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Using the Multi-Domain Spectral Relaxation Method through a Numerical Simulation for the Brusselator System

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Abstract. We introduce the numerical solutions of the Brusselator system by applying the multidomain spectral relaxation method (MSRM). The proposed method is a combination of the Chebyshev pseudo-spectral method and the Gauss-Seidel relaxation approach. This method breaks down the main interval into several small subintervals, finding solutions within each interval. This approach also transforms the model into a set of algebraic equations. We present the error analysis and the order of convergence for the proposed scheme. We validate the effectiveness and precision of the given procedure by utilizing the fourth-order Runge-Kutta method (RK4M), and the variational iteration method. The considered results are tabularly and graphically demonstrated with different values of the model's parameters. From a numerical viewpoint, the given simulations and results indicate that the proposed algorithm is a straightforward and appropriate tool with computational efficiency for such models.

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Key Words and Phrases: Brusselator system, MSRM, Chebyshev pseudo-spectral method, Gauss-Seidel relaxation approach, convergence analysis, RK4M

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1. Introduction

While spectral methods are recognized for their precision, their accuracy diminishes for non-smooth solutions and extensive domain issues, even when more grid points are added ([1], [2]). Domain decomposition has mainly been used with semi-analytical techniques to address the numerical solutions of some systems. Such techniques encompass methods like the multistage Adomian decomposition method [3], multistage variational iteration method [4], and multistage homotopy perturbation method [5]. However, a challenge faced by multi-domain techniques based on analytical approximations is the long and complex process of analytical integration within each sub-domain. Motsa and colleagues ([6], [7]) introduced a spectral method-based multi-domain numerical approach, setting it apart from earlier multi-domain strategies by being entirely numerical. Other numerical strategies that have employed domain decomposition for chaotic systems are the time discretization [8], piecewise successive linearization [9], piecewise spectral homotopy analysis [10], and multi-domain compact finite difference relaxation ([11], [12]). Also, there are numerical algorithms can be applied in many real life problems as in the operation research, data analysis and the financial mathematics ([13], [14]), also in the simulations of some biological models as in ([15],[16]).

In this work, we describe the Brusselator mathematical model, which predicts the oscillations in chemical reactions. We present an argument for why modern thermodynamics is important in analyzing a system that constantly interacts with its environment, and which operates far from thermodynamic equilibrium. The Brusselator model has been used in a wide range of applications in chemical research, where it has been used to study the formation of spatial patterns in chemical systems, such as Turing patterns and spiral waves. It is considered a theoretical model for a type of self-catalytic reaction [17]. It is also considered an example of an autocatalytic, oscillatory chemical reaction, that is, a reaction in which a species increases the rate of its productive reaction [18].

In this paper, we aim to determine and provide the numerical solutions to the Brusselator system using the MSRM. This technique incorporates the Chebyshev spectral method ([19], [20]) and the Gauss-Seidel method process to numerically treat the system across several sub-domains that constitute the entire problem domain. We can confidently assess the effectiveness of the given numerical approach for the model under study. The numerical solutions validate that the proposed technique may effectively tackle the specified model, aligning well with existing solutions. By adding terms from the solution series, we can further minimize relative errors. We highlight the efficiency and vast potential of our proposed numerical method by contrasting the estimated solutions with those obtained from the RK4M. We also illustrate that the multi-domain strategy's strength lies in its reduced error accumulation across sub-domains compared to considering a single domain. The proposed method is a powerful technique that uses an approach of linearization of nonlinear equations for obtaining a better series solution, which provides efficient algorithms for approximate solutions, giving effective precision and convergence. Besides, the solutions converged in a relatively narrow region, and they had sluggish convergence. From the novelty points, the proposed method is considered for the first time for solving the Brusselator system.

2. Basic concepts

2.1. Mathematical formulation

Here, we focus on the Brusselator system, which is formulated as follows [21]:

$$\dot{\theta}_1(t) = \delta - (1 + \gamma)\,\theta_1(t) + (\theta_1(t))^2\,\theta_2(t),\tag{1}$$

$$\dot{\theta}_2(t) = \gamma \,\theta_1(t) - (\theta_1(t))^2 \,\theta_2(t),$$
 (2)

with the following initial conditions:

$$\theta_1(0) = \theta_1^0, \qquad \theta_2(0) = \theta_2^0,$$
 (3)

where θ_1 and θ_2 represent the concentration of the reaction and diffusion processes, respectively, the parameters $\delta > 0$, $\gamma > 0$, and θ_1^0 , θ_2^0 are constants [22].

