ANALYSIS OF A SECOND-ORDER IN TIME IMPLICIT-SYMPLECTIC SCHEME FOR PREDATOR-PREY SYSTEMS

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Abstract. We analyze a second-order accurate implicit-symplectic (IMSP) scheme for reaction-diffusion systems modeling spatio-temporal dynamics of predator-prey populations. We prove stability, errors estimates and positivity of the the semi-discrete in time approximations. The numerical simulations confirm the theoretically derived rates of convergence, and show, at same computational cost, an improved accuracy in the second-order IMSP in comparison with the first-order IMSP.

Key words. Reaction-diffusion predator-prey systems, Semi-discrete in time formulation, Numerical schemes.

1. Introduction.

In this work we focus on predator-prey spatially extended dynamics described by reaction-diffusion systems of the general form

$$\frac{\partial u}{\partial t} = f(u,v) + D_u \Delta u \tag{1.1}$$

$$\frac{\partial v}{\partial t} = g(u,v) + D_v \Delta v \tag{1.2}$$

where $u(x,t)$ and $v(x,t)$ represent population densities of prey and predators at time t and position x. Here Δ denotes the Laplacian operator $\sum_{i=1}^{d} \frac{\partial^2}{\partial {x_i}^2}$, and D_u and D_v are positive diffusion coefficients. The equations evolve in the space-time cylinder $\Omega^T := \Omega \times (0,T)$, where the domain Ω is a bounded and open subset of $\mathbb{R}^d$, $d \leq 3$. The initial densities $u^0(x) = u(x,0)$ and $v^0(x) = v(x,0)$, $x \in \Omega$ are provided, as well as the conditions on the boundary $\partial\Omega \times (0,T)$.

The comprehension of species interaction in ecological systems and spatiotemporal predator-prey behavior is a very active area of research. The modeling reaction-diffusion equations exhibit abundant and rich dynamical features (see e.g., the fundamental paper [16] and references therein). Theoretical analysis is seldom sufficient in the study of these complex dynamics, and important results and conclusions often rely on extensive numerical simulations. This is the case of examining parameter regions of forming patterns, revealing snapshots of spatial patterns, as well as when detection of the onset of chaotic dynamics (see e.g. [15]). Therefore a particular attention is devoted to the choice of accurate, long-time stable numerical schemes, which yield solutions unaffected by numerical artifacts and better preserve properties of the continuous equations.

Two first-order implicit-explicit numerical schemes (IMEX) for reaction-diffusion problems, modeling predator-prey dynamics, were rigorously analyzed in [7], [8], [5], [7]. More recently, it has been proposed in [3] and [4] the use of symplectic integrators for approximating the reaction terms, in conjunction with implicit schemes for the treatment of the diffusive part. The analysis of a first-order implicit-symplectic scheme was performed in [2], where a comparison with a first-order IMEX scheme was also provided. The test examples, widely used in ecological applications ([2]), reveal the advantage of using the implicit-symplectic integrator with respect to the IMEX scheme.

In this paper we analyze the second-order IMSP scheme introduced in [3]. We prove stability and positivity of solutions, provided a timestep restriction, also an a priori error estimate. The fully-discrete approximations, both in finite-difference/finite-element settings, improve in terms of accuracy the results obtained by the first-order IMSP scheme. Our numerical tests confirm the theoretical rates of convergence, and compare the second-order IMSP [3] and first-order IMSP [2] in terms of computational cost.

The paper is organized as follows. In Section 2 we recall some theoretical results from semigroup theory and make some assumptions which delimit the field of application for our results. In Section 3 we present the semi-discrete in time formulation of the first- and second-order IMSP schemes, in

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the framework of partitioned Runge-Kutta methods. The study of positivity for the solutions of the numerical approximations is performed in Section 4. The theoretical results concerning stability and error estimates for the semi-discrete in time formulation of IMSP schemes are presented in Sections 5 and 6, respectively. The fully discrete second-order IMSP algorithm is described in Section 7, and its behavior is exemplified with some numerical simulations in Section 8. Finally, some conclusions are drawn in Section 9.

2. Mathematical preliminaries.

Results from semigroup theory and an a priori estimate were used in [8] to prove the global existence and uniqueness of the classical solutions of the predator-prey system (1.1)-(1.2). We recall that, for the well-posedness of the problem, the reaction terms f, g are assumed to be locally Lipschitz, i.e., $\exists L > 0$ such that

$$|f(u_1, v_1) - f(u_2, v_2)| + |g(u_1, v_1) - g(u_2, v_2)| \leq L(|u_1 - u_2| + |v_1 - v_2|). \tag{2.1}$$

In order to insure the non-negativity of solutions corresponding to biologically meaningful densities, the reaction kinetics are also supposed to satisfy

$$f(0, v), g(u, 0) \geq 0, \qquad \forall u, v \geq 0. \tag{2.2}$$

Consequently, if the initial data $(u^0(x), v^0(x))$ are in $[0, +\infty)^2$ for all $x \in \Omega$ then, by a maximum principle, the solution $(u(x,t), v(x,t))$ 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

$$f(u, v) \leq u(1 - u), \qquad \forall u, v \geq 0, \tag{2.3}$$

and the function g satisfies a sub-linear growth in the second variable, namely $\exists C_g > 0$ such that

$$g(u, v) \leq C_g v, \qquad \forall u, v \geq 0. \tag{2.4}$$

We note that, from the assumptions (2.2), (2.3) and (2.4) it is easy to show that, for all $u, v \geq 0$,

$$g(u, 0) \;=\; f(0, v) = 0. \tag{2.5}$$

Assumptions (2.2), (2.3), (2.4) are not restrictive in that the principal population dynamics models, based on logistic prey growth and 'Holling types' functional predator response (well documented in specialized literature), satisfy the previous requirements (for review, see [9], [13], [18]). This is the case of the well-known Rosenzweig-MacArthur model [17], as well as models which couple logistic prey growth with Holling II and IV functional predator responses [12].

3. IMSP as Partitioned Runge-Kutta schemes.

3.1. Mathematical notations.

Let us introduce some mathematical notations. Consider the Banach space $L^2(\Omega)$ with norm

$$\|u\| := \left(\int_\Omega |u(x)|^2 \, dx \right)^{1/2}$$

and $(\cdot, \cdot)$ is the usual L^2 inner product. We denote by $\langle \cdot, \cdot \rangle$ the duality pairing between $(H^1(\Omega))'$ and $H^1(\Omega)$, where standard notations for the Sobolev space $H^1(\Omega)$ and its dual $(H^1(\Omega))'$ have been used. The norm of $(H^1(\Omega))'$ is denoted by $\| \cdot \|_*$. We also define $L^2(\Omega_T)$ as the Banach space $L^2(0, T, L^2(\Omega))$ of all the functions $u : (0, T) \to L^2(\Omega)$ such that $t \to \|u(t)\|$ is in $L^2(0, T)$, with norm

$$\|u\|_{L^2(\Omega_T)} := \left(\int_0^T \|u(t)\|^2 \, dt \right)^{1/2}.$$

A similar definition is used to denote the space $L^2(0, T, (H^1(\Omega))')$ as the space of all the functions $u : (0, T) \to (H^1(\Omega))'$ such that $t \to \|u(t)\|_*$ is in $L^2(0, T)$ with norm

$$\|u\|_{L^2(0,T,(H^1(\Omega))')} := \left(\int_0^T \|u(t)\|_*^2 \, dt \right)^{1/2}.$$

Let $D = diag(\, D_u,\, D_v \,)$ be a linear matrix operator and consider the vector $G(y) = [f(u,\, v),\; g(u,\, v)]^T$. With the previous notations, the system (1.1)-(1.2) leads to the following continuous-in-time weak formulation: find $y(\cdot,t) = [u(\cdot,t), v(\cdot,t)] \in H^1(\Omega) \times H^1(\Omega)$ such that

$$\big(y_t, \chi\big) + (D\nabla y, \nabla \chi) = (G(y), \chi) \tag{3.1}$$

for all $\chi \in H^1(\Omega) \times H^1(\Omega)$ and for almost every $t \in (0,T)$.

3.2. The algorithms. The implicit-explicit methods, which are widely used for solving (3.1), may be interpreted as partitioned Runge-Kutta methods ([14]). Indeed, by introducing two variables z and w such that $y = z + w$ the equivalent system

$$\big(z_t, \chi\big) + (D\nabla z, \nabla \chi) = 0, \tag{3.2}$$
$$\big(w_t, \chi\big) = (G(z+w), \chi) \tag{3.3}$$

can be solved for $z(\cdot,t)\, w(\cdot,t) \in H^1(\Omega) \times H^1(\Omega)$ in place of (3.1); the solution $y(\cdot,t)$ is then retrieved by adding their values. Then IMEX schemes use a partitioned Runge-Kutta method (see., e.g. [10]) consisting of a pair of implicit/explicit schemes, for finding the approximated solutions of (3.3).

In the same framework, in [4] a three-term splitting for the variable y was proposed, i.e., $y = z + w + q$, and a partitioned Runge-Kutta scheme for solving the system

$$\big(z_t, \chi\big) + (D\nabla z, \nabla \chi) = 0, \tag{3.4}$$
$$\big(w_t, \chi\big) = (G^{(u)}(z+w+q), \chi) \tag{3.5}$$
$$\big(q_t, \chi\big) = (G^{(v)}(z+w+q), \chi) \tag{3.6}$$

where $G = G^{(u)} + G^{(v)}$, $G^{(u)} = [\, f(u,\, v),\, \mathbf{0}\,]^T$, $G^{(v)} = [\,\mathbf{0},\; g(u,\, v)\,]^T$, was considered.

Given α, $\beta \geq 0$, the IMSP approach consists in using an implicit scheme for the variable z (which is related to diffusion)

$$\begin{array}{c|cc} & 0 & 0 \\ & \alpha & \beta \\ \hline & \alpha & \beta \end{array} \tag{3.7}$$

and a partitioned symplectic Runge-Kutta scheme [10] for the variables w and q (which are related to the reaction term)

$$\begin{array}{c|cc} & 0 & 0 \\ & \beta & \alpha \\ \hline & \beta & \alpha \end{array} \qquad \begin{array}{c|cc} & \beta & 0 \\ & \beta & 0 \\ \hline & \beta & \alpha. \end{array} \tag{3.8}$$

Consider a discretization of the temporal horizon $(0,T)$ based on a uniform mesh grid of $N+1$ points $t_n = n\Delta t$, $n = 0, \ldots, N$ with constant stepsize $\Delta t = T/N$. Let $v^0(x)$ and $u^0(x)$ be the predator-prey initial densities $v(x,0)$ and $u(x,0)$, $\forall x \in \Omega$.

