Adapted numerical methods for oscillatory evolutionary problems

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Abstract—It is the purpose of this paper to consider a selection of adapted numerical methods for the solution of evolutionary problems showing a periodic behaviour in their dynamics. The treatise will cover both evolutionary problems in time and space (i.e. reaction-diffusion problems generating a periodic wavefront in time and space) and problems with memory (i.e. Volterra integral equations with periodic solutions), also underlining the necessity to introduce suitable quadrature rules adapted to the problems under investigation. The approach is mainly problem-oriented, in order to match qualitative properties of the problem with the numerical methods, in order to get better accuracy, efficiency and stability properties with respect to existing numerical schemes.

Keywords—Exponential fitting, partial differential equations, reaction-diffusion problem, Volterra integral equations, oscillatory solutions, evolutionary problems.

I. Introduction

Evolutionary problems arising from applications can be modelled by various kinds of mathematical operators, in agreement with the observed dynamics of the phenomenon under investigation. Time discretization of such operators, oriented to provide an accurate and efficient numerical solution, can be led in many different ways that can be ideally divided into two main classed: general and special purpose numerical methods. Classically, a *general purpose* method is constructed in order to be exact (within round-off error) on polynomial solutions up to a certain degree. However, when other a priori known characters are advisable in the exact solution of the problem (e.g. periodicity, oscillations, exponential decay), the computational effort of classical methods could be quite heavy, due to the necessary employ of very small stepsizes needed to accurately reproduce the qualitative behaviour of the solution. In these situations, it may be convenient to use *special purpose* formulae, i.e. numerical methods adapted to the problem, that are exact on functions other than polynomials (see [49], [52] and references therein). The basis functions are chosen according to the information known a priori about the exact solution and belong to a finite-dimensional space called *fitting space*.

Normally, the chosen basis functions also depend on a parameter connected to the solution, whose value is clearly unknown. As a consequence, non-polynomially fitted formulae have variable coefficients relying on this parameter instead of classical formulae that are characterized by constant coefficients.

In summary, an accurate and efficient numerical method based on exponential fitting has to rely on a suitable fitting space and on a cheap - but accurate - procedure for the estimate of the unknown parameters. We show examples of special purpose strategies to solve two families of evolutionary problems exhibiting periodic solutions, i.e. partial differential equations, in Section 2, and Volterra integral equations, in Section 3.

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II. Periodic solutions in reaction-diffusion problems

Let us consider the following λ-ω reaction-diffusion problem [47], [55]

$$\begin{aligned} u_t &= u_{xx} + \lambda(r)u - \omega(r), v \\ v_t &= v_{xx} + \omega(r)u + \lambda(r)v, \end{aligned} \tag{1}$$

where $u, v : [0, \infty) \times [0, T] \longrightarrow \mathbb{R}$, $r = \sqrt{u^2 + v^2}$, $\omega(0) > 0$, $\lambda(0) > 0$.

It is well known (compare [2], [37], [38], [56]–[61] and references therein) that such problem generate travelling waves as fundamental solutions [47], that can be parametrized as follows [47],

$$\begin{aligned} u(x,t) &= \widehat{r}\cos(\omega(\widehat{r})t \pm \sqrt{\lambda(\widehat{r})}x), \\ v(x,t) &= \widehat{r}\sin(\omega(\widehat{r})t \pm \sqrt{\lambda(\widehat{r})}x), \end{aligned} \tag{2}$$

where the unknown parameter $\widehat{r} \in \mathbb{R}$ is such that $\lambda(\widehat{r}) > 0$. Of course, although the presence of the unknown value of $\widehat{r}$ makes (2) incomputable, the expression (2) clarifies the nature of the solution, i.e. the periodic character in time and space with constant shape and speed: such an information can be profitably used to design an accurate and cheap numerical integrator adapted to the problem.

This goal can be achieved, as introduced in Section 1, by means of a special purpose numerical solver more tuned to follow the periodic behavior, in the spirit of the so-called *exponential fitting* technique (compare the review paper on the topic [52] and references therein and the classical monograph [49]; in the case of differential equations, we specifically refer to [30]–[32], [35], [40], [41], [44], [51], [63], [64] and references therein).

Due to the fact that (1) possess a one-parameter family of periodic wave solutions (2), thus oscillating both in space and in time, we propose trigonometrically fitted finite differences for the numerical approximation of the second order space derivative appearing in (1), derived as follows [28], [29].

A. A trigonometrically fitted finite difference

We consider a given function $u(x,t)$ defined on the rectangular domain

$$D = [x_0, X] \times [t_0, T] \subset \mathbb{R}^2.$$

The purpose is that of deriving a numerical approximation of the second derivative with respect to x by the three-point finite difference formula

$$\frac{\partial^2 u}{\partial x^2}(x,t) \approx \frac{1}{h^2}\left(a_0 u(x+h,t) + a_1 u(x,t) + a_2 u(x-h,t)\right), \tag{3}$$

where h is a given spatial stepsize. The unknown coefficients a_0, a_1 and a_2 are derived in correspondence of the fitting space

