomial $L_N(x)$ (2.6) compared with the function (3.10), i.e. the first hand side of (3.13), with different values of ω, and with the limit function (5.1).

The equation (3.13) will be solved by using the Newton's iterative process, by computing the derivative of the function (3.10) by means of the relation (A.4). Theorem 2 guarantees that we can look for simple roots of (3.13), so that the hypothesis of local convergence theorem for Newton's method are satisfied. We use the smallest N positive solutions of

$$\bar{f}_N(x) = 0 \tag{5.5}$$

as initial approximation for the Newton's iterative process applied to the nonlinear equation (3.13). We observe that such initial approximations, differentely from [10], are not $\omega-$dependent, and can be computed once in advance for any fixed N. Moreover, from (5.3), we have that, for sufficiently high values of the frequency, the solutions of (5.5) are close enough to the solutions of (3.13), and the convergence of the Newton's method is guaranteed. In practical situations we had convergence for any $\omega \geq 1$.

Summarizing the procedure, for any fixed N, for $\omega > 1$, we compute the nodes of MEF Gauss-Laguerre quadrature rule by the following steps

1. solve the linear system (5.2);
2. compute the smallest N positive solutions of (5.5), where the function $\bar{f}_N(x)$ is defined by (5.1);
3. solve the linear system (3.6) in correspondence of $Z = -\omega^2$;
4. compute the smallest N positive solutions $\bar{x}_i$ of (3.13), where the function $\bar{f}_N(x, \omega)$ is defined by (3.10), by using as initial approximations for the Newton's iterative process the solutions determined at the step 2;
5. according to (3.12) compute $x_i = \bar{x}_i/\omega$.

We observe as the first two steps are independent of ω for any fixed N.

In the Appendix B we report a Mathematica code for the construction of the functions in (3.10) and (5.1), needed in steps 2 and 4.

Example 1 We consider for example the case $N = 3$, $\omega = 10$.

1. by solving the linear system (5.2) and computing $D_n^3 = (-1)^{\alpha_n} d_n^3$, we obtain $D = [d_0^3, ..., d_6^3]^T = [-14, 46/3, -7/3, 1]^T$.
2. Then the equation (5.5), where the function $\bar{f}_3(x)$ is defined by (5.1), assumes the form

$$\begin{aligned} \bar{f}_3(x) = \eta_{-1}(x) - \frac{x^2}{6}\eta_0(x) = \\ = \cos(x) - \frac{1}{6}x\sin(x) = 0. \end{aligned}$$

The plot of the function $\bar{f}_3(x)$ is reported in Figure 2 (a). By computing the smallest 3 positive solutions of this equation with Newton iterative method with tolerance equal to the machine precision, the solutions are

$$\begin{pmatrix} 1.349552823716614 \\ 4.111617738242456 \\ 6.992351792948499 \end{pmatrix}. \tag{5.6}$$

3. by solving the linear system (3.6) in correspondence of $Z=-\omega^2$, we obtain that the function (3.10) assumes the form
$\bar{f}_3(\text{x},\omega)=\eta_{-1}[x]-\frac{x^2\omega\left(-3+4\omega^2+7\omega^4\right)\eta_0[x]}{2(\omega^3+21\omega^5)}+\frac{x\left(-6\omega^2\eta_0[x]-46\omega^4\eta_0[x]\right)}{2(\omega^3+21\omega^5)}+\frac{x^3\left(-1+8\omega^2+9\omega^4\right)\eta_1[x]}{2(\omega^3+21\omega^5)}$
4. by computing the smallest 3 positive solutions $\bar{x}_i$ of $\bar{f}_3(x,10)=0$, by using as initial approximations for the Newton's iterative process the vector (5.6) we obtain
$$\bar{x}=\begin{pmatrix}1.270745276330846\\4.017590446786748\\6.884277631923562\end{pmatrix}$$
;
5. then we compute
$$x=\bar{x}/10=\begin{pmatrix}0.127074527633085\\0.401759044678675\\0.688427763192356\end{pmatrix}$$

