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Corresponding Author: Dr. Bernardo M Rocha, Ph.D.

Corresponding Author's Institution: Departamento de Ciência da Computação, Universidade Federal de Juiz de Fora

First Author: Ricardo R Pereira, Ph.D.

Order of Authors: Ricardo R Pereira, Ph.D.; Bernardo M Rocha, Ph.D.; Rodrigo W dos Santos, Ph.D.; Abimael F Loula, Ph.D.

Abstract: Several phenomena in life sciences are mathematically modeled as systems of reaction-diffusion partial differential equations. These equations are non-linear and their solutions present complex spatial behavior, such as Turing patterns, which require very fine space discretization and consequently high computational costs. To address these issues we propose second order and unconditionally stable semi-implicit methods, based on an Alternating Direction Implicit (ADI) scheme, suitable for treating non-linear reaction and linear diffusion problems. The schemes are tested in a series of computational experiments to observe their convergence rates and to illustrate computational efficiency in solving the Schnackenberg model and predator-prey models with cross diffusion.

Cover Letter

Dear Editors,

we are very pleased to submit our manuscript entitled "*Second order ADI schemes for nonlinear reaction-diffusion problems*" to *Applied Mathematical Modelling*.

Our manuscript presents to the community second order and unconditionally stable semi-implicit methods, based on an Alternating Direction Implicit (ADI) scheme, suitable for treating nonlinear reaction and linear diffusion problems. Two schemes are presented and tested in a series of computational experiments to observe their convergence rates and to illustrate computational efficiency in solving the Schnackenberg model and predator-prey models with cross diffusion.

In this perspective, our results is of extreme value and significance for the scientific community interested in both reaction-diffusion problems, specially those arising from biological problems, as well as for the numerical methods community.

Briefly, the novelties of our manuscript are:

- Two unconditionally stable, computationally efficient and second order accurate methods based on the Peaceman and Rachford ADI scheme are proposed for the numerical solution of nonlinear reaction-diffusion problems.
- Numerical experiments confirm that the proposed schemes are second order accurate in both space and time are presented in problems with exact solutions. Potential applications of the methods such as for the Schnackenberg model and predator-prey models with cross diffusion are presented.
- A vectorial approach combined with the ADI scheme that results in block tridiagonal systems is proposed to efficiently solve the cross diffusion problems.

In addition, we state that this manuscript is entirely original, has not been copyrighted, published, submitted, or accepted for publication elsewhere.

Sincerely,

Bernardo Martins Rocha

Highlights

- Unconditionally stable and second order accurate methods based on the ADI scheme are proposed for reaction-diffusion problems.
- Numerical experiments concerning nonlinear reaction-diffusion problems are presented to confirm the accuracy of the method.
- Applications of the methods are illustrated for the Schnackenberg model and predator-prey models with cross diffusion.
- To efficiently solve the cross diffusion problems we propose a vectorial approach combined with the ADI scheme.
- Comparisons of the schemes with other methods from the literature are presented to assess the performance of the methods.

Second order ADI schemes for nonlinear reaction-diffusion problems

Ricardo Reis Pereira, Bernardo Martins Rocha, Rodrigo Weber dos Santos, Abimael Fernando Dourado Loula

Abstract

Several phenomena in life sciences are mathematically modeled as systems of reaction-diffusion partial differential equations. These equations are non-linear and their solutions present complex spatial behavior, such as Turing patterns, which require very fine space discretization and consequently high computational costs. To address these issues we propose second order and unconditionally stable semi-implicit methods, based on an Alternating Direction Implicit (ADI) scheme, suitable for treating non-linear reaction and linear diffusion problems. The schemes are tested in a series of computational experiments to observe their convergence rates and to illustrate computational efficiency in solving the Schnackenberg model and predator-prey models with cross diffusion.

Keywords: reaction-diffusion, Turing patterns, ADI, semi-implicit scheme

1. Introduction

In nature a vast amount of biological patterns appear, from specific details of individuals to complex spatial patterns involving an entire population. An interesting pattern, for example, is the distribution of species in the same area due to the presence of a predator, food and water availability. Most of these phenomena have been described mathematically as systems of nonlinear reaction

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*Corresponding author
Email addresses: bernardomartinsrocha@ice.ufjf.br (Bernardo Martins Rocha), aloc@lncc.br (Abimael Fernando Dourado Loula)

and linear diffusion (NRD) partial differential equations (PDEs), as introduced in the pioneering work of Alan Turing [1]. Reaction-diffusion models are the most commonly used to explain and understand biological pattern formation [2]. These models can reproduce a wide range of spatial patterns, and together with mathematical and computational studies they have revealed the required setting for the formation of these patterns. In general, these mathematical models are difficult to be solved numerically for resulting in large non-linear problems that demand robust, accurate and efficient numerical methods.

From the numerical point of view, nonlinear reaction-diffusion equations are challenging. The diffusive part usually requires extremely small time steps, which would be prohibitive in some cases, specially in 3D problems when explicit schemes are adopted. The reaction terms are in general non-linear, stiff and might require an special treatment. Although explicit methods are easy to implement, stability conditions may impose severe restrictions on the size of space and time steps. On the other hand, fully implicit methods require the treatment of the nonlinear reaction terms at each time step, which can be very expensive and hard to handle, since the jacobian matrix is necessary in a Newton-like iterative solver [3].

A class of finite difference methods which has been used in many areas is the classical Alternating Direction Implicit (ADI) method [4, 5, 6, 7]. ADI schemes were introduced for the solution of parabolic and elliptic equations in two space variables by Peaceman and Rachford [7] and Douglas and Rachford [8], and later extended by Douglas to solve efficiently three dimensional problems [4]. The basic idea of the method is to apply a dimension splitting of the Laplacian operator to break down the problem into easier one dimensional problems. The main advantage of the ADI method is unconditional stability with reduced computational cost, since the linear systems resulting from the method are tridiagonal and can be solved very efficiently. But, in the presence of non-linear reaction terms [3], implicit method like ADI requires the computation of the Jacobian matrix and the use of a non-linear equation solver, which increases complexity and computational cost.

In this work we propose unconditionally stable and computationally efficient methods for nonlinear reaction-diffusion problems, based on Peaceman and Rachford ADI scheme. The proposed methods are second order accurate in both space and time as demonstrated in a series of convergence studies concerning nonlinear reaction-diffusion problems with exact solutions. Potential applications of the proposed methodology are illustrated solving the Schnackenberg model and predator-prey models with cross diffusion. To efficiently solve the cross diffusion problems we propose a vectorial approach combined with the ADI scheme which results in block tridiagonal systems and preserves unconditional stability and second order accuracy.

The remainder of this text is organized as follows. In Section 2 some mathematical models of reaction-diffusion phenomena are described. In Section 3 a second-order operator splitting ADI scheme is proposed. In Section 4 a second-order semi-implicit ADI scheme is introduced. Results on convergence studies and examples of possible applications of the propose methodology are presented in Section 5, followed by discussion and conclusions in sections 6 and 7, respectively.

2. Mathematical models

Several phenomena in biology and other areas result in the formation of complex spatial-temporal patterns [1], which in turn give rise to a variety of mathematical models. Most of these mathematical models are described by systems of partial differential equations (PDEs) of nonlinear reaction and linear diffusion (NRD) type.

Let $\Omega \subset \mathbb{R}^2$ be the domain of interest and $\mathbf{u}(\mathbf{x}, t)$ be the solution of the following non-linear reaction-diffusion time-dependent PDE problem:

$$\frac{\partial \mathbf{u}}{\partial t} = \mathcal{A}\mathbf{u} + \mathcal{R}(\mathbf{u}), \quad \mathbf{x} \in \Omega \tag{1}$$

with initial conditions $\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x})$, where $\mathbf{u}$ is the vector of n variables of the problem (*e.g.* vector of chemical component concentrations), $\mathcal{A}$ is a linear

diffusion operator and $\mathcal{R}(\mathbf{u})$ denotes a general non-linear reaction term. The system is closed with either a Dirichlet boundary condition, representing a fixed concentration of $\mathbf{u}$ on the boundary $\partial\Omega$, or Neumann conditions.