$$\mathcal{F} = \{1, \sin(\mu x), \cos(\mu x)\}, \tag{4}$$

with $\mu \in \mathbb{R}$. Hence, we associate to (3) the linear operator

$$\begin{aligned}\mathcal{L}[h, \mathbf{a}]u(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) - \frac{1}{h^2}\big(a_0 u(x+h,t) + a_1 u(x,t) \\ + a_2 u(x-h,t)\big)\end{aligned} \tag{5}$$

and impose its exactness on the functional set (4), leading to the linear system

$$\begin{cases} a_0 + a_1 + a_2 = 0, \\ -a_0 \sin(z) - a_2 \sin(-z) = 0, \\ -z^2 - a_0 \cos(z) - a_1 - a_2 \cos(-z) = 0, \end{cases} \tag{6}$$

with $z = \mu h$, whose solution is given by

$$\begin{aligned} a_0(z) &= -\frac{z^2}{2(\cos(z)-1)}, \quad a_1(z) = \frac{z^2}{\cos(z)-1}, \\ a_2(z) &= -\frac{z^2}{2(\cos(z)-1)}. \end{aligned} \tag{7}$$

The chosen fitting space (4), as it normally happens in function fitting techniques (compare [49], [52] and references therein), explicitly depend on the parameter μ which can be interpreted as the frequency of the oscillations occurring in the solution of (1). As a consequence, the corresponding numerical method will depend on variable coefficients: this is visible, for instance, in the expression of the coefficients (7) of (3). Numerical methods depending on variable-coefficients are effectively useful when a proper estimation of the unknown parameters is actually computable, as it has been clarified in many different situations in the literature (we refer to the review paper [52] and references therein). In our case, we have gained a particular benefit from the knowledge of a parametric representation of the periodic plane wave solutions (2), which clearly shows that sine and cosine are evaluated in $\sqrt{\lambda(\hat{r})}x$. This suggests us to employ as estimation of the parameter $z = \mu h$ in (7) at the mesh point (x_i, t_j) the value

$$z_{ij} = \sqrt{\lambda(r_{ij})}h,$$

where

$$r_{ij} = \sqrt{u_{ij}^2 + v_{ij}^2}.$$

with $u_{ij} \approx u(x_i, t_j)$, $v_{ij} \approx v(x_i, t_j)$. In this way, we have gained an approximation of the fitted parameters without applying optimization techniques or solving nonlinear systems of equations as in [30], [31], [41] and references therein. Thus, the overall computational cost is not compromised, in our case, by the computation of the parameter. This also confirms that, in designing adapted numerical solvers, it is particularly useful to acquire as much theoretical information on the problem as possible.

We observe that the coefficients (7), when z tends to 0, tend to the classical coefficients

$$a_0 = 1, \qquad a_1 = -2, \qquad a_2 = 1, \tag{8}$$

of the corresponding general purpose finite difference, which has second order of accuracy as well. Thus, the trigonometrical fitting adaptation of (3) preserves the order of accuracy of the corresponding general purpose version with coefficients given by (8).

B. Spatial discretization of the operator

We now apply the results developed in the previous sections to the original λ-ω system (1). More precisely, following [55], we are going to consider the system of PDEs (1) in the unbounded domain

$$D = [0, \infty) \times [0, T],$$

equipped by the following boundary conditions

$$\begin{aligned} \frac{\partial u}{\partial x}(0,t) = \frac{\partial v}{\partial x}(0,t) = 0, \\ \lim_{x \to +\infty} u(x,t) = \lim_{x \to +\infty} v(x,t) = 0, \end{aligned} \tag{9}$$

and the initial conditions

$$\begin{aligned} u(x,0) = f_0(x), \\ v(x,0) = g_0(x). \end{aligned} \tag{10}$$

This problem is now aimed to be treated by suitably applying the method of lines (compare [43], [53], [54] and references therein), i.e. through a semi-discretization of the problem along the spatial variable. The periodic nature of the solution, described in Section 1, suggests us to proceed by employing the trigonometrically fitted finite differences derived in Section 2. We now describe in details how the semi-discretized problem is derived.

In the practice, as also suggested in [55], we are going to solve the problem on a domain $[0, X] \times [0, T]$ where X is a large real number. In correspondence of this large value of X, we actually consider as boundary conditions in the right limit X

$$u(X,t) = v(X,t) = 0.$$

More precisely, X is chosen in such a way that further increase on it have negligible effects on the solution, making above zero boundary conditions realistic. In summary, we consider the following boundary conditions in $[0, X]$

$$\begin{aligned} \frac{\partial u}{\partial x}(0,t) = \frac{\partial v}{\partial x}(0,t) = 0, \\ u(X,t) = v(X,t) = 0. \end{aligned} \tag{11}$$

We next consider N equidistant points in the spatial interval $[0, X]$ and denote by h the distance between two consecutive

points. The semi-discretized domain, denoted by D_x, results to be

$$D_x = \left\{ (x_j, t) : x_j = jh,\ j = 0, \ldots, N-1,\ h = \frac{X}{N-1} \right\}.$$

We next denote by $u_j(t) = u(x_j, t)$, $0 \leq j \leq N-1$. As a consequence, the original problem (1) with boundary conditions (11) and initial conditions (10) is transformed in a system of $2N$ first order ordinary differential equations equipped of the initial conditions

$$u_j(0) = f_0(x_j), \quad v_j(0) = g_0(x_j), \quad 0 \leq j \leq N-1.$$

C. Numerical experiments

We now present some numerical results obtained by solving the system of PDEs (1) with $\lambda(r)$ and $\omega(r)$ of the form

$$\lambda(r) = \lambda_0 - r^p, \tag{12}$$

$$\omega(r) = \omega_0 - r^p, \tag{13}$$

with $\lambda_0, \omega_0, p \in \mathbb{R}^+$.

