NUMERICAL SOLUTION OF A COUPLED REACTION-DIFFUSION MODEL USING BARYCENTRIC INTERPOLATION COLLOCATION METHOD

by

Yu ZHANG[a], Wei ZHANG[b*], Chenhui ZHAO[c], and Yulan WANG[c*]

[a] Institute of Mathematics, Jining Normal University, Jining, Inner Mongolia, China
[b] Institute of Economics and Management, Jining Normal University, Jining, Inner Mongolia, China
[c] Department of Mathematics, Inner Mongolia University of Technology, Hohhot, China

Original scientific paper
https://doi.org/10.2298/TSCI2004561Z

In thermal science, chemical and mechanics, the non-linear reaction-diffusion model is very important, and an approximate solution with high precision is always needed. In this article, the barycentric interpolation collocation method is proposed for this purpose. Numerical experiments show that the proposed approach is highly reliable.

Key words: *non-linear reaction-diffusion model, numerical experiments, barycentric interpolation collocation method,*

Introduction

The paper is devoted to the numerical solution of a class of non-linear reaction-diffusion models:

$$\begin{cases} \dfrac{\partial u}{\partial t} = d_1 \dfrac{\partial^2 u}{\partial x^2} + h_1(u,v) \\ \dfrac{\partial v}{\partial t} = d_2 \dfrac{\partial^2 v}{\partial x^2} + h_2(u,v) \end{cases} \quad a \le x \le b, \quad t \ge 0 \tag{1}$$

with the following initial conditions and boundary conditions:

$$\begin{gathered} u(x,0) = f_0(x), v(x,0) = g_0(x), \quad a \le x \le b \\ u(a,t) = f_1(t), u(b,t) = f_2(t), \quad t \ge 0 \\ v(a,t) = g_1(t), v(b,t) = g_2(t), \quad t \ge 0 \end{gathered} \tag{2}$$

where $d_1 > 0$ and $d_2 > 0$ are diffusion coefficients and may also include the parametrizations of turbulence.

The reaction-diffusion model has wide applications in thermal science, chemical and mechanics [1-5]. There are some analytical and numerical methods [6-10] for solving the advection-reaction-diffusion system, among which the barycentric interpolation collocation method [11-17] is a high precision method. In this paper, we mainly employ the Lagrange barycentric interpolation collocation method to solve the reaction-diffusion model (1).

* Corresponding author, e-mail: wylnei@163.com, jnsfxyzw@163.com

The barycentric interpolation formula of the eq. (1)

We give two initial hypothesis functions u_0, v_0 and construct the following linear iterative format:

$$\begin{cases} \dfrac{\partial u_n}{\partial t} = d_1 \dfrac{\partial^2 u_n}{\partial x^2} + h_1(u_{n-1}, v_{n-1}) \\ \dfrac{\partial v_n}{\partial t} = d_2 \dfrac{\partial^2 v_n}{\partial x^2} + h_2(u_{n-1}, v_{n-1}) \end{cases} \quad n = 1, 2, 3, \cdots \tag{3}$$

Next, we give a meshless barycentric interpolation collocation method of eq. (3).

Let $a \le x_1 < x_2 < \cdots < x_M \le b,\ 0 \le t_1 < t_2 < \cdots < t_N \le T$. The barycentric interpolation form of function $u(x, t)$ can be expressed:

$$u(x,t) = \sum_{i=1}^{M} \sum_{j=1}^{N} \xi_i(x) \eta_j(t) u(x_i, t_j) \tag{4}$$

where $\xi_i(x)$ is the barycentric interpolation basis function of M nodes on interval $[a, b]$, $\eta_j(t)$ is the barycentric interpolation basis function of N nodes on interval $[0, T]$.

$$\xi_i(x) = \frac{\prod_{k=1,k\neq i}^{M} (x - x_k)}{\prod_{k=1,k\neq i}^{M} (x_i - x_k)}, \quad i = 1, 2, \cdots, M, \qquad \eta_j(t) = \frac{\prod_{k=1,k\neq j}^{N} (t - t_k)}{\prod_{k=1,k\neq j}^{N} (t_j - t_k)}, \quad j = 1, 2, \cdots, N$$

Using the method of [11-12, 15], eq. (3) can be written in following partitioned matrix form:

$$\begin{bmatrix} D^{(0,1)} - d_1 D^{(2,0)} & 0 \\ 0 & D^{(0,1)} - d_2 D^{(2,0)} \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix} = \begin{bmatrix} \text{diag}[h_1(u_{n-1}, v_{n-1})] \\ \text{diag}[h_2(u_{n-1}, v_{n-1})] \end{bmatrix} \tag{5}$$

where $D^{(0.1)}$, $D^{(0.2)}$, and diag$[h_1(u_{n-1}, v_{n-1})]$ are explained in [11-12, 15]. In this paper, we use displacement method to impose the initial boundary conditions. The detailed procedure can be found in [15].