Several models of NRD problems exhibiting complex Turing pattern dynamic [1] exist in the literature. Common examples are the the Schnakenberg model [9], the Gray-Scott model [10], Fitz-HughNagumo model [11], predator-prey models with spatial diffusion [12]. See also references [13, 14].

Consider $\mathbf{u} = \{u, v\}^T$, in two space dimensions, and the linear operator $\mathcal{A}\mathbf{u}$ given in matrix form by

$$\mathcal{A}\mathbf{u} = \begin{bmatrix} D_u \Delta u & 0 \\ 0 & D_v \Delta v \end{bmatrix}, \tag{2}$$

where D_u and D_v are the diffusion coefficients of u and v, respectively, and $\Delta u = \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}$. In this work we will also consider cross-diffusion between the different concentrations/species, with

$$\mathcal{A}\mathbf{u} = \begin{bmatrix} D_{11} \Delta u & D_{12} \Delta v \\ D_{21} \Delta u & D_{22} \Delta v \end{bmatrix}, \tag{3}$$

where D_{11} and D_{22} are called (self)-diffusion coefficients, whereas D_{12} and D_{21} are known as cross-diffusion coefficients. The next sections recall two important classes of NRD models that are further explored here.

2.1. Schnakenberg model

The Schnakenberg model [9], originally proposed to describe chemical reactions, has also been applied to describe complex pattern formation in biology such as pigmentation patterning in fish [13]; shell markings and others [15]. This model has the following mathematical form

$$\frac{\partial C_a}{\partial t} = \mathcal{D}_1 \Delta C_a + \kappa \left(a - C_a + C_a^2 C_i \right) \tag{4}$$

$$\frac{\partial C_i}{\partial t} = \mathcal{D}_2 \Delta C_i + \kappa \left(b - C_a^2 C_i \right) \tag{5}$$

where C_a and C_i are the concentrations of the activator and inhibitor, respectively; $\mathcal{D}_1$ and $\mathcal{D}_2$ are diffusion coefficients; a, b and κ are constants of the biochemical reactions of the model.

2.2. Predator-Prey model

A predator-prey model with spatial dynamics is another example of nonlinear reaction-diffusion system. In particular, a predator-prey model which includes a term describing refuge dynamics is introduced in [12].

In this complex dynamics preys may prevent being killed by predators either escaping or defending themselves [16]. They may escape by moving to a refuge where the risk of being predated is significantly reduced. The effect of escaping in the population dynamics can be described as a growth in the population of preys and as a decrease in that of the predators, since by escaping the prey mortality is reduced. Other ways of including this dynamics in the models have also been discussed in the literature [17, 18]. The presence of refuge in the model can help to reduce the chance of extinction due to predation and to damp oscillations in predator-prey populations.

Here a two-dimensional and continuous diffusive predator-prey model in a homogeneous environment is considered. Its general form is given by

$$\frac{\partial u}{\partial t} = D_{11}\Delta u + D_{12}\Delta v + R_1(u,v), \tag{6}$$

$$\frac{\partial v}{\partial t} = D_{21}\Delta u + D_{22}\Delta v + R_2(u,v), \tag{7}$$

where D_{11},D_{12},D_{21} and D_{22} are the diffusion coefficients and $R_1(u,v)$ and $R_2(u,v)$ are the reaction terms. A particular example of reaction terms is introduced by Guin and Mandal [12], in the non-dimensional form

$$R_1(u,v) = u(u-1) - \frac{(1-r)uv\epsilon}{(1-r)u+\alpha}, \tag{8}$$

$$R_2(u,v) = \beta v(1-v) + \frac{(1-r)uv\gamma}{(1-r)u+\alpha} - \delta v, \tag{9}$$

where r is the refuge parameter. In these reaction terms it is assumed that the predator (u) follows a logistic growth in case of total extinction of the prey (v) and also that the predator has an alternative source of food rather than only the prey. Also, the model considers a constant proportion of prey refuge ru, where $r \in [0,1)$, *i.e.* a fraction $(1-r)u$ of the prey is available for predation. For

a detailed description, including stability analysis, parameter space and Turing pattern analysis, see [12]

3. A second-order operator splitting scheme

First we recall classical explicit finite difference methods that have been adopted to approximate nonlinear reaction diffusion problems. Then we introduce an unconditionally stable second-order operator splitting ADI scheme. The nonlinearities associated with the reaction terms pose a great challenge, and several methods have been proposed to solve the NRD problem (1). We only consider explicit approximations for the reaction terms as in the classical Euler and second order Runge-Kutta explicit methods which are associated here with the Strang operator splitting scheme [19] to separate the nonlinear reaction terms from the linear diffusion operator.

3.1. Explicit methods

The classical explicit Euler method for the general RD model (1) is given by

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \Delta t(\mathcal{A}\mathbf{u}^n + \mathcal{R}(\mathbf{u}^n)) \tag{10}$$

where $\mathbf{u}^{n+1}$ is the approximate solution to $\mathbf{u}$ at time instant t^{n+1}. Here, the nonlinear reaction term poses no difficulties since it is simply evaluated at the previous time step. However, the method is severely limited due to stability conditions which puts strict restrictions on the size of the time step used [20].

A second order Runge-Kutta method (RK2), for the model problem described by equation (1) is given by

$$\mathbf{u}^{n+1} = \mathbf{u}^n + \frac{\Delta t}{2}(\mathbf{k_1} + \mathbf{k_2}), \tag{11}$$

$$\mathbf{k_1} = \mathcal{A}\mathbf{u}^n + \mathcal{R}(\mathbf{u}^n), \tag{12}$$

$$\mathbf{k_2} = \mathcal{A}\overline{\mathbf{u}} + \mathcal{R}(\overline{\mathbf{u}}), \tag{13}$$

where $\overline{\mathbf{u}} = \mathbf{u}^n + \Delta t\mathbf{k_1}$ was introduced to ease the notation. In this form the RK2 is also known as the Heun method, which is a explicit method as well [20].

3.2. Alternating direction implicit method

We restrict this presentation to the Peaceman-Rachford [7] ADI scheme applied to the scalar version of equation (1) in a two-dimensional domain Ω without the reaction term. Therefore, the equation

$$\frac{\partial u}{\partial t} = \mathcal{A}u + f, \tag{14}$$

where $\mathcal{A}$, representing the Laplacian operator, is split into

$$\mathcal{A}u = \mathcal{A}_1 u + \mathcal{A}_2 u. \tag{15}$$

Besed on the Crank-Nicolson method

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{1}{2}\left(\mathcal{A}_1 + \mathcal{A}_2\right)\left(u^{n+1} + u^n\right) + f^{n+1/2}, \tag{16}$$

the Peaceman-Rachford ADI scheme for equation (16) is presented as

$$\frac{u^{n+1/2} - u^n}{\Delta t} = \tfrac{1}{2}\mathcal{A}_1 u^{n+1/2} + \tfrac{1}{2}\mathcal{A}_2 u^n + \tfrac{1}{2} f^{n+1/2}, \tag{17}$$

$$\frac{u^{n+1} - u^{n+1/2}}{\Delta t} = \tfrac{1}{2}\mathcal{A}_2 u^{n+1} + \tfrac{1}{2}\mathcal{A}_1 u^{n+1/2} + \tfrac{1}{2} f^{n+1/2}. \tag{18}$$

Equations (17) and (18) are usually written in the following compact form:

$$\left(I - \tfrac{1}{2}\Delta t\mathcal{A}_1\right) u^{n+\frac{1}{2}} = \left(I + \tfrac{1}{2}\Delta t\mathcal{A}_2\right) u^n + \tfrac{1}{2}\Delta t f^{n+1/2}, \tag{19}$$

$$\left(I - \tfrac{1}{2}\Delta t\mathcal{A}_2\right) u^{n+1} = \left(I + \tfrac{1}{2}\Delta t\mathcal{A}_1\right) u^{n+\frac{1}{2}} + \tfrac{1}{2}\Delta t f^{n+1/2}. \tag{20}$$

The most attractive features of the Peaceman-Rachford ADI scheme are unconditional stability, second-order accuracy in time ($\mathcal{O}\left(\Delta t^2\right)$) and its remarkable computational performance.