We employ the semi-discretization introduced in Section 3, with initial conditions (10) given by

$$u_j(0) = v_j(0) = A \exp(-\xi x_j), \quad 0 \leq j \leq N-1. \tag{14}$$

In the experiments, as in [55], we will always consider the following values of the above parameters

$$\lambda_0 = 1, \quad \omega_0 = 2, \quad p = 1.8, \quad A = 0.1, \quad \xi = 0.8. \tag{15}$$

We proceed in two different directions: indeed, we consider the spatially semi-discretized version of the problem, by approximating the spatial derivative both with the standard and the trigonometrically fitted finite differences; we next solve the obtained semi-discretized problem by employing a proper time solver.

Figures 1 shows the profile of the solutions originated by applying the trigonometrically fitted spatial semi-discretization with 3 points, i.e through finite differences (3) with coefficients (7), and solving in time with the `ode15s` Matlab routine. Analogously, the solutions of the semi-discretized problem by standard finite differences are depicted in Figure 2; also in this case, the `ode15s` time solver is applied. In both cases, we have considered the spatial variable in [0, 150], while the time integration interval is [0, 60], as in [55], [56]. The space interval is large enough in order to make realistic the use of the boundary conditions (11) instead of (9), as highlighted in [55]. We have involved 50 subinterval in the spatial semi-discretization: hence, the spatial stepsize is $h = 3$. As it is visible from Figure 1, the profile of the obtained solutions is coherent with the expected dynamics and, in particular, with that described in [55], [56]. Such a situation is not visible in Figure 2, since an unstable behavior is visible in the results. Thus, in the comparison between the employ a standard finite difference or a trigonometrically fitted one for the λ-ω problem (1), one can recognize a much more stable behavior of the latter, that is what typically happens in many situations when trigonometrically fitted methods are applied (and this is true in many different situations extensively described, for instance, in [49], [52]).

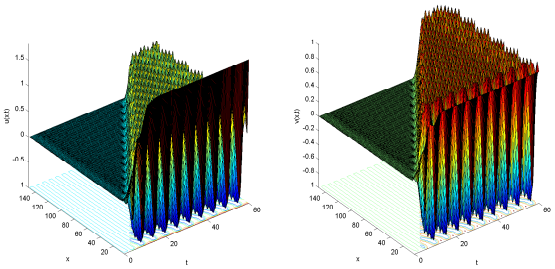

Fig. 1. Numerical solution of (1), with initial conditions (10), boundary conditions (11), with parameters given by (15). The left figure is the plot of $u(x,t)$, the one on the right is $v(x,t)$. The solution is computed by solving the semi-discretized problem obtained by the three-point trigonometrically fitted finite difference (3), with coefficients (7).

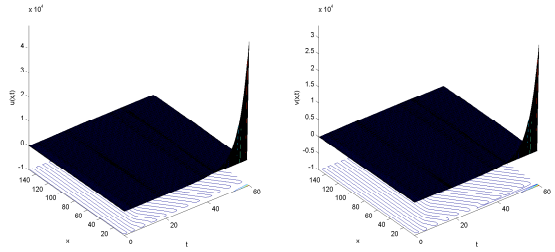

Fig. 2. Numerical solution of (1), with initial conditions (10), boundary conditions (11), with parameters given by (15). The left figure is the plot of $u(x,t)$, the one on the right is $v(x,t)$. The solution is computed by solving the semi-discretized problem obtained by the standard version of the finite difference (3).

III. Volterra integral equations with periodic solutions

We consider the Volterra integral equation

$$\begin{aligned} y(x) &= f(x) + \int_{-\infty}^{x} k(x-s)y(s)ds,\ x \in [0, x_{end}] \\ y(x) &= \psi(x), \qquad\qquad -\infty < x \leq 0, \end{aligned} \tag{16}$$

with $k \in L^1(I\!R^+)$, f continuous and T-periodic on $[0, x_{end}]$, ψ continuous and bounded on $I\!R^-$. Under suitable hypotheses, (16) has a unique T-periodic solution [5]. Some applications which yield to VIEs with periodic solution may be found in [10], [13]. Although an expression of the solution is known, it is of no practical use, since it has not closed form. Therefore a numerical approximation is necessary. As introduced in Section 1, standard numerical procedures are not efficient, especially for high frequency values, thus we propose a specially tuned direct quadrature (DQ) method based on exponential fitting (compare also [9], [12]–[14]).

Following the exponential fitting theory, we formulate a DQ method which is exact whenever the solution $y(x)$ belongs to the fitting space

$$\mathcal{B}_1 := \{1, x, \sin(\omega x), \cos(\omega x)\}, \tag{17}$$

and $k(x) = \exp(\alpha x)$, $\alpha, \omega \in \mathbb{R}$.

