Numerical solution of reaction-diffusion systems of λ-ω type by trigonometrically fitted methods

Raffaele D'Ambrosio, Beatrice Paternoster

Department of Mathematics, University of Salerno, Fisciano (Sa), Italy
e-mail: {rdambrosio, beapat}@unisa.it

Abstract

The numerical solution of reaction-diffusion equations of λ-ω type, which are known to possess a one-parameter family of periodic plane wave solutions, is object of this paper. Due to the periodic character of such solutions, a special purpose numerical integration is here proposed, based on adapted finite differences. The adaptation occurs at the level of the problem, by a suitable spatial semi-discretization based on trigonometrically fitted finite differences. Numerical experiments confirming the effectiveness of the approach are given.

Key words: Reaction-diffusion equations, λ-ω systems, periodic plane wave solutions, exponential fitting, special purpose numerical methods.

1. Introduction

The paper is concerned with the numerical solution of systems of partial differential equations (PDEs), represented in terms of two coupled reaction-diffusion equations of the form

$$\begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix}_t = \begin{bmatrix} D_u & 0 \\ 0 & D_v \end{bmatrix} \begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix}_{xx} + \begin{bmatrix} f_u(u,v) \\ f_v(u,v) \end{bmatrix}, \tag{1.1}$$

with $D_u > 0$ and $D_v > 0$, typically modeling the interactions of two biological species whose concentrations are denoted by $u(x,t)$ and $v(x,t)$. It is known (for instance, refer to [23]) that traveling waves are fundamental solutions of (1.1), of type

$$u(x,t) = U(z), \quad v(x,t) = V(z),$$

where $z = x - at$ denotes the traveling wave coordinate, being a the wave speed.

Many systems of interest in life sciences have been successfully modelled by reaction-diffusion equations, especially for those problems typically exhibiting the generation of periodic waves along their dynamics. For instance, cell cycles are frequently clock-like [8, 17], behaving if they are driven by an autonomous biochemical oscillator.

Among coupled reaction-diffusion equations (1.1), a remarkable interest to λ-ω type equations is visible in the existing literature (for instance, refer to [7, 10, 11, 15,

16, 23, 24] and references therein). λ-ω reaction-diffusion equations are PDEs of the form

$$\begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix}_t = \begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix}_{xx} + \begin{bmatrix} \lambda(r) & -\omega(r) \\ \omega(r) & \lambda(r) \end{bmatrix} \begin{bmatrix} u(x,t) \\ v(x,t) \end{bmatrix}, \tag{1.2}$$

being $r = (u^2 + v^2)^{1/2}$, with $\lambda(0) > 0$ and $\omega(0) > 0$. It is known (refer to [23]) that any isolated zero of $\lambda(\cdot)$ correspond to a limit cycle in the reaction kinetics: this peculiar property has made λ-ω systems a prototype model for reaction-diffusion systems whose kinetics have a limit cycle [23].

A first attempt in analyzing and representing the solution of (1.2) has been given in [16], where the authors proved that the system (1.2) has a one-parameter family of periodic plane waves solutions (thus having constant shape and speed and oscillating both in space and in time), given by

$$\begin{aligned} u(x,t) &= \hat{r}\cos\left(\omega(\hat{r})t \pm \sqrt{\lambda(\hat{r})}x\right), \\ v(x,t) &= \hat{r}\sin\left(\omega(\hat{r})t \pm \sqrt{\lambda(\hat{r})}x\right), \end{aligned} \tag{1.3}$$

for any value of the parameter $\hat{r} \in \mathbb{R}$ satisfying $\lambda(\hat{r}) > 0$. This representation of the plane waves is clearly useless for practical purposes (it depends on the unknown parameter $\hat{r}$), but it will be important hereinafter to assess suitable numerical schemes, see Remark 2.1.

Indeed, the periodic character of the problem suggests to propose a numerical solution of (1.2) which takes into account this qualitative behavior, i.e. 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 (EF, refer to the recent review paper on the topic [20] and references therein and the classical monograph [18]; in the case of differential equations, we specifically refer to [4, 5, 6, 9, 12, 13, 19, 26] and references therein).

The existing literature on EF-based methods has provided a certain number of adaptations of classical numerical methods to better numerically follow known qualitative behaviors (e.g. periodicity, oscillations, exponential decay of the solution). This problem-oriented approach differs from the classical one, given by the employ of *general purpose* methods, which would require a very small stepsize to accurately follow the prescribed dynamics, if compared to problem-based methods, with a subsequent deterioration of the numerical performances, especially in terms of efficiency. For this reason, many classical numerical methods have been adapted in order to more efficiently approach problems with oscillatory solutions (see [20] and references therein).

