A new multi-step pseudo-spectral method for the approximate solution of inverse reaction-diffusion equation

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Abstract. In this paper, we propose a novel multi-step pseudo-spectral method for numerical solution of an inverse reaction-diffusion equation. This method is based on the approximation of the original problem with a sequence of sub-problems. We utilize the collocation method based on a new set of nonclassical basis functions using Chebyshev-Gauss-Radau quadrature points. By using the Pseudo-spectral method, inverse reaction diffusion equation with initial and boundary conditions, would reduce to a system of nonlinear algebraic equations. Due to the ill-posed system of nonlinear algebraic equations, the Tikhonov regularization scheme is employed to obtain a numerical stable solution. The proof the stability and convergence of the method is presented. Some numerical examples are given to show the accuracy of the proposed method and results are compared with those found in literature.

Keywords: reaction-diffusion equation, pseudo-spectral method, multi-step method, inverse problems, regularization.

1. Introduction

Reaction-diffusion systems are mathematical models that explain how the concentration of one or more substances distributed in the space changes under the influence of the two processes. These processes are: local chemical reactions in which the substances are transformed into each other and diffusion that causes the substances to spread out over a surface in space [1]. This description implies that reaction-diffusion systems are naturally applied in chemistry as well

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as biology, geology, physics and ecology [2]. Mathematically, reaction-diffusion systems take the form of the semi-linear parabolic partial differential equations, which are represented in the following general form:

$$u_t = \nabla(\mathbf{D}(u; x, t)\nabla u) + f(u; \nabla u, x, t), \tag{1}$$

where $u = u(x,t)$ represents the concentration of one substance, $\mathbf{D}$ is a diffusion coefficient, and f is the reaction term.

In this paper, we consider the reaction-diffusion problem in the initial and boundary value problem of the following form:

$$\begin{cases} u_t(x,t) = a(t)u_{xx}(x,t) + p(t)u(x,t) + g(x,t), & 0 < x < 1, 0 < t \leq T, \\ u(x,0) = u_0(x), & 0 \leq x \leq 1, \\ u(0,t) = g_0(t), & 0 < t \leq T, \\ u(1,t) = g_1(t), & 0 < t \leq T, \end{cases} \tag{2}$$

where $T \geq 0$ is a constant value and p, g, u_0, g_0 and g_1 are known as functions. A direct problem aims to find a solution that satisfies given partial differential equation with initial and boundary conditions. Moreover, a direct problem aims to find a solution $u(x,t)$ that satisfies Eq. (2). Problems involving the determination of unknown coefficients in partial differential equations by some additional condition are well known in the mathematical literature as "The Inverse Coefficient Problems". The additional condition may be given to the whole domain, on the boundary of the domain, or at the final time [3]. In some problems, the original partial differential equation, initial conditions, and boundary conditions are not sufficient to obtain the solution and some conditions are required. Such problems are called the "Inverse problems" [4].

Here, we assume that the reaction term $a(t)$ is unknown. Therefore, by solving (1) it is aimed to obtain $u(x,t)$ and $a(t)$ at the same time. Accordingly, this problem is an inverse problem, and to solve that problem, we need an additional condition, which is

$$u(x^*, t) = E(t), \qquad 0 < x^* < 1, \quad 0 \leq t \leq T, \tag{3}$$

where $E(t)$ is a known function. Using Eq. (3) and Eq. (2) is written as follows:

$$\begin{cases} u_t(x,t) = a(t)u_{xx}(x,t) + p(t)u(x,t) + g(x,t), & 0 < x < 1,\ 0 < t \leq T, \\ u(x,0) = u_0(x), & 0 \leq x \leq 1, \\ u(0,t) = g_0(t), & 0 < t \leq T, \\ u(1,t) = g_1(t), & 0 < t \leq T, \\ u(x^*,t) = E(t), & 0 < x^* < 1,\ 0 \leq t \leq T. \end{cases} \tag{4}$$

Without the extra measurement (3), the problem (2) is under-determinated and may have an infinite number of solutions. On the other hand, if more than one additional condition is imposed, the solution may not exist.

The existence and uniqueness of the solution of this problem and more applications are discussed in [5, 6]. However, the theory of the numerical solution of this problem is not satisfactory. Cannon [7] and Dehghan [8], reduced the problem to a non-linear integral equation for the coefficient $a(t)$. This approach works well for parabolic equations in one space variable but cannot be easily extended to problem with higher-dimensions because it depends on the explicit form of the fundamental solution of the heat operator. In [9], a backward Euler finite difference scheme is discussed and has been shown that this scheme is stable in the maximum norm and error estimates for u and a and some experimental numerical results are given. The authors of [10], found a numerical solution of the problem for a connected domain in $\mathbb{R}^n$. In [11], this problem has been studied from a different point of view. The authors first transformed a large class of parabolic inverse problems into a non-classical parabolic equation with coefficients, including trace type functional on the solution and with derivatives subjected to some initial and boundary conditions. For the resulted non-classical problem, they introduced a variational form by defining a new function and then employed both continuous and discrete Galerkin procedures to the non-classical problem. Dehghan [12], used several explicit and implicit finite difference methods to solve this problem. In [13], an efficient pseudo-spectral Legendre method is developed to solve the problem given in Eq. (4). The authors of [14], applied Adomian decomposition method to find the solution of this problem. In [15], the numerical solution is also considered by using Chebyshev cardinal functions. The method consists of expanding the required approximate solution as the elements of Chebyshev cardinal functions. This problem is solved by a high-order compact finite difference method in [16]. The authors of [17], applied the collocation method based on the radial basis function (RBF) to find the solution of this problem. They made an effort to solve inverse problem in a class of reaction-diffusion equation using (RBF) as a truly meshless method. The interested reader can see [18, 19, 20] for more research works on this problem. To the best of our knowledge, the above mentioned numerical methods are mainly suited for the small interval, say $T \leq 1$. Besides, it is assumed that the solution is continuous on $[0, T]$. In this study we solve the problem for $T \gg 1$. Moreover the proposed method leads to a suitable approximation for the problems with noncontinuous solution.