The DQ method we propose is based on the quadrature rule

Q, with

$$\int_{X-h}^{X+h} g(x)dx \approx Q[g](X) := h\sum_{k=0}^{1} a_k g(X+\xi_k h) \quad (18)$$

where $X > 0$ and $h > 0$. We impose that such rule is exact on the fitting space

$$\mathcal{B} := \{e^{\alpha x}, xe^{\alpha x}, e^{(\alpha \pm i\omega)x}\}, \quad (19)$$

coming to a nonlinear system of equations in the unknowns weights and nodes. This yields to $a_k = a_k(u,z)$, and $\xi_k = \xi_k(u,z)$, with $u =: \alpha h$, $z := \omega h$. Then it is an easy task to derive the composite quadrature rule based on the formula (18):

$$I[g](X) = \int_a^b g(x)dx \approx Q_m[g] := h\sum_{j=0}^{m-1}\sum_{k=0}^{1} \tilde{a}_k g(t_j + \tilde{\xi}_k h), \quad (20)$$

where $t_j = a + hj$, $j = 0, \ldots, m$, $h = (b-a)/m$, $\tilde{a}_k = a_k/2$, $\tilde{\xi}_k = (1+\xi_k)/2$. By following the exponential fitting theory and suitably adapting its techniques, it is possible to prove that the error $E_m[g] := |I[g] - Q_m[g]|$ of the formula (20) satisfies

$$E_m[g] \leq C(b-a)h^4, \quad (21)$$

whenever $g \in C^4([a,b])$. Here the constant $C > 0$ depends on $\max_{[a,b]} |(D-\alpha)^2((D-\alpha)^2 + \omega^2)g(x)|$, where D stands for the derivative operator..

Given a uniform mesh on $[0, x_{end}]$, $I_h := \{x_n = nh, n = 0, \ldots, N\}$, with $h = x_{end}/N$, the DQ method based on the exponentially fitted formula (20) reads

$$y(x_n) \approx f(x_n) + (I\psi)(x_n) + h\sum_{j=0}^{n-1}\sum_{i=1}^{2} \tilde{a}_i k(x_{n-j} - \tilde{\xi}_i h) y(x_j + \tilde{\xi}_i h), \quad (22)$$

$n = 1, ..., N$, where

$$(I\psi)(x_n) = \int_{-\infty}^{0} k(x_n - s)\psi(s)ds,$$

or is a suitable approximation of such integral, as it will be clarified later. To obtain a fully discretization of (16), an approximation of $y(x_j + \tilde{\xi}_i h)$ is needed. Therefore, similarly to [11], we introduce an approximation by interpolation function $\mathcal{P}$, on the points

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

Two choices are available: the first one is the Lagrange polynomial interpolation, easy but unnatural since we are assuming that the solution is a periodic function. The second one is a mixed-trigonometric interpolation, which is exact on the fitting space (17) by design. In both cases the interpolating function $\mathcal{P}$ can be written as follows

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

where $p_l(s)$ do not depend on x_j but only on r_-, r_+. In particular, in the case of polynomial interpolation $p_l(s)$ are the fundamental Lagrange polynomials. In the case of mixed-trigonometric interpolation, if $r_- + r_+ = 3$, it results $p_l(s) = b_{l+r_-}(s)$, where $b_l(s)$ are the solution of the linear system

$$\begin{cases} b_0(s) + b_1(s) + b_2(s) + b_3(s) = 1, \\ b_1(s) + 2b_2(s) + 3b3_(s) = s + r, \\ b_0(s) + \cos(z)b_1(s) + \cos(2z)b_2(s) + \cos(3z)b_3(s) = \\ \qquad\qquad \cos(z(s+r)), \\ \sin(z)b_1(s) + \sin(2z)b_2(s) + \sin(3z)b_3(s) = \sin(z(s+r)) \end{cases} \quad (23)$$

Therefore $b_l(s)$ are oscillatory functions depending on z.

Once we have approximated the values of the solution $y(x_j + \tilde{\xi}_i h)$ in (22) by the interpolation technique, the fully-discrete method is the following

$$y_n = f(x_n) + (I\psi)(x_n) + h\sum_{j=0}^{n-1}\sum_{i=1}^{2} \tilde{a}_i k(x_{n-j} - \tilde{\xi}_i h) \sum_{l=-r_-}^{r_+} p_l(\tilde{\xi}_i h) y_{j+l}, \quad (24)$$

$n = 1, ..., N$. We set $r_+ \leq 1$ to avoid the use of values of the solution in future mesh points. The method (24) is explicit for $r_+ = 0$, and implicit for $r_+ = 1$.

The error of the DQ method (24) depend on the interpolation error and on the error of the quadrature rule (20). In particular, the following theorem analyzes the error and the convergence of the DQ method

Theorem 3.1: Assume that VIE (16) has a unique periodic solution $y(x) \in C^5([0, x_{end}])$. Let apply the exponentially fitted DQ method (24), where the functions $p_l(s)$ are the Lagrange fundamental polynomials with $r := r_+ + r \geq 3$, or $p_l(s) = b_{l+r_-}(s)$, where $b_l(s)$ are solution of the system (23). Then, if $(I\psi)(x)$ is discretized by $(\bar{I}\psi)(x)$, with $|(I\psi)(x) - (\bar{I}\psi)(x)| \leq C_\psi h^4$, $x \in [0, x_{end}]$, it results

$$\max_{1\leq n\leq N} |y(x_n)y_n| \leq Ch^4, \quad \text{as } h \to 0.$$

We underline that the proposed method has the same order of a DQ method based on standard 2-nodes Gauss quadrature rule. The advantage of the exponentially fitted DQ method with mixed-trigonometric interpolation, is that the error is smaller when periodic problems are treated and the gain is more relevant for high frequency values.

