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Devising efficient numerical methods for oscillating patterns in reaction–diffusion systems

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ABSTRACT

In this paper, we consider the numerical approximation of a reaction–diffusion system 2D in space whose solutions are patterns oscillating in time or both in time and space. We present a stability analysis for a linear test heat equation in terms of the diffusion d and of the reaction timescales given by the real and imaginary parts α and β of the eigenvalues of $J(P_e)$, the Jacobian of the reaction part at the equilibrium point P_e. Focusing on the case $\alpha = 0$, $\beta \neq 0$, we obtain stability regions in the plane (ξ, ν), where $\xi = \lambda(h; d)h_t$, $\nu = \beta h_t$, h_t time stepsize, λ lumped diffusion scale depending also from the space stepsize h and from the spectral properties of the discrete Laplace operator arising from the semi-discretization in space. In space we apply the Extended Central Difference Formulas (ECDFs) of order $p = 2, 4, 6$. In time we approximate the diffusion part in implicit way and the reaction part by a selection of integrators: the Explicit Euler and ADI methods, the symplectic Euler and a partitioned Runge–Kutta method that are symplectic in the absence of diffusion. Hence, by estimating λ, for each method we derive stepsize restrictions $h_t \lessapprox F_{met}(h; d, \beta, p)$ in terms of the stability curve F_{met} depending on diffusion and reaction timescales and from the approximation order in space. For the same schemes, we provide also a dispersion error analysis. We present numerical simulations for the test heat equation and for the Lotka–Volterra PDE system with solutions oscillating only in time for the presence of a centre-type dynamics. In these cases, the implicit-symplectic schemes provide the best choice. We solve also the Schnakenberg model with spatial patterns oscillating in space and time in the presence of an attractive limit cycle due to the Turing–Hopf instability. In this case, all schemes attain closed orbits in the phase space, but the Explicit ADI method is the best choice from the computational point of view.

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1. Introduction

Let us consider the PDE system of reaction–diffusion equations given by

$$\begin{cases} v_t = d\Delta v + f(v, w) \quad (x, y) \in \Omega \subset \mathbb{R}^2, \ t > 0 \\ w_t = d\Delta w + g(v, w) \\ (\mathbf{n} \cdot \nabla v)_{|\partial\Omega} = 0 \qquad (\mathbf{n} \cdot \nabla w)_{|\partial\Omega} = 0 \\ v(x, y, 0) = v_0(x, y) \qquad w(x, y, 0) = w_0(x, y) \end{cases} \tag{1}$$

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where the diffusion coefficient is given by $d > 0$ and zero Neumann boundary conditions (BCs) on a 2D domain Ω are considered.

In this paper we are mainly interested in the numerical approximation of solutions of (1) that are homogeneous or inhomogeneous patterns oscillating in time and also in time and space. It is well known that these oscillations can be caused by different dynamical mechanisms. In particular, we are interested in the spatio-temporal dynamics of: (i) standing oscillations around an equilibrium of centre type (see [1]); (ii) inhomogeneous Turing patterns that are oscillatory in time (weak case) or both in space and time (strong case) that arise in the neighbour of a Turing–Hopf bifurcation point (see [2]). In both cases $J(P_e)$, the Jacobian of the reaction terms in (1) evaluated at the equilibrium point P_e, has complex conjugate eigenvalues.

Concerning the dynamics in (i), where the Jacobian eigenvalues are pure imaginary and typically there exists a time invariant to be preserved, a huge literature can be reported especially in the ODE cases. We can refer to the book [3] for an exhaustive review. Only in recent times the attention has been devoted to the numerical solution of PDEs with this kind of solutions, see e.g. [4,5]. Concerning the dynamics (ii) due to the Turing–Hopf instability, spatio-temporal patterns emerge by the interaction between the so called diffusion-driven or *Turing instability* and the *Hopf instability*. In this case a stable limit cycle in the absence of diffusion becomes unstable in the presence of diffusion leading towards a spatially uniform oscillating solution or an oscillatory inhomogeneous pattern. Reaction–diffusion models with this dynamics have been solved in applied mathematics by different numerical approaches. For example, for time integration, in [6,7] has been used an operator splitting method based on the Explicit Euler; in [8] has been used the code dopri5 based on the Dormand–Prince Runge–Kutta method of order five; in [9] has been used a Peaceman–Rachford Alternating Direction Implicit (ADI) method (see for example [10]) coupled with the Euler method. For the approximation of a reaction–diffusion model for metal growth recently introduced in [11], in [12,13] has been proposed an ADI approach treating implicitly the diffusion terms and explicitly the reaction terms. As far as we know, a numerical analysis of suitable numerical methods for the Turing–Hopf dynamics is not present in the literature.