The reminder of the present work is organized as follows. In the next section, we review some properties of Chebyshev polynomials and explain the function approximation. In Section 3, inspired by the method introduced by Shizgal [21] for solving advection- reaction-diffusion problem, we derive a new spectral approximation. In this method, the domain of the problem is partitioned into a uniform mesh, followed by obtaining the solution on each part, using collocation method. In the next section, we review some properties of Chebyshev polynomials and function approximation. In section 3, we present the computational method for approximating the solution of inverse reaction- diffusion problem.

The convergence analysis of the present method is derived in section 4. Section 5 devoted to numerical finding and in section 6 we give conclusion.

2. Review of Chebyshev polynomials and function approximation

2.1 Chebyshev polynomials

In this section, we give some notation about most commonly used set of the orthogonal polynomials, Chebyshev polynomials [22, 23] that can be determined with the aid of the following recursive relation,

$$\begin{aligned} &T_0(x) = 1, \\ &T_1(x) = x, \\ &T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n \geq 1. \end{aligned} \tag{5}$$

These polynomials are orthogonal on $[-1, 1]$ with respect to the weight function $w(x) = \frac{1}{\sqrt{1-x^2}}$, that is

$$\int_{-1}^{1} T_i(x)T_j(x)w(x)dx = \pi\gamma_i\delta_{ij}, \tag{6}$$

where

$$\gamma_i = \begin{cases} 1, & i = 0, \\ \dfrac{1}{2}, & i > 0, \end{cases} \tag{7}$$

and δ_{ij} is the Kronocker delta. A function $f \in C[-1, 1]$ may be represented by Chebyshev polynomials series as [24, 25]

$$f(x) = \sum_{i=0}^{\infty} f_i T_i(x). \tag{8}$$

If the infinite series in Eq. (8) is truncated, then it can be written as

$$f(x) \simeq \sum_{i=0}^{N} f_i T_i(x) = \mathbf{F}^t \mathbf{T}_N(x), \tag{9}$$

where

$$\mathbf{T}_N(x) = [T_0(x), T_1(x), \ldots, T_N(x)], \quad \mathbf{F} = [f_0, f_1, \ldots, f_N], \tag{10}$$

and

$$f_i = \frac{< f_i, T_i >_{w(x)}}{< T_i, T_i >_{w(x)}}, \qquad i = 0, 1 \ldots, N, \tag{11}$$

where $<,>$ denotes the inner product with respect to suitable weight function $w(x)$. Moreover, if $f \in C^k[-1,1], \quad k \geq 1$, then

$$f^{(k)}(x) \simeq \mathbf{F}^t \mathbf{T}_N^{(k)}(x) = \mathbf{F}^t (P_N^{-1})^k \mathbf{T}_N(x), \tag{12}$$

where $f^{(k)}(x)$ is the k^{th} derivative of $f(x)$ and, P_N is the $(N+1)(N+1)$ operational matrix [26]

$$P_N = \begin{pmatrix} 1 & 1 & 0 & \cdots & 0 & 0 \\ -\frac{1}{4} & 0 & \frac{1}{4} & \cdots & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{2} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{(-i)^{N-1}}{1-(N-1)^2} & 0 & 0 & \cdots & 0 & \frac{1}{2N} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{(-1)^N}{1-N^2} & 0 & 0 & \cdots & -\frac{1}{2N-2} & 0 \end{pmatrix}.$$

2.2 Two dimensional Chebyshev polynomials

In this section, by using Chebyshev polynomials, we define a basis set for $L^2([-1,1] \times [-1,1])$. Let

$$T_{ij}(x) = T_i(x) T_j(x), \qquad i = 0, 1, \ldots, \quad j = 0, 1, \ldots. \tag{13}$$

Then, the the two-dimensional Chebyshev basis vector are as follows:

$$\begin{aligned} \mathbf{T}(x,t) = [&T_0(x)T_0(t), \ldots, T_0(x)T_M(t), T_1(x)T_0(t), \ldots, T_1(x)T_M(t), \ldots, \\ &T_N(x)T_M(t)] \\ = (&\mathbf{T}_N(x) \otimes \mathbf{T}_M(x))^t, \end{aligned} \tag{14}$$

in which $\mathbf{T}_N(x) = [T_0(x), T_1(x), \ldots, T_N(x)]$ and $\mathbf{T}_M(x) = [T_0(x), T_1(x), \ldots, T_M(x)]$ and $\otimes$ is the Kroncher tensor product. The orthogonality property for these polynomials with $w(x,t) = w(x)w(t)$ on the interval $[-1,1] \times [-1,1]$ is stated as

$$< T_{ij}(x,t), T_{kl}(x,t) >_{w(x,t)} = \int_{-1}^{1} \int_{-1}^{1} T_{ij}(x,t) T_{kl}(x,t) w(x,t) dx dt = \pi^2 \gamma_i \gamma_k \delta_{ij} \delta_{kl}.$$

