On quadrature formulas for oscillatory evolutionary problems

Angelamaria Cardone, Dajana Conte, Raffaele D'Ambrosio, Beatrice Paternoster

Abstract—Gaussian-type quadrature rules for oscillatory integrand functions are presented. The weights and nodes depend on the frequency of the problem and they are constructed by following the exponential fitting theory. The error analysis proves that the exponentially fitted Gaussian rules are more accurate than the classical Gaussian rules when oscillatory functions are treated. The numerical approximation to Volterra integral equations with oscillatory solution through these formulas is presented. Some numerical tests are reported.

Keywords—Quadrature, periodic functions, Gaussian rules, exponential fitting

I. Introduction

In this paper we illustrate quadrature rules specially tuned on oscillatory integrand functions. These integrals arise, for example, in the numerical solution of Volterra integral equations (VIEs) with periodic solution, which model a considerable variety of periodic phenomena, as for example seasonal biological phenomena [1] and the response of a nonlinear circuit to a periodic input [74]–[76]. Further examples are furnished in [11], [22], [26], [63], [72].

A successful strategy in the numerical treatment of oscillatory functions has been furnished by the theory of exponential fitting, introduced in [65] (see also the monograph [66]). As a matter of fact several methods for a number of different problems has been proposed so far, from the application to ordinary differential problems [59], [62], [68], [73], to the integral equations [19], [21], [24]–[26], [67], to fractional differential equations [14], to partial differential equations [19], [20], [56], [61] also by means of a special modification of IMEX methods (compare e.g. [2], [3], [29]–[31]).

Following the exponential fitting theory, in [25] authors proposed a Simpson-type formula, called ef-Simpson rule, for integrals over bounded intervals, which is exact on the set of functions $\{1, \cos(\omega s), \sin(\omega s)\}$. As a consequence, the weights of this formula depend on the frequency ω. This formula has the same order of the classical Simpson rule, but has a smaller error constant when periodic integrand functions are treated. Here we describe how to construct more accurate quadrature rules, without increasing the computational cost. In particular we consider exponential fitting quadrature formulas of Gaussian type and analyze the error. We will see that the order is the same as the classical Gauss-Legendre formula, but the error is smaller for oscillatory integrand functions. The first Gauss rule for oscillatory integrands, derived by means of the exponential fitting approach, has been proposed in [67].

These ef-quadrature rules represent a powerful tool to construct highly accurate numerical method for Volterra integral equations (VIEs) with periodic or oscillatory solution. In the sequel, we describe how to derive ef direct quadrature (DQ) methods based on such formulas and analyze the convergence.

The paper is organized as follows. In Sec. 3 and 4 we construct and analyze ef-Gaussian quadrature rules for integrals over a bounded and unbounded intervals, respectively. In Sec. 5, we show the performances of the ef-DQ methods based on such formulas, on some significative test examples. Last section contains some concluding remarks and some ideas on future development of the present work.

II. Quadrature rules on bounded interval

In this section we illustrate the construction and analysis of a family of Gaussian quadrature formulas for an integral on a bounded interval, which are specially tuned for an oscillatory integrand functions. A former example of a similar type of formulas has been derived in [24] and in [34]. In particular we construct a quadrature rule for the integral

$$I[g](X) = \int_{X-h}^{X+h} g(x)dx,$$

where $X > 0$ and $h > 0$, which is exact on the fitting space

$$\mathcal{B} := \{x^k e^{(\alpha \pm i\omega)x}\ ,\ k = 0, \dots, P-1\}. \tag{1}$$

The quadrature formula is of type

$$Q[g](X) := h \sum_{k=0}^{P-1} a_k g(X + \xi_k h) \tag{2}$$

where the weights and nodes

$$a_k = a_k(\alpha h, \omega h), \quad \xi_k = \xi_k(\alpha h, \omega h), \tag{3}$$

$k = 0, 1, \dots, P-1$, will be derived through the exponential fitting theory [65], [66]. To simplify the notation, we will skip the dependence of weights and nodes on αh and ωh. Following the exponential fitting formalism introduced by Ixaru, we introduce the functional $\mathcal{L}$:

$$\mathcal{L}[h, \mathbf{a}, \xi]g(X) := \int_{X-h}^{X+h} g(s)ds - h \sum_{k=0}^{P-1} a_k g(X + \xi_k h)),$$

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A. Cardone, D. Conte, and B. Paternoster are in the Department of Mathematics, University of Salerno, 84084 Fisciano, Italy. (e-mail: {ancardone, dajconte, beapat}@unisa.it.)