The system can exhibit sustained oscillations as δ increases beyond this critical value. The parameter γ controls the balance between the reaction and diffusion processes. The reaction dominates at low values of γ , and the system can exhibit sustained oscillations or spiral waves. As γ increases, diffusion becomes more important, and the system can exhibit Turing patterns.

2.2. The Chebyshev-Lagrange interpolation

The Chebyshev polynomials $T_k(y)$ of order k are generated from the following formula:

$$T_k(y) = \cos(k \arccos(y)), \qquad k \in \mathbb{N}.$$
 (4)

The Chebyshev-Lagrange interpolation of the function $\psi(y)$ at $y=y_i, i=0,1,...,m$ is denoted by $\psi_m(y)$ and defined as follows:

$$\psi_m(y) = \sum_{i=0}^m \psi_i L_i(y), \tag{5}$$

where $L_i(y)$, i = 0, 1, ..., m are the Lagrange's polynomials of degree i. The extreme y_i of $T_m(y)$, which are the Chebyshev-Gauss-Lobatto points (CGLPs), are chosen to be the collocation points, and defined by:

$$\{y_i\}_{i=0}^m = \left\{\cos\left(\frac{\pi i}{m}\right)\right\}_{i=0}^m. \tag{6}$$

Remark 1. This previous choice was made based on our knowledge that the error in Lagrange interpolation is minimized if the interpolation points are zeros of the polynomials.

3. Numerical implementation of the MSRM

The suggested approach will be used to obtain the numerical solutions of the investigated model with the help of the following steps (Algorithm):

(i) Without losing the system's generality, we describe the system (1)-(2) as follows [23]:

$$\dot{\xi} + C\,\xi + \mathbf{N}(\xi) = 0,\tag{7}$$

where $\xi(t) = [\theta_1(t), \theta_2(t)]^T$; C is an 2×2 matrix with entries $c_{i,j}, i, j = 1, 2$ and is defined by:

$$C = \left(\begin{array}{cc} 1 + \gamma & 0 \\ -\gamma & 0 \end{array} \right),$$

here the elements $c_{1,2}$ and $c_{2,2}$ are equal zero, because the equations (1)-(2) do not contain on linear terms of $\theta_2(t)$. Also $\mathbf{N}(\xi)$ is a vector of nonlinear terms of Eq.(7) and is defined by:

$$\mathbf{N}(\xi) = \begin{pmatrix} -\delta - (\theta_1(t))^2 \theta_2(t) \\ (\theta_1(t))^2 \theta_2(t) \end{pmatrix}.$$

(ii) We define the following set of Lagrange polynomials $\{L_i(y)\}_{i=0}^m$ of order i, which are based on the CGLPs as follows:

$$L_i(y) = \frac{(-1)^{i+1} (1 - y^2) T_m(y)}{\hbar_i m^2 (y - y_i)}, \qquad i = 0, 1, \dots, m,$$
 (8)

where $\hbar_0 = \hbar_m = 2, \hbar_i = 1$ for i = 1, 2, ..., m - 1. Also, the Chebyshev polynomial $T_m(y)$, and the CGLPs y_i are defined in (5) and (6), respectively.

(iii) We use the Chebyshev-Lagrange interpolation of the function v(y) at $y = y_i, i = 0, 1, ..., m$, which is denoted by $v_m(y)$ and defined as follows:

$$v_m(y) = \sum_{i=0}^{m} v_i L_i(y),$$
 (9)

where the coefficients $v_i = v(y_i)$.