Similarly to the previous statement, a continuous function $f(x,t)$ on $[-1,1] \times [-1,1]$ can be expanded by the two-dimensional Chebyshev polynomials as the following equation [27]:

$$f(x,t) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} f_{ij} T_{ij}(x,t) = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} f_{ij} T_i(x) T_j(t), \tag{15}$$

$$f_{ij} = \frac{< f(x,t), T_{ij}(x,t) >_{w(x,t)}}{< T_{ij}(x,t), T_{ij}(x,t) >_{w(x,t)}}, \qquad i = 0, 1, \ldots, \qquad j = 0, 1, \ldots, \tag{16}$$

where $< . >$ denotes the inner product with respect to the suitable weight function $w(x,t)$. In practice, only the finite terms of the above series are considered, so we have

$$f(x,t) \simeq \sum_{i=0}^{N} \sum_{j=0}^{M} f_{ij} T_{ij}(x,t). \tag{17}$$

2.3 Shifted Chebyshev polynomials

Let the function $h(x)$ be defined on an arbitrary interval $[a,b]$. Then, it can be approximated by making transformation from $[a,b]$ to $[-1,1]$ as:

$$h(x) \simeq \sum_{i=0}^{N} h_i T_i(\frac{2}{b-a}(x-a)-1) = \mathbf{H}^t \mathbf{T}_{N,[a,b]}(x), \tag{18}$$

where $\mathbf{H} = [h_0, h_1, \ldots, h_N]$ and $\mathbf{T}_{N,[a,b]}$ is Chebyshev polynomials vector that have been shifted from $[-1,1]$ to $[a,b]$. Moreover, for an arbitrary N and M, a continuous function of two variables $u : [a,b] \times [c,d] \longrightarrow \mathbb{R}$ can be approximated by

$$\begin{aligned} u(x,t) &\simeq \sum_{n=0}^{N} \sum_{m=0}^{M} u_{nm} T_{nm}(\frac{2}{b-a}(x-a)+1, \frac{2}{d-c}(t-c)+1) \\ &= \sum_{n=0}^{N} \sum_{m=0}^{M} u_{nm} T_n(\frac{2}{b-a}(x-a)+1) T_m(\frac{2}{d-c}(t-c)+1) \\ &= \mathbf{T}^t_{N,[a,b]}(x) U \mathbf{T}_{M,[c,d]}(x), \end{aligned} \tag{19}$$

where $U = [u_{nm}]$, $n = 0, 1, \ldots, N$ and $m = 0, 1, \ldots, M$.

3. Pseudo-spectral method

In this section, we derive a pseudo-spectral interpolation approximation for functions of two variables and then implement it in a multi-step scheme to approximate the solution of the problem (4). The advantage of this direct interpolation is that it is stable for large mode M and N.

3.1 Function approximation using direct interpolation

The Chebyshev-Gauss-Radau collocation points, $\{x_i\}_{i=0}^{N}$, $\{t_j\}_{j=0}^{M}$ and weights, $\{w_i\}_{i=0}^{N}$, $\{v_j\}_{j=0}^{M}$ provide the approximate quadrature

$$\int_{-1}^{1} \int_{-1}^{1} w(x) v(t) u(x,t) dx dt \simeq \sum_{i=0}^{N} \sum_{j=0}^{M} w_i v_j u(x_i, t_j), \tag{20}$$

where

$$w_i = \begin{cases} \dfrac{\pi}{2N}, & i = 0, N, \\ \dfrac{\pi}{N}, & i = 1, 2, \ldots, N-1, \end{cases}, \quad v_j = \begin{cases} \dfrac{\pi}{2M}, & j = 0, M, \\ \dfrac{\pi}{M}, & j = 1, 2, \ldots, M-1. \end{cases}$$

Further, the solution of Eq. (15), $u \in L^2([0,1] \times [0,1])$, can be expanded in a Chebyshev series. Hence,

$$u(x,t) = \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} u_{nm} T_{nm}(x,t), \tag{21}$$

where

$$u_{nm} = \frac{\gamma_n \gamma_m}{\pi^2} \int_{-1}^{1} \int_{-1}^{1} w(x) v(t) u(x,t) dx dt. \tag{22}$$

By substitution Eq. (20) into Eq. (22), truncated at N and M, we have

$$u_{nm} = \frac{\gamma_n \gamma_m}{\pi^2} \sum_{i=0}^{N} \sum_{j=0}^{M} w_i v_j u(x_i, t_j) T_{nm}(x_i, t_j), \tag{23}$$