IV. Numerical integration of high oscillating functions

In this section we consider the numerical computation of integrals of oscillatory functions over unbounded intervals

$$I = \int_0^\infty e^{-x} f(x)dx, \quad (25)$$

where the integrand $f(x)$ is of the form

$$f(x) = f_1(x)\sin(\omega x) + f_2(x)\cos(\omega x). \quad (26)$$

The coefficients $f_1(x)$ and $f_2(x)$ are assumed smooth enough to be well approximated by polynomials. The accurate computation of integrals of the form (25) is needed in various applications, see e.g. [4], [36], [39], [42].

As in the previous sections we make use of the exponential

fitting strategy in order to derive quadrature formulae of the form

$$I \simeq I_N = \sum_{k=1}^{N} w_k f(x_k), \tag{27}$$

where the unknown weights w_k and nodes x_k depend on the frequency ω, and are derived in correspondence of the fitting space

$$\mathcal{F} = \{x^{n-1}e^{\pm\mu x},\ n = 1, 2, ..., N, \}, \tag{28}$$

as described in [17], [21], [22] for unbounded integration interval, and [45] for bounded integration interval. Hence we associate to the quadrature formula (27) 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 (28). We then obtain the nonlinear system

$$\sum_{k=1}^{N} w_k x_k^{n-1} \frac{\eta_{\lfloor \frac{n-2}{2} \rfloor}(x_k^2 Z)}{\eta_{\lfloor \frac{n-2}{2} \rfloor}(0)} = M_{n-1}(Z), \quad n = 1, \ldots, 2N, \tag{29}$$

where

$$M_n(Z) = \frac{n!}{(1-Z)^{\lceil \frac{n+1}{2} \rceil}} \tag{30}$$

with $Z = \mu^2 = -\omega^2$ and the set of functions $\eta_m(Z)$, $m = -1, 0, 1, 2, ...$ are defined as follows (see for instance [16], [49]).

$$\eta_{-1}(Z) = \begin{cases} \cos(|Z|^{1/2}) & \text{if } Z \leq 0 \\ \\ \cosh(Z^{1/2}) & \text{if } Z > 0 \end{cases}, \tag{31}$$

$$\eta_0(Z) = \begin{cases} \sin(|Z|^{1/2})/|Z|^{1/2} & \text{if } Z < 0 \\ 1 & \text{if } Z = 0 \\ \sinh(Z^{1/2})/Z^{1/2} & \text{if } Z > 0 \end{cases} \tag{32}$$

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

$$\eta_m(Z) = \frac{1}{Z}[\eta_{m-2}(Z) - (2m-1)\eta_{m-1}(Z)], \quad m \geq 1 \tag{33}$$

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

$$\eta_m(0) = \frac{1}{(2m+1)!!}, \quad m \geq 1. \tag{34}$$

Then the Exponentially Fitted (EF) Gauss-Laguerre quadrature formula is of the form (27), with weights and nodes determined as solutions of the nonlinear system (29). 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

$$|I - I_N| = O(\omega^{-N-1}), \quad \omega \to \infty. \tag{35}$$

Then the EF Gauss-Laguerre quadrature rules have the same optimal asymptotic order of steepest descent methods in [50] and complex Gaussian quadrature rules in [1], also maintaining a good accuracy for small values of ω, as they naturally tend to the corresponding classical Gauss-Laguerre formulae for $\omega \to 0$. As proved in [17] the nonlinear system (29) can be solved by splitting it into the following linear system for the weights $w = (w_1, \ldots, w_N)^T$

$$A(Z, x)w = b(Z), \tag{36}$$

and the following nonlinear system for the nodes $x = (x_1, \ldots, x_N)^T$

$$F(Z, w, x) = D(Z, x)w - d(Z) = 0, \tag{37}$$

where

$$A_{ij}(Z, x) = \begin{cases} x_j^{2(i+r-1)} \eta_{i+r-2}(x_j^2 Z), & i = 1, \ldots, s, \\ x_j^{2i-1} \eta_{i-1}(x_j^2 Z), & i = s+1, \ldots, N, \end{cases}$$

for $j = 1, \ldots, N$,

$$b_i(Z) = \begin{cases} \dfrac{2^{i+r-1}(i+r-1)!}{(1-Z)^{i+r}}, & i = 1, \ldots, s, \\ \\ \dfrac{2^{i-1}(i-1)!}{(1-Z)^{i}}, & i = s+1, \ldots, N, \end{cases},$$

$$D_{ik}(Z, x) = \begin{cases} x_k^{2i-2} \eta_{i-2}(x_k^2 Z), & i = 1, \ldots, r, \\ x_k^{2(i-r)-1} \eta_{i-r-1}(x_k^2 Z), & i = r+1, \ldots, N, \end{cases}$$

for $k = 1, \ldots, N$, and

$$d_i(Z) = \begin{cases} \dfrac{2^{i-1}(i-1)!}{(1-Z)^{i}}, & i = 1, \ldots, r, \\ \\ \dfrac{2^{i-r-1}(i-r-1)!}{(1-Z)^{i-r}}, & i = r+1, \ldots, N. \end{cases}$$