Numerical experiments

Experiment 1. We consider the following reaction-diffusion model [3]:

$$\begin{cases} \dfrac{\partial u}{\partial t} = a_1 \dfrac{\partial^2 u}{\partial x^2} - uv^2 + a_2(1 - u) \\ \dfrac{\partial v}{\partial t} = b_1 \dfrac{\partial^2 v}{\partial x^2} + uv^2 - (a_2 + b_2)v \end{cases} \tag{6}$$

with the following initial conditions:

$$u(x,0) = 1 - 0.5 \sin^{100} \frac{\pi(x-50)}{100}, \quad v(x,0) = 0.25 \sin^{100} \frac{\pi(x-50)}{100}, \quad x \in [-50, 50] \tag{7}$$

and the boundary conditions:

$$u(-50,t)=u(50,t)=1, \quad v(-50,t)=v(50,t)=0, \quad t\in[0,400] \tag{8}$$

In tab. 1, we analyze the influence of b_1, b_2 on u and v at t = 100, M = N = 20, with the given parameters a_1 = 1.0, a_2 = 0.064.

Figures 1-3 show the numerical solutions of u and v obtained by the present method, where b_1 = 0.01, b_2 = 0.062, M = 20, N = 20.

Table 1. Comparison of numerical solutions at *t* = 100 for *Experiment 1* (*M* = *N* = 20)

x	$u(x, t)$	$v(x, t)$	$u(x, t)$	$v(x, t)$	$u(x, t)$	$v(x, t)$
	b_1 = 0.01	b_2 = 0.062	b_1 = 0.5	b_2 = 0.062	b_1 = 0.01	b_2 = −0.3
−50	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000
−25	0.5493	–0.0012	0.5156	–0.0090	0.5153	–0.0024
0	0.0006	0.1575	0.2454	0.3662	0.2805	0.2998
25	0.5493	–0.0012	0.5162	–0.0095	0.5153	–0.0024
50	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000