The IMSP scheme (in weak form) is defined as follows: for $n = 0, \ldots, N-1$, find y^{n_1}, y^{n_2}, y^{n_3}, $y^{n+1} \in H^1(\Omega) \times H^1(\Omega)$ such that $\forall \chi \in H^1(\Omega) \times H^1(\Omega)$:

$$\begin{aligned}
&\Big(\frac{y^{n_1} - y^n}{\Delta t}, \chi\Big) = \beta\big(G^{(v)}(y^{n_1}), \chi\big)\\
&\Big(\frac{y^{n_2} - y^{n_1}}{\Delta t}, \chi\Big) + \alpha(D\nabla y^{n_1}, \nabla\chi) = \beta\big(G^{(u)}(y^{n_1}), \chi\big)\\
&\Big(\frac{y^{n_3} - y^{n_2}}{\Delta t}, \chi\Big) + \beta(D\nabla y^{n_3}, \nabla\chi) = \alpha\big(G^{(u)}(y^{n_3}), \chi\big)\\
&\Big(\frac{y^{n+1} - y^{n_3}}{\Delta t}, \chi\Big) = \alpha\big(G^{(v)}(y^{n_3}), \chi\big).
\end{aligned}$$

For $\beta = 1$ and $\alpha = 0$ we recover the first-order accurate IMSP scheme, see e.g., [2]. In this paper we analyze the second-order scheme obtained by setting $\beta = \alpha = 1/2$. We notice that, with this choice of parameters, the triplet (3.7)–(3.8) reduces to the Stormer-Verlet method written in partitioned form ([10]). It is a symplectic second-order procedure which, applied to our problem, provides the second-order IMSP scheme. In terms of the variables u and v, it can be written as follows. For $n = 0, \ldots, N-1$, find v^{n_1}, v^{n_2}, u^{n+1}, $v^{n+1} \in H^1(\Omega)$ such that $\forall \chi \in H^1(\Omega)$:

$$\left(\frac{v^{n_1}-v^n}{\Delta t}, \chi\right) = \frac{1}{2}\big(g(u^n, v^{n_1}), \chi\big) \tag{3.9}$$

$$\left(\frac{v^{n_2}-v^n}{\Delta t}, \chi\right) + \frac{D_v}{2}(\nabla(v^{n_1}+v^{n_2}), \nabla\chi) = \frac{1}{2}\big(g(u^n, v^{n_1}), \chi\big) \tag{3.10}$$

$$\left(\frac{u^{n+1}-u^n}{\Delta t}, \chi\right) + \frac{D_u}{2}(\nabla(u^n+u^{n+1}), \nabla\chi) = \frac{1}{2}\big(f(u^n, v^{n_1}) + f(u^{n+1}, v^{n_2}), \chi\big) \tag{3.11}$$

$$\left(\frac{v^{n+1}-v^n}{\Delta t}, \chi\right) + \frac{D_v}{2}(\nabla(v^{n_1}+v^{n_2}), \nabla\chi) = \frac{1}{2}\big(g(u^n, v^{n_1}) + g(u^{n+1}, v^{n_2}), \chi\big) \tag{3.12}$$

or, equivalently,
find v^{n_1}, u^{n_1}, v^{n_2}, u^{n_2}, v^{n_3}, u^{n+1}, $v^{n+1} \in H^1(\Omega)$ such that $\forall \chi \in H^1(\Omega)$:

$$\left(\frac{v^{n_1}-v^n}{\Delta t}, \chi\right) = \frac{1}{2}\big(g(u^n, v^{n_1}), \chi\big) \tag{3.13}$$

$$\left(\frac{u^{n_1}-u^n}{\Delta t}, \chi\right) + \frac{D_u}{2}(\nabla u^n, \nabla\chi) = 0 \tag{3.14}$$

$$\left(\frac{v^{n_2}-v^{n_1}}{\Delta t}, \chi\right) + \frac{D_v}{2}(\nabla v^{n_1}, \nabla\chi) = 0 \tag{3.15}$$

$$\left(\frac{u^{n_2}-u^{n_1}}{\Delta t}, \chi\right) = \frac{1}{2}\big(f(u^n, v^{n_1}), \chi\big) \tag{3.16}$$

$$\left(\frac{v^{n_3}-v^{n_2}}{\Delta t}, \chi\right) + \frac{D_v}{2}(\nabla v^{n_3}, \nabla\chi) = 0 \tag{3.17}$$

$$\left(\frac{u^{n+1}-u^{n_2}}{\Delta t}, \chi\right) + \frac{D_u}{2}(\nabla u^{n+1}, \nabla\chi) = \frac{1}{2}\big(f(u^{n+1}, v^{n_3}), \chi\big) \tag{3.18}$$

$$\left(\frac{v^{n+1}-v^{n_3}}{\Delta t}, \chi\right) = \frac{1}{2}\big(g(u^{n+1}, v^{n_3}), \chi\big) \tag{3.19}$$

In the following sections we will use either formulations, (3.9)-(3.12) or (3.13)-(3.19), to prove the positivity and stability of solutions, and to provide errors estimates.

4. Positivity. In order to prove positivity of the second-order IMSP solution, we need further assumptions, including a necessary bound on the timestep size.
We denote by $-\Delta_h$ the discrete Laplace operator depending on a (spatial) mesh-size h, used in the weak formulation equations (3.14)-(3.15), and let λ^h_{max} be its largest (non negative) eigenvalue. Then for the stability of the solutions u^{n_1}, v^{n_2} to the forward Euler schemes (3.14) and (3.15) we require the usual CFL condition

$$\Delta t \le 2/(\lambda^h_{max} \max\{D_u, D_v\}).$$

However, for the positivity of the IMSP solutions we need a slightly stronger assumption

$$\Delta t < \Delta t^\circ := \frac{2}{L + \lambda^h_{max} \max\{D_u, D_v\}}. \tag{4.1}$$

Moreover, we assume also that $\forall \Delta t \le \Delta t^\circ$ and $w, v > 0$, the equation

$$u - \Delta t D_u \Delta u = w + \Delta t f(u, v) \tag{4.2}$$

has a unique solution that depends continuously on Δt, D_u, w and v.

THEOREM 4.1. *Assume the timestep $\Delta t < \Delta t^\circ$ and Ω is a domain of class C^1. Provided the initial conditions are positive, i.e., $u^0(x) = u(x, 0) > 0, v^0(x) = v(x, 0) > 0, \forall x \in \Omega$, then the solutions $u^n(x), v^n(x)$ of the second-order scheme (3.13)-(3.19) are positive for all $n \ge 0$.* **Proof.** We will use an induction argument. Suppose that $u^n, v^n > 0$ in Ω, for a fixed arbitrary $n \ge 0$. First we prove that $v^{n_1}(x) \neq 0, \forall x \in \Omega$. Assume by contradiction that $\exists x_\circ \in \Omega$ such that $v^{n_1}(x_\circ) = 0$. Then, from

(3.13), using (2.5), we have that $0 = v^{n_1}(x_\circ) = v^n(x_\circ) + \Delta t g(u^n(x_\circ), v^{n_1}(x_\circ)) = v^n(x_\circ)$, which is in conflict with the positivity of v^n. Moreover, from (3.13), using (2.5), (2.1) and the assumption (4.1) on the timestep $\Delta t \leq \frac{2}{L}$, we also have

$$|v^{n_1} - v^n| = \frac{\Delta t}{2}|g(u^n, v^{n_1}) - g(u^n, 0)| \leq \frac{\Delta t}{2} L|v^{n_1}| \leq |v^{n_1}|.$$

From the above relation, and the induction assumption $v^n(x) > 0$, it follows that $v^{n_1}(x) > 0, \forall x \in \Omega$. To prove that u^{n_1} and v^{n_2} are both positive it is enough to apply the (stronger than the CFL condition) assumption (4.1) to the fully discrete approximations of (3.14)-(3.15). Indeed,

$$\begin{aligned}
u^{n_1} &= u^n + \Delta t \frac{D_u}{2} \Delta_h u^n = \big(1 - \Delta t \frac{D_u}{2} \lambda^h\big) u^n \geq \big(1 - \Delta t \frac{D_u}{2} \lambda^h_{\max}\big) u^n \\
&\geq \big(1 - \frac{2}{L + \lambda^h_{\max} \max\{D_u, D_v\}} \frac{D_u}{2} \lambda^h_{\max}\big) u^n = \big(1 - \frac{\lambda^h_{\max} D_u}{L + \lambda^h_{\max} \max\{D_u, D_v\}}\big) u^n \\
&\geq \big(1 - \frac{\lambda^h_{\max} D_u}{L + \lambda^h_{\max} D_u}\big) u^n > 0,
\end{aligned}$$

and similarly for v^{n_2}.
By (3.16), using (3.14), (2.5), (2.1), the induction assumption $u^n > 0$ and the time step condition (4.1), it follows that

$$\begin{aligned}
u^{n_2} &= u^{n_1} + \frac{\Delta t}{2} f(u^n, v^{n_1}) = u^n + \frac{\Delta t}{2} D_u \Delta_h u^n + \frac{\Delta t}{2} f(u^n, v^{n_1}) \\
&= u^n - \frac{\Delta t}{2} D_u \lambda^h u^n + \frac{\Delta t}{2}\big(f(u^n, v^{n_1}) - f(0, v^{n_1})\big) \\
&\geq u^n - \frac{\Delta t}{2} D_u \lambda^h_{\max} u^n - \frac{\Delta t}{2} L|u^n| = u^n - \frac{\Delta t}{2} D_u \lambda^h_{\max} u^n - \frac{\Delta t}{2} L u^n \\
&> \big(1 - \frac{1}{L + \lambda^h_{\max} \max\{D_u, D_v\}} (D_u \lambda^h_{\max} + L)\big) u^n \geq 0,
\end{aligned}$$

hence $u^{n_2}(x) > 0, \forall x \in \Omega$.
In the continuous-in-space version of the Backward Euler scheme (3.17), the positivity of v^{n_3} is a direct consequence of the maximum principle for elliptic equations with homogeneous Neumann boundary conditions (see e.g. [1, Theorem 3.6.2]). In the fully-discrete case, the proof is contingent to the type of spatial discretization. For example, in the piecewise linear finite-element approximation considered in Section 7, which is equivalent finite-difference representation on rectangular domains using the classical central difference schemes both in one and two dimensions, implemented taking into account zero-flux boundary conditions, the positivity of v^{n_3} follows straightforward from the positivity of v^{n_2}. We illustrate here the proof for the two dimensional case, the five-point stencil (discrete) Laplacian (a similar argument holds for the fourth-order nine-point Laplacian [19, Chapter 12]), when the grid spacing $\Delta x = \Delta y = h$. Let ℓ be the index for the x direction and the index m for the y direction. The standard central difference approximations for the second derivatives lead to the difference formula (corresponding to (3.17))

$$v^{n_3}_{\ell,m} - \Delta t \frac{D_v}{2} \frac{1}{h^2}\big(v^{n_3}_{\ell+1,m} + u^{n_3}_{\ell-1,m} + u^{n_3}_{\ell,m+1} + u^{n_3}_{\ell,m-1} - 4u^{n_3}_{\ell,m}\big) = v^{n_2}_{\ell,m}.$$

