ORIGINAL ARTICLE

Biomath Forum

Numerical solutions of one-dimensional parabolic convection-diffusion problems arising in biology by the Laguerre collocation method

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Received: 2 October 2016, accepted: 4 June 2017, published: 9 June 2017

Abstract—In this work, we present a numerical scheme for the approximate solutions of the onedimensional parabolic convection-diffusion model problems which arise in biological models. The presented method is based on the Laguerre collocation method used for ordinary differential equations. The approximate solution of the problem in the truncated Laguerre series form is obtained by this method. By substituting truncated Laguerre series solution into the problem and by using the matrix operations and the collocation points, the suggested scheme reduces the problem to a linear algebraic equation system. By solving this equation system, the unknown Laguerre coefficients can be computed. The accuracy and efficiency of the method is studied by comparing with other numerical methods when used to solve some numerical experiments.

Keywords-Convection-diffusion equation models, Parabolic problem, Laguerre collocation method.

I. INTRODUCTION

Diffusion models form a reasonable basis for studying insect and animal dispersal and

invasion, which arise from the question of persistence of endangered species, biodiversity, disease dynamics, multi-species competition so on. Convection-diffusion problem is also a form of heat and mass transfer in biological models [1-3].



Fig. 1. (a) Flow between imaginary compartments in a continuous one-dimensional system. (b) Discrete grid system used in two-dimensional transport models. (c) A close-up of five grid points showing the similarity to compartment models.

Compartment models are general framework

Citation: Burcu Gürbüz, Mehmet Sezer, Numerical solutions of one-dimensional parabolic convection-diffusion problems arising in biology by the Laguerre collocation method, Biomath 6 (2017), 1706047, http://dx.doi.org/10.11145/j.biomath.2017.06.047

$$\frac{\partial u(x,t)}{\partial t} = \begin{pmatrix} \text{Convection} \\ \text{In} \end{pmatrix} - \begin{pmatrix} \text{Convection} \\ \text{Out} \end{pmatrix} + \begin{pmatrix} \text{Diffusion} \\ \text{In} \end{pmatrix} - \begin{pmatrix} \text{Diffusion} \\ \text{Out} \end{pmatrix}$$

Fig. 2. A conceptual rate equation with respect to the convection-diffusion model

that has many applications in biology, ecosystems and enzyme kinetics which can be mostly shown by forrester diagrams. The system is decomposed into flows of material as possibly large number of discrete compartments which are very useful. Conversely, it is also useful for the quantities nominally not flow, for instance, blood or water pressure in animal and plant physiological systems. Furthermore, complex interconnection networks can be addressed by these type of models with respect to link many of them together in many different complicated ways (Fig. 1).

On the other hand, in transport models, we have a physical quantity, such as energy i.e. heat or a quantity of matter, that flows from spatial point to point. There are many forces that could influence the flow of the matter, but the following simplified view uses two that will illustrate the qualitative model formulation. Convection moves the substance with a physical flow of water from point to point (i.e. river flow). Diffusion moves a substance in any direction according to the concentration of the substance around each point (Fig. 2) [4-5].

In this study, we consider the one-dimensional parabolic convection-diffusion problem

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + A(x)\frac{\partial u}{\partial x} + B(x)u + f(x,t),$$

$$0 \le x \le l, 0 \le t \le T,$$

(1)

with the initial conditions

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$$u(x,0) = g(x), \quad 0 \le x \le l < \infty,$$
 (2)

and the boundary conditions

$$u(0,t) = h(t), \quad u(l,t) = K(t), \quad 0 \le t \le T < \infty$$
(3)

where f(x,t), A(x), B(x), g(x) and h(t) are functions defined in $[0, l] \times [0, T]$; l and T are appropriate constants. In this study, we develop the Laguerre collocation method given in [9,10] and use to obtain the approximate solution of Eq. (1) in the truncated Laguerre series form

$$u(x,t) = \sum_{r=0}^{N} \sum_{s=0}^{N} a_{r,s} L_{r,s}(x,t); \qquad (4)$$
$$L_{r,s}(x,t) = L_r(x) L_s(t)$$

where $a_{r,s}$, r, s = 0, ..., N, are the unknown Laguerre coefficients and $L_n(x)$, n = 0, 1, 2, ..., N are the Laguerre polynomials defined by [6-8]

$$L_n(x) = \sum_{k=0}^n \frac{(-1)^k}{k!} \binom{n}{k} x^k, n \in \mathbb{N}, \ 0 \le x < \infty.$$
(5)