R. D'Ambrosio is with University of L'Aquila, Department of Engineering and Computer Science and Mathematics, Via Vetoio, Loc. Coppito, 67100 L'Aquila (e-mail: raffaele.dambrosio@univaq.it)

where $\mathbf{a} = (a_0, \dots, a_{P-1})$ and $\xi = (\xi_0, \dots, \xi_{P-1})$ and ask that it annihilates on the fitting space. Since

$$\mathcal{L}[h, \mathbf{a}, \xi] X^k e^{(\alpha+i\omega)X} \text{ and } \mathcal{L}[h, \mathbf{a}, \xi] X^k e^{(\alpha-i\omega)X}$$

are complex conjugate, to annihilate both it is sufficient to impose

$$\mathcal{L}[h, \mathbf{a}, \xi] X^k e^{(\alpha+i\omega)X} = 0. \tag{4}$$

Functions $\mathcal{L}[h, \mathbf{a}, \xi] X^k e^{(\alpha+i\omega)X}$ can be expressed in the compact form:

$$\begin{aligned}
\mathcal{L}[h, \mathbf{a}, \xi] e^{(\alpha+i\omega)X} &= \ell_0 e^{(\alpha+i\omega)X}, \\
\mathcal{L}[h, \mathbf{a}, \xi] X e^{(\alpha+i\omega)X} &= (\ell_0 X + \ell_1) e^{(\alpha+i\omega)X}, \\
\mathcal{L}[h, \mathbf{a}, \xi] X^2 e^{(\alpha+i\omega)X} &= (\ell_0 X^2 + 2\ell_1 X + \ell_2) e^{(\alpha+i\omega)X}, \\
\mathcal{L}[h, \mathbf{a}, \xi] X^3 e^{(\alpha+i\omega)X} &= \\
&\left(\ell_0 X^3 + 3\ell_1 X^2 + 3\ell_2 X + \ell_3\right) e^{(\alpha+i\omega)X}, \\
&\dots
\end{aligned}$$

where ℓ_k are complex coefficients depending on $u = \alpha h, z = \omega h, a_k, \xi_k$, $k = 0, \dots, P-1$. Thus, the quadrature rule (2) is exact on the fitting space $\mathcal{B}$ if and only if

$$\ell_k = 0, \quad \ell = 0, \dots, P-1, \tag{5}$$

i.e. if the real and the imaginary parts of ℓ_k vanish. The system (5) is linear with respect to the weights $\{a_k\}_k$ and non linear with respect to the nodes $\{\xi_k\}_k$, thus the exact solution cannot be derived in a closed form and a numerical method is necessary.

The following theorem analyzes the error of the quadrature formula (2):

$$E[g](X) := \int_{X-h}^{X+h} g(s)ds - Q[g](X).$$

Theorem 2.1: [21] Let assume that $g(x)$ is differentiable indefinitely many times on $[X-h, X+h]$. The error from the quadrature formula $Q[g]$ (2) with weights and nodes given by the system (5) is

$$E[g](X) = \sum_{k=0}^{\infty} h^{2P+1+k} T_k D^k ((D-\alpha)^2 + \omega^2)^P g(X), \tag{6}$$

where D is the derivative operator and $\{T_k\}_k$ depend on $u = \alpha h,\ z = \omega h$, and on $\{a_k, \xi_k\}_{k=0}^{P-1}$. In particular

$$\begin{aligned}
T_0 &= \frac{2 - \sum_{k=0}^{P-1} a_k}{(u^2+z^2)^P} \\
T_1 &= \\
&\frac{2Puz^{2P-2}\left(2 - \sum_{k=0}^{P-1} a_k\right) - (u^2+z^2)^P \sum_{k=0}^{P-1} a_k \xi_k}{(u^2+z^2)^{2P}}
\end{aligned}$$