This leads to the conclusion that at any interior point which is (local) minimum point, $u^{n+1}_{\ell,m} = \min_{i,j} u^{n+1}_{i,j}$ has positive values

$$0 < v^{n_2}_{\ell,m} \leq v^{n_3}_{\ell,m},$$

and then the zero-flux boundary conditions complete the proof of this discrete maximum principle.
To prove that u^{n+1} is positive, since u^{n_2} and v^{n_3} are both positive we can consider the solution of (3.18) as a particular solution of (4.2). Consequently, $u^{n+1} = u^{n+1}(\Delta t)$ depends continuously on the timestep size Δt. Notice that for $\Delta t = 0$, $u^{n+1}(0) = u^{n_2} > 0$. In order to prove that $u^{n+1}(\Delta t)$ is positive for all $\Delta t > 0$, by continuity it is enough to prove that $u^{n+1} \neq 0$ for all $\Delta t > 0$. Suppose,

in contradiction, that $\exists \Delta t_\circ > 0$ such that $u^{n+1}(\Delta t) > 0$ for all $\Delta t < \Delta t_\circ$ and $u^{n+1}(\Delta t_\circ) = 0$. By (3.18) and (2.5) we obtain that

$$u^{n+1}(\Delta t_\circ) - \frac{\Delta t_\circ}{2} D_u \Delta u^{n+1}(\Delta t_\circ) = u^{n_2} + \frac{\Delta t_\circ}{2} f(u^{n+1}(\Delta t_\circ), v^{n_3}) = u^{n_2} > 0;$$

hence, from the strong maximum principle and Hopf's lemma for elliptic equations, the positivity of $u^{n+1}(\Delta t_\circ)$ follows - which is in conflict with the assumption.
Finally, the positivity of v^{n+1} follows by (3.19), using (2.5), (2.1), the positivity of v^{n_3} and the assumption $\Delta t < \frac{2}{L}$

$$\begin{aligned} v^{n+1} &= v^{n_3} + \frac{\Delta t}{2} g(u^{n+1,v^{n_3}}) = v^{n_3} + \frac{\Delta t}{2}\big(g(u^{n+1}, v^{n_3}) - g(u^{n+1}, 0)\big) \\ &\geq v^{n_3} - \frac{\Delta t}{2} L|v^{n_3}| = \big(1 - \frac{\Delta t}{2} L\big) v^{n_3} > 0. \end{aligned}$$

□

5. Stability.

5.1. u^n estimate.

We derive energy estimates for u in a usual manner. First we use $(u^{n+1} + u^n)/2$ as the test function in (3.11) to obtain the following energy equality

$$\begin{aligned} &\frac{1}{2\Delta t}\|u^{n+1}\|^2 - \frac{1}{2\Delta t}\|u^n\|^2 + D_u \|\nabla \frac{u^{n+1} + u^n}{2}\|^2 \\ &= \frac{1}{4}\langle f(u^n, v^{n_1}) + f(u^{n+1}, v^{n_2}), u^{n+1} + u^n \rangle. \end{aligned} \tag{5.1}$$

Remark 5.1. *If f depends linearly only on the first variable (i.e., $f(u, v) = \lambda u$), (5.1) gives the same energy estimate as the Crank-Nicolson method.*

Proposition 5.1. *For all $n = 1, \ldots, N$ we have*

$$\|u^n\| \leq 2|\Omega|^{\frac{1}{2}}. \tag{5.2}$$

Proof. First we multiply (5.1) by $2\Delta t$, then use assumption (2.3), the polarized identity, and that u^n, v^n are non-negative for all n, to get

$$\begin{aligned} &\|u^{n+1}\|^2 - \|u^n\|^2 + 2\Delta t D_u \|\nabla \frac{u^{n+1} + u^n}{2}\|^2 \\ &= \frac{\Delta t}{2}\langle f(u^n, v^{n_1}) + f(u^{n+1}, v^{n_2}), u^{n+1} + u^n \rangle \\ &\leq \frac{\Delta t}{2}\langle u^n(1 - u^n), u^{n+1} + u^n \rangle + \frac{\Delta t}{2}\langle u^{n+1}(1 - u^{n+1}), u^{n+1} + u^n \rangle \\ &= \frac{\Delta t}{2}\langle u^n - |u^n|^2, u^{n+1} + u^n \rangle + \frac{\Delta t}{2}\langle u^{n+1} - |u^{n+1}|^2, u^{n+1} + u^n \rangle \\ &= \frac{\Delta t}{2}\langle u^n - |u^n|^2, u^{n+1} \rangle + \frac{\Delta t}{2}\langle u^n - |u^n|^2, u^n \rangle \\ &\quad + \frac{\Delta t}{2}\langle u^{n+1} - |u^{n+1}|^2, u^{n+1} \rangle + \frac{\Delta t}{2}\langle u^{n+1} - |u^{n+1}|^2, u^n \rangle \\ &= \frac{\Delta t}{2}\langle u^n - |u^n|^2, u^{n+1} \rangle + \frac{\Delta t}{2}\big(\|u^n\|^2 - \|u^n\|^3_{L^3(D)}\big) \\ &\quad + \frac{\Delta t}{2}\big(\|u^{n+1}\|^2 - \|u^{n+1}\|^3_{L^3(D)}\big) + \frac{\Delta t}{2}\langle u^{n+1} - |u^{n+1}|^2, u^n \rangle \\ &\leq \frac{\Delta t}{2}\langle u^n, u^{n+1} \rangle + \frac{\Delta t}{2}\big(\|u^n\|^2 - \|u^n\|^3_{L^3(D)}\big) \\ &\quad + \frac{\Delta t}{2}\big(\|u^{n+1}\|^2 - \|u^{n+1}\|^3_{L^3(D)}\big) + \frac{\Delta t}{2}\langle u^{n+1}, u^n \rangle \\ &= \frac{\Delta t}{2}\big(\|u^n\|^2 + \|u^{n+1}\|^2 - \|u^{n+1} - u^n\|^2\big) + \frac{\Delta t}{2}\big(\|u^n\|^2 - \|u^n\|^3_{L^3(D)}\big) \\ &\quad + \frac{\Delta t}{2}\big(\|u^{n+1}\|^2 - \|u^{n+1}\|^3_{L^3(D)}\big) \end{aligned}$$

$$= \Delta t\big(\|u^n\|^2 + \|u^{n+1}\|^2\big) - \frac{\Delta t}{2}\|u^{n+1} - u^n\|^2 - \frac{\Delta t}{2}\|u^n\|^3_{L^3(\Omega)} - \frac{\Delta t}{2}\|u^{n+1}\|^3_{L^3(\Omega)}$$

which simplifies to

$$\begin{aligned}
&\|u^{n+1}\|^2 - \|u^n\|^2 + \frac{\Delta t}{2}\|u^{n+1} - u^n\|^2 + 2\Delta t D_u\|\nabla \frac{u^{n+1} + u^n}{2}\|^2 \\
&\leq \Delta t\big(\|u^n\|^2 + \|u^{n+1}\|^2\big) - \frac{\Delta t}{2}\|u^n\|^3_{L^3(D)} - \frac{\Delta t}{2}\|u^{n+1}\|^3_{L^3(D)}.
\end{aligned}$$

Using now Hölder's inequality ($\|\phi\|_{L^2(\Omega)} \leq |\Omega|^{\frac{1}{6}}\|\phi\|_{L^3(\Omega)}$) we have

$$\begin{aligned}
&\|u^{n+1}\|^2 - \|u^n\|^2 + \frac{\Delta t}{2}\|u^{n+1} - u^n\|^2 + 2\Delta t D_u\|\nabla \frac{u^{n+1} + u^n}{2}\|^2 \\
&\leq \Delta t\big(\|u^n\|^2 + \|u^{n+1}\|^2\big) - \frac{\Delta t}{2}|\Omega|^{-\frac{1}{2}}\|u^n\|^3_{L^2(D)} - \frac{\Delta t}{2}|\Omega|^{-\frac{1}{2}}\|u^{n+1}\|^3_{L^2(D)} \\
&\leq \Delta t\big(\|u^n\| + \|u^{n+1}\|\big)^2 - \frac{\Delta t}{2}|\Omega|^{-\frac{1}{2}}\big(\|u^n\|^3_{L^2(D)} + \|u^{n+1}\|^3_{L^2(D)}\big) \\
&= \Delta t\big(\|u^n\| + \|u^{n+1}\|\big)^2 - \frac{\Delta t}{2}|\Omega|^{-\frac{1}{2}}\big(\|u^n\| + \|u^{n+1}\|\big)\big(\|u^n\|^2 + \|u^{n+1}\|\|u^n\| + \|u^{n+1}\|^2\big) \\
&\leq \Delta t\big(\|u^n\| + \|u^{n+1}\|\big)^2 - \frac{\Delta t}{2}|\Omega|^{-\frac{1}{2}}\big(\|u^n\| + \|u^{n+1}\|\big)\big(\|u^n\|^2 + \|u^{n+1}\|^2\big) \\
&= \big(\|u^n\| + \|u^{n+1}\|\big)\Big(\Delta t\big(\|u^n\| + \|u^{n+1}\|\big) - \frac{\Delta t}{2}|\Omega|^{-\frac{1}{2}}\big(\|u^n\|^2 + \|u^{n+1}\|^2\big)\Big)
\end{aligned}$$

which dividing by $(\|u^n\| + \|u^{n+1}\|)$ yields

$$\begin{aligned}
&\|u^{n+1}\| - \|u^n\| + \frac{\Delta t}{2}\frac{\|u^{n+1} - u^n\|^2}{\|u^n\| + \|u^{n+1}\|} + 2\Delta t D_u \frac{\|\nabla \frac{u^{n+1}+u^n}{2}\|^2}{\|u^n\| + \|u^{n+1}\|} \\
&\leq \Delta t\big(\|u^n\| + \|u^{n+1}\|\big) - \frac{\Delta t}{2}|\Omega|^{-\frac{1}{2}}\big(\|u^n\|^2 + \|u^{n+1}\|^2\big).
\end{aligned}$$