A special purpose numerical method for the solution of functional equations exactly integrates (within round-off error) problems whose solution lies in a finite dimensional linear space (the so-called *fitting space*) spanned by a set of functions other than polynomials, properly chosen according to the behavior of the solution [18, 20]. The main difference between general and special purpose numerical methods is that the former are characterized by constant coefficients, while the latter depend on variable coefficients, which are functions of the parameters characterizing the solution (e.g. the frequency of the oscillations in case of problems with oscillatory solutions or the rate of decay in case of problems with exponentially decaying solutions).

In this direction, two main problems arise:

(*i*) choosing a fitting space which is as much as possible suitable to represent the solution of the problem;

(*ii*) accurately computing/estimating the parameters on which the numerical method depends.

In the case of λ-ω systems, both problems (*i*) and (*ii*) can be treated by taking into account the existing theoretical studies on the problem, i.e. the possible representation of the periodic plane wave solutions of (1.2), given by (1.3).

The spirit of this paper is that of solving λ-ω reaction-diffusion systems (1.2), by means of special purpose numerical methods based on exponential fitting. To the best of our knowledge, this represents one of the first attempts to apply this technique to partial differential equations, together with [3]. More specifically, we aim to employ finite difference schemes adapted to the qualitative behavior of the problem and, after a spatial semi-discretization based on such formulae, to solve the corresponding system of ordinary differential equations by means of a proper time integrator.

The paper is organized as follows: Section 2 is devoted to the construction and the analysis of adapted finite differences for the approximation of the spatial second derivative appearing in (1.2); the corresponding spatial semi-discretization is introduced in Section 3; the numerical evidence is then described in Section 4. Some conclusions are given in Section 5.

2. Special purpose second order finite differences

As above discussed, we aim to provide a spatial semi-discretization of the system of PDEs (1.2) by means of finite differences adapted to the problem. In particular, due to the fact that (1.2) possess a one-parameter family of periodic wave solutions (1.3), 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 (1.2). We propose here two versions of adapted finite differences, involving three and five consecutive points in the space discretization.

2.1. A three-point trigonometrically fitted finite difference

We review in this subsection part of the results derived in [3] for 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

$$\frac{\partial^2 u}{\partial x^2}(x,t) \approx \frac{1}{h^2}\left(a_0 u(x+h,t) + a_1 u(x,t) + a_2 u(x-h,t)\right), \tag{2.4}$$

of nearest neighbors type (i.e. employing, for any given x, the adjacent meshpoints $x-h$ and $x+h$), where h is a given spatial stepsize.

For our particular purposes, i.e. provide a special purpose spatial semi-discretization of (1.2), we need a trigonometrically fitted version of formula (2.4). Thus, we consider the following fitting space

$$\mathcal{F} = \{1, \sin(\mu x), \cos(\mu x)\}, \tag{2.5}$$

with frequency $\mu \in \mathbb{R}$, whose meaning is clarified in Remark 2.1, and associate to (2.4) the linear operator

$$\mathcal{L}[h, \mathbf{a}]u(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) - \frac{1}{h^2}(a_0 u(x+h,t) + a_1 u(x,t) + a_2 u(x-h,t)). \tag{2.6}$$

The unknown values of a_0, a_1 and a_2 are computed by imposing the exactness of (2.4) on the functional set (2.5) or, equivalently, by annihilating the operator (2.6) on every element of (2.5). This leads to the linear system

$$\begin{cases} a_0 + a_1 + a_2 = 0, \\ a_0 - a_2 = 0, \\ (a_0 + a_2)\cos(z) + a_1 = -z^2, \end{cases} \tag{2.7}$$

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

$$a_0(z) = -\frac{z^2}{2(\cos(z)-1)}, \quad a_1(z) = \frac{z^2}{\cos(z)-1}, \quad a_2(z) = -\frac{z^2}{2(\cos(z)-1)}. \tag{2.8}$$

As usual for trigonometrically fitted formulae, the coefficients are functions of the parameter z which is determined a posteriori (refer to Remark 2.1): this is the main difference with general purpose formulae, which depends on constant coefficients, while special purpose ones are characterized by non-constant coefficients. In general, the value of z is realistically non-zero, since neither the stepsize or the frequency (at least in presence of oscillations or periodicities, which is our case) are equal to zero. This fact has a benefit on the solvability of the system (2.7), whose determinant of the coefficient matrix is given by

$$2(1 - \cos z), \tag{2.9}$$

which annihilates also in $z = 0$. We will also take care in the implementations to avoid values of h such that the corresponding z makes (2.9) equal to zero.

For the derived trigonometrically fitted finite difference, the following accuracy result holds [3].