Also the Jacobian matrix of the Newton iterative method applied to the nonlinear system (37) has been computed in [17] by using the differentiation properties of the $\eta_m(Z)$ functions [16], [49]. The systems (36) and (37) 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, as discussed in [17], [22]. As a matter of fact in the paper [17], 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. In order to overcome this problem Modified EF (MEF) Gauss-Laguerre formulae have been proposed in [21], 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

$$I \simeq I_N = \sum_{i=1}^{N} (a_i f_1(x_i) + b_i f_2(x_i)) \tag{38}$$

where the functions f_1 and f_2 are given in (26). The frequency dependent nodes $x_i = x_i(\omega)$, $i = 1, ..., N$, are defined as the smallest N positive solutions of the nonlinear equation

$$f_N(x, \omega) = 0, \tag{39}$$

where

$$f_N(x, \omega) = \sum_{n=0}^{N} C_n^N(Z) x^n \frac{\eta_{\lfloor \frac{n-1}{2} \rfloor}(x^2 Z)}{\eta_{\lfloor \frac{n-1}{2} \rfloor}(0)}, \quad Z = -\omega^2, \tag{40}$$

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

$$\sum_{j=0}^{N-1} M_{i+j}(Z) C_j^N(Z) = -M_{N+i}(Z), \tag{41}$$

for $i = 0, ..., N-1$, with the moments $M_n(Z)$ defined in (30). 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 (39) has been analyzed in [21], 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 (35).

In order to show the effectiveness of the proposed exponentially fitted formulae, we report in Figure 3 the results obtained by classical, EF and MEF Gauss-Laguerre quadrature rules on the problem

$$\int_0^\infty e^{-x} \cos[(\omega + 1)x] dx = \frac{1}{1 + (1 + \omega)^2}. \tag{42}$$

The integrand $f(x) = \cos[(\omega + 1)x]$ is of form (26) 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 3 the error obtained on problem (42) 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.

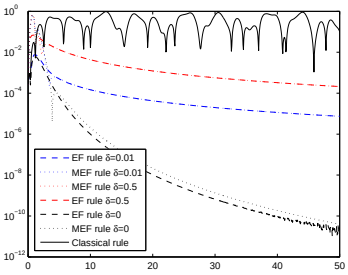

Fig. 3. The $\bar{\omega}$ dependence of the errors on problem (42) with $N = 6$ and $\omega = (1 + \delta)\bar{\omega}$.

V. Conclusion

We have presented a selection of adapted numerical methods for evolutionary problems, by means of the employ of non-polynomially based finite difference methods or quadrature rules resulting to be more efficient than the standard ones based on polynomials.

As regards PDEs, we have considered adapted finite difference schemes based on trigonometrical fitting for λ-ω problems exhibiting a periodic wavefront with constant speed in time and space. The resulting scheme results to be more stable than the classical one based on polynomially fitted finite differences.

For VIEs with periodic solution, we illustrated an exponentially fitted DQ method, whose error is smaller than standard methods when periodic problems are treated. Future developments may concern a further investigation on the collocation method introduced in [5], possibly improved by multistep technique, as done for example in [6]–[8], [15], [18]–[20], [23]–[27].

We moreover described the construction of EF and MEF Gauss-Laguerre quadrature rules for the numerical computation of integrals of high oscillating functions over unbounded domains, providing a massive improvement in accuracy with respect to classical Gauss-Laguere formulae when the frequency of oscillation increases. The MEF quadrature rules can be computed for bigger values of N and ω with respect to the EF ones, and their construction is also less expensive. This approach can be extended also to the case of integral over a bounded interval, and then be used to improve the presented methods for Volterra integral equations.

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References

[1] A. Asheim, D. Huybrechs, *Gaussian quadrature for oscillatory integral transforms*, IMA J. Numer. Anal, 2013.

[2] A. Atri, J. Amundson, D. Clapham, J. Sneyd, *A Single-Pool Model for Intracellular Calcium Oscillations and Waves in Xenopus Iaevis Oocyte*, Biophys. Journal 65, 1727–1739 (1993).

[3] M.J. Berridge, *Calcium oscillations*, J. Biol. Chem. 265, 9583–9586 (1990).

[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] H. Brunner, A. Makroglou, and R. K. Miller, *On mixed collocation methods for Volterra integral equations with periodic solution*, Appl. Numer. Math. **24** (1997), no. 2-3, 115–130, Volterra centennial (Tempe, AZ, 1996).

[6] G. Capobianco, D.Conte, B. Paternoster, *Construction and implementation of two-step continuous methods for Volterra Integral Equations*, submitted.

[7] A. Cardone, D. Conte, *Multistep collocation methods for Volterra integro-differential equations*, Appl. Math. Comput. **221** (2013), 770-785.

[8] A. Cardone, D. Conte, B. Paternoster, *A family of Multistep Collocation Methods for Volterra Integro-Differential Equations*, AIP Conf. Proc. 1168(1), 358-361 (2009).

[9] A. CARDONE, R. D'AMBROSIO, B. PATERNOSTER, *High order exponentially fitted methods for Volterra integral equations with periodic solution*, submitted.