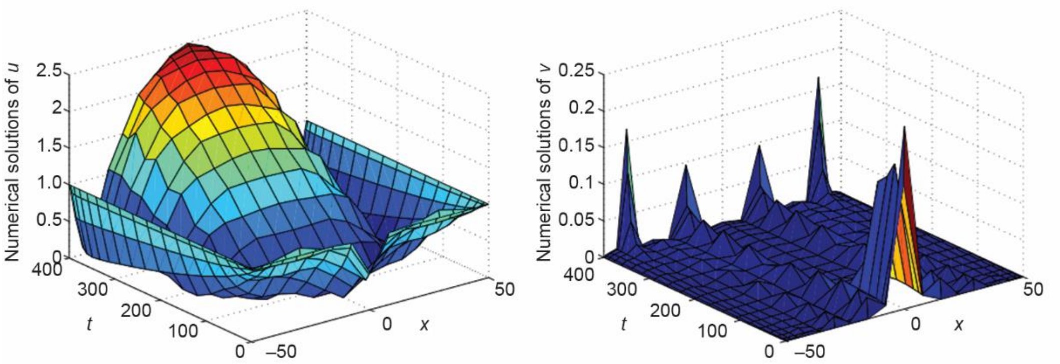

Figure 1. The numerical solution for *Experiment 1* at a_1 = 1.0, a_2 = 0.064

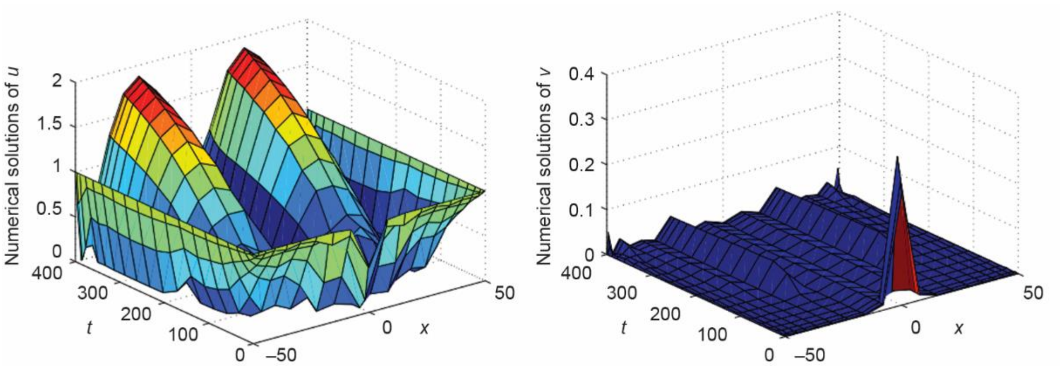

Figure 2. The numerical solution for *Experiment 1* at a_1 = 1.0, a_2 = 0.5

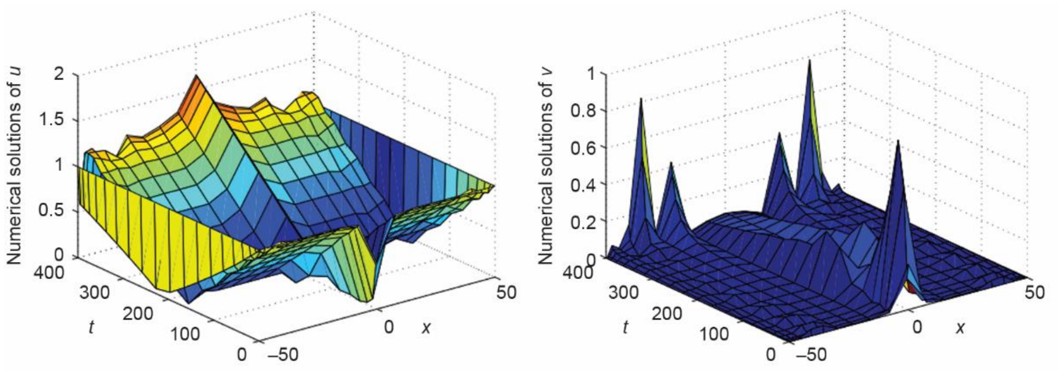

Figure 3. The numerical solution for *Experiment 1* at a_1 = 0.001, a_2 = 0.064

Experiment 2. Consider the following Brusselator model [4, 5]:

$$\begin{cases} \dfrac{\partial u}{\partial t} = 10^{-4}\dfrac{\partial^2 u}{\partial x^2} - 4.4u + u^2 v + 1 \\ \dfrac{\partial v}{\partial t} = 10^{-4}\dfrac{\partial^2 v}{\partial x^2} + 3.4u - u^2 v \end{cases} \tag{9}$$

with the following initial conditions:

$$u(x,0) = 0.5, v(x,0) = 1 + 5x, \quad x \in [0,1] \tag{10}$$

and the boundary conditions:

$$u_x(0,t) = u_x(1,t) = 0, \quad v_x(0,t) = v_x(1,t) = 0, \quad t \in [0,1] \tag{11}$$

The results of *Experiment 2* are given in fig. 4.

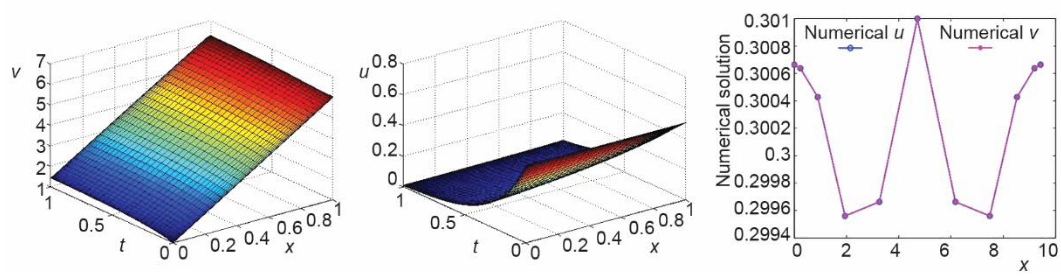

Figure 4. Numerical solutions obtained by the present method for *Experiment 2*

Experiment 3. Consider the Schnakenberg model [1]:

$$\begin{cases} \dfrac{\partial u}{\partial t} = d_1\dfrac{\partial^2 u}{\partial x^2} + a - u + u^2 v \\ \dfrac{\partial v}{\partial t} = d_2\dfrac{\partial^2 v}{\partial x^2} + b - u^2 v \end{cases} \tag{12}$$

- (1) We select the parameter d_1 = 0.2, d_2 = 0.1, a = 0.14, b = 0.66, the initial condition $u(x, 0) = 0.8 + 0.1\cos(x)$, $v(x, 0) = 1.03 + 0.1\cos(x)$ and the boundary condition $u_x(0, t) = 0$, $u_x(3\pi, t) = 0$, $v_x(0, t) = 0$, $v_x(3\pi, t) = 0$.
- (2) We select the parameter d_1 = 0.01, d_2 = 1.0, a = 0.14, b = 0.16 and the initial condition $u(x, 0) = 0.3 + 0.001\sin(3x)$, $v(x, 0) = 1.778 + 0.001\cos(2x)$. The results of *Experiment 3* are given in figs. 5 and 6.