A. Composite quadrature formula

We introduce now a composite quadrature formula based on the rule (2), to approximate the integral

$$I[g] = \int_a^b g(s)ds.$$

We take the equally spaced points $a = t_0 < t_1 < \dots < t_m = b$, with $h = t_{j+1} - t_j = \frac{b-a}{m}$. By applying the quadrature formula (2) on each subinterval $[t_j, t_{j+1}]$, we get the composite formula

$$I[g] \approx Q_m[g] := h \sum_{j=0}^{m-1} \sum_{k=0}^{P-1} \tilde{a}_k g(t_j + \tilde{\xi}_k h), \tag{7}$$

with

$$\tilde{a}_k = \frac{1}{2} a_k, \quad \tilde{\xi}_k = \frac{1}{2} + \frac{1}{2}\xi_k, \quad k = 0, \dots, P-1.$$

If $g \in C^{2P}([a,b])$, it results that the error $E_m[g] = I[g] - Q_m[g]$ satisfy the following inequality

$$|E_m[g]| \le C(b-a)h^{2P}, \tag{8}$$

where C depends on $||((D-\alpha)^2 + \omega^2)^P g||_\infty$.

III. Quadrature rules on unbounded intervals

We now consider quadrature formulae for integrals of oscillatory functions over unbounded intervals. Let $f(x)$ be a function of the form

$$f(x) = f_1(x)\sin(\omega x) + f_2(x)\cos(\omega x), \tag{9}$$

where the coefficients $f_1(x)$ and $f_2(x)$ are assumed smooth enough to be well approximated by polynomials.

Then we consider quadrature formulae of the form

$$I = \int_0^\infty e^{-x} f(x)dx \simeq I_N = \sum_{k=1}^{N} w_k f(x_k). \tag{10}$$

We associate to the quadrature formula (10) 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 $\mathbf{a} = [w_1, w_2, ..., w_N, x_1, x_2, ..., x_N]$ is a vector with $2N$ components which collects the weights and the nodes, and impose its exactness on the fitting space

$$\mathcal{F} = \{x^{n-1} e^{\pm\mu x},\ n = 1, 2, ..., N, \}, \tag{11}$$

as described in [44], [46], [48] for unbounded integration interval, and [67] for bounded integration interval.

Let us define the set of functions $\eta_m(Z)$, $m = -1, 0, 1, 2, ...$ are as follows (see for instance [43], [66]):

$$\eta_{-1}(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \le 0 \\ \\ \cosh(Z^{1/2}) & \text{if } Z > 0 \end{cases}, \tag{12}$$

$$\eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0 \\ 1 & \text{if } Z = 0 \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0 \end{cases} \tag{13}$$

and

$$\eta_m(Z) = \frac{1}{Z}[\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)], \quad m \ge 1 \tag{14}$$

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

$$\eta_m(0) = \frac{1}{(2m+1)!!}, \quad m \geq 1. \tag{15}$$

By imposing the exactness on the fitting space (11) we then obtain the nonlinear system

$$\sum_{k=1}^{N} w_k x_k^{n-1} \frac{\eta_{\lfloor \frac{n-2}{2} \rfloor}(x_k^2 Z)}{\eta_{\lfloor \frac{n-2}{2} \rfloor}(0)} = M_{n-1}(Z), \quad n = 1, \ldots, 2N, \tag{16}$$

where

$$M_n(Z) = \frac{n!}{(1-Z)^{\lceil \frac{n+1}{2} \rceil}} \tag{17}$$

with $Z = \mu^2 = -\omega^2$.

Then the Exponentially Fitted (EF) Gauss-Laguerre quadrature formula is of the form (10), with weights and nodes determined as solutions of the nonlinear system (16). Such formula reduces to classical Gauss-Laguerre quadrature formula as the frequency ω tends to zero. Moreover the error of such formula has the asymptotic decay

$$|I - I_N| = O(\omega^{-N-1}), \quad \omega \to \infty. \tag{18}$$

Then the EF Gauss-Laguerre quadrature rules have the same optimal asymptotic order of steepest descent methods in [70] and complex Gaussian quadrature rules in [4], also maintaining a good accuracy for small values of ω, as they naturally tend to the corresponding classical Gauss-Laguerre formulae for $\omega \to 0$.

In [44] it was proved that the nonlinear system (16) can be solved by splitting it into a linear system for the weights $w = (w_1, \ldots, w_N)^T$ and a nonlinear system for the nodes. Also the Jacobian matrix of the Newton iterative method applied to such nonlinear system has been computed by using the differentiation properties of the $\eta_m(Z)$ functions [43], [66].