II. NUMERICAL METHOD

We first consider the series (4) for N = 2, as follows:

$$u(x,t) = \sum_{r=0}^{2} \sum_{s=0}^{2} a_{r,s} L_r(x) L_s(t)$$

= $a_{00} L_0(x) L_0(t) + a_{10} L_1(x) L_0(t)$
+ $a_{20} L_2(x) L_0(t) + a_{01} L_0(x) L_1(t)$ (6)
+ $a_{11} L_1(x) L_1(t) + a_{21} L_2(x) L_1(t)$
+ $a_{02} L_0(x) L_2(t) + a_{12} L_1(x) L_2(t)$
+ $a_{22} L_2(x) L_2(t)$

Then we can generalize the approximate solution (6) for any truncated limit N and can write the obtained series in the matrix form

$$[u(x,t)] = \mathbf{L}(x)\mathbf{L}(t)\mathbf{A}$$
(7)

where

$$\mathbf{L}(x) = \begin{bmatrix} L_0(x) & L_1(x) & \cdots & L_N(x) \end{bmatrix}$$
$$\overline{\mathbf{L}}(t) = \begin{bmatrix} \mathbf{L}(t) & 0 & \cdots & 0 \\ 0 & \mathbf{L}(t) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{L}(t) \end{bmatrix}$$

and

 $\mathbf{A} = [a_{0,0} \ a_{0,1} \cdots a_{0,N} \cdots a_{N,0} \ a_{N,1} \cdots a_{N,N}]^T$

Also, we can put the matrix $\mathbf{L}(x)$ in the matrix form

$$\mathbf{L}(x) = \mathbf{X}(x)\mathbf{H} \tag{8}$$

where $\mathbf{X}(x)$ and \mathbf{H} are defined as

$$\mathbf{X}(x) = \left[\begin{array}{cccc} 1 & x^1 & \cdots & x^N \end{array} \right]$$

and

$$\mathbf{H} = \begin{bmatrix} \frac{(-1)^0}{0!} \begin{pmatrix} 0 \\ 0 \end{pmatrix} & 0 & \cdots & 0 \\ \frac{(-1)^0}{0!} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & \frac{(-1)^1}{1!} \begin{pmatrix} 1 \\ 1 \end{pmatrix} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \frac{(-1)^0}{0!} \begin{pmatrix} N \\ 0 \end{pmatrix} & \frac{(-1)^1}{1!} \begin{pmatrix} N \\ 1 \end{pmatrix} & \cdots & \frac{(-1)^N}{N!} \begin{pmatrix} N \\ N \end{pmatrix} \end{bmatrix}$$

Moreover, it is clearly seen that the relations between the matrix $\mathbf{X}(x)$ and its derivatives $\mathbf{X}'(x)$ and $\mathbf{X}''(x)$ are

$$\mathbf{X}'(x) = \mathbf{X}(x)\mathbf{B}$$
 and $\mathbf{X}''(x) = \mathbf{X}(x)\mathbf{B}^2$ (9)

where

$$\mathbf{B} = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & N \\ 0 & 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Then, by using the expressions (8) and (9) we easily find the matrix relations

$$\mathbf{L}'(x) = \mathbf{X}(x)\mathbf{B}\mathbf{H}$$
 and $\mathbf{L}''(x) = \mathbf{X}(x)\mathbf{B}^{2}\mathbf{H}(10)$

$$\mathbf{L}(t) = \mathbf{X}(t)\mathbf{H}$$
 and $\mathbf{L}(t) = \mathbf{X}(t)\mathbf{B}\mathbf{H}$ (11)