Now, substituting Eq. (23) into Eq. (21) yields

$$\begin{aligned} u(x,t) &\simeq u_{NM}(x,t) \\ &= \sum_{n=0}^{N} \sum_{m=0}^{M} \sum_{i=0}^{N} \sum_{j=0}^{M} \frac{\gamma_n \gamma_m}{\pi^2} w_i v_j u(x_i, t_j) T_{nm}(x_i, t_j) T_{nm}(x,t). \end{aligned} \tag{24}$$

Due to the values of w_i and v_j, we rewrite Eq. (24) as follows:

$$u(x,t) = \sum_{n=0}^{N} \sum_{m=0}^{M} \sum_{i=0}^{N} \sum_{j=0}^{M} \frac{4\gamma_n \gamma_m}{NM b_i c_j} b_n c_m u(x_i, t_j) T_{nm}(x_i, t_j) T_{nm}(x,t), \tag{25}$$

where

$$b_i = \begin{cases} \frac{1}{2}, & i = 0, N, \\ 1, & i = 1, 2, \ldots, N-1, \end{cases}, \quad c_j = \begin{cases} \frac{1}{2}, & j = 0, M, \\ 1, & j = 1, 2, \ldots, M-1, \end{cases}.$$

With Eq. (25) we obtain the interpolation approximation

$$u_{NM}(x,t) \simeq \sum_{i=0}^{N} \sum_{j=0}^{M} I_{ij}(x,t) u(x_i, t_j), \tag{26}$$

where the interpolating polynomials, $I_{ij}(x,t)$, are defined by

$$I_{ij}(x,t) = \sum_{n=0}^{N} \sum_{m=0}^{M} \frac{4\gamma_n \gamma_m}{NM b_i c_j} b_n c_m T_{nm}(x_i, t_j) T_{nm}(x,t). \tag{27}$$

It can be easily checked that $I_{ij}(x_k, t_l) = \delta_{ik}\delta_{jl}$, because

$$
\begin{aligned}
I_{ij}(x_k, t_l) &= \sum_{n=0}^{N}\sum_{m=0}^{M} \frac{4\gamma_n\gamma_m}{NMb_ic_j} b_n c_m T_{nm}(x_i, t_j) T_{nm}(x_k, t_l) \\
&= \frac{2}{Nb_i}\sum_{n=0}^{N} b_n T_n(x_i)T_n(x_k)\left(\frac{2}{Mc_j}\sum_{m=0}^{M} T_m(t_j)T_m(t_l)\right),
\end{aligned} \tag{28}
$$

and according to [28] $\frac{2}{Mc_j}\sum_{m=0}^{M} T_m(t_j)T_m(t_l) = \delta_{jl}$, therefore

$$I_{ij}(x_k, t_l) = \delta_{ik}\delta_{jl}. \tag{29}$$

Now, by applying Eq. (27) and considering that $z_{ij} = \frac{4}{NMb_ic_j}$, we can write the matrix form of Eq. (26) as follows:

$$u_{NM}(x,t) = \mathbf{U}_{NM}^T.\mathbf{I}_{NM}, \tag{30}$$

where $\mathbf{I}_{NM} = [I_{nm}]$ and $\mathbf{U}_{NM} = [u_{nm}]$ are $(N+1)(M+1)$ matrices and

$$I_{nm} = z_{nm}[B^tT_{N,[a,b]}(x) \otimes C^tT_{M,[c,d]}(t)]^t[T_{N,[a,b]}(x_n) \otimes T_{M,[c,d]}(t_m)], \tag{31}$$

and $B = [b_0, b_1, \ldots, b_N]$, $C = [c_0, c_1, \ldots, c_M]$.

Next, by using Eq. (31) we have

$$
\begin{aligned}
\frac{\partial}{\partial t} I_{nm}(x,t) &= z_{nm}[B^tT_{N,[a,b]}(x) \otimes C^t\frac{\partial}{\partial t}T_{M,[c,d]}(t)]^t[T_{N,[a,b]}(x_n) \otimes T_{M,[c,d]}(t_m)]^T \\
&= \frac{2z_{nm}}{d-c}[B^tT_{N,[a,b]}(x) \otimes C^tP^{-1}MT_{M,[c,d]}(t)]^t[T_{N,[a,b]}(x_n) \otimes T_{M,[c,d]}(t_m)],
\end{aligned} \tag{32}
$$

and

$$
\begin{aligned}
\frac{\partial^2}{\partial x^2} I_{nm}(x,t) &= z_{nm}[B^t\frac{\partial^2}{\partial x^2}T_{N,[a,b]}(x) \otimes C^tT_{M,[c,d]}(t)]^t[T_{N,[a,b]}(x_n) \otimes T_{M,[c,d]}(t_m)] \\
&= \frac{4z_{nm}}{(d-c)^2}[B^t(P_N^{-1})^2T_{N,[a,b]}(x) \otimes C^tT_{M,[c,d]}(t)]^t.[T_{N,[a,b]}(x_n) \otimes T_{M,[c,d]}(t_m)].
\end{aligned} \tag{33}
$$