3.3. Operator splitting

One typical approach to solve non-linear NRD problems is to apply an operator splitting (OS) technique [6] to separate the linear diffusion term from the nonlinear reaction term. Consequently, appropriate methods for diffusion and reaction equations can be used separately, treating the nonlinear reaction

terms efficiently without the need of solving a large nonlinear system of equations, as in the fully implicit scheme. The most used OS techniques for NRD problems are the first-order Godunov scheme [21] and the second-order Strang splitting [19]. These schemes have been applied successfully in a large number of problems [22, 23, 24, 25].

Applied to the NRD problem the Strang splitting separates the reaction and diffusion terms and performs three steps to advance the solution to t^{n+1}. The method starts from the previous solution $\mathbf{u}^n$, applies the reaction operator and advances the solution by $\frac{1}{2}\Delta t$ to obtain an intermediate solution $\mathbf{u}^*$. Then, $\mathbf{u}^*$ is used as the initial condition to solve the diffusion term and obtain a second intermediate solution $\mathbf{u}^{**}$, which is finally used to obtain the solution at t^{n+1} by advancing again by $\frac{1}{2}\Delta t$ the reaction term. The Strang splitting for equation (1) defined as a reaction-diffusion-reaction (RDR) splitting is given by:

$$\frac{d\mathbf{u}^*}{dt} = \mathcal{R}(\mathbf{u}^*), \text{ for } t_n < t \leq t_{n+1/2}, \ \mathbf{u}^*(t_n) = \mathbf{u}^n \tag{21}$$

$$\frac{\partial \mathbf{u}^{**}}{\partial t} = \mathcal{A}\mathbf{u}^{**}, \text{ for } t_n < t \leq t_{n+1}, \ \ \mathbf{u}^{**}(t_n) = \mathbf{u}^*(t_{n+1/2}) \tag{22}$$

$$\frac{d\mathbf{u}^{***}}{dt} = \mathcal{R}(\mathbf{u}^{***}), \text{ for } t_{n+1/2} < t \leq t_{n+1}, \ \mathbf{u}^{***}(t_{n+1/2}) = \mathbf{u}^{**}(t_{n+1}) \tag{23}$$

giving $\mathbf{u}^{n+1} = \mathbf{u}^{***}(t_{n+1})$ as the next approximation; where both $\mathbf{u}^*$ and $\mathbf{u}^{**}$ are intermediate solutions. For each step of the Strang splitting different numerical methods can be used to solve the nonlinear systems of ordinary differential equations (21) and (23), and the linear system of partial differential equations (22). Considering that the Strang splitting (21)-(23) is a second-order approximation of the NRD system (1), consistently, second-order methods should be adopted to approximate each one of the systems (21)-(23) to get a second-order approximation for the original system (1). A second-order finite difference approximation based on the Strang splitting is presented next combining the Runge-Kutta method with the ADI scheme.

3.4. Second-order operator splitting ADI scheme

Adopting the second-order Runge-Kutta method for the reaction systems (21) and (22) combined with the ADI scheme for diffusion system (23) we get

the following second-order splitting scheme:

1. Second order Runge-Kutta scheme for reaction, $t_n < t \leq t_{n+1/2}$

$$\mathbf{u}^* = \mathbf{u}^n + \frac{\Delta t}{4}(\mathbf{R}_1^* + \mathbf{R}_2^*), \tag{24}$$

$$\mathbf{R}_1^* = \mathcal{R}(\mathbf{u}^n), \quad \mathbf{R}_2^* = \mathcal{R}\left(\mathbf{u}^n + \frac{\Delta t}{2}\mathbf{R}_1^*\right), \tag{25}$$

2. Second order ADI scheme for diffusion, $t_n < t \leq t_{n+1}$

$$\left(\mathcal{I} - \frac{\Delta t}{2}\mathcal{A}_1\right)\mathbf{u}^{n+\frac{1}{2}} = \left(\mathcal{I} + \frac{\Delta t}{2}\mathcal{A}_2\right)\mathbf{u}^*, \tag{26}$$

$$\left(\mathcal{I} - \frac{\Delta t}{2}\mathcal{A}_2\right)\mathbf{u}^{**} = \left(\mathcal{I} + \frac{\Delta t}{2}\mathcal{A}_1\right)\mathbf{u}^{n+\frac{1}{2}} \tag{27}$$

3. Second order Runge-Kutta scheme for reaction, $t_{n+1/2} < t \leq t_{n+1}$

$$\mathbf{u}^{***} = \mathbf{u}^{**} + \frac{\Delta t}{4}(\mathbf{R}_1^{**} + \mathbf{R}_2^{**}), \tag{28}$$

$$\mathbf{R}_1^{**} = \mathcal{R}(\mathbf{u}^{**}), \quad \mathbf{R}_2^* = \mathcal{R}\left(\mathbf{u}^{**} + \frac{\Delta t}{2}\mathbf{R}_1^{**}\right) \tag{29}$$

with $\mathbf{u}^{n+1} = \mathbf{u}^{***}$. These scheme, which will be identified here as $Strang_{ADI}$, is second-order and unconditionally stable.

4. A second-order semi-implicit ADI scheme

In this section we introduce the second-order method SSI_{ADI} which is a semi-implicit method based on the Crank-Nicolson combined with the Peaceman-Rachford ADI scheme. The method SSI_{ADI} has unconditional stability inherited from the ADI scheme and converges with $\mathcal{O}(\Delta t^2)$ [7].

4.1. A semi-implicit Crank-Nicolson approximation

To derive the proposed semi-implicit ADI scheme we start from the following second order approximation for the NRD system (1) in the mid-point $n + 1/2$ corresponding to $t_n + \Delta t/2$

$$\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} = \mathcal{A}\mathbf{u}^{n+\frac{1}{2}} + \mathcal{R}(\mathbf{u}^{n+\frac{1}{2}}), \tag{30}$$

where both reaction and diffusion terms are evaluated at $n+1/2$. Then we introduce appropriate approximations for $\mathbf{u}^{n+1/2}$, aiming at preserving the second-order of the approximation in time. First, we approach the linear operator $\mathcal{A}$, associated with diffusion, using the Crank-Nicolson scheme, yielding

$$\frac{\mathbf{u}^{n+1}-\mathbf{u}^{n}}{\Delta t} = \tfrac{1}{2}\left(\mathcal{A}\mathbf{u}^{n+1}+\mathcal{A}\mathbf{u}^{n}\right)+\mathcal{R}(\mathbf{u}^{n+\frac{1}{2}}). \tag{31}$$