Theorem 2.1. *Suppose that $u \in C^4(\Omega)$, where $\Omega = [x-h, x+h] \times [0, T]$, being $h > 0$. Then, the trigonometrically fitted finite difference formula* (2.4)*, whose coefficients are given by* (2.8)*, has second order of accuracy.*

We observe that the coefficients (2.8), when z tends to 0, tend to the classical coefficients

$$a_0 = 1, \qquad a_1 = -2, \qquad a_2 = 1, \tag{2.10}$$

of the corresponding general purpose finite difference, which has second order of accuracy as well. Thus, the trigonometrical fitting adaptation of (2.4) preserves the order of accuracy of the corresponding general purpose version with coefficients given by (2.10).

2.2. A five-point trigonometrically fitted finite difference

We now introduce a new trigonometrically fitted finite difference of order 4 for the numerical approximation of the second order spatial derivative in (1.2). Also in this case we aim to provide a nearest neighbors finite difference formula and, in order to gain higher order of accuracy than the three-point case, we involve five consecutive meshpoints. Thus, the formula we consider has the following form

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2}(x,t) \approx \frac{1}{h^2}(a_0 u(x+2h,t) + a_1 u(x+h,t) + a_2 u(x,t) \\ + a_3 u(x-h,t) + a_4 u(x-2h,t)),\end{aligned} \tag{2.11}$$

where h is a given increment of the x variable. We derive a trigonometrically fitted version of (2.11) in correspondence of the fitting space

$$\mathcal{F} = \{1, \sin(\mu x), \cos(\mu x), x\sin(\mu x), x\cos(\mu x)\}. \tag{2.12}$$

We associate to (2.11) the following linear operator

$$\begin{aligned}\mathcal{L}[h,\mathbf{a}]u(x,t) = \frac{\partial^2 u}{\partial x^2}(x,t) - \frac{1}{h^2}(a_0 u(x+2h,t) + a_1 u(x+h,t) \\ + a_2 u(x,t) + a_3 u(x-h,t) + a_4 u(x-2h,t)),\end{aligned} \tag{2.13}$$

and, in order to derive the unknown coefficients a_0, a_1, a_2, a_3 and a_4, we annihilate it on the chosen space (2.12), i.e.

$$\begin{aligned}\mathcal{L}[h,\mathbf{a}]1 &= 0,\\ \mathcal{L}[h,\mathbf{a}]x^i \sin(\mu x)\Big|_{x=0} &= 0, \quad i = 0,1,\\ \mathcal{L}[h,\mathbf{a}]x^i \cos(\mu x)\Big|_{x=0} &= 0, \quad i = 0,1.\end{aligned}$$

We observe that each evaluation is always referred to the point $(x,t) = (0,0)$, due to the invariance in translation of linear operators, as discussed in [18]. This leads to

$$\begin{aligned}a_0 &= -\frac{z\csc\left(\frac{z}{2}\right)^5 \sec\left(\frac{z}{2}\right)(2-2\cos(z)-z\sin(z))}{32},\\ a_1 &= \frac{z\csc\left(\frac{z}{2}\right)^4 (\sin(z)-z\cos(z))}{4},\\ a_2 &= \frac{z\csc\left(\frac{z}{2}\right)^4 \sec\left(\frac{z}{2}\right)\left(z\cos\left(\frac{z}{2}\right)+2z\cos\left(\frac{3z}{2}\right)-2\sin\left(\frac{3z}{2}\right)\right)}{8},\\ a_3 &= a_1,\\ a_4 &= a_0,\end{aligned} \tag{2.14}$$

with $z = \mu h$.

Remark 2.1. *The chosen fitting spaces* (2.5) *and* (2.12)*, as it normally happens in function fitting techniques (refer to [18, 20] and references therein), explicitly depend on the parameter μ which can be interpreted as the frequency of the oscillations occurring in the solution of* (1.2)*. As a consequence, the corresponding numerical method will depend on variable coefficients: this is visible, for instance, in the expression of the coefficients* (2.8) *and* (2.14) *of the finite differences* (2.4) *and* (2.11)*, respectively. 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 [20] 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* (1.3)*, which clearly shows that sine and cosine are evaluated in $\sqrt{\lambda(\widehat{r})}x$. This suggests us to employ as estimation of the parameter $z = \mu h$ in* (2.8) *and* (2.14) *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 [5, 13] 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.