Now, by means of the relations (7)-(11) we obtain the following matrix forms:

$$[u(x,t)] = \mathbf{L}(x)\overline{\mathbf{L}}(t)\mathbf{A} = \mathbf{X}(x)\mathbf{H}\overline{\mathbf{X}}(t)\overline{\mathbf{H}}\mathbf{A} \quad (12)$$

$$\begin{aligned} [u_x(x,t)] &= \mathbf{L}'(x)\overline{\mathbf{L}}(t)\mathbf{A} \\ &= \mathbf{X}(x)\mathbf{B}\mathbf{H}\overline{\mathbf{X}}(t)\overline{\mathbf{H}}\mathbf{A} \quad (13) \end{aligned}$$

$$[u_{xx}(x,t)] = \mathbf{L}''(x)\overline{\mathbf{L}}(t)\mathbf{A}$$
$$= \mathbf{X}(x)\mathbf{B}^{2}\mathbf{H}\overline{\mathbf{X}}(t)\overline{\mathbf{H}}\mathbf{A} \quad (14)$$

$$[u_t(x,t)] = \mathbf{L}(x)\overline{\mathbf{L}}(t)\mathbf{A}$$

= $\mathbf{X}(x)\mathbf{H}\overline{\mathbf{X}}(t)\overline{\mathbf{BH}}\mathbf{A}$ (15)

By putting the expressions (8), (12), (13), (14) and (15) into Eq. (1), we obtain the matrix equation

$$\{\mathbf{X}(x)\mathbf{H}\overline{\mathbf{X}}(t)\overline{\mathbf{B}} - \mathbf{X}(x)\mathbf{B}^{2}\mathbf{H}\overline{\mathbf{X}}(t) -A(x)\mathbf{X}(x)\mathbf{B}\mathbf{H}\overline{\mathbf{X}}(t)$$
(16)
$$-B(x)\mathbf{X}(x)\mathbf{H}\overline{\mathbf{X}}(\mathbf{t})\}\overline{\mathbf{H}}\mathbf{A} = f(x,t)$$

or briefly,

$$\mathbf{W}(x,t)\mathbf{A} = f(x,t)$$

Besides, by substituting the collocation points defined by

$$x_i = \frac{l}{N}i, \ t_j = \frac{T}{N}j, \ i, j = 0, 1, 2, ..., N,$$

into the Eq.(16), we have the system of the matrix equations $\mathbf{W}(x_i, t_j)\mathbf{A} = f(x_i, t_j)$ or briefly the fundamental matrix equation

$$\mathbf{W}\mathbf{A} = \mathbf{F} \Longrightarrow [\mathbf{W}; \mathbf{F}]$$

By using the same procedure for the initial and boundary conditions we obtain the matrix relations for

$$i, j = 0, 1, ..., N$$
:

$$u(x_i, 0) = \mathbf{X}(x_i)\mathbf{H}\overline{\mathbf{X}}(0)\overline{\mathbf{H}}\mathbf{A} = g(x_i) = \lambda_i$$

$$u(0, t_j) = \mathbf{X}(0)\mathbf{H}\overline{\mathbf{X}}(t_j)\overline{\mathbf{H}}\mathbf{A} = h(t_j) = \mu_j$$

$$u(y, t_j) = \mathbf{X}(y)\mathbf{H}\overline{\mathbf{X}}(t_j)\overline{\mathbf{H}}\mathbf{A} = K(t_j) = \gamma_j$$

or briefly,

$$\mathbf{UA} = [\lambda]; \ [\mathbf{U}; \lambda], \mathbf{VA} = [\mu]; \ [\mathbf{V}; \mu], \mathbf{ZA} = [\gamma]; \ [\mathbf{Z}; \gamma].$$

To obtain the approximate solution of Eq. (1) under conditions (2) and (3), we form the augmented matrix