Equation (31) still depends on the non-linear reaction term evaluated at $\mathbf{u}^{n+1/2}$. To evaluate $\mathcal{R}(\mathbf{u}^{n+1/2})$ we introduce an approximation $\mathcal{R}(\tilde{\mathbf{u}})$, with $\tilde{\mathbf{u}}$ being an explicit approximation for $\mathbf{u}^{n+1/2}$, resulting in the following semi-implicit scheme

$$\frac{\mathbf{u}^{n+1}-\mathbf{u}^{n}}{\Delta t} = \tfrac{1}{2}\left(\mathcal{A}\mathbf{u}^{n+1}+\mathcal{A}\mathbf{u}^{n}\right)+\mathcal{R}(\tilde{\mathbf{u}}). \tag{32}$$

Considering the Taylor expansion

$$\mathbf{u}\left(t_n+\Delta t/2\right) = \mathbf{u}(t_n)+\frac{\Delta t}{2}\frac{\partial \mathbf{u}}{\partial t}(t_n)+\mathcal{O}\left(\Delta t^2\right) \tag{33}$$

and using the NRD system (1) we have

$$\mathbf{u}\left(t_n+\Delta t/2\right) = \mathbf{u}(t_n)+\frac{\Delta t}{2}\left(\mathcal{A}\mathbf{u}(\mathbf{t_n})+\mathcal{R}(\mathbf{u}(t_n))\right)+\mathcal{O}\left(\Delta t^2\right) \tag{34}$$

From the above expansion we conclude that:

1. Choosing $\tilde{\mathbf{u}} = \mathbf{u}^n$ in (32) leads to an unconditionally stable scheme but only first order accurate in time.
2. Choosing
$$\tilde{\mathbf{u}} = \mathbf{u}^n + \tfrac{1}{2}\Delta t(\mathcal{A}\mathbf{u}^n+\mathcal{R}(\mathbf{u}^n)), \tag{35}$$
in (32), which corresponds to predict an approximation for $\mathbf{u}^{n+1/2}$ by the explicit Euler method, leads to a second-order and unconditionally stable semi-implicit Crank-Nicolson scheme.

4.2. The proposed semi-implicit ADI scheme

Equation (32) represents the general form of a linear semi-implicit Crank-Nicolson approximation for the NRD system, independent of the spatial discretization. It can be associated with finite element approximations in the

space domain, for instance, but here we will focus on finite difference methods, in particular on the Peaceman-Rachford ADI scheme. Considering that the linear operator $\mathcal{A}$ represents diffusion, then it can be split in $\mathcal{A}_1$ and $\mathcal{A}_2$ which denotes the diffusion operator in the x and y directions, respectively, the proposed method is presented as:

$$\left(\mathcal{I} - \tfrac{1}{2}\Delta t\mathcal{A}_1\right)\mathbf{u}^{n+\frac{1}{2}} = \left(\mathcal{I} + \tfrac{1}{2}\Delta t\mathcal{A}_2\right)\mathbf{u}^{n} + \tfrac{1}{2}\Delta t\mathcal{R}(\tilde{\mathbf{u}}), \tag{36}$$

$$\left(\mathcal{I} - \tfrac{1}{2}\Delta t\mathcal{A}_2\right)\mathbf{u}^{n+1} = \left(\mathcal{I} + \tfrac{1}{2}\Delta t\mathcal{A}_1\right)\mathbf{u}^{n+\frac{1}{2}} + \tfrac{1}{2}\Delta t\mathcal{R}(\tilde{\mathbf{u}}), \tag{37}$$

where $\mathcal{R}(\tilde{\mathbf{u}})$, given the explict Euler method (35), works as a given source term. When $\mathbf{u}$ is a scalar variable u, this ADI scheme requires the solution of two tridiagonal systems of linear equations at each time step, that are solved efficiently using the classical Thomas algorithm. In the general case of a system of reaction-diffusion equations where $\mathbf{u}$ is a vector of n_s variables the ADI method can also be applied, but in this case it leads to block tridiagonal systems of equations, that still can be solved efficiently by an extension of the Thomas algorithm for block systems [26, 27], as presented next.

4.3. Block tridiagonal ADI scheme

To simplify the presentation we consider $\mathbf{u} = [u, v]$ in the presence of cross-diffusion where the linear operator is given by equation (3). In this case the proposed method results in block tridiagonal systems of equations where each block is a 2 by 2 matrix.

The SSI_{ADI} method first computes a prediction by the explicit Euler scheme using equation (35). The predicted solution is then used to evaluate the reaction term $\mathcal{R}(\tilde{\mathbf{u}})$, which appears in the ADI scheme as a source term. The resulting

system of linear equations, in vector form, corresponds to

$$\frac{\mathbf{u}_{i,j}^{n+\frac{1}{2}} - \mathbf{u}_{i,j}^{n}}{\Delta t} = \tfrac{1}{2}\mathbf{D}\left(\frac{\mathbf{u}_{i-1,j}^{n+\frac{1}{2}} - 2\mathbf{u}_{i,j}^{n+\frac{1}{2}} + \mathbf{u}_{i+1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right) + \tfrac{1}{2}\mathbf{D}\left(\frac{\mathbf{u}_{i,j-1}^{n} - 2\mathbf{u}_{i,j}^{n} + \mathbf{u}_{i,j+1}^{n}}{\Delta y^2}\right) + \tfrac{1}{2}\mathcal{R}(\tilde{\mathbf{u}}) \tag{38}$$

$$\frac{\mathbf{u}_{i,j}^{n+1} - \mathbf{u}_{i,j}^{n+\frac{1}{2}}}{\Delta t} = \tfrac{1}{2}\mathbf{D}\left(\frac{\mathbf{u}_{i,j-1}^{n+1} - 2\mathbf{u}_{i,j}^{n+1} + \mathbf{u}_{i,j+1}^{n+1}}{\Delta y^2}\right) + \tfrac{1}{2}\mathbf{D}\left(\frac{\mathbf{u}_{i-1,j}^{n+\frac{1}{2}} - 2\mathbf{u}_{i,j}^{n+\frac{1}{2}} + \mathbf{u}_{i+1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right) + \tfrac{1}{2}\mathcal{R}(\tilde{\mathbf{u}}) \tag{39}$$

which can be expressed in the following compact form

$$-\boldsymbol{\phi}\mathbf{u}_{i-1,j}^{n+\frac{1}{2}} + (\mathbf{I} - 2\boldsymbol{\phi})\mathbf{u}_{i,j}^{n+\frac{1}{2}} - \boldsymbol{\phi}\mathbf{u}_{i+1,j}^{n+\frac{1}{2}} = \mathbf{F}_i^n, \tag{40}$$

$$-\boldsymbol{\phi}\mathbf{u}_{i,j-1}^{n+1} + (\mathbf{I} - 2\boldsymbol{\phi})\mathbf{u}_{i,j}^{n+1} - \boldsymbol{\phi}\mathbf{u}_{i,j+1}^{n+1} = \mathbf{F}_j^{n+\frac{1}{2}}, \tag{41}$$

where $\mathbf{I}$ is the identity matrix; $\mathbf{D}$ and $\boldsymbol{\phi}$ are 2×2 matrices defined, respectively, as

$$\mathbf{D} = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}, \qquad \boldsymbol{\phi} = \frac{\Delta t}{2\Delta x^2}\mathbf{D}, \tag{42}$$

and $\mathbf{F}_i^n$ and $\mathbf{F}_j^{n+\frac{1}{2}}$ are the following 2×1 vectors

$$\mathbf{F}_i^n = \boldsymbol{\phi}\mathbf{u}_{i,j-1}^{n} + (I + 2\boldsymbol{\phi})\mathbf{u}_{i,j}^{n} + \boldsymbol{\phi}\mathbf{u}_{i,j+1}^{n} + \tfrac{1}{2}\mathcal{R}(\tilde{\mathbf{u}}) \tag{43}$$

$$\mathbf{F}_j^{n+\frac{1}{2}} = \boldsymbol{\phi}\mathbf{u}_{i-1,j}^{n+\frac{1}{2}} + (I + 2\phi)\mathbf{u}_{i,j}^{n+\frac{1}{2}} + \boldsymbol{\phi}\mathbf{u}_{i+1,j}^{n+\frac{1}{2}} + \tfrac{1}{2}\mathcal{R}(\tilde{\mathbf{u}}). \tag{44}$$