A final constructive issue regards the link between the special purpose finite difference (2.11) with coefficients (2.14) and its corresponding classical general purpose version. The latter can be easily recovered by annihilating the linear operator (2.13) on the monomial basis $\{1, x, x^2, x^3, x^4\}$, i.e.

$$\mathcal{L}[h, \mathbf{a}]1 = 0,$$
$$\mathcal{L}[h, \mathbf{a}]x^i\Big|_{x=0,\ t=0} = 0, \quad i = 1, 2, 3, 4.$$

This leads to

$$a_0 = -\frac{1}{12}, \quad a_1 = \frac{4}{3}, \quad a_2 = -\frac{5}{2}, \quad a_3 = \frac{4}{3}, \quad a_4 = -\frac{1}{12}, \tag{2.15}$$

i.e. to the classical five-point finite difference

$$\begin{aligned}\frac{\partial^2 u}{\partial x^2}(x,t) \approx -\frac{1}{12h^2}(u(x+2h,t) - 16u(x+h,t) + 30u(x,t) \\ - 16u(x-h,t) + u(x-2h,t)),\end{aligned} \tag{2.16}$$

which is known to have fourth order of accuracy. We observe that the coefficients (2.14) of the finite difference (2.11), thus obtained with respect to the functional basis (2.12), i.e.

$$\{1, \sin\mu x, \cos\mu x, x\sin\mu x, x\cos\mu x\},$$

when z tends to 0, tend to the classical coefficients (2.15), obtained with respect to the monomial basis

$$\{1, x, x^2, x^3, x^4\}.$$

As a natural consequence, also the expression of the error associated to the trigonometrically fitted formula tends to that of the classical one. Thus, the trigonometrically fitted finite difference (2.11) with coefficients (2.14) retains the same order of accuracy of that based on polynomials with coefficients given by (2.15), i.e. it has order 4. Hence, the non-polynomial version of existing general purpose formulae do not deteriorate their order of accuracy (this also happens in many other contexts, such as interpolation, quadrature, numerical solution of ordinary differential equations [18, 20]).

Remark 2.2. *The choices of the fitting spaces* (2.5) *and* (2.12) *reveal a similarity with the Fourier spectral method of lines [25]. Actually, in a more general sense, one could recognize a close similarity among trigonometrically fitted method of lines, based on suitably truncating the mixed basis*

$$\{1, \sin \mu x, \cos \mu x, x \sin \mu x, x \cos \mu x, ...\} \tag{2.17}$$

or the trigonometrical basis

$$\{1, \sin \mu x, \cos \mu x, \sin 2\mu x, \cos 2\mu x, ...\} \tag{2.18}$$

and the Fourier spectral method of lines, obtained in correspondence of the functional basis

$$\{1, \sin x, \cos x, \sin 2x, \cos 2x, ...\}. \tag{2.19}$$

We point out here two similarities and one significant difference. A clear similarity is given by the form of the chosen basis functions, especially in (2.18) *and* (2.19)*, as well as by the fact that the number of chosen basis functions influence the order of convergence. For instance, formula* (2.4) *with coefficients* (2.8) *attains order 2 (3 basis functions are employed for its construction, i.e. those in* (2.5)*), while formula* (2.11) *with coefficients* (2.14) *attains order 4 (5 basis functions are employed for its construction, i.e. those in* (2.12)*). As one can easily expect, higher orders can be achieved by coherently augmenting, at the same time, the number of points in the finite difference as well as the number of basis functions. A significant difference is given by the gained level of adaptation to the problem: indeed, the standard Fourier basis* (2.19) *does not contain an explicit reference to the problem under consideration, while the trigonometrically fitted ones* (2.17) *and* (2.18) *depends on the parameter μ which is closely connected to the solution of the problem. This makes the trigonometrically fitted approach more problem oriented and, thus, more accurate, as observed in Section 4.*

3. Semi-discretization of the operator

We now apply the results developed in the previous sections to the original λ-ω system (1.2). More precisely, following [23], we are going to consider the system of PDEs (1.2) in the unbounded domain

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

equipped by the following boundary conditions

$$\frac{\partial u}{\partial x}(0,t) = \frac{\partial v}{\partial x}(0,t) = 0, \tag{3.20a}$$

$$\lim_{x\to+\infty} u(x,t) = \lim_{x\to+\infty} v(x,t) = 0, \tag{3.20b}$$

and the initial conditions

$$\begin{aligned} u(x,0) &= f_0(x), \\ v(x,0) &= g_0(x). \end{aligned} \tag{3.21}$$

This problem is now aimed to be treated by suitably applying the method of lines (refer to [14, 21, 22] 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 [23], we are going to solve the problem on a bounded domain $[0, X] \times [0, T]$ where X is a large real number. In correspondence of this large value of X, instead of (3.20b), we actually consider the following boundary conditions