Finally, Eqs. (32)-(33) together with Eq. (30), yield

$$u_{NM,t}(x,t) = \frac{\partial}{\partial t}(U_{NM}^t I_{NM}(x,t)) = U_{NM}^t I_{NM,t}(x,t), \tag{34}$$

and

$$u_{NM,xx}(x,t) = \frac{\partial^2}{\partial x^2}(U_{NM}^t I_{NM}(x,t)) = U_{NM}^t I_{NM,xx}(x,t), \tag{35}$$

where

$$I_{NM,t}(x,t) = \left[\frac{\partial}{\partial t} I_{nm}(x,t)\right]_{n=0,m=0}^{N,M}, \qquad I_{NM,xx}(x,t) = \left[\frac{\partial^2}{\partial x^2} I_{nm}(x,t)\right]_{n=0,m=0}^{N,M}.$$

3.2 The multi-step collocation method

In the previous section, with the aid of Chebyshev polynomials and Chebyshev-Gauss-Lobatto quadrature points, a direct interpolation scheme for approximating $u(x,t)$ with reference to the pseudo-spectral method were represented. In this subsection, a multi-step collocation method is presented for approximating the solution of the problem (4). In the proposed method, we divide the interval of the problem into a set of sub-intervals and then approximate the solution of the sub-problem for each sub-intervals. An important point in this approach is that, since the original problem is solved independently on each sub-interval, it would be a useful approximation for large T, i.e., on large domains. As stated before, we consider a step size and then divide the interval $(0,T]$ to a sequence of subintervals with length equal to the considered step size. For this purpose, we first assume $\frac{T}{l}$ as the step size of the interval $(0,T]$, and l as a positive integer number. Then we divide interval $(0,T]$ into l sub-interval

$$R_k = \left(\frac{(k-1)T}{l}, \frac{kT}{l}\right], \qquad k = 1, 2, \ldots, l. \tag{36}$$

Furthermore, we define the restriction of $u(x,t)$ on each R_k by a piecewise function as follows:

$$u(x,t)|_{R_k} = u^k(x,t), \qquad k = 1, 2, \ldots, l, \qquad x \in (0,1), \qquad t \in R_k, \tag{37}$$

where $u^k(x,t)$, is solution of Eq. (4) on the area $\Omega_k = \{(x,t)|\ x \in [0,1],\ t \in R_k\}$. Now, we can rewrite Eq.(4) on Ω_k as follows:

$$\begin{cases} u_t^k(x,t) = a(t)u_{xx}^k(x,t) + p(t)u^k(x,t) + g(x,t), & x \in (0,1),\ t \in R_k, \\ u^k(x,0) = u_k(x), & x \in [0,1], \\ u^k(0,t) = g_0(t), & t \in R_k, \\ u^k(1,t) = g_1(t), & t \in R_k, \\ u^k(x^*,t) = E(t), & x^* {\in} (0,1), t {\in} R_k {\cup} \{0\}. \end{cases} \tag{38}$$

Here, we suppose that $u^k(x,t)$, $k = 0, 1, \ldots, l$, approximates the solution of the problem (4) on Ω_k. So, we divide the problem (4) into l independent problems, and then we solve them consecutively. It is worth mentioning that, when we solve the problem on the Ω_k area, it means that, we have already solved it on the previous area Ω_{k-1}. So, the approximation of $u^{k-1}(x, \frac{(k-1)T}{l})$ in k^{th} step is known.

Here, we use Chebyshev-Gauss-Radau collocation points and pseudo-spectral method for approximating of $u(x,t)$. According to [28], we represent Chebyshev polynomials series of $a(t)$ on the interval R_k as follows:

$$a^k(t) \simeq \sum_{j=0}^{M} a_j I_j(t) = \mathbf{I}_{M,R_k}^T(t)\mathbf{A}^k. \tag{39}$$

where $\mathbf{I}_{M,R_k}(t) = [I_{l,R_k}]$ and $I_{l,R_k}(t) = \sum_{l=0}^{M} T_l(t)T_l(t_l)$.

To solve the sub-problem (38), first by using Eqs. (34)-(35) and Eq. (30) we rewrite this problem as the following matrix form

$$
(40)\quad \begin{cases}
(U_{NM}^k)^t.\mathbf{I}_{NM,t}(x_i,t_j) = \mathbf{I}_{M,R_k}^t(t_j)\mathbf{A}^k(U_{NM}^k)^t\mathbf{I}_{NM,xx}(x_i,t_j) \\
+P(t_j)(U_{NM}^k)^t\mathbf{I}_{NM}(x_i,t_j)+g(x_i,t_j), i{=}1,2,\ldots,N{-}1,\ j=1,\ldots,M, \\
(U_{NM}^k)^t.\mathbf{I}_{NM}(x_i,0) = u^k(x_i), \qquad i=1,\ldots,N, \\
(U_{NM}^k)^t.\mathbf{I}_{NM}(0,t_j) = g_0(t_j), \qquad j=1,\ldots,M, \\
(U_{NM}^k)^t.\mathbf{I}_{NM}(1,t_j) = g_1(t_j), \qquad j=1,\ldots,M, \\
(U_{NM}^k)^t.\mathbf{I}_{NM}(x^*,t_j) = E(t_j), \qquad j=0,1,\ldots,M.
\end{cases}
$$