Note that the matrices associated to each system of equations (40) and (41) are block tridiagonal, where each block is a 2×2 matrix. For example, the block

tridiagonal system from equation (40) has the following form:

$$\begin{bmatrix} \mathbf{I}-2\boldsymbol{\phi} & -\boldsymbol{\phi} & \dots & \dots & \mathbf{0} \\ -\boldsymbol{\phi} & \mathbf{I}-2\boldsymbol{\phi} & -\boldsymbol{\phi} & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & -\boldsymbol{\phi} & \mathbf{I}-2\boldsymbol{\phi} & -\boldsymbol{\phi} \\ \mathbf{0} & \dots & \dots & -\boldsymbol{\phi} & \mathbf{I}-2\boldsymbol{\phi} \end{bmatrix} \begin{bmatrix} \mathbf{X}_1^{n+\frac{1}{2}} \\ \mathbf{X}_2^{n+\frac{1}{2}} \\ \vdots \\ \mathbf{X}_N^{n+\frac{1}{2}} \\ \mathbf{X}_{N+1}^{n+\frac{1}{2}} \end{bmatrix} = \begin{bmatrix} \mathbf{F}_1^n \\ \mathbf{F}_2^n \\ \vdots \\ \mathbf{F}_N^n \\ \mathbf{F}_{N+1}^n \end{bmatrix} \tag{45}$$

where $\mathbf{X}_k$ for $k = 1, \dots, N+1$ is the solution of the system.

Note that the matrix associated to the system (41) has a similar structured and therefore is not presented here. To solve these block tridiagonal systems, a modified version of the Thomas algorithm for block matrix is considered [26], which involves the inverse of $\boldsymbol{\phi}$. The matrix $\boldsymbol{\phi}^{-1}$ is easily obtained if the number of variables n_s is small, such as the case considered here for $n_s = 2$.

In summary, the proposed technique combined with the ADI method for a two-dimensional problem results in two block tridiagonal systems to be solved at each time step, which can be treated efficiently. Otherwise, if the backward Euler or the Crank-Nicolson scheme is used, then one would have to treat the entire sparse system of the linear equations which would require other solvers such as, for instance, the conjugate gradient method. Thus, the ADI scheme combined with the block tridiagonal solver is a robust and efficient numerical method for NRD problems with cross diffusion.

5. Numerical Experiments

This section reports on the numerical results obtained in a series of studies using the SSI_{ADI} scheme. We begin with simple nonlinear NRD problems without and with cross diffusions where an exact solution can be used to estimate the convergence rate of the proposed method. Detailed comparison in terms of accuracy and performance of the SSI_{ADI} method and other methods are presented for the models studied here. More complex models such as the Schnakenberg

and predator-prey with cross diffusion are simulated and the resulting Turing patterns are considered for different paramenter settings.

5.1. Convergence study for a nonlinear RD problem

Consider the nonlinear reaction-diffusion system given by

$$\frac{\partial u}{\partial t} - \nu \Delta u + u^2 v = f_1(u_e, v_e), \tag{46}$$

$$\frac{\partial v}{\partial t} - \nu \Delta v + u v^2 = f_2(u_e, v_e), \tag{47}$$

where ν is the constant diffusion coefficient, f_1 and f_2 are source terms. This system was solved numerically in $\Omega = [0,1]^2$ to check the convergence of the proposed method. The following exact solution was considered:

$$u_e(x,y,t) = e^{x+y-t}, \quad v_e(x,y,t) = \sin(\pi x)\sin(\pi y)e^{-t}. \tag{48}$$

The analytical expressions for the forcing terms f_1 and f_2 are not shown here, but can easily be found by substituting equations (48) in (46) and (47), respectively. Neumann boundary conditions were imposed and initial conditions were prescribed from the exact solution (48).

Table 1: Convergence study for u variable of the nonlinear reaction-diffusion problem using the SSI_{ADI} method: Δx the space discretization, Δt time step, L^∞ and L^2 the errors at the respective norm and the observed rate of convergence r.

Grid	Δx	Δt	L^∞-error	L^2-error	r^∞	r^2
10×10	0.100E+00	0.500E-05	0.501E-06	0.232E-06	-	-
20×20	0.500E-01	0.250E-05	0.136E-06	0.621E-07	1.88	1.90
40×40	0.250E-01	0.125E-05	0.347E-07	0.160E-07	1.97	1.95
80×80	0.125E-01	0.625E-06	0.891E-08	0.405E-08	1.96	1.98
160×160	0.625E-02	0.313E-06	0.226E-08	0.102E-08	1.98	1.99

The results of the semi-implicit predictor method for solving the problem defined by equations (46)-(47) with $\nu = 1$ at the time $t = 0.5 \times 10^{-4}$ for the u variable are shown in Table 1. The table presents the numerical errors against

the exact solution u_e in the L^∞ and L^2, norms and the respective convergence rates, denoted by r^∞ and r^2, respectively. The results for the v variable are similar and are not shown for the sake of brevity. One can observe from the results that the SSI_{ADI} method presents a second order convergence rate as expected.

5.2. Converge study for a nonlinear RD with cross diffusion

A nonlinear reaction-diffusion problem with the inclusion of a cross diffusion operator has also been considered for a convergence study. The model problem is given by:

$$\frac{\partial u}{\partial t} - D_{11}\Delta u - D_{12}\Delta v + u^2 v = f_1(u_e, v_e), \tag{49}$$

$$\frac{\partial v}{\partial t} - D_{21}\Delta u - D_{22}\Delta v + uv^2 = f_1(u_e, v_e), \tag{50}$$

where D_{11} and D_{22} are the self-diffusion coefficients, whereas D_{12} and D_{21} are the cross diffusion coefficients. The reaction terms were defined as $R_1 = u^2 v$ and $R_2 = uv^2$, as in the previous example.

In this study the following exact solution

$$u_e(x, y, t) = (1 - e^{-t}) \cos(\pi x) \cos(\pi y), \tag{51}$$

$$v_e(x, y, t) = (1 - e^{-t}) \cos(2\pi x) \cos(2\pi y), \tag{52}$$

was considered for the numerical experiments. Given the exact solution, the forcing terms f_1 and f_2 can be easily determined by substituting u_e and v_e in the model problem (49)-(50). Additionally, as in the previous case, homogeneous Neumann boundary conditions were considered and the initial conditions are given from the exact solution.

Table 2 shows the numerical errors computed against the exact solution and the resulting rate of convergence for the variable u evaluated at time $t = 1$. As expected, we observe a second order of convergence for this non-linear RD problem even with the inclusion of the cross diffusion operator.

Table 2: Convergence study for u variable of the nonlinear reaction-diffusion problem with cross diffusion operator using the SSI_{ADI} method: Δx the space discretization, Δt time step, L^∞ and L^2 the errors at the respective norm and the observed rate of convergence r.