The above mentioned systems can be affected by ill-conditioning as 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. In order to overcome these problems Modified EF (MEF) Gauss-Laguerre formulae have been proposed in [46], 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 MEF Gauss-Laguerre quadrature rule is defined by

$$I \simeq I_N = \sum_{i=1}^{N} (a_i f_1(x_i) + b_i f_2(x_i)) \tag{19}$$

where the functions f_1 and f_2 are given in (9). The frequency dependent nodes $x_i = x_i(\omega)$, $i = 1, ..., N$, are defined as the smallest N positive solutions of the nonlinear equation

$$f_N(x, \omega) = 0, \tag{20}$$

where

$$f_N(x, \omega) = \sum_{n=0}^{N} C_n^N(Z) x^n \frac{\eta_{\lfloor \frac{n-1}{2} \rfloor}(x^2 Z)}{\eta_{\lfloor \frac{n-1}{2} \rfloor}(0)}, \quad Z = -\omega^2, \tag{21}$$

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

$$\sum_{j=0}^{N-1} M_{i+j}(Z) C_j^N(Z) = -M_{N+i}(Z), \tag{22}$$

for $i = 0, ..., N-1$, with the moments $M_n(Z)$ defined in (17). Moreover $a_i(\omega)$, $b_i(\omega)$ 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, $i = 1, ..., N$. The solvability of the nonlinear equation (20) has been analyzed in [46], together with the choice of a suitable initial approximation for the Newton iterative process, which allows to construct formulae with a larger number of nodes with respect to EF Gauss-Laguerre formulae. Moreover the error of the MEF Gauss-Laguerre quadrature formulae has the same asymptotic decay as in (18).

In order to show the effectiveness of the proposed exponentially fitted formulae, we report in Figure 1 the results obtained by classical, EF and MEF Gauss-Laguerre quadrature rules on the problem

$$\int_0^\infty e^{-x} \cos[(\omega+1)x] dx = \frac{1}{1+(1+\omega)^2}. \tag{23}$$

The integrand $f(x) = \cos[(\omega+1)x]$ is of form (9) with $f_1(x) = \sin(x)$ and $f_2(x) = \cos(x)$. We moreover suppose not to know the frequency exactly, i.e. by considering 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 1 the error obtained on problem (23) with different values 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.

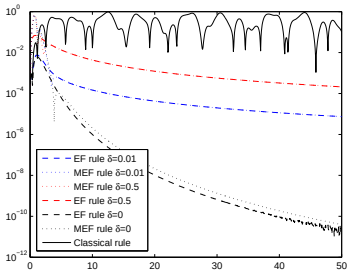

Fig. 1. The $\bar{\omega}$ dependence of the errors on problem (23) with $N = 6$ and $\omega = (1+\delta)\bar{\omega}$.

IV. Numerical treatment of Volterra integral equations with periodic solution

We focus our attention on VIEs with periodic solution of the type

$$\begin{aligned} y(x) = &\quad f(x) + \int_{-\infty}^{x} k(x-s)y(s)ds,\ x \in [0, x_{end}] \\ y(x) = &\quad \psi(x), \quad -\infty < x \leq 0, \end{aligned} \tag{24}$$

where $k \in L^1(I\!R^+)$, f is continuous and periodic on $[0, x_{end}]$, ψ is continuous and bounded on $I\!R^-$. Main results on the existence and uniqueness of a periodic solution of (24) are given in [11], [12]. The first attempts to the numerical solution of eq. (24) are given by [6], [11], [12] For an overview on the numerical treatment of VIEs of general type compare [10], [13].

Consider the uniform mesh $I_h := \{x_0 = 0 < x_1 < \cdots < x_N = x_{end}\}$, with $x_n = nh$, $\forall n$, $h = x_{end}/N$. The equation (24) at $x = x_n$ takes the form

$$y(x_n) = f(x_n) + (I\psi)(x_n) + \int_0^{x_n} k(x_n - s)y(s)ds, \tag{25}$$

where $(I\psi)(x)$ is the known part of the integral:

$$(I\psi)(x) = \int_{-\infty}^{0} k(x-s)\psi(s)ds, \quad x \in [0, x_n].$$

If we cannot evaluate $(I\psi)(x)$ analytically, we may approximate it numerically without compromising the accuracy of the overall method. As a matter of fact, we may adopt a technique similar to that applied in [33]. Since the integrand $k(x-s)y(s)$ vanishes as $s \to -\infty$, we can approximate the integration interval $]-\infty, 0]$ with a bounded one $]-M(h), 0]$, where $M(h)$ can be a priori estimated, in such a way that the order of convergence of the DQ method is preserved. Further details may be found in [21], [25], [26].