(iv) We calculate the first derivative of the approximate solution (9) at the collocation points y_i as follows:

$$\frac{dv_m(y)}{dy} = \sum_{k=0}^{m} v(y_k) \frac{dL_k(y_i)}{dy} = \sum_{k=0}^{m} D_{ik} v(y_k) = \mathbb{D}V_i, \qquad i = 0, 1, \dots, m, \quad (10)$$

the elements of the first-order Chebyshev differentiation matrix D_{ik} can be evaluated for i, k = 0, 1, ..., m at the collocation points y_i (6) as follows [24]:

$$D_{ik} = \frac{dL_k(y_i)}{dy} = \begin{cases} \frac{h_i(-1)^{k+i}}{h_k(y_k - y_i)}, & i \neq k, \\ -\frac{y_i}{(1 - y_i^2)}, & (i = k) \neq 0, m, \\ \frac{2m^2 + 1}{6}, & i, k = 0, \\ -\frac{2m^2 + 1}{6}, & i, k = m. \end{cases}$$
(11)

(v) We divide the interval I = [0, T] into n subdomains with a uniform length $\frac{T}{n} = t_j - t_{j-1}$, where $I_j = [t_{j-1}, t_j]$ has the characteristic that:

$$\bigcup_{j=1}^{n} [t_{j-1}, t_j] = [0, T]. \tag{12}$$

Now, by using the following linear transformation, we can convert each subdomain of the form $[t_{i-1}, t_i]$ to the domain of the CGLPs [-1, 1], which is specified in Eq.(6):

$$\hat{t} = 0.5(t_j - t_{j-1})y + 0.5(t_{j-1} + t_j) = 0.5(T/n)y + 0.5(t_{j-1} + t_j), \quad j = 1, 2, \dots, n.$$

(vi) We estimate the derivatives of the first term in the system of ODEs (7) with the help of the Chebyshev differentiation matrix, to reduce it to a system of algebraic equations. We use $\Theta_s^j = \left[\theta_s\left(y_0^j\right), \theta_s\left(y_1^j\right), \cdots, \theta_s\left(y_m^j\right)\right]^T$, and y_k^j , k = 0, 1, ..., m to represent the approximate solution and the collocation points in each subdomain, respectively. These considerations lead us to the following matrix form system:

$$\left(\frac{2n}{T}\mathbb{D} + c_{s,s}I\right)\Theta_s^j + \sum_{\substack{i=1\\i\neq s}}^2 c_{s,i}\Theta_i^j + \mathbf{N}_s^j(\Theta) = 0, \qquad s = 1, 2,$$
(13)

where $c_{s,i}$ are the elements of the matrix C defined in (7), and:

$$\Theta = \left[\Theta_1, \Theta_2\right]^T, \quad \mathbf{N}_s(\Theta) = \left[\mathbf{N}_s\left(\Theta\left(y_0\right)\right), \, \mathbf{N}_s\left(\Theta\left(y_1\right)\right), \, \dots, \, \mathbf{N}_s\left(\Theta\left(y_m\right)\right)\right]^T.$$

(vii) By using the Gauss-Seidel method to solve the algebraic equations (13) in each subdomain I_i , we can reduce it to the following iteration formula:

$$\left(\frac{2n}{T}\mathbb{D} + c_{s,s}I\right)\Theta_{s,p+1}^{j} = -\sum_{i=1}^{s-1}c_{s,i}\Theta_{i,p}^{j} - \sum_{i=s+1}^{2}c_{s,i}\Theta_{i,p}^{j} - \mathbf{N}_{s,p}^{j}, \qquad s = 1, 2, (14)$$

where $\Theta_{s,p+1}$ is the numerical estimation of θ_s at the $(p+1)^{\text{th}}$ iteration, and $\mathbf{N}_{s,p}^j = \mathbf{N}_s\left(\Theta_{1,p}^j,\Theta_{2,p}^j,\ldots,\Theta_{s-1,p}^j,\Theta_{s,p}^j\right)$ are used to evaluate the nonlinear terms.

(viii) In light of the above, the numerical solution can be obtained as follows:

$$\Theta_{s,p+1}^{j} = A_s^{-1} B_s^{j}, \tag{15}$$

where

$$A_s = \frac{2n}{T}\mathbb{D} + c_{s,s}I,$$
 $B_s^j = -\sum_{i=1}^{s-1} c_{s,i}\Theta_{i,p}^j - \sum_{i=s+1}^2 c_{s,i}\Theta_{i,p}^j - \mathbf{N}_{s,p}^j.$

We will use the initial conditions in the first iteration at p = 0, of the iteration matrix form (15).