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

More precisely, X is chosen in such a way that any further increase on it have negligible effects on the solution, thus making above zero boundary conditions realistic and coherent with (3.20b). In summary, we consider the following boundary conditions in $[0, X]$

$$\frac{\partial u}{\partial x}(0,t) = \frac{\partial v}{\partial x}(0,t) = 0, \tag{3.22a}$$

$$u(X,t) = v(X,t) = 0. \tag{3.22b}$$

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 $u_j(t) = u(x_j, t)$, $0 \le j \le N-1$. As a consequence, the original problem (1.2) with boundary conditions (3.22a)-(3.22b) and initial conditions (3.21) is transformed in the following system of $2N$ ordinary differential equations

$$u'_0(t) = u'_2(t), \tag{3.23a}$$

$$v'_0(t) = v'_2(t), \tag{3.23b}$$

$$u'_i(t) = \Delta_n[u_i(t), h] + \lambda(r)u_i(t) - \omega(r)v_i(t), \quad 1 \le i \le N-2 \tag{3.23c}$$

$$v'_i(t) = \Delta_n[v_i(t), h] + \omega(r)u_i(t) + \lambda(r)v_i(t), \quad 1 \le i \le N-2 \tag{3.23d}$$

$$u'_{N-1}(t) = 0, \tag{3.23e}$$

$$v'_{N-1}(t) = 0. \tag{3.23f}$$

This system of ordinary differential equations is then equipped of the initial conditions

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

We observe that Equations (3.23a) and (3.23b) arise from the boundary conditions (3.22a), taking into account that

$$\frac{\partial u}{\partial x}(0,t) \approx \frac{u_0(t) - u_2(t)}{2h} = 0, \quad \frac{\partial v}{\partial x}(0,t) \approx \frac{v_0(t) - v_2(t)}{2h} = 0,$$

which implies that $u_0(t) = u_2(t)$ and $v_0(t) = v_2(t)$. On the other hand, Equations (3.23c) and (3.23d) are obtained by approximating the second spatial derivative $\frac{\partial^2 u}{\partial x^2}(x,t)$ with the chosen finite difference $\Delta_n[u(x,t),h]$, depending on n consecutive meshpoints. Finally, Equations (3.23e) and (3.23f) are obtained by considering the boundary conditions (3.22b).

4. Numerical experiments

We now present some numerical results obtained by solving the system of PDEs (1.2) with $\lambda(r)$ and $\omega(r)$ of the form

$$\lambda(r) = \lambda_0 - r^p, \tag{4.24}$$

$$\omega(r) = \omega_0 - r^p, \tag{4.25}$$

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

By employing the semi-discretization introduced in Section 3, we are specifically considering the system of ODEs (3.23a)-(3.23f) with boundary conditions (3.22a)-(3.22b) and initial conditions (3.21) given by

$$u_j(0) = v_j(0) = A\exp(-\xi x_j), \quad 0 \le j \le N-1. \tag{4.26}$$

In the experiments, as in [23], we will always consider the following values of the above parameters

$$\lambda_0 = 1, \quad \omega_0 = 2, \quad p = 1.8, \quad A = 0.1, \quad \xi = 0.8. \tag{4.27}$$

We proceed in two different directions: indeed, we consider the spatially semi-discretized version (3.23a)-(3.23f) 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 and 2 show the profiles of the solutions originated by applying the trigonometrically fitted spatial semi-discretization (with 3 and 5 points, i.e. through finite differences (2.4) and (2.11) with coefficients (2.8) and (2.14), respectively) and solving in time with the `ode15s` Matlab routine. The solutions of the semi-discretized problem by standard finite differences are also depicted in Figures 1 and 2; also in this case, the `ode15s` time solver is applied. The problem is solved for $(x,t) \in [0,150] \times [0,60]$, as in [23]. The space interval is large enough in order to make the use of the boundary conditions (3.22a)-(3.22b) instead of (3.20a)-(3.20b) realistic, as highlighted in [23].

We have involved 50 subintervals in the spatial semi-discretization with 3 points (Figure 1) and 20 subintervals in the spatial semi-discretization with 5 points (Figure 2): hence, the spatial stepsizes are $h = 3$ and $h = 7.5$, respectively.

As it is visible from Figures 1 and 2, the profiles of the solutions obtained via the trigonometrically fitted method of lines are coherent with the expected dynamics and, in particular, with that described in [23]. Such a situation is not visible for the classical method of lines, since an unstable behavior is visible in Figure 1 for the three-point semi-discretization, while a total loss of the periodic character of the solution is evident in Figure 2 for the five-point semi-discretization: this is also pointed out by the range of variability of the solutions shown in Tables 1 and 2. Thus, in the comparison between a standard finite difference and a trigonometrically fitted one for the λ-ω problem (1.2), one can recognize a much more stable behavior of the latter and a clear ability to retain the periodic character of the solutions.

As highlighted by the representation (1.3) of the periodic plane waves solutions, the range of variability is given by $[-\hat{r}, \hat{r}]$, suggesting that we should expect symmetric values of the boundary of such interval with respect to the origin. As shown in Tables 1 and 2, the best results in this sense are obtained by employing the trigonometrically fitted finite difference depending on 5 points. This aspect gives us a measure of the accuracy of our approach which, in comparison with the classical one, results to be more accurate and stable.