Next, let $d = (M+1)(N+3)$ is the dimension of the above system of nonlinear algebraic equations (NAEs). The NAEs (40) can be represented in the general form

$$
(41)\quad \begin{cases}
\mathbb{F}(.) : \mathbb{R}^d \longrightarrow \mathbb{R}^d, \\
\mathbb{F}(\mathbf{Z}) = 0,
\end{cases}
$$

where $\mathbb{F} = (F_1, F_2, \ldots, F_d)$, $\mathbf{Z} = (z_1, z_2, \ldots, z_d)$ and $F_i(z_1, z_2, \ldots, z_d) = 0$, $i = 1, 2, \ldots, d$. By applying a proper method for solving the nonlinear system (41), we can obtain $(M{+}1)(N{+}3)$ unknown coefficients u_{ij} and a_j, $i = 1, \ldots, N$, $j = 0, 1, \ldots, M$, and consequently $\mathbf{U}_{NM}^T.\mathbf{I}_{NM}$ and $\mathbf{I}_{M,R_k}^t(t)\mathbf{A}^k$ as the approximate solutions of the inverse problem (4) on Ω_k.

Since the original inverse reaction diffusion (4) is ill-posed, the NAEs (41) my be unstable. In other words, for the ill-posed problem or some special cases, the inverse of Jacobian matrix of $\mathbb{F}$ does not exist or cannot be found in the numerical sense. So the optimal searching direction used in the iteration process or Newton's method is not proposed [14]. So in order to stabilize the solution, we use the Tikhonov regularization scheme.

4. Convergence analysis

The propose of the present section is to obtain an error bound for the best approximation of the function u based on interpolation functions and to describe the convergence behavior of the proposed numerical method.

We suppose

$$
(42)\qquad u(x,t) = \sum_{k=1}^{l} u^k(x,t),
$$

where $u^k = u\chi_{\Omega_k}$.

Recall that $(\mathbf{U}^k)^T\mathbf{I}_{NM}(x,t)$ is interpolation function of $u^k(x,t)$ on the Ω_k, hence, it is the best approximation of $u^k(x,t)$ [25].

Theorem 4.1. *Suppose that $u \in C^r([0,1] \times [0,T])$ then $\boldsymbol{U}^T \boldsymbol{I}_{NM}(x,t)$ approximates $u(x,t)$ with the following error bound*

$$\|u(x,t) - \mathbf{U}^T \mathbf{I}_{NM}(x,t)\|_2 \leq (\frac{\lambda\sqrt{T}}{r!})(1 + \frac{T}{l})^r, \qquad \lambda = \max_{\substack{x\in[0,T]\\ 0\leq j\leq r}} |\frac{\partial^r u(x,t)}{\partial x^j \partial t^{r-j}}|. \tag{43}$$

Proof. Let $p(x,t)$ be the Taylor expansion for the function $u^k(x,t)$, it is known as [23]:

$$| u^k(x,t) - p(x,t) | \leq \frac{\lambda}{r!}(x + (t - \frac{(k-1)T}{l}))^r, \ k = 1, 2, \ldots, l. \tag{44}$$

Since, $(\mathbf{U}^k)^T \mathbf{I}_{NM}(x,t)$ is the best approximation of $u^k(x,t)$, hence by using Eq. (44) we obtain

$$\begin{aligned}\|u^k(x,t) - (\mathbf{U}^k)^T \mathbf{I}_{NM}(x,t)\|_2^2 &\leq \| u^k(x,t) - \tilde{u}^k(x,t) \|_2^2 \\ &\leq \int_0^1 \int_{\frac{(k-1)T}{l}}^{\frac{kT}{l}} (\frac{\lambda}{r!})^2 (x + (t - \frac{(k-1)T}{l}))^{2r} dxdt \\ &\leq (\frac{\lambda}{r!})^2 \int_0^1 \int_{\frac{(k-1)T}{l}}^{\frac{kT}{l}} (1 + \frac{T}{l})^{2r} dxdt \\ &= (\frac{\lambda}{r!})^2 \frac{T}{l} (1 + \frac{T}{l})^{2r}.\end{aligned} \tag{45}$$

Now,

$$\begin{aligned}\|u(x,t) - u_{NM}(x,t)\|_2^2 &\leq \sum_{k=1}^{l} \|u^k(x,t) - (\mathbf{U}^k)^T \mathbf{I}_{NM}(x,t)\|_2^2 \\ &\leq (\frac{\lambda}{r!})^2 T (1 + \frac{T}{l})^{2r}\end{aligned} \tag{46}$$

and, we have

$$\|u(x,t) - u_{NM}(x,t)\| \leq (\frac{\lambda\sqrt{T}}{r!})(1 + \frac{T}{l})^r. \tag{47}$$

□

5. Numerical examples

In this section, the theoretical considerations introduced in the previous sections will be illustrated with some examples. In the process of computation, all the symbolic and numerical computations were performed by using the package of Maple 16. We tested the accuracy and the stability of the method which was presented in this paper by performing the mentioned method for different values of N and M. To study the convergence behavior of the multi-step pseudo-spectral method, we apply the root mean square (RMS) that is

$$RMS(u) = \sqrt{\frac{1}{NM}\sum_{i=0}^{N}\sum_{j=0}^{M}|u(x_i,t_j) - u^k(x_i,t_j)|^2}.$$