6 Numerical illustrations

In this section we show numerical experiments which confirm as the new MEF formulae produce an error of the same order of magnitude with respect to the EF ones. The advantage of these formulae is that their weights and nodes can be determined in a more efficient way with respect to classical EF ones, and for bigger values of N and ω.
Test case 1. We consider the function
$$f(x)=x\cos(\omega x)+x\sin(\omega x), \tag{6.7}$$
for which we have
$$\int_0^\infty e^{-x}f(x)dx=\frac{1+2\omega-\omega^2}{(1+\omega^2)^2}. \tag{6.8}$$
In Table 1 we compare the absolute errors $|I_{exact}-I_{comput}|$ of the results from classical, EF Gauss-Laguerre [10] and MEF Gauss-LAguerre rules for $N=3,4$ and various values of ω. We observe that, as for the EF method, the MEF method is affected only by round-off error for all ω. This is what we expected as the test function belongs to the EF basis.
Test case 2. The function
$$f(x)=\cos[(\omega+1)x] \tag{6.9}$$
is of form (1.2) with $f_1(x)=\sin(x)$ and $f_2(x)=\cos(x)$, and
$$\int_0^\infty e^{-x}f(x)dx=\frac{1}{1+(1+\omega)^2}. \tag{6.10}$$

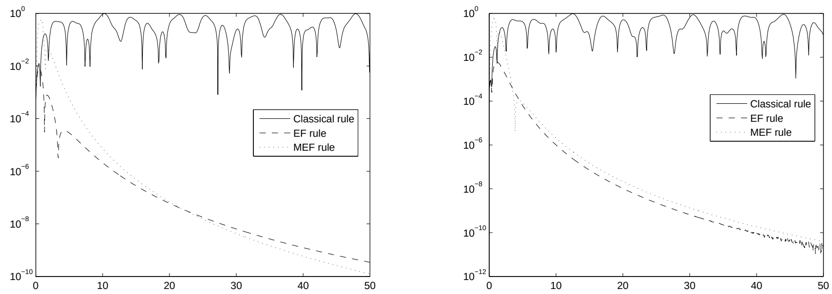
In Table 2 we report the results obtained by the classical, the EF and the MEF rule with $N=5$ and $N=6$ for different values of ω. In Fig. 3 we plot

N	rules	$\omega = 0$	$\omega = 10$	$\omega = 20$	$\omega = 30$	$\omega = 40$	$\omega = 50$
3	Classic	1.11e-16	1.22e+00	6.04e-01	7.77e-01	1.23e+00	8.62e-01
	EF	1.11e-16	4.51e-17	1.64e-17	4.98e-18	6.18e-18	5.69e-18
	MEF	1.11e-16	6.94e-18	8.67e-19	1.08e-18	7.59e-19	3.79e-19
4	Classic	2.24e-12	4.95e-01	6.74e-01	2.62e-01	1.13e+00	8.14e-02
	EF	2.24e-12	3.58e-15	1.35e-16	2.09e-16	2.50e-17	1.46e-16
	MEF	2.24e-12	3.47e-17	9.11e-18	6.51e-19	9.76e-19	7.05e-19

Table 1: Error produced by the MEF Gauss-Laguerre rule with $N = 3, 4$ on problem (6.7).

N	rules	$\omega = 0$	$\omega = 10$	$\omega = 20$	$\omega = 30$	$\omega = 40$	$\omega = 50$
5	Classic	5.41e-04	9.32e-01	3.88e-01	2.30e-01	1.05e-01	3.52e-02
	EF	5.41e-04	2.10e-06	6.04e-08	6.39e-09	1.24e-09	3.44e-10
	MEF	5.41e-04	7.29e-06	6.89e-08	4.28e-09	5.87e-10	1.25e-10
6	Classic	2.62e-04	1.70e-02	5.04e-01	6.49e-01	5.34e-01	1.00e-01
	EF	2.62e-04	9.96e-07	1.03e-08	6.47e-10	9.35e-11	3.16e-11
	MEF	2.62e-04	2.07e-06	2.14e-08	1.34e-09	1.84e-10	3.93e-11

Table 2: Error produced by the MEF Gauss-Laguerre rule with $N = 5, 6$ on problem (6.9).



(a) (b)

Fig. 3: The ω dependence of the errors produced by classic (solid), EF (dashed) and MEF (dot) Gauss-Laguerre quadrature rule for $N = 5$ (a) and $N = 6$ (b) on problem (6.9).

the variation with ω of the errors from the three rules. We observe as the MEF rule reaches the same order of accuracy fo the EF one.