	TCM	LCM	TCM	LCM
х	E_{25}	E_{25}	E_{50}	E_{50}
0.0	0.69500E-17	7.00000E-13	0.10000E-18	0.0000000000
0.1	0.15886E-03	3.681538E-06	0.15886E-03	1.040134E-07
0.2	0.63428E-03	2.207214E-05	0.63428E-03	4.157153E-08
0.3	0.14208E-02	4.966673E-05	0.14208E-02	9.332459E-08
0.4	0.25078E-02	5.150761E-05	0.25078E-02	1.652982E-05
0.5	0.38799E-02	2.543790E-11	0.38799E-02	2.569605E-15
0.6	0.55168E-02	1.324508E-04	0.55168E-02	3.676180E-06
0.7	0.73934E-02	3.734395E-04	0.73934E-02	4.964259E-06
0.8	0.94802E-02	7.505606E-04	0.94802E-02	6.423988E-06
0.9	0.11744E-01	1.291408E-03	0.11744E-01	8.044241E-07
1.0	0.14146E-01	2.023575E-03	0.14146E-01	9.812752E-07

TABLE I Comparison of the absolute errors with TCM and LCM for N = 25, 50 in Example 2.

$$[ilde{\mathbf{W}}; ilde{\mathbf{F}}] = \left[egin{array}{c} \overline{\mathbf{W}}; \mathbf{F} \ \mathbf{U}; \lambda \ \mathbf{U}; \mu \ \mathbf{Z}; \gamma \end{array}
ight.$$

Hence, the unknown Laguerre coefficients are computed by

$$\mathbf{A} = (\tilde{\tilde{\mathbf{W}}})^{-1} \tilde{\tilde{\mathbf{F}}}$$

where $[\tilde{\tilde{\mathbf{W}}}; \tilde{\tilde{\mathbf{F}}}]$ is obtained by using the Gauss elimination method and then removing zero rows of augmented matrix $[\tilde{\mathbf{W}}; \tilde{\mathbf{F}}]$ [9-11]. By substituting the determined coefficients into Eq. (4), we have the Laguerre series solution

$$u_N(x,t) = \sum_{r=0}^{N} \sum_{s=0}^{N} a_{r,s} L_{r,s}(x,t), L_{r,s}(x,t) = L_r(x) L_s(t)$$

III. NUMERICAL RESULTS

Test case[11]

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + (2x+1)\frac{\partial u}{\partial x} + x^2 u + \frac{e^{x+t}}{\epsilon}, \\ 0 \le x \le 1, 0 \le t \le 1,$$
(17)

with conditions

$$u(x,0) = \frac{e^x}{\epsilon}, \quad 0 \le x \le 1$$

$$u(0,t) = \frac{e^t}{\epsilon}, \quad u(y,t) = \frac{e^{1+t}}{\epsilon} \quad 0 \le t \le 1,$$

with $\epsilon = 2.10^{-4}$ and the exact solution of the problem is $u(x,t) = \frac{e^{x+t}}{\epsilon}$. From Table 1, it is seen that the errors from Laguerre Collocation Method (LCM) are in general less than Taylor Collocation Method (TCM).

Table I. shows the comparison between absolute errors of LCM solutions and TCM solutions for different N values.

IV. CONCLUSION

We have presented and illustrated the Laguerre collocation method is based on computing the coefficients in the Laguerre expansion of solution of a one dimensional parabolic convection-diffusion model problems. A considerable advantage of the method is that the Laguerre polynomial coefficients of the solution are found very easily by using computer programs; Maple and Matlab.

Illustrative example is included to show the validity and applicability of the technique. Shorter computation time and lower operation count results in reduction of cumulative truncation errors and improvement of overall accuracy.

As a result, the method can also be extended to the system of reaction-diffusion-advection model problems with their residual error analysis, but some modifications are required.

ACKNOWLEDGMENT

This work was financially supported by Society for Mathematical Biology for during the Bio-Math 2016, The annual International Conference on Mathematical Methods and Models in Biosciences and it is performed within the "Numerical Solutions of Partial Functional Integro Differential Equations with respect to Laguerre Polynomials and Its Applications" project, Manisa Celal Bayar University Department of Scientific Research Projects, with grant ref. 2014-151.

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