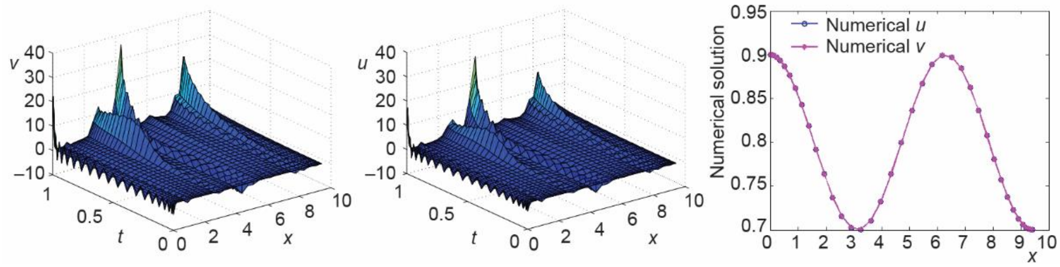

Figure 5. Numerical solutions obtained by the present method for *Experiment 3* (1)

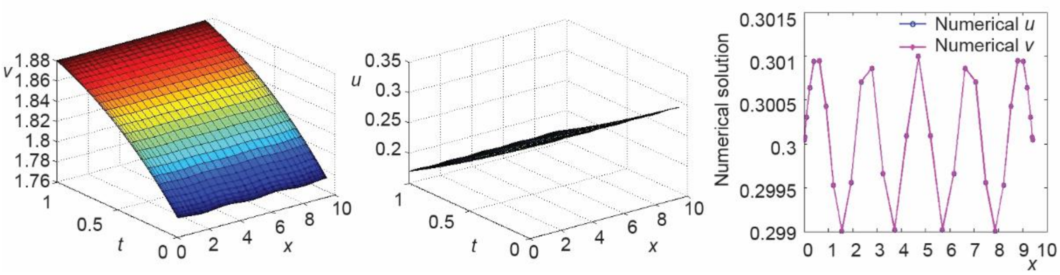

Figure 6. Numerical solutions obtained by the present method for *Experiment 3* (2)

Experiment 4. Consider the isothermal chemical model [2]:

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} - uv \\ \dfrac{\partial v}{\partial t} = \dfrac{\partial^2 v}{\partial x^2} - kv + uv \\ u(x,0) = 1, \quad v(x,0) = \exp(-x^2), \quad 0 \le x \le 200 \\ u_x(0,t) = 0, \quad u(200,t) = 1, \quad v_x(0,t) = 0, \quad u(200,t) = 0 \end{cases} \tag{13}$$

We select the parameter k = 0.1, 0.3, 0.5, 0.7, 0.9. The results of *Experiment 4* are given in fig. 7 and tab. 2.

Table 2. Comparison of numerical solution with the *k* for *Experiment 4*

k	Numerical solution of *u*	Numerical solution of *v*	*k*	Numerical solution of *u*	Numerical solution of *v*
0.1	0.0038529	0.0053738	0.7	0.0046887	0.0049609
0.3	0.0037315	0.0050254	0.9	0.0050133	0.0051748
0.5	0.0042162	0.0043605			