By applying the composite quadrature rule (7) to (25), we get:

$$\begin{aligned} y(x_n) \approx f(x_n) + (I\psi)(x_n) \\ + h\sum_{j=0}^{n-1}\sum_{i=0}^{P-1} \tilde{a}_i k(x_{n-j} - \tilde{\xi}_i h)y(x_j + \tilde{\xi}_i h) \end{aligned} \tag{26}$$

$n = 1, \ldots, N$. Then we adopt a suitable interpolation technique to approximate $y(x_j + \tilde{\xi}_i h)$:

$$y(x_j + \tilde{\xi}_i h) \approx \mathcal{P}(x_j + \tilde{\xi}_i h), \tag{27}$$

where $\mathcal{P}$ is the either algebraic or ef interpolating polynomial constructed on the points:

$$(x_{j+l}, y_{j+l}), \quad l = -r_-, ..., r_+, \tag{28}$$

with $y_n \approx y(x_n)$, $\forall n$. This idea follows the lines of what has been done in [23] in the context of double delay VIEs. By using (27) we have:

$$\begin{aligned} y_n = f(x_n) + (I\psi)(x_n) + \\ h\sum_{j=0}^{n-1}\sum_{i=0}^{P-1} \tilde{a}_i k(x_{n-j} - \tilde{\xi}_i h)\mathcal{P}(x_j + \tilde{\xi}_i h), \end{aligned}$$

$n = 1, ..., N$. Both in the case of algebraic and ef interpolation, we can write

$$\mathcal{P}(x_j + sh) = \sum_{l=-r_-}^{r_+} p_l(s)y_{j+l} \tag{29}$$

where $p_l(s)$ does not depend on x_j but only on r_-, r_+. Therefore we have:

$$\begin{aligned} y_n = f(x_n) + (I\psi)(x_n) + \\ h\sum_{j=0}^{n-1}\sum_{i=0}^{P-1} \tilde{a}_i k(x_{n-j} - \tilde{\xi}_i h)\sum_{l=-r_-}^{r_+} p_l(\tilde{\xi}_i)y_{j+l}, \end{aligned} \tag{30}$$

$n = 1, ..., N$. We impose $r_+ \leq 1$ to avoid the use of future mesh points. The method is explicit for $r_+ = 0$, and implicit for $r_+ = 1$.

The order of convergence is the same, using both the algebraic interpolation and the exponentially fitting interpolation [21], nevertheless the error constant is smaller in the latter case when periodic problems are treated.

The following theorem analyzes the convergence of the method.

Theorem 4.1: Assume that the equation (24) satisfies the hypotheses for the existence and uniqueness of solution, and assume that $y(x) \in C^{2P}([0, x_{end}])$. Let $\{y_n\}_{n=1}^N$ be the numerical solution of (24) obtained by the ef-DQ method (30) with $r_+ + r_- = 2P - 1$, where the polynomial $\mathcal{P}$ is either the Lagrange polynomial or the ef-based interpolation polynomial. Then, the error $e_n = y(x_n) - y_n$ satisfies:

$$\max_{1 \leq n \leq N} |e_n| = \mathcal{O}(h^{2P}) \quad as \quad h \to 0.$$

V. Numerical examples

In this section we illustrate the performances of the ef-DQ method (30) on some test examples. The numerical experiments have been carried out by Matlab®. The nodes $\{\xi_i\}_i$ have been computed by solving the nonlinear system by Matlab routine fsolve with maximal accuracy. Now we consider the problem of type (24), with $X = 5$,

$$k(x) = e^{\bar{\alpha}x},$$

and $f(x)$ is such that

$$y(x) = x^3 \cos(\bar{\omega}x),$$

provided the same expression is adopted for $\psi(x)$. We take $\bar{\alpha} = -1$.

We apply the efDQ method (30) with $P = 3$ and $r_- = 5$, $r_+ = 0$, which is convergent of order six. We plotted in Fig. 2 the error of the efDQ method and of the classical DQ method of the same order six. We observe that the error of the efDQ method is considerably smaller, at the same computational cost.