Example 5.1. As the first example, we consider the inverse reaction- diffusion equation that can be found in [17]:

$$\begin{cases} u_t(x,t) = a(t)u_{xx}(x,t), & 0 < x < 1, \quad 0 < t \leq T, \\ u(x,0) = e^{\frac{x}{2}}, & 0 \leq x \leq 1, \\ u(0,t) = \frac{1+2t^3}{1+t^3} + \sin(\frac{t}{2}), & 0 < t \leq T, \\ u(1,t) = \sqrt{e}(\frac{1+2t^3}{1+t^3} + \sin(\frac{t}{2})), & 0 < t \leq T, \\ u(x^*,t) = 1.13315(\frac{1+2t^3}{1+t^3} + \sin(\frac{t}{2})), & 0 < x^* < 1, \quad 0 \leq t \leq T. \end{cases} \tag{48}$$

The exact solution to this problem is $u(x,t) = e^{\frac{x}{2}}(\frac{1+2t^3}{1+t^3} + \sin(\frac{t}{2}))$, $a(t) = \frac{2[6t^2+(1+t^3)^2\cos(\frac{t}{2})]}{(1+t^3)[1+2t^2+(1+t^3)\sin(\frac{t}{2})]}$. We solved this example by using the method described in this paper for $N = M = 9, 10$ with the number of sub-interval $l = 10$, $x^* = 0.25$ and $T = 1$. Table 1 shows the absolute value of errors, using the proposed method and compares the result with the results obtained by using the technique in [17]. Table 2 shows the RMS errors for various values of M and N. In addition, the graphs of the error functions are plotted in Figs. 1-4 with $N = M = 10$.

Table 1: Numerical results of Example 4.1

	Method [17]		Presented Method	
t	$N=9, M=9$	$N=10, M=10$	$N=9, M=9$	$N=10, M=10$
0.1	4.9E-6	1.0E-7	6.1E-13	3.7E-17
0.3	1.3E-6	1.0E-7	8.3E-12	2.2E-18
0.5	2.2E-6	1.9E-7	5.0E-12	7.1E-15
0.7	2.6E-6	2.1E-7	8.1E-11	8.3E-14
0.9	2.6E-6	2.1E-7	2.6E-10	2.9E-13

Table 2: The RMS error for $u(x,t)$ and $a(t)$ for Example 4.1

	Method [17]		Presented Method	
x	$N=5, M=5$	$N=8, M=8$	$N=5, M=5$	$N=8, M=8$
RMS(u)	5.2E-4	6.2E-5	8.4E-7	9.4E-11
RMS(a)	3.9E-2	4.2E-3	3.3E-5	2.1E-10

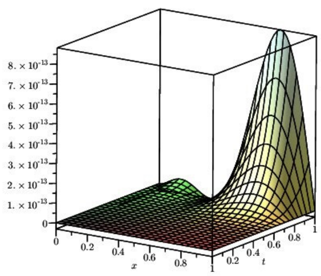

Figure 1: Graph of $u(x,t) - u_{NM}(x,t)$ for $N = M = 10$

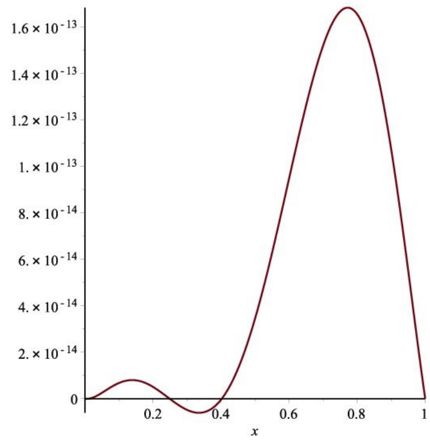

Figure 2: Graph of $u(x,t) - u_{NM}(x,t)$ for $t = 0.9$ and $N = M = 10$

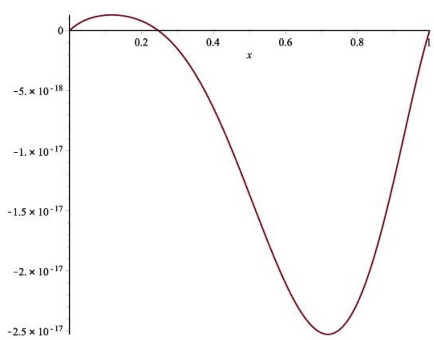

Figure 3: Graph of $u(x,t) - u_{NM}(x,t)$ for $t = 0.1$ and $N = M = 10$

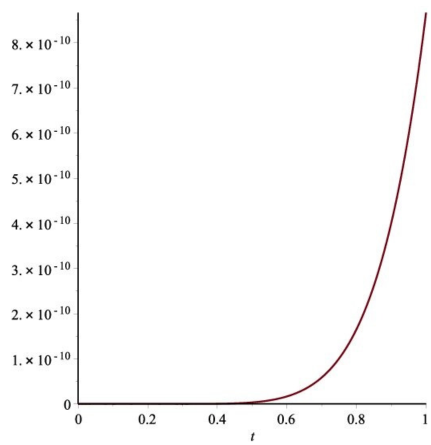

Figure 4: Graph of $a(t) - a_{app}(t)$ for $N = M = 10$

Example 5.2. In this example, we solve the problem (4) with $T = 3$ and $x^* = \frac{2}{7}$ and the initial boundary and the extra measurement condition as following:

$$\begin{cases} u_t(x,t) = a(t)u_{xx}(x,t) + (-2t^2 - 1)u(x) + 2t(x+t)e^{(t^2+1)x}, \\ \qquad\qquad\qquad\qquad 0 < x < 1, \quad 0 < t \leq T, \\ u(x,0) = e^x, \qquad\qquad 0 \leq x \leq 1, \\ u(0,t) = 1, \qquad\qquad 0 < t \leq T, \\ u(1,t) = e, \qquad\qquad 0 < t \leq T, \\ u(x^*,t) = e^{\frac{2(t^2+1)}{7}}, \\ \qquad\qquad\qquad\qquad 0 < x^* < 1, \quad 0 \leq t \leq T. \end{cases} \tag{49}$$