Furthermore, division by $\|u^n\|\|u^{n+1}\|$ yields

$$\frac{1}{\|u^{n+1}\|} - \frac{1}{\|u^n\|} + \Delta t\big(\frac{1}{\|u^n\|} + \frac{1}{\|u^{n+1}\|}\big) \geq |\Omega|^{-\frac{1}{2}}\Delta t + \Delta t\mathcal{E}_n, \tag{5.3}$$

where

$$\mathcal{E}_n := \frac{1}{\|u^n\|\|u^{n+1}\|(\|u^n\| + \|u^{n+1}\|)}\Big(\frac{1}{2}\big(\|u^{n+1} - u^n\|^2\big) + 2D_u\|\nabla \frac{u^{n+1} + u^n}{2}\|^2\Big).$$

Now we multiply (5.3) by $\frac{(1+\Delta t)^n}{(1-\Delta t)^n}$ and sum for $n = 0, \ldots, N-1$ to obtain

$$\begin{aligned}
\frac{1}{\|u^N\|}\frac{(1+\Delta t)^N}{(1-\Delta t)^{N-1}} - \frac{1}{\|u^0\|}(1-\Delta t) \geq \qquad & \frac{1}{2}|\Omega|^{-\frac{1}{2}}(1-\Delta t)\Big(\Big(\frac{1+\Delta t}{1-\Delta t}\Big)^N - 1\Big) \\
+ \Delta t\sum_{n=0}^{N-1} \frac{(1+\Delta t)^n}{(1-\Delta t)^n}\mathcal{E}_n.
\end{aligned}$$

Next we multiply by $\frac{(1-\Delta t)^{N-1}}{(1+\Delta t)^N}$

$$\begin{aligned}
&\frac{1}{\|u^N\|} - \frac{1}{\|u^0\|}(1-\Delta t)\frac{(1-\Delta t)^{N-1}}{(1+\Delta t)^N} \geq \frac{1}{2}|\Omega|^{-\frac{1}{2}}\Big(1 - \frac{(1-\Delta t)^N}{(1+\Delta t)^N}\Big) \\
&+ \Delta t\frac{(1-\Delta t)^{N-1}}{(1+\Delta t)^N}\sum_{n=0}^{N-1} \frac{(1+\Delta t)^n}{(1-\Delta t)^n}\mathcal{E}_n
\end{aligned}$$

and rearrange

$$\|u^N\| \leq \frac{1}{\frac{1}{\|u^0\|}\frac{(1-\Delta t)^N}{(1+\Delta t)^N} + \frac{1}{2}|\Omega|^{-\frac{1}{2}}\Big(1 - \frac{(1-\Delta t)^N}{(1+\Delta t)^N}\Big) + \Delta t\frac{(1-\Delta t)^{N-1}}{(1+\Delta t)^N}\sum_{n=0}^{N-1} \frac{(1+\Delta t)^n}{(1-\Delta t)^n}\mathcal{E}_n}$$

which finally gives (5.2). □

5.2. v^n estimate. We will derive now energy estimates for v. First, subtract (3.10) from (3.12) to get

$$\frac{v^{n+1}-v^{n_2}}{\Delta t}=\frac{1}{2}g(u^{n+1},v^{n_2}), \tag{5.4}$$

then multiply by v^{n+1} and integrate over the space domain to obtain

$$\frac{1}{2\Delta t}\|v^{n+1}\|^2-\frac{1}{2\Delta t}\|v^{n_2}\|^2+\frac{1}{2\Delta t}\|v^{n+1}-v^{n_2}\|^2=\frac{1}{2}\langle g(u^{n+1},v^{n_2}),v^{n+1}\rangle. \tag{5.5}$$

Next subtract (3.9) from (3.10) to get

$$\frac{v^{n_2}-v^{n_1}}{\Delta t}=\frac{1}{2}\big(D_v\Delta_h v^{n_1}+D_v\Delta_h v^{n_2}\big), \tag{5.6}$$

which, when tested with $(v^{n_2}+v^{n_1})/2$, gives

$$\frac{1}{2\Delta t}\|v^{n_2}\|^2-\frac{1}{2\Delta t}\|v^{n_1}\|^2+D_v\|\nabla_h\frac{v^{n_1}+v^{n_2}}{2}\|^2=0. \tag{5.7}$$

Multiplying (3.9) with v^{n_1} yields

$$\frac{1}{2\Delta t}\|v^{n_1}\|^2-\frac{1}{2\Delta t}\|v^{n}\|^2+\frac{1}{2\Delta t}\|v^{n_1}-v^{n}\|^2=\frac{1}{2}\langle g(u^{n},v^{n_1}),v^{n_1}\rangle. \tag{5.8}$$

Finally add (5.5), (5.7) and (5.8) and obtain

$$\begin{aligned}&\frac{1}{2\Delta t}\|v^{n+1}\|^2-\frac{1}{2\Delta t}\|v^{n}\|^2\\&+\frac{1}{2\Delta t}\|v^{n+1}-v^{n_2}\|^2+\frac{1}{2\Delta t}\|v^{n_1}-v^{n}\|^2+D_v\|\nabla_h\frac{v^{n_1}+v^{n_2}}{2}\|^2\\&=\frac{1}{2}\langle g(u^{n+1},v^{n_2}),v^{n+1}\rangle+\frac{1}{2}\langle g(u^{n},v^{n_1}),v^{n_1}\rangle.\end{aligned} \tag{5.9}$$

Since the nonlinearity g depends heavily on the intermediary time steps n_1, n_2, bounding the RHS of (5.9) in terms of v^{n+1}, v^n requires manipulation of the intermediary relations (5.5), (5.7), (5.8).

PROPOSITION 5.2. *For all $m=1,\dots,N$ we have*

$$\begin{aligned}&\|v^m\|^2+\frac{1}{1-\frac{1}{2}C_g\Delta t}\sum_{n=0}^{m-1}\|v^{n+1}-v^{n_2}\|^2+\frac{1+\frac{1}{2}C_g\Delta t}{(1-C_g\Delta t)(1-\frac{1}{2}C_g\Delta t)}\sum_{n=0}^{m-1}\|v^{n_1}-v^{n}\|^2\\&\quad+\Delta tD_v\frac{2+C_g\Delta t}{1-\frac{1}{2}C_g\Delta t}\|\nabla_h\sum_{n=0}^{m-1}\frac{v^{n_1}+v^{n_2}}{2}\|^2+\frac{\frac{1}{2}C_g\Delta t}{1-\frac{1}{2}C_g\Delta t}\sum_{n=0}^{m-1}\big|\|v^{n_2}\|-\|v^{n+1}\|\big|^2\\&\le\|v^0\|^2\exp\Big(\frac{2C_gN\Delta t}{(1-\frac{1}{2}C_g\Delta t)(1-C_g\Delta t)}\Big).\end{aligned} \tag{5.10}$$

Proof. From (5.7) we deduce

$$\|v^{n_2}\|^2+2\Delta tD_v\|\nabla_h\frac{v^{n_1}+v^{n_2}}{2}\|^2\le\|v^{n_1}\|^2,$$

while using assumptions (2.4), (4.1) and Theorem 4.1, relation (5.8) yields

$$\|v^{n_1}\|^2+\frac{1}{1-C_g\Delta t}\|v^{n_1}-v^{n}\|^2\le\frac{1}{1-C_g\Delta t}\|v^{n}\|^2, \tag{5.11}$$

and therefore

$$\|v^{n_2}\|^2+2\Delta tD_v\|\nabla_h\frac{v^{n_1}+v^{n_2}}{2}\|^2+\frac{1}{1-C_g\Delta t}\|v^{n_1}-v^{n}\|^2\le\frac{1}{1-C_g\Delta t}\|v^{n}\|^2. \tag{5.12}$$

Multiplying (5.9) by Δt, using (2.4), the Cauchy-Schwarz inequality, (5.11)-(5.12), we obtain

$$
\begin{aligned}
&\|v^{n+1}\|^2-\|v^n\|^2+\frac{1}{1-\frac{1}{2}C_g\Delta t}\|v^{n+1}-v^{n_2}\|^2+\frac{1+\frac{1}{2}C_g\Delta t}{(1-C_g\Delta t)(1-\frac{1}{2}C_g\Delta t)}\|v^{n_1}-v^n\|^2\\
&\quad+\Delta t D_v\frac{2+C_g\Delta t}{1-\frac{1}{2}C_g\Delta t}\|\nabla_h\frac{v^{n_1}+v^{n_2}}{2}\|^2+\frac{\frac{1}{2}C_g\Delta t}{1-\frac{1}{2}C_g\Delta t}\big|\|v^{n_2}\|-\|v^{n+1}\|\big|^2\\
&\le\frac{2C_g\Delta t}{(1-\frac{1}{2}C_g\Delta t)(1-C_g\Delta t)}\|v^n\|^2.
\end{aligned}
$$

Summation from $n=0$ to $m-1$ and use of Gronwall's inequality consequently gives (5.10). □

6. Error estimates. Let $\varepsilon_u^{n+\frac{1}{2}},\varepsilon_v^{n+\frac{1}{2}}\in(H^1(\Omega))'$ denote the following local truncation errors for scheme (3.11)-(3.10)

$$
\begin{aligned}
\langle\varepsilon_u^{n+\frac{1}{2}},\chi\rangle&:=\frac{1}{\Delta t}\langle u(t_{n+1})-u(t_n),\chi\rangle-\frac{1}{2}\big\langle f(u(t_n),v(t_n))\\
&\quad+f(u(t_{n+1}),v(t_{n+1})),\chi\big\rangle+D_u(\nabla\frac{u(t_{n+1})+u(t_n)}{2},\nabla\chi),
\end{aligned}\tag{6.1}
$$

$$
\begin{aligned}
\langle\varepsilon_v^{n+\frac{1}{2}},\chi\rangle&:=\frac{1}{\Delta t}\langle v(t_{n+1})-v(t_n),\chi\rangle-\frac{1}{2}\big\langle g(u(t_n),v(t_n))\\
&\quad+g(u(t_{n+1}),v(t_{n+1})),\chi\big\rangle+D_v(\nabla\frac{v(t_{n+1})+v(t_n)}{2},\nabla\chi),
\end{aligned}\tag{6.2}
$$

where $\chi\in H^1(\Omega)$, and $e_u^n,e_v^n\in H^1(\Omega)$ denote the pointwise errors

$$
e_u^n=u(t_n)-u^n,\qquad e_v^n=v(t_n)-v^n.
$$

LEMMA 6.1. *Assume the classical solution of* (1.1)-(1.2) *has the following regularity*

$$
\frac{d^2u}{dt^2},\frac{d^2v}{dt^2}\in L^2(0,T,H^1(\Omega)),\qquad\frac{du}{dt},\frac{dv}{dt},\frac{d^3u}{dt^3},\frac{d^3v}{dt^3}\in L^2(0,T,(H^1(\Omega))').\tag{6.3}
$$