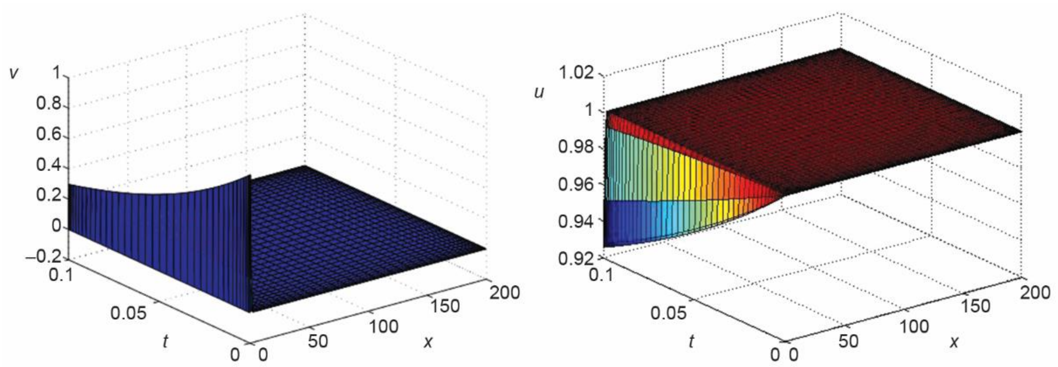

Figure 7. Numerical solutions obtained by the present method for *Experiment 4*

Conclusion

In this paper, a class of reaction-diffusion systems have been solved by using the barycentric interpolation collocation method. The numerical experiments show that the algorithm is highly accurate. All computations are performed by a mathematical software.

Acknowledgment

This paper is supported by the Natural Science Foundation of Inner Mongolia [2017MS0103], Inner Mongolia maker collaborative innovation center of Jining Normal University, the Doctoral Program of Jining Normal University [jsbsjj1704] and the National Natural Science Foundation of China [11361037].

References

[1] Schnakenberg, J., Simple Chemical Reaction Systems with Limit Cycle Behaviour, *Journal of theory biological, 81* (1979), 3, pp. 389-400
[2] Merkin, J. H., Needham, D. J., The Development of Travelling Waves in a Simple Isothermal Chemical System, Cubic Autocatalysis with Quadratic and Linear Decay, *Proc R Soc Lond*, *A 430* (1990), 1879, pp. 315-345
[3] Jiwari, R., *et al.,* Numerical Simulation to Capture the Pattern Formation of Coupled Reaction-Diffusion Models, *Chaos, Solitons and Fractals, 103* (2017), Oct., pp. 422-439
[4] Nicolis, G., Prigogine, I., *Exploring Complexity*, Freeman, New York, USA, 1989
[5] Lefever, R., Nicolis, G., Chemical Instabilities and Sustained Oscillations, *Journal of Theory Biological, 30* (1971), 2, pp. 267-284
[6] He, J. H., Ji, F. Y., Taylor Series Solution for Lane-Emden Equation, *Journal of Mathematical Chemistry, 57* (2019), 8, pp. 1932-1934
[7] He, J. H., The Simplest Approach to Non-Linear Oscillators, *Results in Physics, 15* (2019), 102546
[8] He, J. H., A Simple Approach to One-Dimensional Convection-Diffusion Equation and Its Fractional Modification for E Reaction Arising in Rotating Disk Electrodes, *Journal of Electroanalytical Chemistry, 854* (2019), 113565
[9] He, J. H., Homotopy Perturbation Method: A New Non-Linear Analytical Technique, *Applied Mathematics and Computation*, *135* (2003), 1, pp. 73-79
[10] He, J. H., Wu, X. H., Construction of Solitary Solution and Compacton-Like Solution by Variational Iteration Method, *Chaos Solitons Fractals*, *29* (2006), 1, pp. 108-113
[11] Li, S. P., Wang, Z. Q., *Barycentric Interpolation Collocation Method for Non-Linear Problems*, National Defense Industry Press, Beijing China, 2015
[12] Li, S. P., Wang, Z. Q., *High-Precision Non-Grid Center of Gravity Interpolation Collocation Method: Algorithm, Program and Engineering Application*, Science Press*,* Beijing China, 2012

[13] Li, J. M., *et al*., Numerical Simulation of the Lorenz-Type Chaotic System Using Barycentric Lagrange Interpolation Collocation Method, *Adv. Math. Phys., 2019* (2019), ID 1030318
[14] Zhou, X. F., *et al*., Numerical Simulation of a Class of Hyperchaotic System Using Barycentric Lagrange Interpolation Collocation Method, *Complexity*, *2019* (2019), ID 1739785
[15] Liu, F. F., Wang, Y. L., Barycentric Interpolation Collocation Method for Solving the Coupled Viscous Burgers' Equations, *International Journal of Computer Mathematics, 95* (2018), 11, pp. 2162-2173
[16] Wang, Y. L.,Tian, D., *et al.*, Numerical Method for Singularly Perturbed Delay Parabolic Partial Differential Equations, *Thermal Science, 21* (2017), 4, pp. 1595-1599
[17] Du, M. J., *et al*., Numerical Simulation of a Class of Three-Dimensional Kolmogorov Model with Chaotic Dynamic Behavior by Using Barycentric Interpolation Collocation Method, *Complexity, 2019* (2019), ID 3426974

Paper submitted: April 24, 2019
Paper revised: November 1, 2019
Paper accepted: November 1, 2019