NUMERICAL TREATMENT OF GRAY-SCOTT MODEL WITH OPERATOR SPLITTING METHOD

BERAT KARAAGAC*
Faculty of Mathematics and Statistics
Ton Duc Thang University, Ho Chi Minh City, Vietnam
Department of Mathematics Education
Adiyaman University, Adiyaman, Turkey

Abstract. This article focuses on the numerical solution of a classical, irreversible Gray Scott reaction-diffusion system describing the kinetics of a simple autocatalytic reaction in an unstirred ow reactor. A novel finite element numerical scheme based on B-spline collocation method is developed to solve this model. Before applying finite element method, “strang splitting” idea especially popularized for reaction-diffusion PDEs has been applied to the model. Then, using the underlying idea behind finite element approximation, the domain of integration is partitioned into subintervals which is sought as the basis for the B-spline approximate solution. Thus, the partial derivatives are transformed into a system of algebraic equations. Applicability and accuracy of this method is justified via comparison with the exact solution and calculating both the error norms $L_2$ and $L_\infty$. Numerical results arising from the simulation experiments are also presented.

1. Introduction. With a simple definition a reaction-diffusion systems are a set of partial differential equations representing reacting, diffusing and transporting of constituents with the aid of chemical reactions. Also, reaction-diffusion systems are related to many research areas and they can be applied in biology, medicine, epidemiology etc. For example, in biology, the systems are used to explain the stripe patterns of zebras, leopards, jaguars, snakes and seashells [42] and constructing a model for simulating the hepatitis B virus (HBV) infection with spatial dependence[44]. In medicine, it is used in diffusion of drugs in body streams[41]. In epidemiology, it is used in modelling the evolution dynamics of infectious and process spreading of infection disease[40]. There are several different and attractive studies on numerical or theoretical aspect of reaction diffusion models in the literature. Some of them are, in [28], a mathematical model for investigating the hepatitis B virus disease in fractional medium is derived using fractional-in-space reaction–diffusion equations and obtained some useful biological results. Owolabi and Patidar [29] integrated directly some systems of reaction–diffusion equations using fourth-order finite difference scheme (in space) coupled with fourth-order time-stepping methods. Hasnain and Shahid [12] used three finite difference implicit schemes for enhancing consistency. A meshfree algorithm is developed for solving

2020 Mathematics Subject Classification. Primary: 65L60, 35Q68; Secondary: 65D07.
Key words and phrases. Gray Scott model, finite element method, B-spline, collocation, strang splitting.

* Corresponding author: Berat Karaagac(beratkaraagac@tdtu.edu.vn).
1D and 2D Brusselator models. The method based on radial basis multiquadric functions and differential quadrature (DQ) technique in [19]. There exists more specialized models for Reaction Diffusion systems to interpret particular experimental situations such as Belousov-Zhabotinsky reaction system (a simplification of Noyes-field model), Lotka-Volterra competition diffusion system, Gray-Scott model, two- and three-component models for quadratic solitons. Recently, increasing interest in fractional order differential equations yields introduce a new parameter which is a fractional derivative depending on the time and(or) space derivatives index to Reaction Diffusion systems. Solutions to the fractional diffusion equation have been spread at a same rate with the classical diffusion equation. In order to contribute to the literature, when a brief knowledge is given, we can acquaint several studies such as; Owolabi [30, 31] has used two separate mathematical techniques and formulate a Fourier spectral discretization method to solve fractional reaction-diffusion problems and several reaction diffusion models are solved numerically with finite difference approximation for the spatial discretization. Also in [32], the author applied an efficient and viable alternative approach to low order schemes for solving fractional-in-space reaction-diffusion equations. Guo et al [11] have developed a finite difference/Hermite–Galerkin spectral method for solving the time-fractional nonlinear reaction–diffusion equation. Cheng et al [4] constructed and analyzed a new linearized compact ADI scheme to obtain solutions of the 2D Riesz space fractional nonlinear reaction–diffusion equations. Further important knowledge about numerical aspect of fractional differential equations with different kernels see in [32, 26, 37, 33].

In this article, we investigate the application of the collocation method combined with Strang splitting technique to the irreversible Gray-Scott (GS) model, a very well-known reaction-diffusion system. The GSM was first presented by Gray and Scott in [10]. Pearson [35] have computed solutions of the two-dimensional Gray-Scott, numerically and revealed a rich and complex structure in the solutions for the Gray-Scott model. The model involves two reactants, one of them is an activator and other is a substrate and it is a model of chemical reaction between two substances. In dimensionless, the model equations are as follows [38]:

\[
\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2 u(x,t)}{\partial x^2} - u(x,t)v(x,t)^2 + a(1 - u(x,t)), \quad x \in [x_l, x_r], T > 0
\]

where the two unknown variables \(u(x,t)\) and \(v(x,t)\) describe concentration of two substances, \(\tilde{a}, \tilde{b}\) and \(\tilde{d}\) are constants. \(\tilde{d}\) is the normalized diffusivity of second substance, \(\tilde{a}\) denotes the rate which the first substance is fed from the reservoir into the reactor and \(\tilde{b}\) is the general decay rate of second one. One can encounter many studies and analysis about the Gray Scott (GS) model [7, 8, 36, 6]. In numerical aspect, Manaa and Rasheed [21] has solved the problem numerically for finding an approximate solution by Successive approximation method and finite difference method. Yadav and Jiwari [46] used Galerkin finite element method to obtain approximation of solutions with Lagrange basis. Owolabi et al [34] investigated numerical simulations of coupled one-dimensional Gray-Scott model using a combination of higher order exponential time differencing Runge-Kutta scheme, higher-order symmetric finite difference scheme and higher-order ETDRK method. Önarcan et al [25] investigated numerical solutions of the model via the trigonometric quintic B-spline finite element collocation method and linearized the term \(uv\) and \(uv^2\). Korkmaz et
al. [18] obtained the numerical simulations of the problem sinc differential quadrature combined with third-fourth order implicit Rosenbrock and exponential B-spline collocation methods. In [46, 25, 18], the authors consider the Gray Scott model with initial conditions given by $u(x,0) = 1 - \frac{1}{2} \sin^{100}(\pi x)$ and $v(x,0) = \frac{1}{4} \sin^{100}(\pi x)$ and obtained numerical simulations, successfully.