Then the truncation errors satisfy the following bound:

$$
\begin{aligned}
&\Delta t\sum_{n=0}^{N-1}\Big(\frac{1}{D_u}\|\varepsilon_u^{n+\frac{1}{2}}\|_*^2+\frac{1}{D_v}\|\varepsilon_v^{n+\frac{1}{2}}\|_*^2\Big)\\
&\le\frac{\Delta t^4}{2^4}\int_{t_0}^{t_N}\Big[\frac{1}{5D_u}\|u'''(t)\|^2+\frac{1}{5D_v}\|v'''(t)\|^2\\
&\quad+\frac{1}{3}\Big(\frac{1}{D_u}\|\nabla f\Big\|^2_{L^\infty(0,T;L^\infty(\Omega))}+\frac{1}{D_v}\|\nabla g\|^2_{L^\infty(0,T;L^\infty(\Omega))}\Big)(\|u''(t)\|^2+\|v''(t)\|^2)\\
&\quad+\Big(\frac{1}{D_u}\|\nabla^2 f\|^2_{L^\infty(0,T;L^\infty(\Omega))}+\frac{1}{D_v}\|\nabla^2 g\|^2_{L^\infty(0,T;L^\infty(\Omega))}\Big)(\|u'(t)\|^4_{L^4(\Omega)}+\|v'(t)\|^4_{L^4(\Omega)})\\
&\quad+\frac{1}{12}\big(D_u\|\nabla u''(t)\|^2+D_v\|\nabla v''(t)\|^2\big)\Big]dt.
\end{aligned}\tag{6.4}
$$

Proof. Using Taylor's formula to expand $v(t_n),v(t_{n+1}),u(t_n),u(t_{n+1})$ about $t_{n+\frac{1}{2}}$ we have

$$
\begin{aligned}
\langle\varepsilon_u^{n+\frac{1}{2}},\chi\rangle&\le\frac{\Delta t^{3/2}}{8\sqrt{5}}\Big(\int_{t_n}^{t_n+\Delta t}\|u'''(t)\|^2dt\Big)^{1/2}\|\chi\|\\
&\quad+\frac{\Delta t^{3/2}}{8\sqrt{3}}\|\nabla f\|_{L^\infty(0,T;L^\infty(\Omega))}\Big(\int_{t_n}^{t_{n+1}}(\|u''(t)\|^2+\|v''(t)\|^2)dt\Big)^{1/2}\|\chi\|\\
&\quad+\frac{\Delta t^{3/2}}{8}\|\nabla^2 f\|_{L^\infty(0,T;L^\infty(\Omega))}\Big(\int_{t_n}^{t_{n+1}}(\|u'(t)\|^4_{L^4(\Omega)}+\|v'(t)\|^4_{L^4(\Omega)})dt\Big)^{1/2}\|\chi\|\\
&\quad+\frac{\Delta t^{3/2}}{16\sqrt{3}}D_u\Big(\int_{t_n}^{t_n+\Delta t}\|\nabla u''(t)\|^2dt\Big)^{1/2}\|\nabla\chi\|,
\end{aligned}
$$

and

$$\langle \varepsilon_v^{n+\frac{1}{2}}, \chi\rangle \le \frac{\Delta t^{3/2}}{8\sqrt{5}}\Big(\int_{t_n}^{t_n+\Delta t} \|v'''(t)\|^2 dt\Big)^{1/2}\|\chi\|$$
$$+ \frac{\Delta t^{3/2}}{8\sqrt{3}}\Big\|\nabla g\Big\|_{L^\infty(0,T;L^\infty(\Omega))}\Big(\int_{t_n}^{t_{n+1}} (\|u''(t)\|^2 + \|v''(t)\|^2)dt\Big)^{1/2}\|\chi\|$$
$$+ \frac{\Delta t^{3/2}}{8}\Big\|\nabla^2 g\Big\|_{L^\infty(0,T;L^\infty(\Omega))}\Big(\int_{t_n}^{t_{n+1}} (\|u'(t)\|^4_{L^4(\Omega)} + \|v'(t)\|^4_{L^4(\Omega)})dt\Big)^{1/2}\|\chi\|$$
$$+ \frac{\Delta t^{3/2}}{16\sqrt{3}}D_v\Big(\int_{t_n}^{t_n+\Delta t} \|\nabla v''(t)\|^2 dt\Big)^{1/2}\|\nabla\chi\|,$$

which yields (6.4) in a standard manner. $\square$

To establish the error estimate for the numerical solution, we also need an energy-type bound for the errors in terms of local truncation errors. We start by proving a preliminary estimate.

LEMMA 6.2. *Assume that the reaction terms and the solution to the system (3.9)-(3.12) are sufficiently regular. Then, the following inequalities hold*

$$\Big\|\nabla\frac{(v^{n+1}+v^n)-(v^{n_2}+v^{n_1})}{2}\Big\| \le C\Delta t^2, \tag{6.5}$$

$$\begin{aligned}&\big\|f(u^n,v^n)-f(u^n,v^{n_1})+f(u^{n+1},v^{n+1})-f(u^{n+1},v^{n_2})\big\|\\ &\quad+\big\|g(u^n,v^n)-g(u^n,v^{n_1})+g(u^{n+1},v^{n+1})-g(u^{n+1},v^{n_2})\big\| \le C\Delta t^2.\end{aligned} \tag{6.6}$$

Proof. First add (3.9) and (3.10), then subtract the result from (3.12) to get

$$(v^{n+1}+v^n)-(v^{n_2}+v^{n_1}) = \frac{\Delta t}{2}\big(g(u^{n+1},v^{n_2})-g(u^n,v^{n_1})\big).$$

Next we use Taylor expansion, assume that the gradient and the Hessian of g are uniformly bounded, and that the sequences $\{u^n\},\{v^{n_1}\},\{v^{n_2}\}$ are uniformly bounded in $H^1(\Omega)$, to obtain

$$\Big\|\nabla\frac{(v^{n+1}+v^n)-(v^{n_2}+v^{n_1})}{2}\Big\| \le C\Delta t\Big(\|u^{n+1}-u^n\|_{H^1(\Omega)} + \|v^{n_2}-v^{n_1}\|_{H^1(\Omega)}\Big).$$

Finally, provided that $\{u^n\},\{v^{n_1}\},\{v^{n_2}\}$ are uniformly bounded in $H^3(\Omega)$ and $f,\nabla f$ are bounded, the equations (3.11) and (5.6) imply the estimate (6.5).

To prove (6.6), we proceed similarly. We note that subtracting (3.10) from (3.12) gives

$$\frac{v^{n+1}-v^{n_2}}{\Delta t} = \frac{1}{2}g(u^{n+1},v^{n_2}). \tag{6.7}$$

Then a combination of Taylor expansions and manipulation of equations (3.9), (6.7), (3.11) and (5.6) yields the estimate (6.6), and concludes the argument. $\square$

LEMMA 6.3. *For a sufficiently small timestep, the error in the implicit-symplectic scheme (3.11)-(3.9) satisfies the following stability property*

$$\begin{aligned}&\|e_u^N\|^2+\|e_v^N\|^2+\Delta t\sum_{n=0}^{N-1}\Big(D_u\big\|\nabla\frac{e_u^{n+1}+e_u^n}{2}\big\|^2 + D_v\big\|\nabla\frac{e_v^{n+1}+e_v^n}{2}\big\|^2\Big)\\ &\le \exp\big(\tfrac{CT}{1-C\Delta t}\big)\Big(\|e_u^0\|^2+\|e_v^0\|^2+\Delta t\sum_{n=0}^{N-1}\big(\frac{1}{D_u}\|\varepsilon_u^{n+\frac{1}{2}}\|_*^2+\frac{2}{D_v}\|\varepsilon_v^{n+\frac{1}{2}}\|_*^2\big)+CT\Delta t^4\Big).\end{aligned} \tag{6.8}$$

Proof. We subtract (3.11), (3.12) from (6.1)-(6.2) to obtain

$$\frac{1}{\Delta t}\langle e_u^{n+1}-e_u^n,\chi\rangle + D_u(\nabla\frac{e_u^{n+1}+e_u^n}{2},\nabla\chi) = \langle\varepsilon_u^{n+\frac{1}{2}},\chi\rangle$$
$$+\frac{1}{2}\big\langle f(u(t_n),v(t_n))-f(u^n,v^{n_1})+f(u(t_{n+1}),v(t_{n+1}))-f(u^{n+1},v^{n_2}),\chi\big\rangle,$$

$$\frac{1}{\Delta t}\langle e_v^{n+1}-e_v^n,\chi\rangle + D_v(\nabla\frac{e_v^{n+1}+e_v^n}{2},\nabla\chi)$$
$$+ D_v(\nabla\frac{(v^{n+1}+v^n)-(v^{n_1}+v^{n_2})}{2},\nabla\chi)$$
$$= \langle \varepsilon_v^{n+\frac{1}{2}},\chi\rangle + \frac{1}{2}\big\langle g(u(t_n),v(t_n)) - g(u^n,v^{n_1}) + g(u(t_{n+1}),v(t_{n+1})) - g(u^{n+1},v^{n_2}),\chi\big\rangle.$$

Next we test with $\frac{e_u^{n+1}+e_u^n}{2}$, $\frac{e_v^{n+1}+e_v^n}{2}$, respectively, add up, use the Cauchy-Schwarz inequality and rearrange to obtain

$$\begin{aligned}
&\frac{1}{2\Delta t}\big(\|e_u^{n+1}\|^2+\|e_v^{n+1}\|^2-\|e_u^n\|^2-\|e_v^n\|^2\big) \\
&\quad+\frac{D_u}{2}\big\|\nabla\frac{e_u^{n+1}+e_u^n}{2}\big\|^2+\frac{D_v}{2}\big\|\nabla\frac{e_v^{n+1}+e_v^n}{2}\big\|^2 \\
&\le \frac{1}{2D_u}\|\varepsilon_u^{n+\frac{1}{2}}\|_*^2+\frac{1}{D_v}\|\varepsilon_v^{n+\frac{1}{2}}\|_*^2+\frac{D_u}{2}\big\|\frac{e_u^{n+1}+e_u^n}{2}\big\|^2+\frac{D_v}{4}\big\|\frac{e_v^{n+1}+e_v^n}{2}\big\|^2 \\
&\quad+D_v\Big\|\nabla\frac{(v^{n+1}+v^n)-(v^{n_1}+v^{n_2})}{2}\Big\|^2 \\
&\quad+\frac{1}{2}\big\|f(u(t_n),v(t_n))-f(u^n,v^{n_1})+f(u(t_{n+1}),v(t_{n+1}))-f(u^{n+1},v^{n_2})\big\|\big\|\frac{e_u^{n+1}+e_u^n}{2}\big\| \\
&\quad+\frac{1}{2}\|g(u(t_n),v(t_n))-g(u^n,v^{n_1})+g(u(t_{n+1}),v(t_{n+1}))-g(u^{n+1},v^{n_2})\|\big\|\frac{e_v^{n+1}+e_v^n}{2}\big\|.
\end{aligned} \tag{6.9}$$

