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#### ABSTRACT

The numerical solution of reaction-diffusion systems modelling predator-prey dynamics using implicit-symplectic (IMSP) schemes is relatively new. When applied to problems with chaotic dynamics they perform well, both in terms of computational effort and accuracy. However, until the current paper, a rigorous numerical analysis was lacking. We analyse the semi-discrete in time approximations of a first-order IMSP scheme applied to spatially extended predator-prey systems. We rigorously establish semi-discrete *a priori* bounds that guarantee positive and stable solutions, and prove an optimal *a priori* error estimate. This analysis is an improvement on previous theoretical results using standard implicit-explicit (IMEX) schemes. The theoretical results are illustrated via numerical experiments in one and two space dimensions using fully-discrete finite element approximations.

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#### 1. Introduction

In spatial ecology the deterministic description of population densities that are continuous in space and time are modelled by reaction-diffusion systems, which can be analysed by means of the well-developed theories of differential equations and dynamical systems [1]. We focus on spatially-extended predator-prey models described by reaction-diffusion systems in the following general form

$$\frac{\partial u}{\partial t} = f(u, v) + D_u \Delta u,$$
(1.1a)
$$\frac{\partial v}{\partial t} = g(u, v) + D_v \Delta v,$$
(1.1b)

where u(x, t) and v(x, t) represent population densities of prey and predators at time t and position x and  $D_u$  and  $D_v$  are positive constant diffusion coefficients. The equations evolve in  $\Omega_T := \Omega \times (0, T)$  where the domain  $\Omega$  is a bounded and open subset of  $\mathbb{R}^d$ ,  $d \leq 3$ . The boundary of the domain  $\partial \Omega$  is assumed to belong to the class of  $C^1$ . The system is augmented with initial conditions

$$u_0(x) := u(x, 0), \quad v_0(x) := v(x, 0), \quad x \in \Omega,$$
 (1.1c)

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and the homogeneous Neumann boundary conditions

$$\frac{\partial u}{\partial v} = \frac{\partial v}{\partial v} = 0 \quad \text{on } \partial \Omega \times (0, T).$$
(1.1d)

In the above equations  $\nu$  denotes the outward unit normal to  $\partial \Omega$  and  $\Delta$  denotes the Laplacian operator  $\sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$ .

Results from semigroup theory and an *a priori* estimate were used in Garvie and Trenchea [2] to prove the global existence and uniqueness of the classical solutions of the predator–prey system (1.1a)-(1.1d) on two specific systems. For the well-posedness of the problem, we assume the nonlinearities f, g are globally Lipschitz, i.e., there exists L > 0 such that

$$|f(u_1, v_1) - f(u_2, v_2)| + |g(u_1, v_1) - g(u_2, v_2)| \le L(|u_1 - u_2| + |v_1 - v_2|),$$
(1.2)

for all  $u_i$  and  $v_i$  in a compact subset of  $\mathbb{R}^+ \times \mathbb{R}^+$  and, in order to assure the non-negativity of solutions corresponding to biologically meaningful densities, the reaction kinetics satisfy

$$f(0, v), g(u, 0) \ge 0, \quad \forall u, v \ge 0.$$
 (1.3)

Consequently, if the initial data  $(u_0(x), v_0(x))$  is chosen in  $[0, +\infty)^2$  for all  $x \in \Omega$ , then by a maximum principle the solution (u(x, t), v(x, t)) also lies in  $[0, +\infty)^2$ , which is a positively invariant region for the system.

Moreover, we assume that f(u, v) has *logistic* dominated growth in the first variable, namely

$$f(u,v) \le u(1-u), \quad \forall u,v \ge 0, \tag{1.4}$$

and the function g satisfies a sub-linear growth in the second variable, i.e., there exists  $C_g > 0$  such that

$$g(u,v) \le C_g v, \quad \forall u,v \ge 0.$$
(1.5)

Notice that from the assumptions (1.3)–(1.5) it is easy to show that for all  $u, v \ge 0$ 

$$g(u, 0) = f(0, v) = 0.$$
 (1.6)

The assumptions (1.3)-(1.5) are not overly restrictive as the principal population dynamics models, based on logistic prey growth and 'Holling type' functional response of the predators, satisfy these conditions [3–5]. This is the case of models that couple logistic prey growth with Holling II and IV functional predator responses [6] as well as the well-known Rosenzweig–MacArthur model [7].

The reaction-diffusion system (1.1a)-(1.1d) includes a class of predator-prey models exhibiting instabilities [8]. Reaction-diffusion systems with logistic prey growth and 'Holling type' functional response of the predators exhibit spiral waves, target waves, and spatiotemporal chaos. However, diffusion induced instability is not possible for systems of this type. Numerical schemes used to approximate such dynamics should be sufficiently robust to reproduce the correct behaviour of the continuous solutions. Stability, high-order consistency and preservation of geometric properties form three pillars on which numerical methods for differential equations rest [9]. The need for a rigorous error analysis of the numerical schemes to approximate the reaction-diffusion dynamics was highlighted in the papers by M. Garvie, C. Trenchea and their co-authors in [10,2,11]. In particular, two implicit–explicit schemes (IMEX) have been extensively analysed by the authors in Garvie and Trenchea [10] using the standard Galerkin finite element method with piecewise linear continuous basis functions.

The preservation of properties of the exact flow under numerical discretization is a more recent field of research. For an exhaustive study of geometric integrators, especially for ordinary differential systems, we refer to the monograph by Hairer et al. [12]. Recently, attention has been devoted to the geometric integration of reaction–diffusion equations. For example, splitting methods were introduced by Hansen et al. [9] to preserve positivity of the numerical approximations.

Implicit-symplectic (IMSP) schemes are numerical integrators based on an implicit scheme for the stiff diffusive term and a geometric integrator for the reaction function. In Diele et al. [13,14] IMSP schemes were proposed as novel numerical schemes for the simulation of population and metapopulation predator-prey dynamics. Symplectic partitioned Runge-Kutta schemes based on composition of Symplectic Euler steps were implemented for approximating Lotka-Volterra (LV) reaction-diffusion dynamics. The authors were motivated by the classical results for the local Poisson nature of the LV dynamics (see, for example, Hairer et al. [12]). Poisson integrators (for example, Symplectic Euler method and composition of symplectic Euler steps) reproduce the correct qualitative behaviour of the theoretical solution and achieve an accurate long-time numerical approximation [12,15]. A stability analysis of IMSP schemes in terms of the diffusion and the reaction time-scales was recently developed in Settanni and Sgura [16]. Their numerical simulations reveal that IMSP schemes provide the best choice for spatio-temporal dynamics of standing oscillations around an equilibrium of centre type (see e.g. Guckenheimer and Holmes [17]).

In this paper we undertake the rigorous numerical analysis of the semi-discrete in time approximations of a first-order IMSP scheme applied to the spatially extended predator-prey system (1.1a)-(1.1d). In Diele et al. [13,14] the method of lines was used. Here, we consider a more technical methodology based on the analysis of a semi-discrete in time formulation of the scheme. We do not undertake the numerical analysis of the fully-discrete problems, however, the analysis of the semi-discrete problems provides the basis on which such a task could be carried out. A novel aspect of the current work is the use of the IMSP approach in conjunction with the standard Galerkin finite element method to solve reaction-diffusion systems.

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