For our aim, firstly we develop the Strang splitting approach for Eq. (1). This approach converts the solution of GSM into four differential equations involving two linear and two nonlinear equations. Then, for unknown variables $u(x,t)$ and $v(x,t)$, two approximate solutions are defined as a linear combination of cubic B-spline basis with unknown time parameters. Substituting the trial solution in the model problem with finite difference approximations which are forward finite difference and Cranck Nicolson formula lead us to formulate linear algebraic equations, easily. Also, the nonlinear terms in the third and fourth equations are discretized using Rubin Graves finite difference approach [39].

This article is structured as follows; Section 2 introduces Strang splitting technique, section 3 describes the application of finite element approximation to the GSM and obtaining numerical scheme. Stability analysis of the numerical scheme is discussed in section 4. Numerical results, tables and graphics are given in section 5. Finally, conclusion is presented in section 6.

2. Strang splitting for Gray-Scott model. Splitting methods are powerful methods for numerical investigation of complex models and used in computing numerical solutions to partial differential equations. The main idea of the method is splitting the original problem into different sub-problems and using specialized numerical algorithms and different discretization techniques for each sub-problems. The splitting methods are efficient and easily applicable methods and they lead usually reduced of the computational costs to solve the problem. Strang splitting is one of the well-known and the second order splitting methods. It was investigated by Strang for the improvement of accuracy of the splitting algorithm [43]. Let us consider the problem given as

$$u_t = A(u) \quad (2)$$

where $A(u)$ depends on $u$ and its spatial and time derivatives of different orders. Assuming the exact solution of the problem given in (2) is defined on the time interval $[0,T]$ where $T > 0$ and partition of the time interval as $P = \{t_n : n = 0,1,\ldots,M\}$ for $\Delta t = t_{n+1} - t_n$. The splitting method for the case of $A = A_1 + A_2$, we get the following differential equations

$$u_t = A_1(u) \quad \text{(3)}$$

$$u_t = A_2(u) \quad \text{(4)}$$

The Strang splitting process can be written in the form:

$$u_t = A_1(u), \quad t \in [t_n, t_{n+\frac{1}{2}}] \quad (3)$$

$$u_t = A_2(u), \quad t \in [t_n, t_{n+1}] \quad (4)$$

$$u_t = A_1(u), \quad t \in [t_n, t_{n+\frac{1}{2}}] \quad (5)$$

where $\Delta t$ is step length of the time interval. This means that; instead of solving Eq. (2) for time $\Delta t$, first of all, we solve Eq. (3) for $\Delta t/2$. Then, we solve the Eq. (4) for $\Delta t$. At the end, for purpose of complete time step, Eq. (5) is solved for $\Delta t/2$. 

Applying the idea of Strang splitting technique the Gray Scott model, we get the following form of the equations

\[ u_t = u_{xx} + \tilde{a}(1 - u) \]  
\[ v_t = \tilde{d}v_{xx} - \tilde{b}v \]  
\[ u_t = -uv^2 \]  
\[ v_t = uv^2 \]

Now, we can begin to apply finite element collocation method to the above equations.

3. **Application of the collocation method to Gray-Scott model.** Collocation method is a powerful tool for solving partial differential equations using generally interpolation functions (for different application of the method see in [27, 23, 14, 5, 9, 15]). This section covers the application of the method for the solution of the Gray-Scott model given in Eqs. (6)-(9) using cubic B-spline basis functions. Let us present a brief summary of the collocation method with application of the method through to the model problem following

**Step 1.** The basic idea of numerical methods is the discretization of given partial differential equations. For finite element approximation discretization process is different. Solution interval have to be divided into a suitable sets of finite elements, because of the approximate solution going to be defined on each elements. Let \( \{x_m\}_{m=1}^N \) be interior points or nodal points of interval \([x_{left}, x_{right}]\) and assume that

\[ x_0 = x_{left} < x_1 < \cdots < x_{N-1} < x_{right} = x_N \]

where \( m \) is a relative integer, \( N \) total number collocation points and \( x_m = mh \).

**Step 2.** The collocation method assumes the exact solutions \( u(x, t) \) and \( v(x, t) \) given in Eq. (1) can be interpolated and approximated by the linear combination of B-spline basis functions with unknown time dependent parameters at nodal points as follows

\[ u(x, t) \approx u_{apprx}(x, t) = \sum_{m=-1}^{N+1} \alpha_m(t) \phi_m(x) \]

\[ v(x, t) \approx v_{apprx}(x, t) = \sum_{m=-1}^{N+1} \beta_m(t) \phi_m(x) \]

where the expression of \( \phi_m(x) \) are cubic B-spline basis and \( \alpha_m(t), \beta_m(t) \) are time dependent unknown parameters. Cubic splines are 3rd degree polynomials whose restriction on the knots \( x_{m-2}, x_{m-1}, x_m, x_{m+1}, x_{m+2} \) and zero except on the interval \([x_{m-2}, x_{m+2}]\). We define cubic B-splines as [20]

\[
\phi_m(x) = \begin{cases} 
\frac{(x-x_{m-2})^3}{h^3}, & \text{if } x_{m-2} \leq x < x_{m-1}, \\
\frac{h^3 + 3h^2(x-x_{m-1}) + 3h(x-x_{m-1})^2}{h^3}, & \text{if } x_{m-1} \leq x < x_m, \\
\frac{-3(x-x_{m-1})^3}{h^3}, & \text{if } x_m \leq x < x_{m+1}, \\
\frac{h^3 + 3h^2(x_{m+1}-x) + 3h(x_{m+1}-x)^2}{h^3}, & \text{if } x_{m+1} \leq x < x_{m+2}, \\
(x_{m+2}-x)^3, & \text{if } x_{m+2} \leq x, \\
0, & \text{otherwise}. 
\end{cases}
\]