The third-to-last term in the right-hand-side is going to be handled by the estimate (6.5) in the Lemma 6.2. The last two terms are treated with a triangle inequality and the following estimate, which is again a consequence of the Taylor expansion and equations (3.11), (3.12)

$$\begin{aligned}
&\|f(u(t_{n+1}),v(t_{n+1}))+f(u(t_n),v(t_n)-\big(f(u^{n+1},v^{n+1})+f(u^n,v^n)\big)\| \\
&\quad+\|g(u(t_{n+1}),v(t_{n+1}))+g(u(t_n),v(t_n)-\big(g(u^{n+1},v^{n+1})+g(u^n,v^n)\big)\| \\
&\le L(\|e_u^{n+1}+e_u^n\|+\|e_v^{n+1}+e_v^n\|)+C\Delta t^2.
\end{aligned} \tag{6.10}$$

Hence using (6.5), (6.6) and (6.10) in (6.9) we obtain

$$\begin{aligned}
&\frac{1}{2\Delta t}\big(\|e_u^{n+1}\|^2+\|e_v^{n+1}\|^2-\|e_u^n\|^2-\|e_v^n\|^2\big) \\
&\quad+\frac{D_u}{2}\big\|\nabla\frac{e_u^{n+1}+e_u^n}{2}\big\|^2+\frac{D_v}{2}\big\|\nabla\frac{e_v^{n+1}+e_v^n}{2}\big\|^2 \\
&\le \frac{1}{2D_u}\|\varepsilon_u^{n+\frac{1}{2}}\|_*^2+\frac{1}{D_v}\|\varepsilon_v^{n+\frac{1}{2}}\|_*^2+C\Big(\|e_u^{n+1}\|^2+\|e_v^{n+1}\|^2+\|e_u^n\|^2+\|e_v^n\|^2\Big)+C\Delta t^4.
\end{aligned}$$

Summing for $n=0$ to $N-1$ yields

$$\begin{aligned}
&\|e_u^N\|^2+\|e_v^N\|^2+D_u\Delta t\sum_{n=0}^{N-1}\big\|\nabla\frac{e_u^{n+1}+e_u^n}{2}\big\|^2+D_v\Delta t\sum_{n=0}^{N-1}\big\|\nabla\frac{e_v^{n+1}+e_v^n}{2}\big\|^2 \\
&\le \|e_u^0\|^2+\|e_v^0\|^2+\frac{1}{D_u}\Delta t\sum_{n=0}^{N-1}\|\varepsilon_u^{n+\frac{1}{2}}\|_*^2+\frac{2}{D_v}\Delta t\sum_{n=0}^{N-1}\|\varepsilon_v^{n+\frac{1}{2}}\|_*^2+CT\Delta t^4 \\
&\quad+C\Delta t\sum_{n=0}^{N}\Big(\|e_u^n\|^2+\|e_v^n\|^2\Big).
\end{aligned}$$

Then under a small timestep condition, the discrete Gronwall inequality [11] yields (6.8). □

The error estimate of the semi-discrete-in time approximation (3.9)-(3.12) follows necessarily, proving the second-order accuracy in time.

PROPOSITION 6.4. *Under the assumptions of Lemmata 6.1-6.3, suppose also that the error in the initial data is second-order accurate. Then, there exists a positive constant $C_\circ$ such that*

$$\|e_u^N\|^2+\|e_v^N\|^2+\Delta t\sum_{n=0}^{N-1}\Big(D_u\big\|\nabla\frac{e_u^{n+1}+e_u^n}{2}\big\|^2+D_v\big\|\nabla\frac{e_v^{n+1}+e_v^n}{2}\big\|^2\Big)\le C_\circ\Delta t^4.$$

7. A fully discrete approximation. For the numerical implementation of the second-order IMSP scheme, we follow [7] and use the Galerkin finite-element approximation with piecewise linear basis functions (which has an equivalent standard finite-difference representation on rectangular domains). Let T^h be a quasi-uniform partitioning of Ω into disjoint open simplices $\{\tau\}$ with $h_\tau :=$diam τ and $h :=\max_{\tau\in T^h} h_\tau$, so that $\bar{\Omega} = \cup_{\tau\in T^h}\bar{\tau}$. We use the standard Galerkin finite element space of piecewise linear continuous functions defined by:

$$S^h := \{v \in C(\bar{\Omega}) : v|_\tau \text{ is linear } \forall \tau \in \Omega^h\} \subset H^1(\Omega).$$

We shall also need the Lagrange interpolation operator $\pi^h : C(\bar{\Omega}) \to S^h$ s.t. $\pi^h(v(x_j) = v(x_j)$ for all $j = 0, \dots, M$ where $\{x_j\}_{j=0}^M$ are the nodesof the triangulation. Let $\{\phi\}_{j=0}^M$ be the standard basis for S^h, satisfying $\phi_j(x_i) = \delta_{ij}$, where $\{x_j\}_{j=0}^M$ is the set of nodes of T^h. A discrete L^2 inner product on $C(\bar{\Omega})$ is then defined by

$$(u, v)^h := \int_\Omega \pi^h(u(x)v(x))\, dx \equiv \sum_{j=0}^{M} \hat{M}_{jj} u(x_j)v(x_j),$$

where $\hat{M}_{jj} := (1, \phi_j) \equiv (\phi_j, \phi_j)^h$, corresponding to the (diagonal) lumped mass matrix $\hat{M}$. Then, the fully discrete finite-element second-order IMSP approximation can be formulated as follows. Starting with $U_h^0 = \pi^h(u(x, 0))$, and $V_h^0 = \pi^h(v(x, 0))$ for all $x \in \Omega_h$, for $n = 0, \dots, N-1$ find $U_h^{n_1}$, $V_h^{n_1}$, U_h^{n+1} and V_h^{n+1} so that for all $\chi_h \in S^h$

$$\Big(\frac{V_h^{n_1} - V_h^n}{\Delta t}, \chi\Big)^h = \big(g(U_h^n, V_h^{n_1}), \chi\big)^h \tag{7.1}$$

$$\Big(\frac{U_h^{n_1} - U_h^n}{\Delta t}, \chi\Big)^h + \frac{D_u}{2}(\nabla U_h^n, \nabla\chi) = 0 \tag{7.2}$$

$$\Big(\frac{V_h^{n_2} - V_h^{n_1}}{\Delta t}, \chi\Big)^h + \frac{D_v}{2}(\nabla V_h^{n_1}, \nabla\chi) = 0 \tag{7.3}$$

$$\Big(\frac{U_h^{n_2} - U_h^{n_1}}{\Delta t}, \chi\Big)^h = \frac{1}{2}\big(f(U_h^n, V_h^{n_1}), \chi\big)^h \tag{7.4}$$

$$\Big(\frac{V_h^{n_3} - V_h^{n_2}}{\Delta t}, \chi\Big)^h + \frac{D_v}{2}(\nabla V_h^{n_3}, \nabla\chi) = 0 \tag{7.5}$$

$$\Big(\frac{U_h^{n+1} - U_h^{n_2}}{\Delta t}, \chi\Big)^h + \frac{D_u}{2}(\nabla U_h^{n+1}, \nabla\chi) = \frac{1}{2}\big(f(U_h^{n+1}, V_h^{n_3}), \chi\big)^h \tag{7.6}$$

$$\Big(\frac{V_h^{n+1} - V_h^{n_3}}{\Delta t}, \chi\Big)^h = \frac{1}{2}\big(g(U_h^{n+1}, V_h^{n_3}), \chi\big)^h \tag{7.7}$$

Choosing $U_h^n = \sum_{j=0}^h U_j^n \phi_j$, $V_h^n = \sum_{j=0}^h V_j^n \phi_j$, $\chi_h = \phi_i$, $i = 0, \dots T$, where $U_j^n \approx u(x_j, t_n)$, $V_j^n \approx v(x_j, t_n)$, the above finite-element scheme has an equivalent finite-difference representation on rectangular domains. Indeed, we let the set of nodes $\{x_j\}_{j=0}^M$ correspond to a rectangular grid $\Omega_h \subset \bar{\Omega}$, with mesh width h. Consider L the approximation of the Laplacian operator Δ acting on the element of Ω_h, obtained by classical central difference schemes both in one and two dimensions, with zero-flux boundary conditions. Denoting I the identity matrix, the finite difference IMSP approximation leads to the same steps provided by the finite element scheme (7.1-7.6) for the vectors $\{\mathbf{U}^n\}_i = U_i^n$, $\{\mathbf{V}^n\}_i = V_i^n$:

1. solve the nonlinear system for the vector $\mathbf{V}^{n_1}$

$$\mathbf{V}^{n_1} - \frac{\Delta t}{2}\, g(\mathbf{U}^n, \mathbf{V}^{n_1}) = \mathbf{V}^n,$$

2. evaluate the entries of the vectors $\mathbf{U}^{n_1}$, $\mathbf{U}^{n_2}$, $\mathbf{V}^{n_2}$

$$\mathbf{U}^{n_1} = (I + \frac{\Delta t}{2} D_u\, L)\mathbf{U}^n$$

$$\mathbf{U}^{n_2} = \mathbf{U}^{n_1} + \frac{\Delta t}{2}\, f(\mathbf{U}^n, \mathbf{V}^{n_1})$$

$$\mathbf{V}^{n_2} = (I + \frac{\Delta t}{2} D_v\, L)\mathbf{V}^n$$

3. solve the linear system for $\mathbf{V}^{n_3}$

$$(I - \frac{\Delta t}{2} D_v\, L)\mathbf{V}^{n_3} = \mathbf{V}^{n_2}$$

4. solve the nonlinear system for the vector $\mathbf{U}^{n+1}$

$$(I - \frac{\Delta t}{2} D_u\, L)\mathbf{U}^{n+1} - \frac{\Delta t}{2} f(\mathbf{U}^{n+1}, \mathbf{V}^{n_3}) = \mathbf{U}^{n_2}. \tag{7.8}$$

5. evaluate the entries of the vectors $\mathbf{V}^{n+1}$

$$\mathbf{V}^{n+1} = \mathbf{V}^{n_3} + \frac{\Delta t}{2} g(\mathbf{U}^{n+1}, \mathbf{V}^{n_3})$$

Comparing the above algorithm with the first-order IMSP scheme, we notice that the second-order accuracy requires a major computational effort due to the solution of the nonlinear (7.8). Provided that for all n, $\mathbf{U}_0^{n+1} = \mathbf{U}^n$ is a good approximation of the solution $\mathbf{U}^{n+1}$, iterative schemes based on the evaluation of the Jacobian of the function

$$F(\mathbf{U}) \,=\, (I - \frac{\Delta t}{2} D_u\, L)\mathbf{U} - \frac{\Delta t}{2} f(\mathbf{U}, \mathbf{V}^{n_3}) - \mathbf{U}^{n_2}.$$

given by

$$J_F(\mathbf{U}) = I - \frac{\Delta t}{2} D_u\, L - \frac{\Delta t}{2} \frac{\partial f}{\partial U}(\mathbf{U}, \mathbf{V}^{n_3})$$

can be implemented. Moreover, in order to cut down the computational effort for updating the Jacobian, the algorithms may be modified in such a way that, during the iterations, the value of the Jacobian is kept constant. In the next Section 8 we will show the results of the application of the modified Newton algorithm where the same LU decomposition of the Jacobian has been used for every step of the iteration and only back substitutions were performed.