A further comparison is then provided with respect to Matlab `pdepe` routine, which acts as an authomatic solver for a class of PDEs of the type

$$c\left(x, t, \varphi, \frac{\partial \varphi}{\partial x}\right) \frac{\partial \varphi}{\partial t} = x^{-m} \frac{\partial}{\partial x} \left(x^m f(x, t, \varphi, \frac{\partial \varphi}{\partial x}) \right) + s\left(x, t, \varphi, \frac{\partial \varphi}{\partial x}\right),$$

suitably equipped by initial and boundary conditions. Problem (1.2) falls into this class of equations, by assuming

$$\begin{aligned} c\left(x, t, \varphi, \frac{\partial \varphi}{\partial x}\right) &= [1,\ 1]^\intercal, \\ f\left(x, t, \varphi, \frac{\partial \varphi}{\partial x}\right) &= \left[\frac{\partial u}{\partial x},\ \frac{\partial v}{\partial x}\right]^\intercal, \\ s\left(x, t, \varphi, \frac{\partial \varphi}{\partial x}\right) &= [\lambda(r)u - \omega(r)v,\ \omega(r)u + \lambda(r)v]^\intercal, \\ m &= 0. \end{aligned}$$

The routine `pdepe` is based on employing finite differences depending on a number of points which is automatically selected by the solver. Figure 3 shows the profiles of the solution of (1.2), with initial conditions (3.21), boundary conditions (3.22a)-(3.22b), in correspondence of several values of the spatial stepsize h. From a first glance, one can easily recognize that an accurate computation of the solution through `pdepe` requires a severe mesh refinement: indeed, for $h = 15$ or $h = 7.5$ the wavefront is very irregular and badly approximated; for $h = 3$, the wavefront appear more regular, but it is not accurately matched with the zero boundary condition. A much better situation occurs for $h = 1.5$. This is absolutely coherent with the description provided by the developers

in the inline guide: they clearly state the routine is able to solve problems with a modest accuracy, thus severe mesh refinements are needed in order to accurately reproduce the profiles of the solutions. This gap does not occur in employing trigonometrically fitted finite differences, which look accurate also with larger values of the stepsize, as shown.

Type of finite difference	$\min_{(x,t)\in[0,150]\times[0,60]} u(x,t)$	$\max_{(x,t)\in[0,150]\times[0,60]} u(x,t)$
Standard on 3 points	-0.9697	70.0670
Standard on 5 points	$-2.8550 \cdot 10^{-4}$	0.1000
Trigonometrically fitted on 3 points	-0.9912	1.3403
Trigonometrically fitted on 5 points	-1.0379	1.0366

Table 1: Range of variability of the values of the numerical approximation of the solution $u(x,t)$ of (1.2), with initial conditions (3.21), boundary conditions (3.22a)-(3.22b), in correspondence of the parameters given by (4.27), by various finite differences for the spatial semi-discretization.

Type of finite difference	$\min_{(x,t)\in[0,150]\times[0,60]} v(x,t)$	$\max_{(x,t)\in[0,150]\times[0,60]} v(x,t)$
Standard on 3 points	-3.7892	$4.9338 \cdot 10^{4}$
Standard on 5 points	$-4.0383 \cdot 10^{-4}$	0.1000
Trigonometrically fitted on 3 points	-1.1873	1.0837
Trigonometrically fitted on 5 points	-1.0416	1.0376

Table 2: Range of variability of the values of the numerical approximation of the solution $v(x,t)$ of (1.2), with initial conditions (3.21), boundary conditions (3.22a)-(3.22b), in correspondence of the parameters given by (4.27), by various finite differences for the spatial semi-discretization.

5. Conclusions

We have proposed an alternative approach for the numerical solution of reaction-diffusion systems of λ-ω type (1.2), based on the employ of trigonometrically fitted finite differences. This approach is problem-oriented: since it is known from the literature [23] that the problem has a one-parameter family of periodic plane wave solutions, an adapted numerical approach taking into account this qualitative behavior has been preferred. Clearly, the numerical solution of other problems than that considered in this paper can be handled by non-polynomially fitted methods as well, but they would need to be suitably adapted to the problem under investigation. In developing the special purpose approach, the theoretical knowledge of many aspects of the problem have been taken into account: they have guided, in particular, the choice of the fitting space and that of the fitted parameters. Numerical evidence highlights that this approach is promising in solving partial differential equations whose solutions are periodic plane waves or, more in general, have an a priori known qualitative behavior, which can be exploited in developing a proper numerical scheme. Further efforts will be thus oriented in this direction, i.e. introducing and analyzing adapted numerical techniques in order to approach other differential operators and providing techniques of parameter estimations.