For our problem, we have a set of linear and nonlinear partial differential equations. It is also sensible to perform the linearization of the nonlinear terms before the spatial discretization. For this purpose, we are going to present forward difference
formula with Rubin Graves linearization technique for the terms $uv^2$ in Eqs. (8) and (9).

$$uv^2 = \frac{(uv^2)^{n+1} + (uv^2)^n}{2}$$

$$= \frac{(u^n)^2v^{n+1}}{2} + u^n v^n v^{n+1} - \frac{u^n (v^n)^2}{2}$$

In order to obtain numerical solutions and simulations iteratively, the governing
equations must be discretized in both space and time. Temporal discretization
is obtained by forward difference formula in time and Crank Nicolson formula,
respectively

$$\frac{\partial u}{\partial t} = \frac{u^{n+1} - u^n}{\Delta t}, \quad \frac{\partial v}{\partial t} = \frac{v^{n+1} - v^n}{\Delta t}$$

Thus, we get

$$\frac{u^{n+1} - u^n}{\Delta t} = \frac{(u_{xx})^{n+1} + (u_{xx})^n}{2} + \tilde{a} \left[ 1 - \left( \frac{u^{n+1} + u^n}{2} \right) \right]$$

$$\frac{v^{n+1} - v^n}{\Delta t} = \frac{(v_{xx})^{n+1} + (v_{xx})^n}{2} - \tilde{b} \left( \frac{v^{n+1} + v^n}{2} \right),$$

$$\frac{u^{n+1} - u^n}{\Delta t} = - \left( \frac{(v^n)^2}{2} u^{n+1} - \Delta t u^n v^n v^{n+1} + \frac{\tilde{a}}{2} u^n (v^n)^2 \right)$$

$$\frac{v^{n+1} - v^n}{\Delta t} = \frac{(u^n)^2}{2} u^{n+1} + \Delta t u^n v^n v^{n+1} - \frac{\tilde{b}}{2} u^n (v^n)^2$$

Substituting (10) into Eq. (6)-(9) with values of $u_{\text{apprx}}$, $v_{\text{apprx}}$ and their second
derivatives at the $x_m$ knot points using the terms of the parameters $\alpha_m(t), \beta_m(t)$
given following form

$$u_{\text{apprx}} = \alpha_{m-1} + 4\alpha_m + \alpha_{m+1}$$

$$u'_{\text{apprx}} = \frac{6}{\Delta t} (\alpha_{m-1} - 2\alpha_m + \alpha_{m+1})$$

$$v_{\text{apprx}} = \beta_{m-1} + 4\beta_m + \beta_{m+1}$$

$$v'_{\text{apprx}} = \frac{6}{\Delta t} (\beta_{m-1} - 2\beta_m + \beta_{m+1})$$

After some arrangements, we get an algebraic equation system which can be expressed in the following form

$$\alpha_{m-1} \left( 1 - \Delta t \left( \frac{3}{\Delta x^2} - \frac{3}{2} \right) \right) + \alpha_m \left( 4 + \Delta t \left( \frac{3}{\Delta x^2} + 2\tilde{a} \right) \right)$$

$$+ \alpha_{m+1} \left( 1 - \Delta t \left( \frac{3}{\Delta x^2} - \frac{3}{2} \right) \right) = \alpha_{m-1} \left( 1 + \Delta t \left( \frac{3}{\Delta x^2} - 2\tilde{a} \right) \right)$$

$$\beta_{m-1} \left( 1 - \Delta t \left( \frac{3\tilde{d}}{\Delta x^2} - \frac{3}{2} \right) \right) + \beta_m \left( 4 + \Delta t \left( \frac{3\tilde{d}}{\Delta x^2} + 2\tilde{b} \right) \right)$$

$$+ \beta_{m+1} \left( 1 - \Delta t \left( \frac{3\tilde{d}}{\Delta x^2} - \frac{3}{2} \right) \right) = \beta_{m-1} \left( 1 + \Delta t \left( \frac{3\tilde{d}}{\Delta x^2} - 2\tilde{b} \right) \right)$$

$$+ \beta_{m+1} \left( 4 - \Delta t \left( \frac{3\tilde{d}}{\Delta x^2} + 2\tilde{b} \right) \right) + \beta_{m+1} \left( 1 + \Delta t \left( \frac{3\tilde{d}}{\Delta x^2} - \frac{3}{2} \right) \right)$$
\begin{align*}
\alpha_{m-1}^{n+1} 
&= \alpha_{m-1}^{n+1} \left(1 + \frac{\Delta t g_m^2}{2}\right) + \beta_{m-1}^{n+1} (z_m g_m \Delta t) + \alpha_{m+1}^{n+1} \left(1 + \frac{\Delta t g_m^2}{2}\right) \\
&+ \beta_{m-1}^{n+1} (z_m g_m \Delta t) + \beta_{m+1}^{n+1} (z_m g_m \Delta t) \\
&= \alpha_{m-1}^{n+1} + 4\alpha_m^{n+1} + \alpha_{m+1}^{n+1} + \frac{z_m g_m^2 \Delta t}{2} \\
&+ \beta_{m-1}^{n+1} (1 - z_m g_m \Delta t) + \beta_{m+1}^{n+1} (1 - z_m g_m \Delta t) \\
&= \beta_{m-1}^{n+1} + 4\beta_m^{n+1} + \beta_{m+1}^{n+1} + \frac{z_m g_m^2 \Delta t}{2}
\end{align*}

where \(z_m = u_m^n\) and \(g_m = v_m^n\) known values of functions at the knots points \(x_m\). Collocation method yields a system of algebraic equations. The first and second equations consist of \((N + 1)\) equation and \((N + 2)\) unknown variables. we are going to consider the third and fourth equations together. Thus, the equation systems given in (13) and (14) consist of \((2N + 2)\) equation and \((2N + 4)\) unknown variables such as

\[
\{\alpha_{-1}, \alpha_0, \alpha_1, \ldots, \alpha_N, \alpha_{N+1}\} \\
\{\beta_{-1}, \beta_0, \beta_1, \ldots, \beta_N, \beta_{N+1}\}
\]