The numerical approximation of the above dynamics is a challenging task for several reasons: (a) long-time integration is required to obtain the pattern corresponding to the steady state solution; (b) in order to identify the pattern structure, highly accurate discretization in space is needed, that is very fine meshes on large domain of integration must be used; (c) to track oscillatory solutions and related closed limit cycle in the phase space suitable time integrators must be used often with very small timesteps. The main goal of this paper is to provide a flexible mathematical tool to devise efficient methods dealing with all above points (a)–(c).

To provide high accuracy in space for point (b), here we apply the Method of Lines (MOL) and consider the semi-discretization by high order finite differences given by the Extended Central Difference Formulas (ECDF$_p$) that approximate Neumann BCs with the same order of accuracy $p = 2, 4, 6$. To deal with points (a) and (c), we provide a stability analysis including information from the diffusion scale d, the reaction timescales given by the real and imaginary parts α and β of the eigenvalues of $J(P_e)$, and from the spectral properties of the discrete Laplace operator $\widetilde{\Delta}$ arising from the space semi-discretization. The basic idea was firstly introduced to study the numerical approximation of stationary Turing patterns in [14], where we have introduced a linear test heat equation with a real (positive and negative) reaction scale α, that is for $\beta = 0$. Stepsize restrictions for the 2-SBDF scheme were found, while the best method highlighted was the semi-implicit ADI-ECDF scheme. Here we extend this approach by considering the more general test problem corresponding to the linear heat equation with a *complex* reaction term and the equivalent real reaction–diffusion (RD) system.

Towards this aim, we consider an implicit (IM) approximation for the diffusion part (Laplacian) and different time integrators for the discretization of the reaction part. In particular, we will consider the classical explicit and implicit Euler methods; two methods of first order that are symplectic in the absence of diffusion, i.e. the classical symplectic Euler method reported in [3], here called IMSP_IE, and the Runge–Kutta partitioned scheme introduced in [4] for the predator–prey dynamics, called IMSP; the explicit and semi-implicit ADI methods.

If h_t is the time stepsize, for each method we find stability volumes wrt the 3D axes (ξ, μ, ν), $\xi = \lambda(d, h)h_t$ where λ is a lumped diffusion scale depending also from the space stepsize $h = \max(h_x, h_y)$ and from the spectral properties of the discrete Laplace operator; $\mu = \alpha h_t$ accounts for α, the dissipative or unstable contribution of the reaction term; $\nu = \beta h_t$ accounts for the oscillatory contribution of the reaction term. For simplicity, we focus on the case $|\alpha|$ small, $\alpha \geq 0$ and $|\alpha| \ll |\beta|$. In particular, we consider $\alpha = 0$ and we analyse in detail the stability regions that are projections of the above volumes on the plane (ξ, ν). As a consequence, if the methods *stay* inside the regions they will approximate well solutions with damped oscillations, while if they stay on the boundaries of the represented regions they will be able to approximate solutions with standing oscillations. By using information on the spectral properties of the discrete Laplace operator $\widetilde{\Delta}$ for the ECDF$_p$, we specialize the expression of λ and we deduce stepsize restrictions in the space (h, h_t), such that $h_t \lessapprox F_{met}(h; d, \beta, p)$, where for each method analysed $F_{met}(h; d, \beta, p)$ is a stability curve that depends from the space stepsize, the PDE parameters d, β and from the order p of the space discretization. Hence, given a problem (1), we calculate the stability curves F_{met}, we compare the methods in terms of the obtained stepsize restrictions and then we devise the more efficient schemes (in terms of dissipation) for the oscillatory dynamics of interest. Moreover, for the same schemes applied to the test PDE problem, we present an analysis of the dispersion error. We prove that all of them have dispersion order $q = 2$ for $d \to 0$, but the symplectic methods have the smallest error constants.

The second part of the paper concerns numerical experiments. To study the behaviour of the numerical schemes, we calculate the space mean values $\langle v(t)\rangle$, $\langle w(t)\rangle$ of the numerical solution of (1) and we compare them in the phase plane. First of all, we solve the test heat equation and we provide a numerical study of dissipation and dispersion errors for

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