Grid	Δx	Δt	L^∞-error	L^2-error	r^∞	r^2
40×40	0.250E-01	0.250E-01	0.140E-03	0.641E-04	-	-
80×80	0.125E-01	0.125E-01	0.377E-04	0.154E-04	1.90	2.06
160×160	0.625E-02	0.625E-02	0.976E-05	0.381E-05	1.95	2.02
320×320	0.313E-02	0.313E-02	0.248E-05	0.949E-06	1.98	2.00
640×640	0.156E-02	0.156E-02	0.626E-06	0.237E-06	1.99	2.00

5.3. Comparison of the numerical methods

To compare the performance of the SSI_{ADI} method we considered the nonlinear RD with cross diffusion from the previous section. For simplicity, the total execution time was used as a metric of comparison against other methods implemented in this work. In particular two classical explicit schemes were considered: first order Euler method and the second-order Runge-Kutta (RK2) method. In addition, the second order Strang operator splitting was used for comparisons with the proposed method. The Strang operator splitting was used with the ADI method for the diffusion combined with the Runge-Kutta 2 for the reaction terms. This method is referred as to $Strang_{ADI}$ to remark the fact that the diffusion is treated implicitly with the ADI method and the block tridiagonal solver.

The numerical solutions were obtained using a grid of 640×640 nodes and with successive refinements in the time step, starting from $\Delta t = 0.02$. The following values for the self- and cross-diffusion coefficients were used in the simulations: $D_{11} = D_{22} = 10^{-4}$ and $D_{12} = D_{21} = 10^{-5}$. This particular choice of very small diffusion was made to mitigate the stability condition of the explicit methods (Euler and RK2). For high diffusion parameters a comparison of the methods becomes very difficulty due to the conditional stability of the fully explicit methods. We computed the error against the exact solution provided

by equation (51) and (52) to allow a fair comparison of the methods not only in terms of execution time but also based on accuracy.

Table 3 presents the numerical results. For each case, numerical simulations were carried out 3 times and the average execution times are reported in Table 3. In all cases the standard deviation of the execution time was smaller than 1 second.

Table 3: Performance comparison of the methods for problem (51)-(52) average execution time, measured in seconds, and the numerical error within the parenthesis.

Δt	Expl. Euler	RK2	Strang$_{ADI}$	SSI$_{ADI}$
2.00E-2	-	-	13.23 (3.43E-06)	7.83 (5.37E-06)
1.00E-2	-	-	26.08 (8.57E-07)	15.38 (1.34E-06)
5.00E-3	11.74 (8.18E-04)	26.03 (8.59E-07)	52.52 (2.15E-07)	30.40 (3.35E-07)
2.50E-3	22.34 (4.09E-04)	52.88 (2.16E-07)	103.87 (5.48E-08)	60.68 (8.35E-08)
1.25E-3	43.35 (2.04E-04)	103.02 (5.49E-08)	210.05 (1.48E-08)	123.15 (2.07E-08)

Due to stability restriction of the explicit methods (Euler and RK2), for the first two cases with larger time steps the methods were not able to obtain an approximate solution. For these cases the average execution times and errors are not reported, as indicated by the symbol (-).

For the explicit approaches (Euler and RK2) the results show that the time step has to be, at least, smaller than 5×10^{-3}, to obtain a stable solution. Also, with respect to these methods, note that due to the second order accuracy of the RK2 method its error is much smaller than the one obtained with the explicit Euler method, which in turn resulted in a more expensive numerical solution as reflected in the execution time of the RK2 method.

The results show that for a given time step, the explicit Euler method is the fastest among the methods studied, as expected, since it involves less operations per time step. Note that all the second order methods obtained errors of similar magnitude. With respect to the performance of the implicit approaches, the SSI$_{ADI}$ method is about 70% faster than the Strang splitting scheme with ADI for diffusion and RK2 for reaction method (Strang$_{ADI}$).

Considering the error obtained by the methods for different time step sizes, one can note that the SSI_{ADI} scheme is quite competitive. For instance, with a larger time step size such as $\Delta t = 0.02$ the SSI_{ADI} method is much faster and more accurate than the explicit Euler method with $\Delta t = 0.00125$. When comparing the Strang_{ADI} and the SSI_{ADI} schemes, one observes that the SSI_{ADI} method has an improved accuracy and performance.

5.4. Applications to biological models

In this section we present the results of experiments considering the SSI_{ADI} for the numerical solution of well known mathematical models such as the Schnakenberg and a predator-prey with refuge.

5.4.1. Schnakenberg

An initial study was performed considering the following parameters [25]: $a = 0.1305$, $b = 0.7695$, $\kappa = 100$, $\mathcal{D}_1 = 0.05$ and $\mathcal{D}_2 = 1$. A unit square domain with homogeneous Neumann boundary conditions was considered and the following initial conditions were used:

$$C_a(x, y, 0) = a + b + 10^{-3} e^{-100((x-1/3)^2+(y-1/2)^2)}, \tag{53}$$

$$C_i(x, y, 0) = \tfrac{b}{(a+b)^2}. \tag{54}$$

The numerical solution was carried out by the SSI_{ADI} method considering a time step of $\Delta t = 10^{-5}$ and a grid of 200×200 nodes. The spatial distribution of C_a at different time instants until the $t_f = 10$ was reached, are shown in Figure 1.

To check whether the dynamics has reached a steaty-state pattern, we computed the norm of the increment in the solution $\|C^{n+1} - C^n\|_2$, where C could be either the activator or inhibitor $C = \{C_a, C_i\}$. Figure 2 shows the behavior of the norm of the increment in the solution for both the activator and inhibitor as a function of time. Assuming a tolerance of $tol = 10^{-6}$, one can observe that the steady state was achieved at about $t = 8$. Therefore, Figure 1(f) shows the final steady state pattern obtained for this simulation.

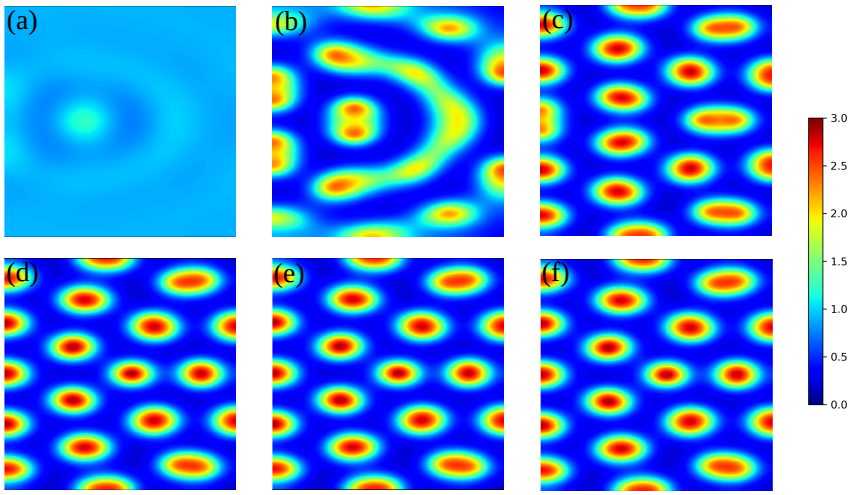

Figure 1: Spatial patterns obtained with the Schnakenberg model using the SSI_{ADI} method at different time instants: (a) $t = 0.03$, (b) $t = 0.05$, (c) $t = 1.5$, (d) $t = 4.5$, (e) $t = 7.5$ and (f) $t = 10.0$.

Next, a convergence study of the approximated solution using the SSI_{ADI} method is presented. The errors were computed considering a reference solution obtained in a very fine grid of 1600×1600 nodes. The errors were computed using the L^∞ norm at time instant $t = 2.0$ of the simulation, when the stationary pattern was not reached yet.

Table 4: Schnakenberg model: L^∞-errors and the observed rate of convergence r^∞ when compared to a reference solution computed in a refined grid of 1600×1600 nodes.