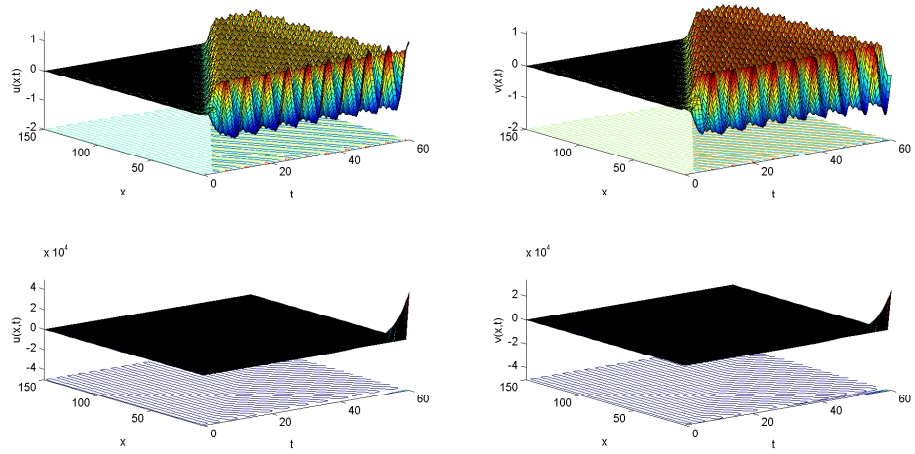

Figure 1: Numerical solution of (1.2), with initial conditions (3.21), boundary conditions (3.22a)-(3.22b), with parameters given by (4.27). The left figures are the profiles of $u(x,t)$ computed by solving the semi-discretized problem (3.23a)-(3.23f) obtained by the three-point trigonometrically fitted finite difference (2.4) with coefficients (2.8) (top) and the classical one with coefficients (2.10) (bottom). Analogously, the right figures are the profiles of $v(x,t)$.

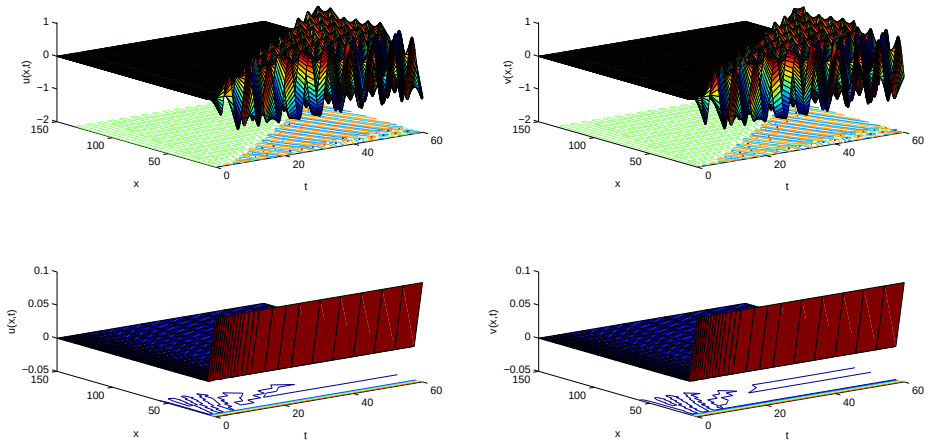

Figure 2: Numerical solution of (1.2), with initial conditions (3.21), boundary conditions (3.22a)-(3.22b), with parameters given by (4.27). The left figures are the profiles of $u(x,t)$ computed by solving the semi-discretized problem (3.23a)-(3.23f) obtained by the five-point trigonometrically fitted finite difference (2.11) with coefficients (2.14) (top) and the classical one with coefficients (2.15) (bottom). Analogously, the right figures are the profiles of $v(x,t)$.

Acknowledgments
This work was supported by the Italian National Group of Computing Science (GNCS-INDAM). We truly express our appreciation to the anonymous referees for the high quality comments, which have remarkably improved the paper.

References

[1] 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).

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

[3] 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).

[4] R. D'Ambrosio, B. Paternoster, *Exponentially fitted singly diagonally implicit Runge-Kutta methods*, J. Comput. Appl. Math. 263, 277-287 (2014).

[5] 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).

[6] 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).

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

[8] J.E. Ferrell, T.Y. Tsai, Q. Yang, *Modeling the cell cycle: why do certain circuits oscillate?*, Cell. 144(6), 874–885 (2011).

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

[10] 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).

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

[12] D. Hollevoet, M. Van Daele, *Exponentially-fitted methods and their stability functions*, J. Comput. Appl. Math. 236(16), 4006–4015 (2012).

[13] 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).