**Step 3.** As seen from step 2, the number of equations is less than the number of unknown variables. In order to obtain a solvable system, the first thing that we need to do is applying boundary conditions at the boundary of the interval which are the most important step in implementing FEM. This will yield us to eliminate unknown variables from the above systems i. e. when we use boundary conditions with approximate solution constructed in (10), we can obtain following equations.

\[
\begin{align*}
\alpha_{-1} &= u(x_{left}, 0) - 4\alpha_0 - \alpha_1 \\
\beta_{-1} &= v(x_{left}, 0) - 4\beta_0 - \beta_1 \\
\alpha_{N+1} &= u(x_{right}, 0) - 4\alpha_N - \alpha_{N-1} \\
\beta_{N+1} &= v(x_{right}, 0) - 4\beta_N - \beta_{N-1}
\end{align*}
\]

So, \(\alpha_{-1}, \alpha_{N+1}, \beta_{-1}\) and \(\beta_{N+1}\) can be removed from systems. Now, we applied our boundary condition, we can solve our systems given in (11)-(14). At the end, the first and second systems consists of \((N + 1)\) equations and \((N + 1)\) unknown variables and third and fourth systems consists of \((2N + 2)\) equations and \((2N + 2)\) unknown variables.

These systems are going to be solved via iterative procedure, the process of each loop is a single iteration and outcome of each loop generates starting point of next iteration process. Thus, each \((n + 1) - th\) approximation is derived from the \(n - th\) approximation.

According to Strang splitting algorithm, only the first and last time steps need to involve half time steps. Therefore, Eqs.(11) and (12) are going to be solved for half step by individual because the first and second system consist of only parameters \(\alpha_m\).
and $\beta_m$, respectively. Since the systems Eqs. (13) and (14) are consist of parameters $\alpha_m$ and $\beta_m$ with together, they going to compute in parallel.

**Step 4.** An iterative method starts with an initial vector and improving this initial vector until the solution of system is achieved up to predefined time step. This step of the method consist of obtaining initial vector \( \{\alpha_0^{(0)}, \alpha_1^{(0)}, \ldots, \alpha_{N-1}^{(0)}, \alpha_N^{(0)}\} \), \( \{\beta_0^{(0)}, \beta_1^{(0)}, \ldots, \beta_{N-1}^{(0)}, \beta_N^{(0)}\} \) at time \( t = 0 \). Initial conditions of the problem will help us to obtain our initial vector in this step. Now, let us obtain an algebraic equation system using initial condition of the problem and approximate solution given in (10) at knots points \( x_m \) as follows

\[
\begin{align*}
  u(x_0, 0) &= \alpha_0 - 1 + 4\alpha_0 + \alpha_1 \\
  u(x_1, 0) &= \alpha_0 + 4\alpha_1 + \alpha_2 \\
  \vdots \\
  u(x_{N-1}, 0) &= \alpha_{N-2} + 4\alpha_{N-1} + \alpha_N \\
  u(x_N, 0) &= \alpha_{N-1} + 4\alpha_N + \alpha_{N+1}
\end{align*}
\]

and

\[
\begin{align*}
  v(x_0, 0) &= \beta_0 - 1 + 4\beta_0 + \beta_1 \\
  v(x_1, 0) &= \beta_0 + 4\beta_1 + \beta_2 \\
  \vdots \\
  v(x_{N-1}, 0) &= \beta_{N-2} + 4\beta_{N-1} + \beta_N \\
  v(x_N, 0) &= \beta_{N-1} + 4\beta_N + \beta_{N+1}
\end{align*}
\]

It is seen from the above system, we have encountered the same situation with step 3. There are more unknowns than equations. Using equations given in (15), we can deal with this situation. At the end, we get initial vector, solving following system of equation

\[
\begin{bmatrix}
  4 & 2 & 0 & 0 & \cdots & 0 & 0 & 0 \\
  1 & 4 & 1 & 0 & \cdots & 0 & 0 & 0 \\
  0 & 0 & \ddots & \ddots & \ddots & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 1 & 4 & 1 \\
  0 & 0 & 0 & 0 & 0 & 2 & 4 \\
\end{bmatrix}
\begin{bmatrix}
  \alpha_0 \\
  \alpha_1 \\
  \vdots \\
  \alpha_N \\
\end{bmatrix}
= \begin{bmatrix}
  u(x_0, 0) \\
  u(x_1, 0) \\
  \vdots \\
  u(x_N, 0) \\
\end{bmatrix}
\]

and

\[
\begin{bmatrix}
  4 & 2 & 0 & 0 & \cdots & 0 & 0 & 0 \\
  1 & 4 & 1 & 0 & \cdots & 0 & 0 & 0 \\
  0 & 0 & \ddots & \ddots & \ddots & 0 & 0 & 0 \\
  0 & 0 & 0 & 0 & 1 & 4 & 1 \\
  0 & 0 & 0 & 0 & 0 & 2 & 4 \\
\end{bmatrix}
\begin{bmatrix}
  \beta_0 \\
  \beta_1 \\
  \vdots \\
  \beta_N \\
\end{bmatrix}
= \begin{bmatrix}
  v(x_0, 0) \\
  v(x_1, 0) \\
  \vdots \\
  v(x_N, 0) \\
\end{bmatrix}
\]

and the iteration procedure goes to until the result at desired time level are obtained with the help of third step.