Grid	L^∞-error	r^∞
50×50	0.808709	-
100×100	0.134374	2.1
200×200	0.030492	2.1
400×400	0.007154	2.3

From the results one observe that the expected second order of convergence was achieved for this complex problem involving pattern formation where no

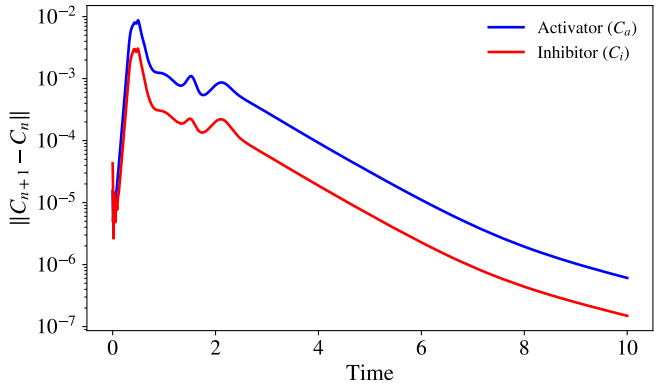

Figure 2: Behavior of the increment $\|C^{n+1} - C^n\|_2$, where $C = \{C_a, C_i\}$, to show that the stationary pattern is attained at about $t_f = 8$ (within a tolerance of 10^{-6}).

exact solution is available.

5.4.2. Predator-Prey with refuge

Next, we describe the application of the SSI_{ADI} method for the numerical solution of a predator-prey model. The model defined by equations (6)-(7) was studied for the particular problem introduced by Guin and Mandal [12] where the reaction terms F_1 and F_2 are defined by equations (8) and (9). For the simulations presented here a square domain $\Omega = [0, 100]^2$ was considered and the following set of parameters was used: $\alpha = 0.59$, $\beta = 0.0327$, $\gamma = 0.15$, $\delta = 0.05$, $\epsilon = 1.0$, $D_{11} = 0.1$, $D_{12} = 0.01$, $D_{21} = 0.8$, $D_{22} = 1.0$. Different values for the refuge parameter were considered: $r = \{0.0, 0.02, 0.12, 0, 18, 0.24\}$. In all cases presented next, homogeneous Neumann boundary conditions were imposed.

For the initial conditions two cases were considered: one considers random perturbations of about 10^{-2} around the local equilibrium of the reaction terms, whereas the other is a deterministic initial condition. The former case was used to explore the different patterns resulting from the model, whereas the later case was used to perform a grid independence test.

First, we present an initial example of the solution and the spatial pattern obtained with the predator-prey model with cross diffusion considering $r = 0$ (no

refuge). The simulation was performed until a spatial steady state pattern was formed, as indicated by the norm of the increment in the solution $\|u^{n+1} - u^n\|_2$ as a function of time.

Figure 3 shows the steady-state spatial patterns obtained for the preys and predators (panels (a) and (b), respectively). In both cases one can observe a spotted-like pattern, which is typical for the case without refuge ($r = 0$), as discussed in [12]. For this case, we considered the steady state was achieved within a tolerance of 10^{-4} in terms of the norm of the increment of the solution, as shown in Figure 3(c).

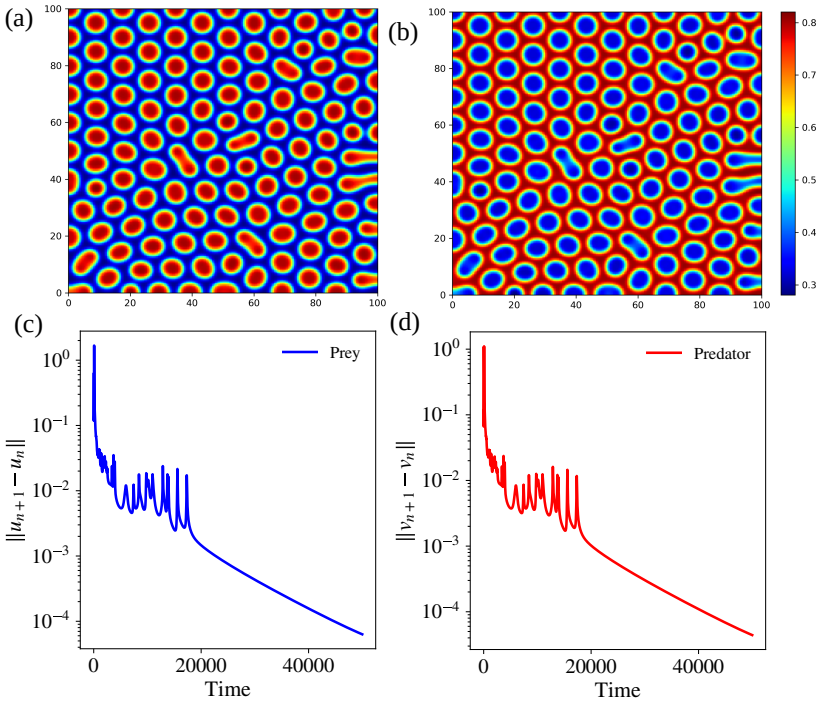

Figure 3: Example of steady state pattern obtained for the predator-prey model with cross-diffusion operator. Panels (a) and (b) show the spatial distribution of prey and predators, respectively, whereas panel (c) shows the norm of the increment of each variable u and v.

Next, to check that the implementation of the method for this particular problem was correct and the obtained approximated solution was independent of the grid resolution we carried out another set of simulations. The idea is to

check whether by refining the grid the same spatial pattern is recovered. However, instead of considering a random perturbation field around the equilibrium values (u^*, v^*) of the reaction terms, a deterministic initial condition was used. The following functions were chosen for the initial conditions of the preys and predators:

$$u_0(x, y, 0) = u^* + \varepsilon g(x, y), \tag{55}$$

$$v_0(x, y, 0) = v^* + \varepsilon g(x, y), \tag{56}$$

$$g(x, y) = \sin(8\pi x/L)\sin(8\pi y/L), \tag{57}$$

where $\varepsilon = 10^{-3}$ is a parameter to scale the perturbation to the initial condition given by the g function.

Simulations were carried using the SSI_{ADI} method with refuge $r = 0.02$, a time step of $\Delta t = 0.05$ and considering a sequence of grid refinements of $N_x \times N_x$ nodes where $N_x = \{100, 200, 400\}$. The results for the prey variable are shown in Figure 4, and the results for the predators are qualitatively similar and, therefore, omitted for the sake of clarity. One can note that the spatial pattern achieved with the 400×400 grid is the same as the other two obtained with coarser grids. Thus, it is clear that the results obtained are not grid dependent and given the same initial conditions converge to the same spatial pattern.

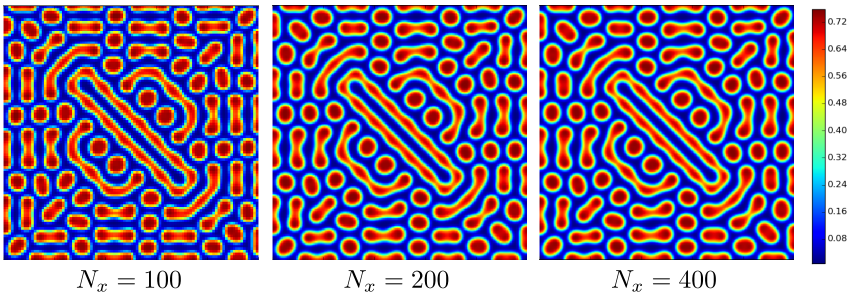

Figure 4: Grid independence test for the predator-prey model with refuge for grid discretizations with 100×100, 200×200 and 400×400 nodes.

Finally, the effect of the refuge parameter on the stationary Turing patterns was explored for $r = 0.02$, $r = 0.12$ and $r = 0.18$ using the SSI_{ADI} method

and the parameter set described before. The spatial steady-state patterns are shown in Figure 5 for both preys (variable u, top row) and predators (variable v, bottom row).