We plot in Figure 4 the error produced on problem (6.9) by the MEF rule with increasing values of N and ω. we observe that for these values it was not possible in [10] to determine the weights and nodes. We note as for increasing N the error decreases more rapidly as ω increases, as we expected from the $O(\omega^{-N-1})$ behaviour.

We next show what happens if we suppose not to know the frequency exactly. More precisely we consider the exact frequency given by $\omega = (1+\delta)\bar{\omega}$, and we derive the MEF and EF methods in correspondence of the frequency $\bar{\omega}$. We plot in Figure 5 the error obtained on problem (6.9) with different values

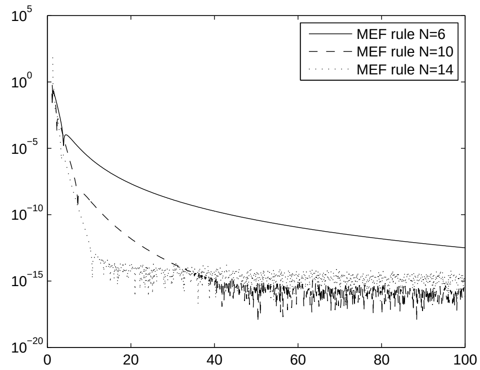


Fig. 4: The ω dependence of the errors on problem (6.9).

of δ. We observe as the MEF error is in any case smaller than the classical error, and behaves in the same way as the EF error.

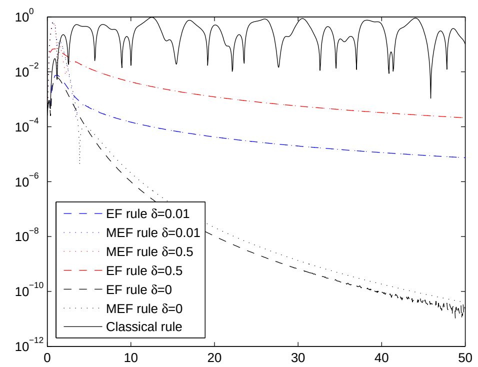


Fig. 5: The $\bar{\omega}$ dependence of the errors on problem (6.9) with $N = 6$ and $\omega = (1 + \delta)\bar{\omega}$.

7 Conclusions

We constructed a class of modified EF Gauss-Laguerre rules for the computation of integrals of oscillatory functions over infinite intervals. We proved as these new formulae behave as the EF Gauss-Laguerre quadrature rules [10], providing a massive improvement in accuracy with respect to the classical Gauss-Laguerre formulae when the frequency of oscillation increases. The advantage of MEF Gauss-Laguerre formule is that they can be computed for bigger values of N and ω with respect to the EF ones, and their construction is also less expensive. Numerical experiments confirm the theoretical expectations.

This approach can be directly extended also to the case of integrals over a bounded interval, thus improving the results of the paper [29], where standard EF Gauss-Legendre methods have been constructed, and of the paper [31], where the quadrature nodes are determined with an heuristic dependence on ω, and also providing a good alternative to formulae constructed in the paper [2], which are not easy to determine when the number of nodes increases, and their existence is not guaranteed. As a matter of fact, in the case of bounded interval, the weights and nodes of the Gauss EF quadrature rule in [29] can be reformulated as in (3.2) with a different form for the moments in (3.3). This will be object of future research. The approach described in this paper can be useful also to improve the methods constructed in [7] for Volterra integral equations.

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Appendix A

The set of functions $\eta_m(Z)$, $m = -1, 0, 1, 2, \ldots$ has been originally introduced in [26] in the context of CP methods for the Schrödinger equation. The functions $\eta_m(Z)$ with $m = -1, 0$ are first defined by some formulae, namely:

$$\eta_{-1}(Z) = \begin{cases} \cos(|Z|^{1/2}) \text{ if } Z \leq 0 \\ \\ \cosh(Z^{1/2}) \text{ if } Z > 0 \end{cases}, \; \eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0 \\ 1 & \text{if } Z = 0 \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0 \end{cases} \tag{A.1}$$

and those with $m > 0$ are further generated by recurrence

$$\eta_m(Z) = \frac{1}{Z}[\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)], \quad m = \; 1, \; 2, \; 3, \ldots \tag{A.2}$$

if $Z \neq 0$, and by following values at $Z = 0$:

$$\eta_m(0) = \frac{1}{(2m+1)!!}, \quad m = \; 1, \; 2, \; 3, \ldots \tag{A.3}$$

The differentiation of these functions is of direct concern for this paper. The rule is

$$\eta_m'(Z) = \frac{1}{2}\eta_{m+1}(Z)\,, \; m = -1, \, 0, \, 1, \, 2, \, 3, \ldots \tag{A.4}$$

For more details on these functions see [9,26,30].