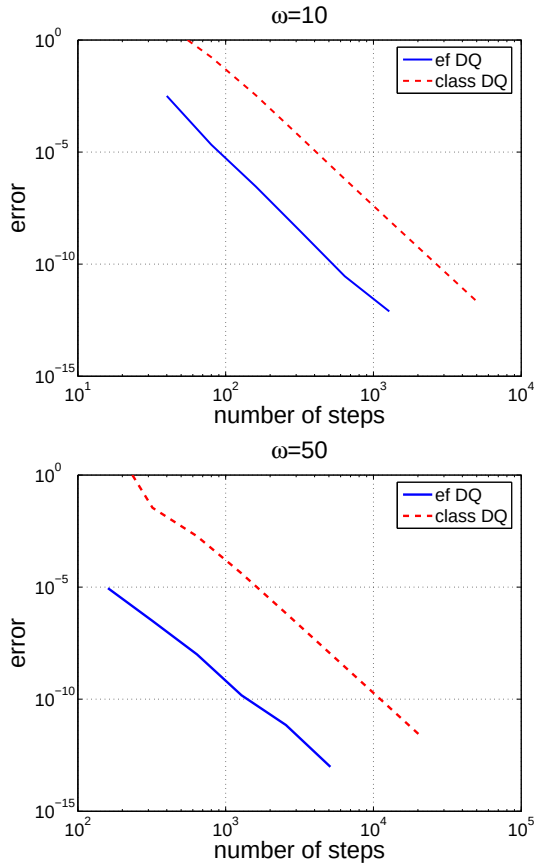

Fig. 2. Error versus number of steps of the classical DQ method and by efDQ method (30) on the test problem 2, with $\bar{\omega} = 10$ on the top and $\bar{\omega}$ at the bottom. Logarithmic scale on the x- and y-axis.

VI. Conclusions

We described a specially tuned approach to quadrature problems involving oscillatory problems. The parameters of the method depend on an estimate of the frequency of the integrand functions, by means of the exponential fitting technique. The proposed methods find an effective application to periodic or oscillatory evolutionary problems, as VIEs with periodic solution, as the theoretical and experimental analysis proved.

The research is open to many further developments. An issue to be addressed regards the numerical stability of ef-DQ methods, which should be analyzed starting from the basic test equation from the literature [5], [13], [36], [69], [71], [77], [78], and which may take advantage from some techniques used for ordinary differential equations, as for example the Runge-Kutta, the quadratic and the algebraic stability [7], [8], [27], [28], [37], [39], [40], [79]. Moreover new specially tuned methods can be formulated, as for example multistep collocation methods (see e.g. [16]–[18], [41], [45]) on a suitable functional basis, considering as a starting point the one-step collocation methods proposed in [11], [12]. More efficient numerical methods can also be obtained by ecploiting a parallel environment [35], [42], [47]. Another possibility to explore new methods is to consider a special version of general linear methods [7]–[9], [15], [27], [32], [49]–[55], [57], [58], [60], [79].

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Angelamaria Cardone is researcher in Numerical Analysis of University of Salerno, Italy. She received her PhD in Computational sciences and applied mathematics in 2004, from University of Naples Federico II, Italy. Her research interests regard the numerical treatment of Volterra integral equations, ordinary differential equations and more recently fractional differential equations. Part of the research deals with the development of mathematical software, also in parallel environment.

Dajana Conte is Associate Professor in Numerical Analysis at University of Salerno, Italy. Her research activity concerns the development and analysis of efficient and stable numerical methods for the solution of evolutionary problems, also with memory, modeled by ordinary differential equations and Volterra integral and integro-differential equations. She was involved also on problems related to the numerical solution of the many-body Schrodinger equation in quantum molecular dynamics.

Raffaele D'Ambrosio is Associate Professor at the Department of Engineering and Computer Science and Mathematics of University of L'Aquila. He has been Fulbright Research Scholar in the Academic Year 2014-15 at Georgia Institute of Technology. His research topics mainly interest numerical methods for evolutionary problems of several kind (ordinary and partial differential equations, integral equations, Hamiltonian problems, stochastic differential equations, piecewise smooth dynamical systems), with particular emphasis to structure-preserving numerical integration.

Beatrice Paternoster is Full Professor of Numerical Analysis at University of Salerno, Italy. In her research she has been involved in the analysis and derivation of new and efficient numerical methods for functional equations, in particular differential and integral Equations. She is also involved in parallel computation, with concerns to the development of mathematical software for evolutionary problems.