8. Numerical examples. In a previous article, [2], we tested the first-order IMSP scheme on dynamics of both ecological and numerical interest. Among these, we recall the well-known spatially explicit Rosenzweig-MacArthur (RM) model [17], as well as models that couple logistic prey growth with Holling II and IV functional predator responses [12]. In this paper we test the second-order accurate scheme on the same examples as in [2], in order to numerically verify the increment in accuracy and to evaluate the advantage of the augmented accuracy with respect to the increased computational cost.

8.1. A one-dimensional example. In this section we present the results related to a one-dimensional problem with Holling II type dynamics governing the reaction term:

$$\begin{aligned} \frac{\partial u}{\partial t} &= u(1-u) - v(1 - e^{-\gamma u}) + \Delta u \\ \frac{\partial v}{\partial t} &= \beta v(\alpha - 1 - \alpha e^{-\gamma u}) + \Delta v \end{aligned}$$

The parameters $\alpha = 1.5$, $\beta = 1$ and $\gamma = 5$ were chosen in order to guarantee a stable limit cycle in the reaction kinetics surrounding an unstable steady state. Thus, the densities of predators and prey are oscillatory, which is the situation of primary interest from an ecological point of view, and which can be better treated with the IMSP schemes. The initial densities for prey and predator population were set to 0.2 and 0.0328.

In order to numerically verify the second-order in time convergence rate of the IMSP scheme, we considered as reference solution, the solution at $T = 20$ of the continuous in time approximation

$$\frac{dU}{dt} = D_u L\, U + U(1-U) - V(1 - e^{-\gamma U}),$$

$$\frac{dV}{dt} = D_v L\,V + \beta V(\alpha - 1 - \alpha e^{-\gamma U})$$

obtained with the Matlab code `ode45` with absolute and relative tolerance set to 10^{-15} and 10^{-13}, respectively. The solution $U(20)$ and $V(20)$ are the vectors of prey and predators densities on the uniform grid $x_j = j\,h$ (for $j = 0, \dots M = 1/h$) of space step $h = 1/1024$ embedded into the domain $\Omega = [0, 1]$. The initial values are given by the vectors with entries $U_j(0) = u(x_j, 0)$ and $V_j(0) = v(x_j, 0)$ for $j = 0, \dots M$. The matrix L is obtained by approximating the second order derivatives with central differences and imposing zero flux boundary conditions (see [2]).

We set as initial step size $\Delta t_0 = 1/2$; then, we successively halved this value obtaining a decreasing sequences of stepsizes $\Delta t_i = 1/2^{i+1}$ for $i = 1, \dots, 8$. We compared the reference solutions $U(20)$ and $V(20)$ with the approximations $\mathbf{U}^{N_i}$ and $\mathbf{V}^{N_i}$, with $N_i = 20/\Delta t_i$, obtained advancing in time for $n = 0, 1, \dots N_i - 1$ according to the IMSP second order steps

$$\begin{aligned}
&V_j^{n_1} = \frac{{V_j}^n}{1 - \frac{\Delta t_i}{2}\beta(\alpha - 1 - \alpha e^{-\gamma {U_j}^n})} \qquad j = 0, \dots, M \\
&\mathbf{U}^{n_1} = (I + \frac{\Delta t_i}{2} D_u\, L)\mathbf{U}^n \\
&U_j^{n_2} = U_j^{n_1} + \frac{\Delta t_i}{2}\left(U_j^n(1 - U_j^n) - V_j^{n_1}(1 - e^{-\gamma U_j^n})\right) \qquad j = 0, \dots, M \\
&\mathbf{V}^{n_2} = (I + \frac{\Delta t_i}{2} D_v\, L)\mathbf{V}^n \\
&(I - \frac{\Delta t_i}{2} D_v\, L)\mathbf{V}^{n_3} = \mathbf{V}^{n_2} \\
&(I - \frac{\Delta t_i}{2} D_u\, L)\mathbf{U}^{n+1} - \frac{\Delta t_i}{2}\Big(\mathbf{U}^{n+1}(1 - \mathbf{U}^{n+1}) - \mathbf{V}^{n_3}(1 - e^{-\gamma \mathbf{U}^{n+1}})\Big) = \mathbf{U}^{n_2} \\
&V_j^{n+1} = V_j^{n_3} + \frac{\Delta t_i}{2}\beta V_j^{n_3}(\alpha - 1 - \alpha e^{-\gamma U_j^{n+1}}) \qquad j = 0, \dots, M.
\end{aligned} \tag{8.1}$$

Notice that in (8.1) the mathematical operations between vectors are defined as vectors with entries given by the elementwise operations.

In order to solve the nonlinear system (8.1) we implemented, for each n, a modified Newton-Rhapson procedure with an LU decomposition of the Jacobian frozen at U_n, given by

$$J_F(\mathbf{U}^n) = diag\Big(1 - \frac{\Delta t_i}{2}\big(1 - 2\,U_j^n - \gamma V_j^{n_3} e^{-\gamma U_j^n}\big)\Big)_{j=0,\dots M} - \frac{\Delta t_i}{2} D_u\, L. \tag{8.2}$$

The errors in the prey densities $E_i^{(U)} = \|U(20) - \mathbf{U}^{N_i}\|_1 = \max_{0 \le j \le M} |U_j(20) - {U_j}^{N_i}|$ are plotted in Figure 8.1 (left) with respect to Δt_i for $i = 1, \dots, 8$ using logarithmic scales for both axes. The slope of the segments joining the different points of the IMSP2 curve, which denote the second-order scheme, confirms the second-order rate of convergence. For comparison, in Figure 8.1 (left), we also report the results of the first-order IMSP approximation, denoted by IMSP1 curve.

In Figure 8.1 (right) we report the previous errors in prey densities versus the cputimes evaluated by means of Matlab counters `tic` and `toc`. We notice that, reducing the stepsize, the first-order scheme requires an increment of computational time that is is greater than the one corresponding to the second-order method. This means that for values of stepsize below a threshold, using the same computational time, the second-order scheme provides more accurate approximations compared to the first-order scheme. [1].

8.2. A two-dimensional example. We compare the results of the first-order and second-order IMSP schemes on the test case proposed in [6], for the spatially extended predator-prey interactions of Rosenzweig-MacArthur form:

$$\frac{\partial u}{\partial t} = u(1 - u) - \frac{uv}{u + \alpha} + D_u \Delta u \tag{8.3}$$

[1]Matlab codes implementing first (`fd1dKin1IMSP1`) and second order (`fd1dKin1IMSP2`) IMSP schemes applied to the above example are downloadable from *http://www.uoguelph.ca/ mgarvie/PredPrey_files/*.

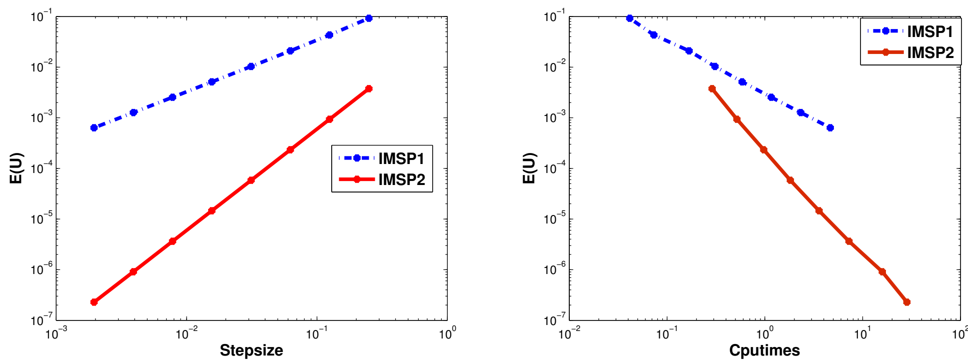

FIG. 8.1. *On the left: Convergence rate and accuracy comparison between first- and second-order IMSPs schemes at $T = 20$. The two curves have different slopes, suggesting the different orders of convergence. The slope of the IMSP1 curve is approximately 1, validating the first-order accuracy, while IMSP2 slope is approximately 2, verifying the second-order accuracy. On the right: comparison between numerical errors and cputime for the first- and second-order IMSP schemes.*

$$\frac{\partial v}{\partial t} = \frac{\beta uv}{u+\alpha} - \gamma v + D_v \Delta v. \tag{8.4}$$

We consider the same spatial domain given in [6], a hypothetical lake with an island. The unstructured mesh grid given by a coarse triangularization of $M = 427$ nodes generated by the authors with `Mesh2d v2.4` Matlab routine was used in our example for providing comparisons not affected by different spatial discretization. Parameters were set as follows: $D_u = D_v = 1$, $\alpha = 0.4$, $\beta = 0.2$ and $\gamma = 0.6$, $u_0 = 6/35 - 2 \cdot 10^{-7}(x - 0.1 \cdot y - 225)(x - 0.1 \cdot y - 675)$ and $v_0 = 116/245 - 3 \cdot 10^{-5} \cdot (x - 450) - 1.2 \cdot 10^{-4}(y - 150)$. We ran our code several times, with different time steps, and we compare the performance of IMSP second-order scheme with respect to the first-order method.