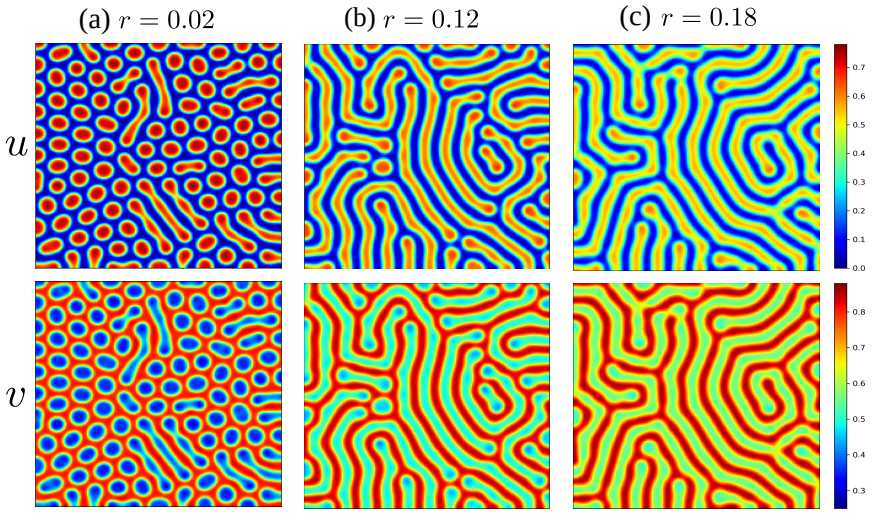

Figure 5: Effects of refuge parameter on pattern formation of the predador-prey model with cross diffusion. Top and bottom rows show, respectively, the spatial distribution of u (prey) and v (predator) for the following values of refuge: (a) $r = 0.02$, (b) $r = 0.12$ and (c) $r = 0.18$.

The results show that as the value of the refuge parameter r increases, the obtained Turing pattern changes from a predominantly spot-like pattern, to a mix of spot- and strip-like pattern ($r = 0.02$), and then to a predominantly strip-like pattern ($r = 0.18$).

6. Discussion

6.1. Comparison of the methods

For the systems of reaction-diffusion studied in this work the proposed semi-implicit predictor method (SSI_{ADI}) demonstrated to be more efficient than the Strang_{ADI} scheme, which is based on RK2 for reaction and ADI with the block tridiagonal solver. Here, the Strang splitting was implemented using the reaction-diffusion-reaction scheme, which required a total of 4 evaluations of the

reaction term per time step. The semi-implicit predictor method only requires 2 evaluations of the reaction terms, one during the prediction step and the other at $t_{n+1/2}$. In both methods, the ADI block tridiagonal solver is used once at each time step. Thus, even in the problem used in this comparison which has a simple reaction term the semi-implicit predictor outperformed the Strang$_{ADI}$ scheme.

We expect that for more complicated problems, such as in cardiac electrophysiology, where the reaction terms are very stiff [28, 29] and contains several variables that the performance of the semi-implicit predictor method will be even better than the Strang$_{ADI}$ scheme which requires more evaluations of the reaction terms.

6.2. Comparison with methods from the literature

To the best of our knowledge, no previous works have been found in the literature which is exactly the same as the SSI$_{ADI}$ or the Strang$_{ADI}$ method. Next, we discuss the schemes introduced in this work and their relation to other schemes from the literature.

In the work of Jim Douglas [4], where an ADI scheme for three space variables was presented, a method similar to the SSI$_{ADI}$ for nonlinear parabolic problems was introduced. The Douglas method consists of a predictor-corrector scheme that uses the ADI scheme to compute an approximation to $\mathbf{u}^{n+\frac{1}{2}}$ required for the evaluation of the nonlinear reaction term $\mathcal{R}(\mathbf{u}^{n+\frac{1}{2}})$ from equation (31). As discussed in [4] (see Section 5, page 48), the computational costs in terms of floating point arithmetic per time step is doubled using the ADI scheme as the predictor. However, the increases in accuracy justifies this extra work. The SSI-ADI approach is based on the explicit Euler method to compute an approximation to $\mathbf{u}$ at time $t^{n+1/2}$, which requires less computations than the ADI scheme used by Douglas and still results in a second order accurate method even regardless of using a first order method for the prediction.

With respect to the Strang$_{ADI}$ method, a similar approach was used by [30] to solve the Allen-Cahn equation where the Strang splitting was employed and

the ADI scheme was used in the intermediate step to solve a fractional partial differential equation. At this point we remark that the Strang$_{ADI}$ scheme discusses here uses the ADI method for a system of PDEs with a block tridiagonal system of equations solver.

Alternative methods such as an Implicit-Explicit scheme (IMEX) have been proposed for NRD models in which the reaction term is treated explicitly whereas the diffusive term is treated implicitly. In [3] some variants of the IMEX scheme are presented and applied to problems of pattern formation. In its classic form the IMEX method is only first order accurate, however more complex versions based on the Backward Differentiation Formula (BDF) method [31] are also presented in [3].

For predator-prey models, a second order time discretization scheme was presented by Gambino *et al.* [32] which uses the Peaceman-Rachford ADI method [7] combined with an operator splitting approach. In their scheme the solution in a new time step requires an explicit step of the reaction term, then a implicit step of the diffusion, followed by an explicit step of diffusion and, finally, an implicit step of reaction. As discussed by Gambino *et al.* [32] this scheme guarantees second order accuracy in time.

Other works present different methods for reaction-diffusion with cross diffusion: in [33] finite difference schemes for predator-prey models are presented; a high order exponential scheme based on the ADI method is presented for convection and diffusion problems in [34]; also non-standard finite difference scheme have been applied for the problem of predator-prey with cross diffusion in [35].

Other numerical techniques such as discontinuous Galerkin finite element methods (DG) have been proposed for reaction-diffusion models such as the Schnakenberg in [25]. Whereas the finite element method is flexible for treating complex geometries, as demonstrated in the mentioned work, the particular case of discontinuous Galerkin method involves system of equations with a large number of degrees of freedom, requiring a large amount of processing power [25]. Other works using advanced numerical techniques such as the finite volume [36] and spectral methods [37] have been proposed for reaction-diffusion problems.

7. Conclusions

In this work we presented second order ADI schemes for the numerical solution of partial differential equations, in particular, non-linear reaction-diffusion models with applications in biology. The proposed SSI_{ADI} method considers the reaction and diffusion terms at $n + \frac{1}{2}$ and, in particular, uses a prediction of the solution to evaluate the reaction term and the average of the solutions at n and $n + 1$ to treat the diffusion. Thus, the reactions are handled explicitly avoiding the need to solve a system of non-linear equations, whereas the diffusion term is treated implicitly in an efficient form using the ADI method. The numerical scheme is second order accurate and unconditionally stable, as demonstrated through a series of numerical experiments.

In addition to that, we presented the combination of the second-order Strang operator splitting scheme with the ADI scheme ($Strang_{ADI}$) for a system of reaction-diffusion equations with two variables. In this case the use of the ADI scheme results in two block tridiagonal linear systems that can be solved efficiently using an extension of the Thomas algorithm. The block version of this method only requires computation of the inverse of small matrices, such as 2×2 in the present case, obtained analytically.

Simulations of complex reaction-diffusion problems such as the Schnakenberg and prey-predator model with cross diffusion were carried out to assess the numerical accuracy and computational performance of the methods compared with other well established methods. Also, the SSI_{ADI} method is as efficient as the second-order and unconditionally stable $Strang_{ADI}$ method, which is based on the Strang operator splitting and ADI scheme. In summary, we showed that the proposed methods SSI_{ADI} and $Strang_{ADI}$ are efficient, accurate, and attractive alternatives for the numerical solution of non-linear reaction-diffusion problems.

Acknowledgments

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