Some recent advances in the numerical solution of differential equations

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Abstract. The purpose of the talk is the presentation of some recent advances in the numerical solution of differential equations, with special emphasis to reaction-diffusion problems, Hamiltonian problems and ordinary differential equations with discontinuous right-hand side. As a special case, in this short paper we focus on the solution of reaction-diffusion problems by means of special purpose numerical methods particularly adapted to the problem: indeed, following a problem oriented approach, we propose a modified method of lines based on the employ of finite differences shaped on the qualitative behavior of the solutions. Constructive issues and a brief analysis are presented, together with some numerical experiments showing the effectiveness of the approach and a comparison with existing solvers.

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PERIODIC PLANE WAVES IN REACTION-DIFFUSION PROBLEMS

We focus on reaction-diffusion problems modeled by coupled partial differential equations (PDEs) of the type

$$\begin{aligned}\frac{\partial u}{\partial t} &= D_u \frac{\partial^2 u}{\partial x^2} + f_u(u,v),\\ \frac{\partial v}{\partial t} &= D_v \frac{\partial^2 v}{\partial x^2} + f_v(u,v),\end{aligned} \tag{1}$$

with $D_u > 0$ and $D_v > 0$. This problem exhibits traveling waves as fundamental solutions [19], thus it has been widely used in Life Science to model problems generating periodic waves along their dynamics: this is typical of cell cycles [9, 16], behaving as a biochemical oscillator.

These situations are also typically encountered in intracellular calcium signaling [20]: indeed, calcium shows many differrent types of oscillations in time and space, in response to various extracellular signals [2]. Among many existing mathematical models, that described in [20] is based on the release of calcium from intracellular stores through channels that are sensitive to the regulatory molecule IP_3: the main idea, first presented in [1], is that external stimuli produce increased concentrations of IP_3, causing the release of calcium from these internal stores. Under the mathematical point of view, in the model provided in [1, 20], the dynamics of this process is governed by two partial differential equations

$$\begin{aligned}\frac{\partial c}{\partial t} &= D_c \frac{\partial^2 c}{\partial x^2} + k_{flux}\mu n\left(b + \frac{1-b}{k_1 + c}\right) - \frac{\gamma c}{k_\gamma + c},\\ \tau_n \frac{\partial n}{\partial t} &= \frac{k_2^2}{k_2^2 + c^2} - n.\end{aligned} \tag{2}$$

in the unknowns $c(x,t)$ and $n(x,t)$, respectively denoting the local calcium concentration and the fraction of receptors that have not been inactivated by calcium. As it arises from [1], D_c denotes the cytosolic diffusion coefficient of calcium, k_{flux} is the maximum total calcium flux, b represents a basal current through sensitive channels, γ gives the rate of calcium pumping out of the cytosol, k_γ is the calcium concentration at which the rate of calcium pumping from the cytosol is at half-maximum, τ_n is the time constant for the dynamics of $n(x,t)$, k_2 is the rate of production of new receptors. Coherently with the biological evidence, the solutions derived in [20] under suitable initial and boundary conditions, exhibit an oscillatory dynamics both in space and in time.

A special case of (1) is given by λ-ω problems [8, 10, 11, 14, 15, 19, 23]

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} + \lambda(r)u - \omega(r)v, \\ \frac{\partial v}{\partial t} &= \frac{\partial^2 v}{\partial x^2} + \omega(r)u + \lambda(r)v, \end{aligned} \tag{3}$$

with $r = (u^2+v^2)^{1/2}$, $\lambda(0) > 0$ and $\omega(0) > 0$, having a one-parameter family of periodic plane waves solutions [15]

$$\begin{aligned} u(x,t) &= \hat{r}\cos\left(\omega(\hat{r})t \pm \sqrt{\lambda(\hat{r})}x\right), \\ v(x,t) &= \hat{r}\sin\left(\omega(\hat{r})t \pm \sqrt{\lambda(\hat{r})}x\right), \end{aligned} \tag{4}$$

for any $\hat{r} \in \mathbb{R}$ such that $\lambda(\hat{r}) > 0$. Though incomputable, this parametrization is very useful to develop a problem oriented numerical scheme that gains a significant benefit from the a priori knowledge of the qualitative behavior of the solution: this point of view deeply falls in the spirit of *exponential fitting* technique (EF, see [17, 18, 21, 22] and references therein).