[10] A. CARDONE, I. DEL PRETE, H. BRUNNER, *Asymptotic periodicity of nonlinear discrete Volterra equations and applications*, J. Difference Equ. Appl. **18**(9) 1531-1543 (2012).

[11] A. CARDONE, I. DEL PRETE, C. NITSCH, *Gaussian Direct Quadrature methods for double delay Volterra integral equations*, Electron. Trans. Numer. Anal. 35, 201-216 (2009).

[12] A. CARDONE, L. GR. IXARU, AND B. PATERNOSTER, *Exponential fitting direct quadrature methods for Volterra integral equations*, Numer. Algorithms **55** (2010), no. 4, 467–480.

[13] A. CARDONE, L. GR. IXARU, B. PATERNOSTER, AND G. SANTOMAURO, *Ef-Gaussian direct quadrature methods for Volterra integral equations with periodic solution*, Math. Comput. Simulation **110** (2015), 125–143.

[14] A. CARDONE, B. PATERNOSTER, AND G. SANTOMAURO, *Exponential fitting quadrature rule for functional equations*, AIP Conf. Proc. **1479** (2012), no. 1, 1169–1172.

[15] Conte, D., D'Ambrosio, R., and Paternoster, B., *Two–step diagonally–implicit collocation based methods for Volterra Integral Equations*, Appl. Numer. Math. 62, 1312–1324 (2012).

[16] 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.

[17] 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.

[18] Conte, D., Jackiewicz, Z., and Paternoster, B., *Two-step almost collocation methods for Volterra integral equations*, Appl.Math. Comput. 204, 839–853 (2008).

[19] Conte, D. and Paternoster, B., *Multistep collocation methods for Volterra Integral Equations*, Appl. Numer. Math. 59, 1721–1736 (2009).

[20] D. Conte, B. Paternoster, *A Family of Multistep Collocation Methods for Volterra Integral Equations*, in: AIP Conference Proceedings, Numerical Analysis and Applied Mathematics, T.E.Simos, G. Psihoyios, Ch. Tsitouras (Eds.) 936, 128–131, Springer (2007).

[21] D. Conte, B. Paternoster, *Modified Gauss-Laguerre exponential fitting based formulae*, J. Sci. Comput., doi:10.1007/s10915-016-0190-0, in press.

[22] D. Conte, B. Paternoster, G. Santomauro, *An exponentially fitted quadrature rule over unbounded intervals*, AIP Conf. Proc. 1479, 1173–1176 Springer, 2012.

[23] R. D'Ambrosio, M. Ferro, B. Paternoster, Collocation-Based Two-Step Runge-Kutta Methods for Ordinary Differential Equations, Lecture Notes in Comput. Sci. 5073, 736–751(2008).

[24] R. D'Ambrosio, M. Ferro, Z. Jackiewicz, B. Paternoster, Two-step almost collocation methods for ordinary differential equations, Numer. Algor. 53(2-3), 195–217 (2010).

[25] R. D'Ambrosio, Z. Jackiewicz, Continuous two-step Runge-Kutta methods for ordinary differential equations, Numer. Algor. 54(2), 169–193 (2010).

[26] R. D'Ambrosio, Z. Jackiewicz, Construction and implementation of highly stable two-step continuous methods for stiff differential systems, Math. Comput. Simul. 81(9), 1707–1728 (2011).

[27] R. D'Ambrosio, B. Paternoster, Two-step modified collocation methods with structured coefficients matrix for Ordinary Differential Equations, Appl. Numer. Math. 62(10), 1325–1334 (2012).

[28] R. D'AMBROSIO, B. PATERNOSTER, *Numerical solution of a diffusion problem by exponentially fitted finite difference methods*, SpringerPlus 3:425, doi:10.1186/2193-1801-3-425 (2014).

[29] R. D'AMBROSIO, B. PATERNOSTER, *Numerical solution of reaction-diffusion systems of lambda-omega type by trigonometrically fitted methods*, J. Comput. Appl. Math. 294, 436–445 (2016).

[30] R. D'AMBROSIO, E. ESPOSITO, B. PATERNOSTER, *Parameter estimation in two-step hybrid methods for second order ordinary differential equations*, J. Math. Chem. 50 (1), 155–168 (2012).

[31] R. D'AMBROSIO, E. ESPOSITO, B. PATERNOSTER, *Exponentially fitted two-step Runge-Kutta methods: Construction and parameter selection*, Appl. Math. Comp. 218 (14), 7468–7480 (2012).

[32] R. D'AMBROSIO, M. FERRO, B. PATERNOSTER, *Trigonometrically fitted two-step hybrid methods for special second order ordinary differential equations*, Math. Comput. Simul. 81, 1068–1084 (2011).

[33] G.B. ERMENTROUT, *Small amplitude stable wavetrains in reaction-diffusion systems*, Lecture Notes Pure Appl. Math. 54, 217–228 (1980).

[34] J.E. FERRELL, T.Y. TSAI, Q. YANG, *Modeling the cell cycle: why do certain circuits oscillate?*, Cell. 144(6), 874–885 (2011).

[35] J.M. FRANCO, I. GOMEZ, *Trigonometrically fitted nonlinear two-step methods for solving second order oscillatory IVPs*, Appl. Math. Comp. 232, 643–657 (2014) .