4. **Stability analysis.** The stability problem is a common issue in seeking numerical solutions of evolution equations. A numerical scheme \( L(u^n_m) \) for an evolution equation on \([0, T]\) is stable if the accumulated error in the scheme remains bounded with time. The aim of this section is to examine von Neumann stability analysis of the numerical approach for Gray-Scott model. For this analysis, we assume that coefficients of the difference equations increase so slowly as to be considered constant in space and time. In that case, the solutions of the difference equations are all of the form:

\[
\begin{align*}
  u^n_m &= \xi^n_1 e^{ikm\Delta x} \\
  v^n_m &= \xi^n_2 e^{ikm\Delta x}
\end{align*}
\]

where \( k \) is spatial wave number and \( \xi \) is the amplification factor. Therefore, the difference equations are stable if \( |\xi| \leq 1 \).
Now, we are going to obtain stability condition for numerical schemes given in (11)-(12) according to time level. For this purpose, substituting (16) and (17) into Eq. (11) and (12), respectively, we get

\[
\xi_1^{n+1/2} e^{i k m \Delta x} \left\{ \left(1 - \Delta t \left( \frac{3}{h^2} - \frac{b}{2} \right) \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 + \Delta t \left( \frac{g_m}{h^2} + 2 \tilde{a} \right) \right\} \\
= \xi_1^{n} e^{i k m \Delta x} \left\{ \left(1 + \Delta t \left( \frac{3}{h^2} - \frac{b}{2} \right) \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 - \Delta t \left( \frac{g_m}{h^2} + 2 \tilde{a} \right) \right\}
\]

\[
\xi_1^{1/2} \left\{ \left(2 + \cos (k \Delta x) \right) \left( 2 + \tilde{a} \Delta t \right) + \frac{12 \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right) \right\} \\
= \left\{ \left(2 + \cos (k \Delta x) \right) \left( 2 - \tilde{a} \Delta t \right) - \frac{12 \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right) \right\}
\]

\[
\xi_1^{1/2} = \frac{\left(2 + \cos (k \Delta x) \right) \left( 2 + \tilde{a} \Delta t \right) - \frac{12 \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right)}{\left(2 + \cos (k \Delta x) \right) \left( 2 + \tilde{a} \Delta t \right) + \frac{12 \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right)} \Rightarrow |\xi_1^{1/2}| \leq 1 \quad (18)
\]

and

\[
\xi_2^{n+1/2} e^{i k m \Delta x} \left\{ \left(1 - \Delta t \left( \frac{3d}{h^2} - \frac{b}{2} \right) \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 + \Delta t \left( \frac{g_d}{h^2} + 2 \tilde{b} \right) \right\} \\
= \xi_2^{n} e^{i k m \Delta x} \left\{ \left(1 + \Delta t \left( \frac{3d}{h^2} - \frac{b}{2} \right) \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 - \Delta t \left( \frac{g_d}{h^2} + 2 \tilde{b} \right) \right\}
\]

\[
\xi_2^{1/2} \left\{ \left(2 + \cos (k \Delta x) \right) \left( 2 + \tilde{b} \Delta t \right) + \frac{12d \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right) \right\} \\
= \left\{ \left(2 + \cos (k \Delta x) \right) \left( 2 - \tilde{b} \Delta t \right) - \frac{12d \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right) \right\}
\]

\[
\xi_2^{1/2} = \frac{\left(2 + \cos (k \Delta x) \right) \left( 2 + \tilde{b} \Delta t \right) - \frac{12d \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right)}{\left(2 + \cos (k \Delta x) \right) \left( 2 + \tilde{b} \Delta t \right) + \frac{12d \Delta t}{h^4} \sin^2 \left( k \Delta x/2 \right)} \Rightarrow |\xi_2^{1/2}| \leq 1 \quad (19)
\]

to obtain stability condition for numerical schemes given in (13)-(14) simultaneous, if we substitute \( u_m^n = P \xi^n e^{i k m \Delta x} \) and \( u_m^n = W \xi^n e^{i k m \Delta x} \) in the equations, we get the following

\[
P \xi_3^{n+1} e^{i k m \Delta x} \left\{ \left(1 + \Delta t \frac{g_m^2}{2} \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 + 2 \Delta t g_m^2 \right\} \\
+ W \xi_3^{n+1} e^{i k m \Delta x} \left\{ \left(1 - z_m g_m \Delta t \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 z_m g_m \Delta t \right\} \\
= P \xi_3^{n} e^{i k m \Delta x} \left\{ \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 \right\}
\]

\[
P \xi_3^{n+1} e^{i k m \Delta x} \left\{ \left(-\frac{g_m^2 \Delta t}{2} \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) - 2 \Delta t g_m^2 \right\} \\
+ W \xi_3^{n+1} e^{i k m \Delta x} \left\{ \left(1 - z_m g_m \Delta t \right) \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 - 4 z_m g_m \Delta t \right\} \\
= W \xi_3^{n} e^{i k m \Delta x} \left\{ \left( e^{-i k \Delta x} + e^{i k \Delta x} \right) + 4 \right\}
\]

\[
P \left[ \xi_3 \left( 2 + g_m^2 \Delta t \right) - 2 \right] + W \left[ 2 \xi_3 z_m g_m \Delta t \right] = 0 \\
P \left[ -\xi_3 g_m^2 \Delta t \right] + W \left[ 2 \xi_3 \left(1 - z_m g_m \Delta t \right) - 2 \right] = 0 
\]

where \( P \) and \( W \) are the harmonic amplitudes. In order to obtain at least one non-trivial solution of the above system, the determinant of the coefficient matrix of the system must be zero. Therefore,

\[
\xi_3^2 \left( g_m^2 \Delta t - 2 z_m g_m \Delta t + 2 \right) - \xi_3 \left( g_m^2 \Delta t - 2 z_m g_m \Delta t + 4 \right) + 2 = 0 \quad (21)
\]

and discriminant \( D \) of the quadratic equation given in (21) is

\[
D = \left( g_m^2 \Delta t - 2 z_m g_m \Delta t + 4 \right)^2 - 4 \left( g_m^2 \Delta t - 2 z_m g_m \Delta t + 2 \right) + 4 \\
= \left( \left( g_m^2 \Delta t - 2 z_m g_m \Delta t + 2 \right) - 2 \right)^2 \\
= \left( g_m^2 \Delta t - 2 z_m g_m \Delta t \right)^2.
\]
Hence, when we denote the roots of Eq. (21) as $\xi_{3,1}$ and $\xi_{3,2}$, we obtain

$$\xi_{3,1} = \frac{(g_m^2 \Delta t - 2z_m g_m \Delta t + 4) - (g_m^2 \Delta t - 2z_m g_m \Delta t)}{2(g_m^2 \Delta t - 2z_m g_m \Delta t + 2)} = 2 \left(\frac{2}{g_m^2 \Delta t - 2z_m g_m \Delta t + 2}\right) \leq 1,$$

when we chose maximum value of the $\tilde{u}$ at the $x_m$ nodal point, $\tilde{v}$ has its minimum value. So, we get

$$|\xi_{3,1}| = \left| \frac{2}{\Delta t \ (\tilde{v} - u) + 2} \right| \leq 1,$$

and

$$|\xi_{3,2}| = |1| \leq 1.$$

To find the condition for $\xi$ according to the Strang splitting method, it yields [3]

$$|\xi| \leq |\xi_1|^{1/2} |\xi_2|^{1/2} |\xi_3|^{1/2} |\xi_4|^{1/2} \leq 1.$$

Thus, it has been shown that the numerical scheme is stable in the sense of von Neumann.