Classically, EF based numerical methods arise from the adaptation of existing methods, in order to let them exactly integrate (within round-off error) problems having solutions in a functional space spanned by basis functions other than polynomials, to be chosen in accordance with the behavior of the solution [17, 18, 21, 22]. The corresponding methods are characterized by on non-constant coefficients, since they depend on parameters related to the solutions which need to be suitably computed. Choosing a proper fitting space and accurately providing and estimate of the unknown parameters is a crucial problem [5, 6, 12, 13], still unsolved in many situations; however, for λ-ω problems, the parametrization (4) turns to be useful in order to approach the aforementioned two issues.

In the remainder of the treatise, we provide a spatial semi-discretization of problem (3) through adapted finite differences properly developed taking into account the nature of the solutions (4) and solve in time the resulting system of ordinary differential equations.

ADAPTED FINITE DIFFERENCES

We proposed in [4] an adapted three-point finite difference formula

$$\frac{\partial^2 u}{\partial x^2}(x,t) \approx \frac{1}{h^2}\left(a_0 u(x+h,t) + a_1 u(x,t) + a_2 u(x-h,t)\right), \tag{5}$$

where h is a given spatial stepsize and $u(x,t)$ is defined on the rectangular domain

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

Taking into account the parametrization (4) of the plane waves solutions, we compute the coefficients a_0, a_1 and a_2 of (5) in order to make it exact on the linear space spanned by [4, 3, 7]

$$\mathscr{F} = \{1, \sin(\mu x), \cos(\mu x)\}. \tag{6}$$

Hence, we obtain

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

where $z = \mu h$. One can easily recognize that the coefficients are now non-constant, but functions of z. Such a parameter can be estimated by analogy with (4), which shows that sine and cosine in the solution are evaluated in $\sqrt{\lambda(\hat{r})}x$. Thus, we estimate z in the mesh point (x_i, t_j) by

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

where

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

with $u_{ij} \approx u(x_i,t_j)$, $v_{ij} \approx v(x_i,t_j)$. This is a cheap estimate arising from the computation of the solution in any mesh point and without additional function evaluations.

It was proved in [4] that the trigonometrically fitted finite difference formula (5) with coefficients (7), has second order of accuracy, as it happens in the classical case, i.e. for the formula (5) with constant coefficients

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

Hence, the trigonometrical fitting adaptation of (5) retains the same order of accuracy of the corresponding constant coefficient version.

SPATIAL SEMI-DISCRETIZATION OF THE OPERATOR

Following [19], we solve problem (3) in the unbounded domain $D = [0,\infty) \times [0,T]$, and consider the following boundary conditions

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

and the initial conditions

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

In many practical situations [19], the problem is solved on a bounded domain $[0,X] \times [0,T]$, where X is a large real number chosen in such a way that any further increase on it have negligible effects on the solution, and we consider the following zero boundary conditions in $[0,X]$

