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Adapted numerical methods for advection–reaction–diffusion problems generating periodic wavefronts

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ABSTRACT

The paper presents an adapted numerical integration for advection–reaction–diffusion problems. The numerical scheme, exploiting the a-priori knowledge of the qualitative behaviour of the solution, gains advantages in terms of efficiency and accuracy with respect to classic schemes already known in literature. The adaptation is here carried out through the so-called trigonometrical fitting technique for the discretization in space, giving rise to a system of ODEs whose vector field contains both stiff and non-stiff terms. Due to this mixed nature of the vector field, an Implicit–Explicit (IMEX) method is here employed for the integration in time, based on the first order forward–backward Euler method. The coefficients of the method here introduced rely on unknown parameters which have to be properly estimated. In this work, such an estimate is performed by minimizing the leading term of the local truncation error. The effectiveness of this problem-oriented approach is shown through a rigorous theoretical analysis and some numerical experiments.

1. Introduction

The treatise is devoted to the numerical integration of nonlinear advection–reaction–diffusion problems having periodic waves as fundamental solutions. The general expression of such systems is the following:

$$\begin{aligned} \frac{\partial u}{\partial t} &= d_1 \frac{\partial^2 u}{\partial x^2} + a_1 \frac{\partial u}{\partial x} + f_1(u, v), \\ \frac{\partial v}{\partial t} &= d_2 \frac{\partial^2 v}{\partial x^2} + a_2 \frac{\partial v}{\partial x} + f_2(u, v), \end{aligned} \tag{1.1}$$

with proper initial and boundary conditions. The functions $u, v : \mathcal{D} = [0, X] \times [0, \infty) \longrightarrow \mathbb{R}$ are state variables denoting, for example, the concentrations of certain interacting biological species; the advection coefficients a_1 and a_2 represent the velocities of the transport medium, such as water or air; the terms $d_1 > 0$ and $d_2 > 0$ are diffusion coefficients and may also include the parametrizations of turbulence. The reaction term $[f_1(u, v),\ f_2(u, v)]^{\mathsf{T}}$ is linked to the interactions between the various involved species and generally models the results of their chemical interactions. These systems are widely used in the applications: for instance, they are employed to model air pollution phenomena [1] or to understand morphogenesis [2].

For the numerical integration of such problems, classic methods could require a very small stepsize to accurately follow the oscillatory behaviour of the exact solution because they are based on general purpose formulae constructed in order to

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be exact (within round-off error) on polynomials up to a certain degree. Since we focus on systems having an oscillating exact solution, it may be more convenient to employ fitted formulae developed in order to be exact on functions other than polynomials: this strategy is nowadays well-known as *trigonometrical fitting* (see [3,4] and references therein) and the basis functions are typically supposed to belong to a finite-dimensional space called fitting space. The choice of a suitable fitting space is suggested by the a-priori known information about the exact solution, so the coefficients of the resulting adapted method are no longer constant as in the classic case, but rely on a parameter characterizing the exact solution, whose value is clearly unknown. As a result, the trigonometrical fitting strategy implies two main challenges: the choice of a suitable fitting space and the accurate estimate of the unknown parameters. In this paper, the oscillatory dynamics of the considered problems suggests the adoption of a trigonometrically fitted space and the minimization of the leading term of the local truncation error allows to accurately estimate the parameter.

Extending the ideas introduced in [5], we present a numerical scheme which spatially discretizes the system (1.1) by means of trigonometrically fitted finite differences and employs an Implicit–Explicit (IMEX) method, based on the first order forward–backward Euler method, to integrate in time the resulting system of ordinary differential equations

$$y' = Ay + f(y),$$

where A is a matrix whose size depends on the number of spatial grid points and $f(y)$ is a vector-valued function.

The choice of a time integration scheme based on IMEX method is suggested by the mixed nature of such system actually composed by stiff components (arising from the diffusion term) and nonlinear ones (coming from the reaction and the advection terms). Indeed, an IMEX numerical method implicitly integrates the stiff terms and explicitly integrates the others [6–8], obtaining benefits in terms of efficiency and stability.

The paper is organized as follows: in Section 2 we develop a problem-oriented numerical scheme for the general advection–reaction–diffusion system (1.1); Section 3 concerns the rigorous analysis of accuracy and stability properties of the introduced method, whereas Section 4 is focused on the estimate of the parameters appearing in the coefficients of the method and Section 5 provides some numerical experiments. Finally, Section 6 is devoted to present some conclusions.

2. An adapted numerical scheme

We aim to solve system (1.1), equipped by the following initial conditions

$$u(x,0) = \psi_1(x), \qquad v(x,0) = \psi_2(x), \quad x \in [0, X], \tag{2.1}$$

and periodic boundary conditions

$$\begin{aligned} &u(0,t) = u(X,t), \qquad v(0,t) = v(X,t),\\ &\frac{\partial u}{\partial t}(0,t) = \frac{\partial u}{\partial t}(X,t), \quad \frac{\partial v}{\partial t}(0,t) = \frac{\partial v}{\partial t}(X,t). \end{aligned} \tag{2.2}$$

Following the method of lines (see [9–11] and references therein), we spatially discretize the domain $\mathcal{D}$ in

$$\mathcal{D}_h = \{(x_i, t) : x_i = ih,\ i = 0, \dots, N-1,\ h = X/(N-1)\},$$

where h is the chosen spatial stepsize. The resulting semi-discrete system of ordinary differential equations has the following expression

$$u'_0(t) = u'_{N-1}(t), \tag{2.3a}$$

$$u'_i(t) = d_1 \Delta_n^{(II)}[u_i(t), h] + a_1 \Delta_n^{(I)}[u_i(t), h] + f_1(u_i(t), v_i(t)), \quad i = 1, \dots, N-2, \tag{2.3b}$$

$$v'_0(t) = v'_{N-1}(t), \tag{2.3c}$$

$$v'_i(t) = d_2 \Delta_n^{(II)}[v_i(t), h] + a_2 \Delta_n^{(I)}[v_i(t), h] + f_2(u_i(t), v_i(t)), \quad i = 1, \dots, N-2, \tag{2.3d}$$

where

$$u_i(t) = u(x_i, t), \qquad v_i(t) = v(x_i, t), \quad i = 0, \dots, N-1,$$

while $\Delta_n^{(II)}[\phi_i(t), h]$ and $\Delta_n^{(I)}[\phi_i(t), h]$ (with $\phi_i(t) = u_i(t)$ or $\phi_i(t) = v_i(t)$) are the n-point fitted finite difference formulae used to approximate the second spatial derivatives and the first spatial derivatives, respectively. The system (2.3) is also joined with the initial conditions

$$u_i(0) = \psi_1(x_i), \qquad v_i(0) = \psi_2(x_i), \quad i = 0, \dots, N-1. \tag{2.4}$$

For the approximation of the spatial derivatives, we follow the well-known trigonometrical fitting procedure (see, for instance, [3,4]) which consists in constructing formulae in order to be exact on basis functions belonging to a finite-dimensional space called *fitting space*. Such functions are chosen according to the a-priori information about the qualitative behaviour of the exact solution. Since we focus on problems having periodic solutions, we choose the following trigonometric fitting space

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

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