[14] E. Isaacson, H.B.Keller, *Analysis of Numerical Methods*, Dover Publications, New York (1994).

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

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

[17] A.W. Murray, M.W. Kirschner, *Dominoes and clocks: the union of two views of the cell cycle*, Science 246, 614621 (1989).

[18] L. Gr. Ixaru, G. Vanden Berghe, *Exponential Fitting*, Kluwer, Boston-Dordrecht-London (2004).

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

[20] 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).

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

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

[23] 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).

[24] 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).

[25] Lloyd 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).

[26] 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).

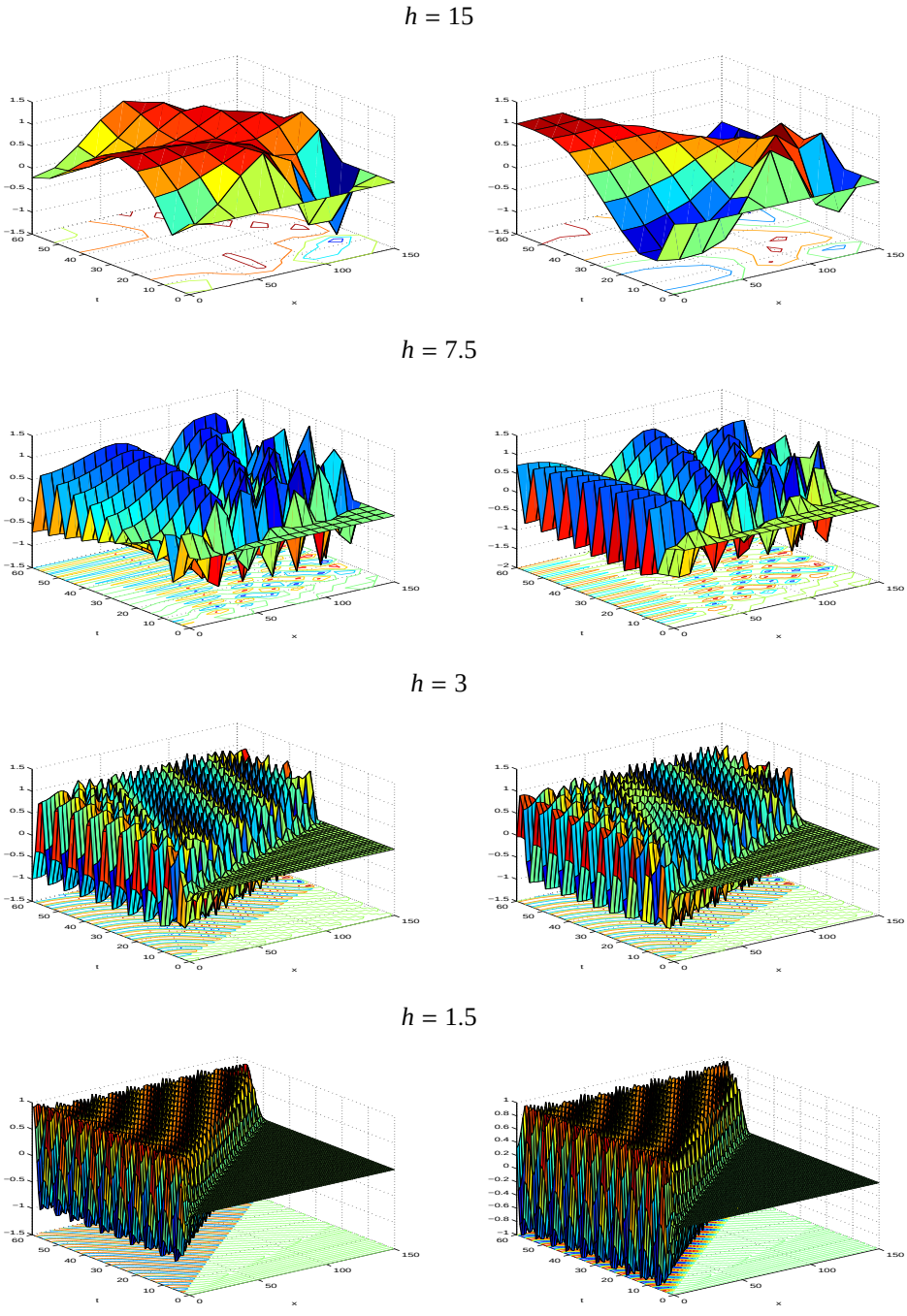

Figure 3: Profile of the solutions of (1.2), with initial conditions (3.21), boundary conditions (3.22a)-(3.22b) computed by `pdepe` Matlab routine with different values of the spatial stepsize. The left column depicts the profiles of $u(x,t)$, while in the right one the graphs of $v(x,t)$ are drawn.