The solution of the system (7) is then given by [25]:

$$\theta_s = \bigcup_{j=1}^n \Theta_s^j(y_j). \tag{16}$$

4. Convergence and error analysis

We describe how domain decomposition affects MSRM convergence and error estimates. Eq.(15) can be expressed as a block matrix system as follows:

$$A\Theta = B, (17)$$

where

$$A = \begin{pmatrix} \frac{2n}{T} \mathbb{D} + c_{1,1} I & c_{1,2} I \\ c_{2,1} I & \frac{2n}{T} \mathbb{D} + c_{2,2} I \end{pmatrix}, \quad \Theta^j = \begin{pmatrix} \Theta_1^j \\ \Theta_2^j \end{pmatrix}, \quad \text{and} \quad B^j = \begin{pmatrix} -\mathbf{N}_1^j \\ -\mathbf{N}_2^j \end{pmatrix}.$$

Theorem 1.

The sequence of solutions $\{\Theta^{(k)}\}_{k=0}^{\infty}$, which is generated from (15) by $\Theta = A^{-1}B$ with any choice of $\Theta^{(0)} \in \mathbb{R}^{\bar{n}}$, converges to the unique solution $\bar{\Theta}$ if the matrix A is strictly diagonally dominant.

Proof. The details of the proof of this theorem can be found in [26].

Theorem 2. [27]

Let $\Theta_s(t)$ be a polynomial of degree $\leq m$ that interpolates the function $\theta_s(t) \in C^{m+1}[0,T]$ at m+1 various points $y_0,y_1,\ldots,y_m \in [t_j,t_{j+1}]$, with the property (12). According to (8), if the nodes y_i are used as the CGLPs, the error term for the polynomial interpolation in [0,T] using the nodes y_i in each sub-domain is estimated as follows:

$$E(t) = |\theta_s(t) - \Theta_s(t)| \le \frac{\lambda T^{m+1}}{(4n)^m (m+1)!}, \qquad \lambda \ne 0.$$
(18)

Remark 2. It can be shown that the error in the multi-domain situation is significantly smaller than the single domain example, n = 1, due to the factor $\left(\frac{1}{n}\right)^m << 1$ for large n.

5. Numerical simulation

By addressing the system (1)-(2) in the range [0,3] with various values of m, δ , γ with initial conditions $\theta_1^0 = \theta_2^0 = 1$, we will show a numerical simulation on a test example to demonstrate the accuracy of the provided numerical scheme. Figure 1 (a,b) shows the behavior of the obtained approximate solutions using different values of the order of the used polynomials, m = 3, m = 7, at $\delta = 0.25$, $\gamma = 1$. We compared the results to those obtained using the RK4M (as a reference solution) with $\delta = 0.0$, and $\gamma = 1$ in Figure 2 (a,b). This comparison demonstrates that the proposed method is appropriate for solving the suggested model. The behavior of the approximate solution via distinct values of $\gamma = 0.5$, 1.0, 1.5 with m = 5, $\delta = 0$ is presented in Figure (a,b). From this figure, we can confirm that the parameter γ controls the balance between the reaction and diffusion processes. Figure (a,b) also displays the behavior of the numerical solutions with various

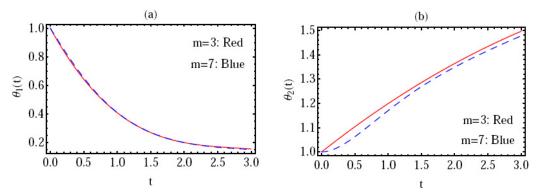


Fig. 1: The approximate solution $\theta_1(t)$, $\theta_2(t)$ via various values of m.

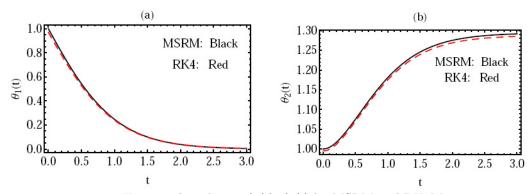


Fig. 2: The solution $\theta_1(t)$, $\theta_2(t)$ by MSRM and RK4M.

values of $\delta = 0.0, 0.5, 1.0$, at $m = 5, \gamma = 0.75$. From this figure, we can confirm that the system can exhibit sustained oscillations as δ increases beyond this critical value.

Through the above results (Figures 1-4), we can see how the numerical solution behaves when the proposed approach is applied to the values of m, γ , δ . From Figure 3, we can confirm that as the value of parameter γ increases, the value of $\theta_1(t)$ decreases, and the value of $\theta_2(t)$ increases, and this is consistent with the nature of the effect of this parameter on chemical reactions of this type. From Figure 4, we find that as the value of δ increases, the value of $\theta_1(t)$ increases, and the value of $\theta_2(t)$ decreases, and this is consistent with the nature of the effect of this parameter on chemical reactions of this type.