5. Numerical results. In the several scientific areas, nonlinear phenomena are often modeled with four main solitary wave forms: solitons, kinks, peakons, and cuspons [45]. In this section, the focus is going to be on tanh-kink shaped solutions of GSM given in (1) with the initial and boundary conditions given as respectively

$$u(x, 0) = \frac{3 - \sqrt{3}}{4} - \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} x\right),$$

$$v(x, 0) = \frac{1 + \sqrt{3}}{4} + \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} x\right),$$

and

$$u(x_{left}, t) = \frac{3 - \sqrt{3}}{4} - \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} (x_{left} - ct)\right),$$

$$u(x_{right}, t) = \frac{3 - \sqrt{3}}{4} - \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} (x_{right} - ct)\right),$$

$$v(x_{left}, t) = \frac{1 + \sqrt{3}}{4} + \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} (x_{left} - ct)\right),$$

$$v(x_{right}, t) = \frac{1 + \sqrt{3}}{4} + \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} (x_{right} - ct)\right).$$

The exact solution of the GSM is [38]

$$u(x, t) = \frac{3 - \sqrt{3}}{4} - \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} (x - ct)\right),$$

$$v(x, t) = \frac{1 + \sqrt{3}}{4} + \frac{\sqrt{2}}{4} \tanh \left(\frac{\sqrt{2}}{4} (x - ct)\right),$$

where $\tilde{a} = \tilde{b} = 1/8, \tilde{d} = 1, \mu = 1 - 4\tilde{a}, \xi = 1 + \sqrt{2} - 2\tilde{a}$ and $c = \sqrt{2} (1 - 3\sqrt{3}) / 4$.

As the following section, interval is chosen as $[-20, 20]$, final time $T = 1$. The number of time partitioning are changed using collocation numbers $N = 400, N =
10 BERAT KARAAGAC

\[ u(x,t) \quad v(x,t) \]

\[ h \quad L_2 \times 10^6 \quad L_\infty \times 10^6 \quad L_2 \times 10^6 \quad L_\infty \times 10^6 \]

0.1 16.255794672 8.8693520879 16.255794674 8.8693521167
0.05 4.7212245929 3.5788660872 4.7212245653 3.578860765
0.025 3.1114886810 3.6707532707 3.1114889322 3.6707531289
0.0125 3.3850799985 9.7614962725 3.3850788862 9.7614970661

Table 1. Gray Scott model: The error norms for \( \Delta t = 0.01 \) and various values of \( h \) at \( T = 1 \)

\[ h \quad L_2 \times 10^6 \quad L_\infty \times 10^6 \quad L_2 \times 10^6 \quad L_\infty \times 10^6 \]

0.1 16.339991746 8.7969669421 16.339991702 8.7969670275
0.05 4.8404628306 3.5790496331 4.8404627644 3.5790495422
0.025 2.9993515295 3.6711268925 2.9993514761 3.6711268910
0.0125 2.9168925317 3.7175342072 2.9168926962 3.7175350072

Table 2. Gray Scott model: The error norms for \( \Delta t = 0.0025 \) and various values of \( h \) at \( T = 1 \).

\[ h \quad L_2 \times 10^6 \quad L_\infty \times 10^6 \quad L_2 \times 10^6 \quad L_\infty \times 10^6 \]

0.1 16.374721220 8.7933451145 16.374721299 8.7933453672
0.05 4.9049725941 3.5790587130 4.9049726730 3.5790587406
0.025 2.9993515295 3.6711268925 2.9993514761 3.6711268910
0.0125 2.9168925317 3.7175342072 2.9168926962 3.7175350072

Table 3. Gray Scott model: The error norms for \( \Delta t = 0.00125 \) and various values of \( h \) at \( T = 1 \).

800, \( N = 1600 \) and \( N = 3200 \) and the error norms are calculated by using formula given as

\[ L_2 = \| u - U_N \|_2 = \left( \sum_{j=0}^{N} h \left| u_j - (U_N)_j \right|^2 \right)^{1/2}, \]

\[ L_\infty = \| u - U_N \|_\infty = \max_{0 \leq j \leq N} \left| u_j - (U_N)_j \right|. \]  

(22)

We present both of the results \( u(x,t) \) and \( v(x,t) \) in Tables 1-4 via error norms. In Table 1, while the step size changing, time step is fixed to \( t = 0.01 \). The rest of the tables include decreasing time step which are fixed in the each table and changing the step sizes. Therefore, the newly obtained numerical results give us a chance to investigate numerical behaviours of the solutions according to number of partition.

The Collocation method has many advantages. The well-known advantage of the method over other finite element approaches is that calculation of the coefficients in the equations is very fast because of lack of evaluate integrals [22, 24, 2, 1]. Also, choice of the collocation points is an important and sensitive part of the collocation method. It can be seen from the tables, as expected from the method that nodal points effected solutions in a good way and the convergence of the collocation method is quite rapid with increasing values of partition number of the interval. Moreover, discretization in time also effect the behaviour of the numerical solutions,
GRAY-SCOTT MODEL WITH OPERATOR SPLITTING METHOD

\[ u(x,t) \quad v(x,t) \]

| h   | \( L_2 \times 10^6 \) | \( L_\infty \times 10^6 \) | \( L_2 \times 10^6 \) | \( L_\infty \times 10^6 \) |
|-----|------------------------|-----------------------------|------------------------|-----------------------------|
| 0.1 | 16.382770949           | 8.7929105788                | 16.382270862           | 8.7929107112                |
| 0.05| 4.9186006922           | 3.5790599957                | 4.9186005560           | 3.5790598445                |
| 0.025| 3.062445954            | 3.6711482907                | 3.0624458638           | 3.6711480981                |
| 0.0125| 2.9466605008         | 3.7175784792                | 2.9466601800           | 3.717579681                 |

Table 4. Gray Scott model: The error norms for \( \Delta t = 0.001 \) and various values of \( h \) at \( T = 1 \).