Table 3: Maximum error of numerical solution to $u(x,t)$ for Example 4.2

Sub-interval on t axes	$N=7, M=7$	$N=10, M=10$
$[0.0, 0.3]$	1.0E-11	1.0E-14
$[0.6, 0.9]$	2.2E-11	1.3E-13
$[0.9, 1.2]$	2.6E-11	2.3E-13
$[1.2, 1.5]$	2.6E-11	2.4E-13
$[1.5, 1.8]$	2.6E-10	2.4E-12
$[1.8, 2.1]$	1.5E-10	1.7E-12
$[2.1, 2.4]$	1.9E-10	3.5E-12
$[2.4, 2.7]$	1.1E-9	3.7E-11
$[2.7, 3.0]$	3.6E-9	3.8E-11

The exact solution of (49) is $u(x,t) = e^{(t^2+1)x}$ and $a(t) = \frac{1}{(1+t^2)^2}$. The propose of this example is to show that the approximate solution have a good degree of accuracy even for large values of T. The data in Table 3 shows the maximum errors between the calculated and the exact solution of $u(x,t)$ with $M = N = 7, 10$ and $l = 10$. The graphs of the error functions are plotted in Figs. 5-8 with $N = M = 10$. It is seen that the approximate solutions have a good degree of accuracy even for large values of T.

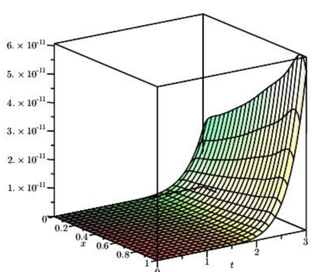

Figure 5: Graph of $u(x,t) - u_{app}(x,t)$ for $N = M = 10$

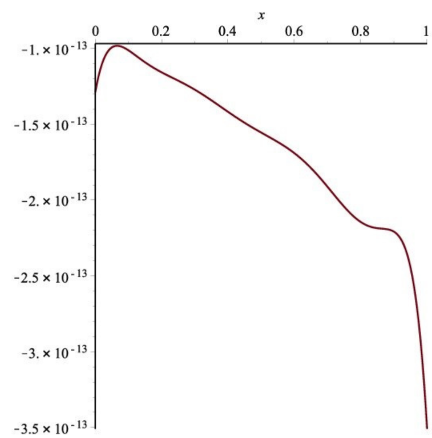

Figure 6: Graph of $u(x,t) - u_{NM}(x,t)$ for $t = 1$ and $N = M = 10$

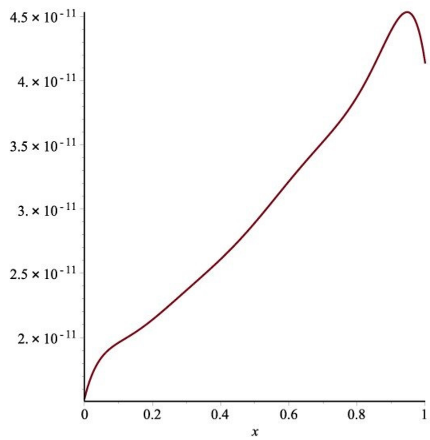

Figure 7: Graph of $u(x,t) - u_{NM}(x,t)$ for $t = 2.9$ and $N = M = 10$

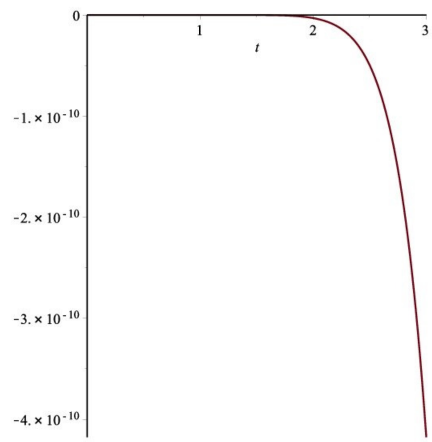

Figure 8: Graph of $a(t) - a_{app}(t)$ for $N = M = 10$

6. Conclusion

The main objective of this work is to construct a new approximation to the solution of the inverse reaction-diffusion equations system. For this purpose, the pseudo-spectral multi-step method with two-dimensional Chebyshev interpolation, are implemented. The main advantage of our method is that, since the main problem is solved independently on the subintervals, it provides reasonable approximations for large T. In addition, the proposed method is numerically stable. Numerical findings show that there is a good agreement between the obtained results and the exact values that demonstrates the validity and the accuracy of the proposed method for such problems and gives the method a wider applicability.

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Accepted: March 15, 2020