[36] 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.

[37] M.R. GARVIE, J.F. BLOWEY, *A reaction-diffusion system of λ-ω type. Part II: Numerical analysis*, Euro. J. Appl. Math. 16, 621–646 (2005).

[38] J.M. GREENBERG, *Spiral waves for λ-ω systems*, Adv. Appl. Math. 2, 450–455 (1981).

[39] S. M. Hasheminejad and M. Aghabeigi, *Liquid sloshing in half-full horizontal elliptical tanks*,J. of Sound and Vibration 324, 332–349, 2009.

[40] D. HOLLEVOET, M. VAN DAELE, *Exponentially-fitted methods and their stability functions*, J. Comput. Appl. Math. 236(16), 4006–4015 (2012).

[41] D. HOLLEVOET, M. VAN DAELE, G. VANDEN BERGHE, *Exponentially-fitted methods applied to fourth order boundary value problems*, J. Comput. Appl. Math. 235(18), 5380–5393 (2011).

[42] D. Huybrechs, S. Vandewalle, *A sparse discretization for integral equation formulations of high frequency scattering problems*, SIAM J. Sci. Comput. 29, 2305–2328, 2007.

[43] E. ISAACSON, H.B.KELLER, *Analysis of Numerical Methods*, Dover Publications, New York (1994).

[44] L.GR. IXARU, *Runge-Kutta method with equation dependent coefficients*, Comput. Phys. Commun. 183(1), 63–69 (2012).

[45] L. Gr. Ixaru, B. Paternoster, *A Gauss quadrature rule for oscillatory integrands*, Comput. Phys. Commun. 133, 177–188, 2001.

[46] S. KOGA, *Rotating spiral waves in reaction-diffusion systems. Phase singularities of multiarmed waves*, Prog. Theor. Phys. 67, 164–178 (1982).

[47] N. KOPELL, L.N. HOWARD, *Plane wave solutions to reaction-diffusion equations*, Stud. Appl. Math. 52, 291–328 (1973).

[48] A.W. MURRAY, M.W. KIRSCHNER, *Dominoes and clocks: the union of two views of the cell cycle*, Science 246, 614?621 (1989).

[49] L. GR. IXARU, G. VANDEN BERGHE, *Exponential Fitting*, Kluwer, Boston-Dordrecht-London (2004).

[50] H. Majidian, Numerical approximation of highly oscillatory integrals on semi-finite intervals by steepest descent method, Numer. Algor. 63 (3), 537–548, 2013.

[51] A. PARIS, L. RANDEZ, *New embedded explicit pairs of exponentially fitted Runge-Kutta methods*, J. Comput. Appl. Math. 234(3), 767–776 (2010).

[52] 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).

[53] W.E. SCHIESSER, *The Numerical Method of Lines: Integration of Partial Differential Equations*, Academic Press, San Diego (1991).

[54] W.E. SCHIESSER, G.W. GRIFFITHS, *A Compendium of Partial Differential Equation Models: Method of Lines Analysis with Matlab*, Cambridge University Press (2009).

[55] J.A. SHERRATT, *On the evolution of periodic plane waves in reaction-diffusion systems of λ-ω type*, SIAM J. Appl. Math. 54(5), 1374–1385 (1994).

[56] J.A. SHERRATT, *Periodic waves in reaction-diffusion models of oscillatory biological systems*, FORMA 11, 61–80 (1996).

[57] M.J. SMITH, J.D.M. RADEMACHER, J.A. SHERRATT, *Absolute stability of wavetrains can explain spatiotemporal dynamics in reaction–diffusion systems of lambda-omega type*, SIAM J. Appl. Dyn. Systems 8, 1136–1159 (2009).

[58] J.A. Sherratt, M.J. Smith, Transition to spatiotemporal chaos via stationary branching shocks and holes, Physica D: Nonlinear Phenomena 241(15), 1671–1679 (2012).

[59] J.A. Sherratt, M.J. Smith, Periodic travelling waves in cyclic populations: field studies and reaction?diffusion models, J. Roy. Soc. Interface 5, 483–505 (2008).

[60] M.J. Smith, J.A. Sherratt, X. Lambin, The effects of density-dependent dispersal on the spatiotemporal dynamics of cyclic populations, J. Theor. Biol. 254(2), 264–274 (2008).

[61] M.J. Smith, J.A. Sherratt, The effects of unequal diffusion coefficients on periodic travelling waves in oscillatory reaction-diffusion systems, Physica D: Nonlinear Phenomena 236(2), 90–103 (2007).

[62] L. N. TREFETHEN, *Finite Difference and Spectral Methods for Ordinary and Partial Differential Equations*, unpublished text, available at http://people.maths.ox.ac.uk/trefethen/pdetext.html (1996).

[63] G. VANDEN BERGHE, M. VAN DAELE, H. VANDE VYVER, *Exponentially fitted Runge-Kutta methods of collocation type: fixed or variable knot points?*, J. Comput. Appl. Math 159, 217–239 (2003).

[64] G. VANDEN BERGHE, L.GR. IXARU, H. DE MEYER, *Frequency determination and step-length control for exponentially-fitted Runge-Kutta methods*, J. Comput. Appl. Math. 132(1), 95–105 (2001).

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