![Figure 1](image1.png)

(a) \( u_{\text{approx}}(x,t) \)

Figure 1. Numerical simulation of Gray Scott model

generally. It is pointed out in tables that the errors of the mentioned technique has an important effect on numerical solutions.

As the second step, as a numerical illustration, we consider \( a = b = 1/8, \bar{d} = 1, \mu = 1 - 4\bar{a}, \xi = 1 + \sqrt{\mu - 2\bar{a}}, c = \sqrt{\frac{1}{2}(1 - 3\sqrt{\mu})}/4 \), for \( x \in [-20, 20] \), \( T = 1, \Delta t = 0.01 \) and \( h = 0.1 \).

Then, we plot numerical simulations of Gray Scott model for different times in Figure 1-3. As it is seen from the figure, these type of solutions resemble upward and downward steps and rises or descending from one asymptotic state to another. The amplitude of the kink waves is independent of its velocity. Some of the main application area of kink solutions are nonlinear optics, water waves, atomic Bose-Einstein condensates and so on [16, 13, 17]. Finally, it can concluded from the tables and figures that new approach is significantly convergent to exact solution and the collocation method is considerably robust and accurate.

6. Conclusion. A cubic B-spline based on finite element collocation method in conjunction with Strang splitting technique is formulated for solving the Gray-Scott reaction-diffusion system. With the idea of Strang splitting technique, GS model is divided into a set of problems which each problem is more simpler and application of any method is more practical. Using collocation method yields us represent the solution in a form which is a linear combination of B-spline basis and time dependent unknown parameter and application of the method to GS model yields an algebraic equation system. At the end, solving the algebraic equation system carries us to the focus of our article. Additionally, the performance and accuracy of the proposed method is measured by the error norms \( L_2 \) and \( L_\infty \).

The power and electivity of the aforesaid methods is justified by presented in tables
and figures. It should be noted that the proposed numerical technique used in this paper can be extended to solve a range on nonlinear reaction-advection-diffusion problems encountered in applied sciences and engineering. Application to solve high dimensional real-life phenomena is left for future research.

Acknowledgments. I would like to express my sincere thanks to the anonymous referees for their useful suggestions and to my supervisor, Prof. Dr. Alaattin ESEN, for his continuous guidance and support.

REFERENCES

[1] E. N. Aksan, H. Karabenli and A. Esen, An application of finite element method for a moving boundary problem, Thermal Science, 22 (2018), 25–32.
[2] A. H. A. Ali, G. A. Gardner and L. R. T. Gardner, A collocation solution for Burgers’ equation using cubic B-spline finite elements, Comput. Methods Appl. Mech. Engrg., 100(1992), 325–337.
[3] İ. Çelikkaya, Operator splitting solution of equal width wave equation based on the Lie-Trotter and strang splitting method, Konuralp J. Math. 6 (2018), 200–208.
[4] X. Cheng, J. Duan and D. Li, A novel compact ADI scheme for two-dimensional Riesz space fractional nonlinear reaction-diffusion equations, *Appl. Math. Comput.*, **346** (2019), 452–464.

[5] M. Dehghan and A. Shokri, A numerical method for solution of the two-dimensional sine-Gordon equation using the radial basis functions, *Math. Comput. Simulation*, **79** (2008), 700–715.

[6] F. Dkhil, E. Logak and Y. Nishiura, Some analytical results on the Gray–Scott model, *Asymptot. Anal.*, **39** (2004), 225–261.

[7] A. J. Doelman, T. J. Kaper and P. Zegeling, Pattern formation in the one-dimensional Gray Scott model, *Nonlinearity*, **10** (1997), 523–563.

[8] A. J. Doelman, R. A. Gardner and T. J. Kaper, Stability analysis of singular patterns in the 1D Gray-Scott model: A matched asymptotics approach, *Phys. D*, **122** (1998), 1–36.

[9] A. Esen, O. Tasbozan, Y. Ucar and N. M. Yagmurlu, A B-spline collocation method for solving fractional diffusion and fractional diffusion-wave equations, *Tbilisi Math. J.*, **8** (2015), 181–193.

[10] P. Gray and S. K. Scott, Autocatalytic reactions in the isothermal, continuous stirred tank reactor: Oscillations and instabilities in the system $A + 2B \rightarrow 3B; B \rightarrow C$, *Chem. Eng. Sci.*, **39** (1984), 1087–1097.

[11] S. Guo, L. Mei, Z. Zhang, J. Chen, Y. He and Y. Li, Finite difference/Hermite-Galerkin spectral method for multi-dimensional time-fractional nonlinear reaction-diffusion equation in unbounded domains, *Appl. Math. Model.*, **70** (2019), 246–263.

[12] S. Hasnain, M. Saqib, M. F. Afzaal and N. A. Harbi, Numerical study to coupled three dimensional reaction diffusion system, *IEEE Access*, **7** (2019), 46695–46705.

[13] R. S. Johnson, *A Modern Introduction to The Mathematical Theory of Water Waves*, Cambridge Texts in Applied Mathematics, Cambridge University Press, Cambridge, 1997.

[14] B. Karaagac and A. Esen, The Hunter-Saxton: A numerical approach using collocation method, *Numer. Methods Partial Differential Equations*, **34** (2018), 1637–1644.

[15] A. H. Khater, R. S. Temsah and M. M. Hassan, A Chebyshev spectral collocation method for solving Burgers-type equations, *J. Comput. Appl. Math.*, **222** (2008), 333–350.

[16] Y. S. Kivshar and G. P. Agrawal, *Optical Solitons: From Fibers to Photonic Crystals*, Academic Press, San Diego, 2003.