References

1. G. Arfken, Mathematical Methods for Physicists, third ed., Academic Press, Orlando, FL, 1985.
2. A. Asheim, A. Deaño, D. Huybrechs, H. Wang, *A Gaussian quadrature rule for oscillatory integrals on a bounded interval*, Discret. Contin. Dyn. S. 34 (3), 883–901, 2014.
3. A. Asheim, D. Huybrechs, *Gaussian quadrature for oscillatory integral transforms*, IMA J. Numer. Anal, 2013.
4. G. Bao, W. Sun, *A fast algorithm for the electromagnetic scattering from a large cavity*, SIAM J. Sci. Comput. 27, 553–574, 2005.
5. A. Cardone, M. Ferro, L. Gr. Ixaru and B. Paternoster, *A Family of Exponential Fitting Direct Quadrature Methods for Volterra Integral Equations*, AIP Conf. Proc. 1281, 2204-2207 (2010).
6. A. Cardone, L. Gr. Ixaru and B. Paternoster, *Exponential fitting direct quadrature methods for Volterra integral equations*, Numerical Algorithms 55, 467–480, 2010.
7. A. Cardone, L.Gr. Ixaru, B. Paternoster, G. Santomauro, *Ef-Gaussian direct quadrature methods for Volterra integral equations with periodic solution*, Math. Comput. Simulation, in press.
8. A. Cardone, B. Paternoster, G. Santomauro, *Exponential fitting quadrature rule for functional equations*, AIP Conference Proceedings, AIP Conf. Proc. 1479, 1169-1172 Springer (2012).
9. D. Conte, E. Esposito, B. Paternoster, L. Gr. Ixaru, *Some new uses of the $\eta_m(Z)$ functions*, Comput. Phys. Commun. 181, 128–137, 2010.
10. D. Conte, L.Gr.Ixaru, B. Paternoster, G. Santomauro, *Exponentially-fitted Gauss-Laguerre quadrature rule for integrals over an unbounded interval*, J.Comput.Appl.Math 255, 725–736, 2014.
11. D. Conte, B. Paternoster, G. Santomauro, *An exponentially fitted quadrature rule over unbounded intervals*, AIP Conf. Proc. 1479, 1173–1176 Springer, 2012.
12. R. D'Ambrosio, E. Esposito, B. Paternoster, *Exponentially fitted two-step hybrid for $y'' = f(x, y)$*, Journal Comp. and Appl. Math. 235, 4888-4897, 2011.
13. R. D'Ambrosio, E. Esposito, B. Paternoster, *Parameter estimation in exponentially fitted hybrid methods for second order differential problems*, J. Math. Chem. 50 (1), 155-168 (2012).
14. R. D'Ambrosio, E. Esposito, B. Paternoster, *Exponentially fitted two-step Runge-Kutta methods: construction and parameter selection*, Appl. Math. Comput 218 7468-7480 (2012).
15. R. D'Ambrosio, M. Ferro, B. Paternoster, *Two-step hybrid collocation methods for $y'' = f(x, y)$*, Appl. Math. Lett. 22 (2009), 1076-1080.
16. R. D'Ambrosio, M. Ferro, B. Paternoster, *Trigonometrically fitted two-step hybrid methods for special second order ordinary differential equations*, Mathematics and Computers in Simulation, 81, 1068–1084, 2011
17. R. D'Ambrosio, L. Gr. Ixaru, B. Paternoster, *Construction of the ef-based Runge- Kutta methods revisited*, Comput. Phys. Commun. 182, 322-329, 2011.
18. R. D'Ambrosio, B. Paternoster, *Numerical solution of a diffusion problem by exponentially fitted finite difference methods.* SPRINGERPLUS. 3:425, 1–7 (2014).
19. R. D'Ambrosio, B. Paternoster, *Exponentially fitted singly diagonally implicit Runge-Kutta methods*, J.Comput.Appl.Math , 263, 277–287 (2014).
20. R. D'Ambrosio, B. Paternoster, G. Santomauro, *Revised exponentially fitted Runge-Kutta-Nystrom methods*, Appl. Math. Lett., 30, 56–60 (2014).
21. P.J. Davies, D.B. Duncan, *Stability and convergence of collocation schemes for retarded potential integral equations*, SIAM J. Numer. Anal. 42, 1167–1188, 2004.
22. P. J., Davis, P. Rabinowitz, *Methods of numerical integration*, Computer Science and Applied Mathematics. Academic Press [A subsidiary of Harcourt Brace Jovanovich, Publishers] New York-London, 1975.
23. R. Frontczak and R. Schoebel, *On modified Mellin transforms, Gauss-Laguerre quadrature, and the valuation of American call options*, J. Comput. Appl. Math. 234, 1559–1571, 2010.