In addition, to validate our numerical solutions, we present a comparison of the relative error (RE) in Table 1 with those solutions obtained by the variational iteration method (VIM) [22] with integer derivative $\alpha=1$. We considered the system (1)-(2) in the range [0,2] with initial conditions $\theta_1^0=\theta_2^0=1$, $\delta=0.25$, $\gamma=1$, and m=5. Here, to evaluate the RE, we took the numerical solutions obtained by the RK4 method as reference solutions. This is due to the lack of knowledge of the exact solutions of the proposed model. This comparison shows the thoroughness of the proposed method and has the largest convergence interval compared to the VIM. Finally, we can confirm that the proposed method in this article addressed and overcame the shortcomings of the VIM method.

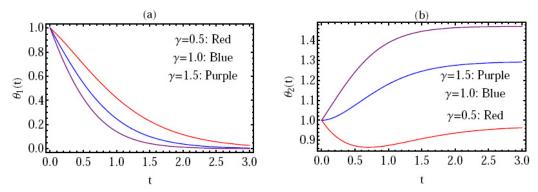


Fig. 3: The approximate solution $\theta_1(t)$, $\theta_2(t)$ via various values of γ .

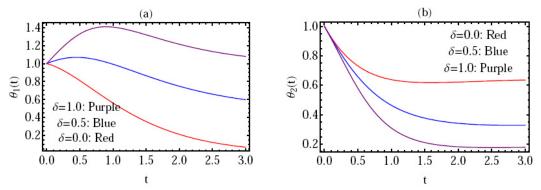


Fig. 4: The approximate solution $\theta_1(t)$, $\theta_2(t)$ via various values of δ .

Table 1. The relative error for numerical solutions by using MSRM and VIM [22] at m=5.

	Relative error- $\theta_1(t)$ at $m=5$		Relative error- $\theta_2(t)$ at $m=5$	
t	MSRM	VIM	MSRM	VIM
0.00	5.15975E-06	2.15671E-04	8.00145E-06	2.31456E-05
0.25	2.75961E-06	6.32587E-04	3.25874E-06	8.02145E-04
0.50	0.18523E- 05	3.25874E-04	6.65402 E-05	2.01597E-04
0.75	7.13289E-06	2.32104E-03	0.01478E-06	0.23145E-03
1.00	6.28410E-06	4.01573E-03	2.01478E-07	1.25489E-03
1.25	2.63985E-06	7.25890E- 02	3.25874E-06	2.32014E-02
1.50	8.02514E-05	0.21546E-02	0.25641E- 05	0.02546E-02
1.75	7.01478E-05	0.21456E-01	6.02587E-06	0.56479E-01
2.00	6.52041E- 05	0.25643E- 00	0.21478E-05	0.36547E-00

6. Conclusions

Through this work, the multi-domain approach, known as the MSRM, is modified to solve the given Brusselator system. The numerical simulation of the model under study

was investigated by calculating the relative error with various values of the approximation order m. By including more terms from the approximation solution series, or by raising m, we may also regulate the precision of the error and lower it. By assessing the relative error, we can ensure that the proposed technique is accurate and efficient. The proposed method shows its advantage in that calculations are relatively easy to follow and understand. The results obtained by the MSRM are accurate, valid for a longer period, and highly compatible with those obtained by the RK4M and the VIM (but in small intervals). Hence, this technique can be used to solve many other nonlinear problems that appear in the applied sciences and engineering applications. The outcomes additionally demonstrate the proposed MSRM's accuracy, computational effectiveness, and dependability as a solution for solving this model. All the numerical results were obtained with the help of the Mathematica software program. As future work and an attempt to generalize the results obtained in this paper, we will try to treat one or all of the following suggestions:

- (i) We deal with the same problem, but using a different type of polynomial.
- (ii) We consider the model in its fractional form and solve it numerically with the help of a suitable numerical/approximate method.
- (iii) We try to modify the proposed method in the current work to treat some weaknesses of the method, such as the low accuracy of the resulting solutions compared to other methods, and then use it for solving numerically some other models.

Competing interests: There is no conflict of interest.

Authors' contributions: This study was written in collaboration the authors.

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