The first test evaluates the rates of convergence. Since no exact solution is known we considered as reference solutions the approximation at $T = 50$ on a fine temporal mesh $\Delta t = 1/2^{10}$ of the second-order IMSP scheme applied to the ODE system

$$\begin{aligned}
\frac{dU}{dt} &= D_u L\, U + U(1-U) - \frac{U\, V}{U+\alpha},\\
\frac{dV}{dt} &= D_v L\, V + \frac{\beta U\, V}{U+\alpha} - \gamma V.
\end{aligned}$$

The solution $U(50)$ and $V(50)$ are the vectors of prey and predators densities on the considered unstructured mesh grid. The explicit expression of the approximated Laplacian L on the considered spatial triangularization and imposing zero flux boundary conditions can be found in [6].

In our tests we used a decreasing sequences of stepsizes $\Delta t_i = 1/2^i$ for $i = 1, \dots, 6$. We compared the reference solutions $U(50)$ and $V(50)$ with the approximations $\mathbf{U}^{N_i}$ and $\mathbf{V}^{N_i}$, with $N_i = 50/\Delta t_i$, obtained advancing in time for $n = 0, 1, \dots N_i - 1$ according to the IMSP second-order steps

$$\begin{aligned}
V_j^{n_1} &= \frac{V_j{}^n}{1 - \frac{\Delta t_i}{2}\big(\frac{\beta U_j{}^n}{U_j{}^n+\alpha} - \gamma\big)} \qquad j = 0, \dots M\\
\mathbf{U}^{n_1} &= (I + \frac{\Delta t_i}{2} D_u\, L)\mathbf{U}^n\\
U_j^{n_2} &= U_j^{n_1} + \frac{\Delta t_i}{2}\,\big(U_j^n(1-U_j^n) - \frac{U_j{}^n\, V_j^{n_1}}{U_j{}^n+\alpha}\big) \qquad j = 0, \dots M\\
\mathbf{V}^{n_2} &= (I + \frac{\Delta t_i}{2} D_v\, L)\mathbf{V}^n\\
(I - \frac{\Delta t_i}{2} D_v\, L)\mathbf{V}^{n_3} &= \mathbf{V}^{n_2}\\
(I - \frac{\Delta t_i}{2} D_u\, L)\mathbf{U}^{n+1} - \frac{\Delta t_i}{2}\Big(\mathbf{U}^{n+1}(1-\mathbf{U}^{n+1}) &- \frac{\mathbf{U}^{n+1}\,\mathbf{V}^{n_3}}{\mathbf{U}^{n+1}+\alpha}\Big) = \mathbf{U}^{n_2}
\end{aligned} \tag{8.5}$$

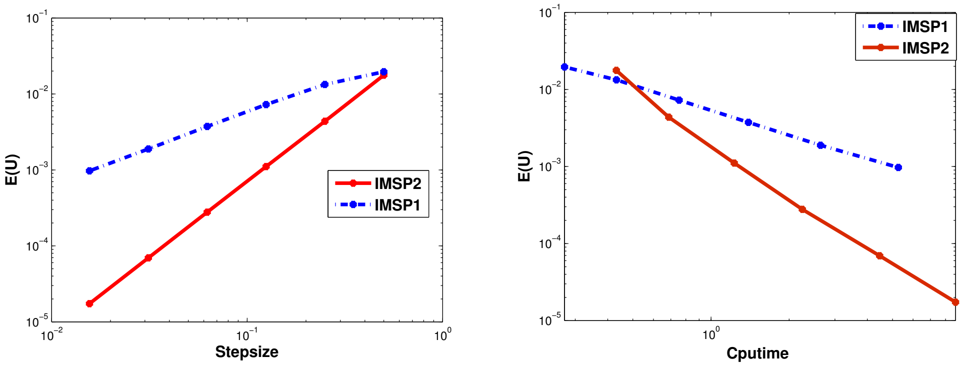

FIG. 8.2. *On the left: Convergence rate and accuracy comparison between first and second order IMSPs schemes at $T = 50$. The two curves have different slopes, this confirming the different order of convergence; the slope of IMSP1 curve is approximately 1 denoting a first order accuracy while IMSP2 slope is approximately equal to 2 denoting a second order accuracy. On the right: comparison between numerical error and cputime for first and second order IMSP schemes*

$$V_j^{n+1} = V_j^{n_3} + \frac{\Delta t_i}{2} V_j^{n_3} \big(\frac{\beta U_j^{n+1}}{U_j^{n+1} + \alpha} - \gamma \big) \qquad j = 0, \dots M$$

As for the previous example, in (8.5) the operations among vectors are defined as vectors with entries given by the corresponding elementwise operation. In order to solve the nonlinear system (8.5) we implemented, for each n, a modified Newton-Rhapson procedure with LU decomposition of the Jacobian frozen at U_n and given by

$$J_F(\mathbf{U}^n) = diag\Big(1 - \frac{\Delta t_i}{2}\big(1 - 2\,U_j^n - \alpha \frac{V_j^{n_3}}{(U_j^n + \alpha)^2}\big)\Big)_{j=0,\dots M} - \frac{\Delta t_i}{2} D_u\, L.$$

The errors in the prey densities $E_i^{(U)} = \|U(50) - \mathbf{U}^{N_i}\| = \max_{0 \le j \le M} |U_j(50) - U_j{}^{N_i}|$ are plotted in Figure 8.2 (left) with respect to Δt_i for $i = 1, \dots, 6$, using logarithmic scales for both axes. The slopes of the segments joining the different points confirm the theoretically predicted rates of convergence for the first- and second-order IMSP schemes. In Figure 8.2 (right) we report the previous errors in prey densities versus the cputimes evaluated by means of Matlab counters `tic` and `toc`. The results show that, reducing the stepsize, the first-order scheme requires an increased computational time in comparison with the second-order scheme. Hence, using the same amount of computational time, the second-order scheme with stepsizes below a threshold value provides more accurate approximations than the first-order scheme. [2]

Finally, we show the spatial distribution of prey densities on the two-dimensional domain obtained by using IMSP first- and second-order approaches. On the left column of Figure 8.3 we display the successive approximations at $T = 150$ using the IMSP first-order scheme with stepsizes $\Delta t = 1/3,\ 1/24,\ 1/384$. On the right, we report the approximations of the second-order IMSP scheme corresponding to the same temporal stepsizes. Again, we emphasize the faster convergence of the IMSP second-order scheme versus the first-order approximation.

9. Conclusion. A semi-discrete in time formulation of a second-order implicit-symplectic scheme for reaction-diffusion systems modeling predator-prey dynamics has been analyzed. We proved stability of the algorithm, an optimal a priori error estimate, and the positivity of solutions, provided the temporal stepsize is small. These results extend the study developed in [2] for the first-order IMSP scheme, and constitute the basis for the analysis of the fully-discrete approximations in finite-difference and finite-element settings. The numerical examples confirm that the IMSP second-order approximations, applied with stepsizes below a suitable threshold value, provide an improvement in terms of accuracy compared the corresponding first-order algorithm, at same computational cost.

[2]Matlab codes implementing first (`IMSP1fe2dnfast`) and second order (`IMSP2fe2dnfast`) IMSP schemes applied to the above example are downloadable from *http://www.uoguelph.ca/ mgarvie/PredPrey_files/*.

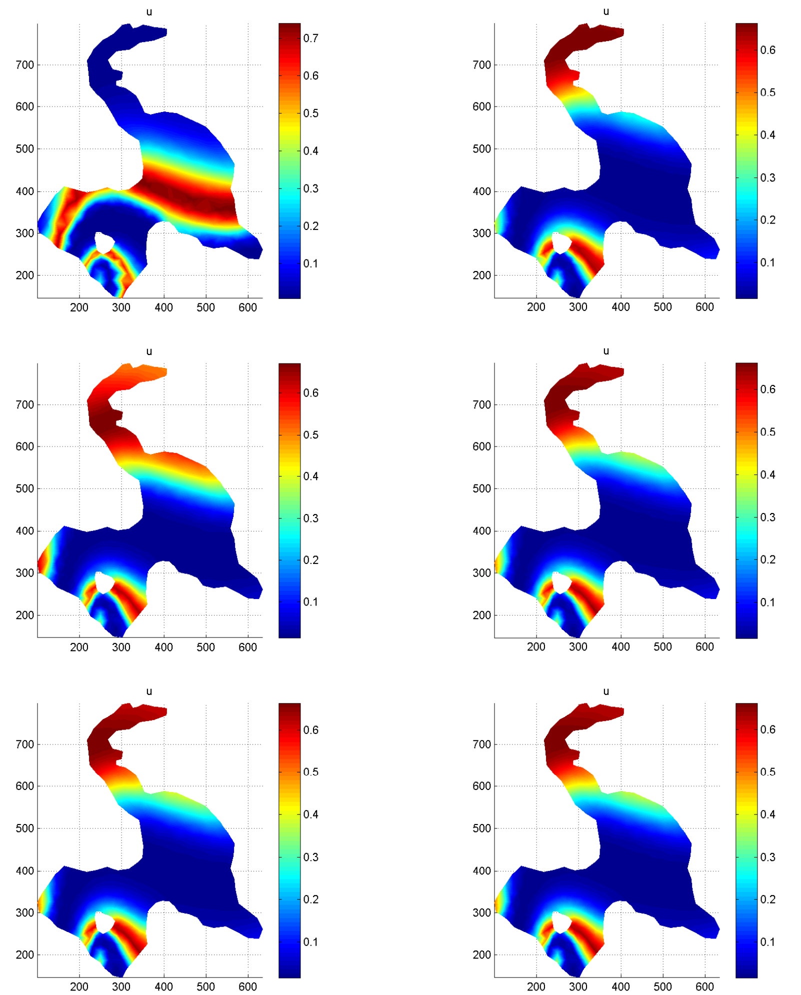

FIG. 8.3. *RM model* (8.3)-(8.4). *Spatial distribution of prey densities in the domain: on the left column IMSP first order approximations with* $\Delta t = 1/3,\ 1/24,\ 1/384$, *on the right column the approximation with IMSP second order scheme in correspondence of the same temporal stepsizes. Parameters:* $D_u = D_v = 1$, $\alpha = 0.4$, $\beta = 0.2$, $\gamma = 0.6$. *Initial conditions:* $u_0 = 6/35 - 2\cdot 10^{-7}(x - 0.1\cdot y - 225)(x - 0.1\cdot y - 675)$ *and* $v_0 = 116/245 - 3\cdot 10^{-5}\cdot(x - 450) - 1.2\cdot 10^{-4}(y - 150)$. *Notice that IMSP2 approximation reaches convergence more quickly than IMSP1 scheme.*

Matlab codes, downloadable from *http://www.uoguelph.ca/ mgarvie/PredPrey_files/*, have been developed to implement the considered schemes on two examples.

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