24. S. M. Hasheminejad and M. Aghabeigi, *Liquid sloshing in half-full horizontal elliptical tanks*,J. of Sound and Vibration 324, 332–349, 2009.
25. D. Huybrechs, S. Vandewalle, *A sparse discretization for integral equation formulations of high frequency scattering problems*, SIAM J. Sci. Comput. 29, 2305–2328, 2007.
26. L. Gr. Ixaru, *Numerical methods for differential equations and applications*, Reidel, Dordrecht-Boston-Lancaster, 1984.
27. L. Gr. Ixaru, *Operations on Oscillatory Functions*, Comput. Phys. Commun. 105, 1–19, 1997.
28. L. Gr. Ixaru, *Runge-Kutta method with equation dependent coefficients*, Comput. Phys. Commun. 183, 63–69, 2012.
29. L. Gr. Ixaru, B. Paternoster, *A Gauss quadrature rule for oscillatory integrands*, Comput. Phys. Commun. 133, 177–188, 2001.
30. L. Gr. Ixaru and G. Vanden Berghe, *Exponential Fitting*, Kluwer, Boston - Dordrecht - London, 2004.
31. V. Ledoux and M. Van Daele, Interpolatory quadrature rules for oscillatory integrals, J. Sci. Comput., 53, 586–607, 2012.
32. K. J. Kim *Quadrature rules for the integration of the product of two oscillatory functions with different frequencies*, Comput. Phys. Commun. 153, 135–144, 2003.
33. K. J Kim, *Two-frequency-dependent Gauss quadrature rules*, J. Comput. Appl. Math. 174, 43–55, 2005.
34. K. J Kim, R. Cools, L. Gr. Ixaru, *Quadrature rules using first derivatives for oscillatory integrands*, J. Comput. Appl. Math. 140, 479–497, 2002.
35. K. J Kim, R. Cools, L. Gr. Ixaru, *Extended quadrature rules for oscillatory integrands*, Appl. Numer. Math. 46, 59–73, 2003.
36. H. Majidian, Numerical approximation of highly oscillatory integrals on semi-finite intervals by steepest descent method, Numer. Algor. 63 (3), 537–548, 2013.
37. G.V. Milovanovic, A.S. Cvetkovic, M.P. Stanic,*Gaussian quadratures for oscillatory integrands*, Appl. Math. Lett. 20, 853-860, 2007.
38. B.Paternoster, *Present state-of-the-art in exponential fitting. A contribution dedicated to Liviu Ixaru on his 70-th anniversary*, Comput. Phys. Commun. 183, 2499–2512, 2012.
39. T. E. Simos, *An exponentially-fitted Runge-Kutta method for the numerical integration of initial-value problems with periodic or oscillating solutions*. Comput. Phys. Comm. 115, 1–8, 1998.
40. W. Sun, N.G. Zamani, *Adaptive mesh redistribution for the boundary element method in elastostatics*, Comput. Struct. 36, 1081–1088, 1990.
41. M. Van Daele, G. Vanden Berghe, H. Vande Vyver, *Exponentially fitted quadrature rules of Gauss type for oscillatory integrands*. Appl. Numer. Math. 53, 509–526, 2005.
42. M. Van Daele, T. Van Hecke, G. Vanden Berghe, H. De Meyer, *Deferred correction with mono-implicit Runge-Kutta methods for first-order IVPs. Numerical methods for differential equations* (Coimbra, 1998). J. Comput. Appl. Math. 111 (1999), no. 1-2, 37–47.