[17] V. V. Konotop, Dark solitons in Bose-Einstein condensates: Theory, *Springer*, (2008), 65–83.

[18] A. Korkmaz, O. Ersoy Hepson and I. Dag, Motion of patterns modeled by the Gray-Scott autocatalysis system in one dimension *MATCH Commun. Math. Comput. Chem.*, **77** (2017), 507–526.

[19] S. Kumar, R. Jiwari and R. C. Mittal, Numerical simulation for computational modelling of reaction-diffusion Brusselator model arising in chemical processes, *J. Math. Chem.*, **57** (2019), 149–179.

[20] S. Kutluay, Y. Ucar and N. M. Yagmurlu, Numerical solutions of the modified Burgers equation by a cubic B-spline collocation method, *Bull. Malays. Math. Sci. Soc.*, **39** (2016), 1603–1614.

[21] S. A. Manaa and J. Rasheed, Successive and finite difference method for gray Scott model, *Science Journal of University of Zakho*, **1** (2013), 862–873.

[22] G. Micula and S. Micula, *Handbook of Splines*, Mathematics and its Applications, 462, Kluwer Academic Publishers, Dordrecht, 1999.

[23] R. C. Mittal and R. K. Jain, Numerical solutions of nonlinear Burgers equation with modified cubic B-splines collocation method, *Appl. Math. Comput.*, **218** (2012), 7839–7855.

[24] A. K. Mittal and V. K. Kukreja, Solution of Burger’s equations by orthogonal collocation on finite elements hermite basis, *6th Int. Conference On Advances in Engineering Sciences and Applied Mathematics (Icaesam’2016) Dec. Kuala Lumpur (Malaysia)*, 2016, 40–45.

[25] A. T. Onarcan, N. Adar and I. Dag, Numerical solutions of reaction-diffusion equation systems with trigonometric quintic B-spline collocation algorithm, preprint, *arXiv:1701.04558*.

[26] A. B. Orovio, D. Kay and K. Burrage, Fourier spectral methods for fractional-in-space reaction-diffusion equations, *BIT*, **54** (2014), 937–954.

[27] O. Oruc, A. Esen and F. Bulut, A Haar wavelet collocation method for coupled nonlinear Schrödinger- KdV equations, *Internat. J. Modern Phys.*, **27** (2016), 1650103, 16 pp.

[28] K. M. Owolabi, Numerical solution of diffusive HBV model in a fractional medium, *Springer-Plus*, **5** (2016), 2–19.

[29] K. M. Owolabi and K. C. Patidar, Higher-order time-stepping methods for time-dependent reaction-diffusion equations arising in biology, *Appl. Math. Comput.*, **240** (2014), 30–50.
[30] K. M. Owolabi, Numerical analysis and pattern formation process for space-fractional superdiffusive systems, *Discrete Contin. Dyn. Syst. Ser. S*, **12** (2019), 543–566.

[31] K. M. Owolabi, Robust IMEX schemes for solving two-dimensional reaction-diffusion models, *Int. J. Nonlinear Sci. Numer. Simul.*, **16** (2015), 271–284.

[32] K. M. Owolabi and A. Atangana, Numerical simulations of chaotic and complex spatiotemporal patterns in fractional reaction-diffusion systems, *Comput. Appl. Math.*, **37** (2018), 2166–2189.

[33] K. M. Owolabi and E. Pindza, Mathematical and computational studies of fractional reaction-diffusion system modelling predator-prey interactions, *J. Numer. Math.*, **26** (2018), 97–110.

[34] K. M. Owolabi and K. C. Patidar, Numerical solution of singular patterns in one-dimensional Gray-Scott-like models, *Int. J. Nonlinear Sci. Numer. Simul.*, **15** (2014), 437–462.

[35] J. E. Pearson, Complex patterns in a simple system, *Science*, **261** (1993), 189–192.

[36] L. A. Peletier, Pulses, kinks and fronts in the Gray-Scott model, *Nonlinear Diffusive Systems-dynamics and Asymptotic Analysis (Japanese) (Kyoto, 2000)*, Surikaisekikenkyusho Kokyuroku, **1178** (2000), 16–28.

[37] S. Z. Rida, A. M. A. El-Sayed and A. A. M. Arafa, On the solutions of time-fractional reaction-diffusion equations, *Commun. Nonlinear Sci. Numer. Simul.*, **15** (2010), 3847–3854.

[38] M. Rodrigo and M. Mimura, Exact solutions of reaction-diffusion systems and nonlinear wave equations, *Japan J. Indust. Appl. Math.*, **18** (2001), 657–696.

[39] S. G. Rubin and R. A. Graves, *A Cubic Spline Approximation for Problems in Fluid Mechanics*, NASA TR R-436, Washington, DC, 1975.

[40] N. Stollenwerk and J. P. Boto, Reaction-superdiffusion systems in epidemiology, an application of fractional calculus, *AIP Conf. Proc.*, **1168** (2009), 1548–1551.

[41] V. Tuoi, *Mathematical Analysis of Some Models for Drug Delivery*, Phd thesis, National University of Ireland, 2012.

[42] A. M. Turing, The chemical basis of morphogenesis, *Bulletin of Mathematical Biology*, **52** (1990), 153–197.

[43] Y. Ucar, N. M. Yagmurlu and I. Çelikkaya, Operator splitting for numerical solution of the modified Burgers’ equation using finite element method, *Numer. Methods Partial Differential Equations*, **35** (2019), 478–492.

[44] K. Wang and W. Wang, Propagation of HBV with spatial dependence, *Math. Biosci.*, **210** (2007), 78–95.

[45] A. M. Wazwaz, New solitary wave solutions to the modified Kawahara equation, *Phys. Lett. A.*, **360** (2007), 588–592.

[46] O. P. Yadav and R. Jiwari, A finite element approach for analysis and computational modelling of coupled reaction diffusion models, *Numer. Methods Partial Differential Equations*, **35** (2019), 830–850.

Received March 2019; revised April 2019.

E-mail address: beratkaraagac@tdtu.edu.vn