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

Chosen a fixed spatial stepsize h, the semi-discretized domain is given by $D_x = \{(x_j,t) : x_j = jh,\ j = 0,\dots,N-1\}$. By denoting $u_j(t) = u(x_j,t)$, $0 \le j \le N-1$, the original problem (3) with boundary conditions (11) and initial conditions (10) leads to the following system of $2N$ ordinary differential equations

$$u'_0(t) = u'_2(t), \quad v'_0(t) = v'_2(t), \tag{12a}$$

$$u'_i(t) = \Delta_n[u_i(t),h] + \lambda(r)u_i(t) - \omega(r)v_i(t), \quad 1 \le i \le N-2 \tag{12b}$$

$$v'_i(t) = \Delta_n[v_i(t),h] + \omega(r)u_i(t) + \lambda(r)v_i(t), \quad 1 \le i \le N-2 \tag{12c}$$

$$u'_{N-1}(t) = 0, \quad v'_{N-1}(t) = 0. \tag{12d}$$

with 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 now provide a numerical evidence in correspondence of

$$\lambda(r) = 1 - r^{1.8}, \quad \omega(r) = 2 - r^{1.8}, \tag{13}$$

and initial conditions (10) given by

$$u_j(0) = v_j(0) = 0.1\exp(-0.8x_j), \quad 0 \le j \le N-1. \tag{14}$$

Figure 1 shows the profiles of the solutions originated by applying the trigonometrically fitted spatial semi-discretization by (5) with coefficients (7) and (8), with the same spatial stepsize $h = 15$. 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 [19]. Such a situation is not visible for the classical method of lines, since an unstable behavior is visible in Figure 1. Thus, in the comparison between a standard finite difference and a trigonometrically fitted one for the λ-ω problem (3), one can recognize a much more stable behavior of the latter and a clear ability to retain the periodic character of the solutions. More results are reported in [3].

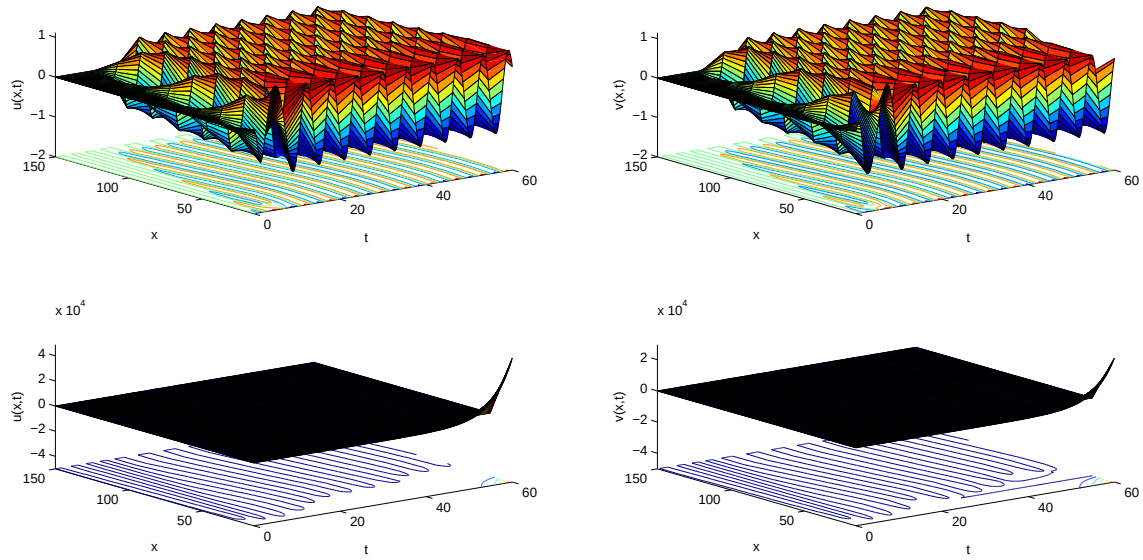

FIGURE 1. Numerical solution of (3) in $(x,t) \in [0,150] \times [0,60]$, with initial conditions (10) and boundary conditions (11). The left figures are the profiles of $u(x,t)$ computed by solving the semi-discretized problem (12a)-(12d) obtained by the three-point trigonometrically fitted finite (top) and the classical one (bottom). Analogously, the right figures are the profiles of $v(x,t)$. The applied time solver is Matlab `ode15s`.

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