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On the solution of one-dimensional heat equation with higher-order non-central finite difference method of lines

Gour Chandra Paul*,[1] and Md. Emran Ali [1,2]
[1]*Department of Mathematics, University of Rajshahi, Rajshahi 6205, Bangladesh,*
[2]*Department of Textile Engineering, Northern University Bangladesh, Dhaka 1230, Bangladesh*

E-mail: pcgour2001@yahoo.com (G. C. Paul)*; emran.ru.math.bd@gmail.com (M. E. Ali)

ABSTRACT

In this paper, a one-dimensional heat equation with Dirichlet boundary condition is solved using the method of lines where the discretization is made with the help of higher-order non-central finite difference approximation method. During imposing higher-order approximation method, the specification of the values of the field variable at some exterior points outside the domain are required which are made using proper assumption. It is found that the attained results agree well with the exact solution on the basis of the root mean square errors.

Keywords: Heat equation, Boundary condition, Method of lines, Higher-order finite difference approximation.

INTRODUCTION

Partial differential equations (PDEs) are effective tools for explaining natural phenomena. As most of the PDEs do not have an analytical solution, numerical solutions with more efficient and faster techniques are therefore highly required. The numerical solution of PDEs has got good popularity to the research community after John von Neumann from mid-1940 (Tadmor, 2012). Nowadays, several tools such as Fourier transform, Laplace transform, finite difference method (FDM), finite element method, finite volume method, first recursive marching method, boundary matching method, homotopy perturbation method, method of lines (MOLs) have been developed in solving PDEs both analytically and numerically. In recent decades, the MOLs, advocated in the past, has been made great attraction to the research community for its simplicity in computation (Paul and Ali, 2019; Bakodah, 2011; Hicks and Wei, 1967; Paul et al., 2014; Pregla, 1987; Pregla and Pascher, 1989; Sadiku and Obiozor, 2000; Schiesser and Griffiths, 2009). It is a semi-analytic technique that transforms PDEs to a set of ordinary differential equations (ODEs) by discretizing all derivatives leaving one continuous. Normally, the time derivative, if exists, is kept continuous (Bakodah, 2011; Paul et al., 2014; Pregla, 1987; Sadiku and Obiozor, 2000; Schiesser and Griffiths, 2009; Paul et al., 2018). Sometimes, it is regarded as a special type of FDM with more flexibility in accuracy, computational cost, and stability (Sadiku and Obiozor, 2000).

Generally, it is seen in several studies, such as Pregla (1987), Pregla and Pascher (1989), Sadiku (2000), Paul et al. (2014, 2018), second-order 3-point forward, backward, and central finite difference approximations (FDAs) are being used in making discretization of spatial variables during computation with MOLs, but higher-order FDAs, such as 5-point, 7-point, 9-point, 11-point forward, backward and central differences possess local truncation error of higher-order resulting from a higher step size (Bakodah, 2011; Chapra and Canale, 2015; Paul and Ali, 2019; Ahmed and Yaacob, 2013). Thus, a smaller step size with a higher-order FDA method (FDAM) may return a more accurate result. On the other hand, according to Hicks (1967), 5-point non-central FDA with MOLs makes the computation much faster and more efficient. So, it is our interest to solve a very simple one-dimensional diffusion equation, viz. one-dimensional heat equation is solved using the higher-order backward finite difference approximation MOLs in coordination with some sophisticated ODE solvers, which in turn will help to solve other PDEs. But the problem of implementing the higher-order approximation method is that the speciation of the values of the field variables at some points outside of the boundary are to be supplied (Paul and Ali, 2019). The problem has been solved in Hicks (1967) which is applicable only for homogeneous type boundary with a higher grid resolution (Paul and Ali, 2019). However, the assumption that outside the domain, some neighboring points will preserve the same temperature as that of the respective boundary does (Paul and Ali, 2019). The assumption works so easily in homogeneous and non-homogeneous boundary conditions (BCs) as well as every type of BC (Paul and Ali, 2019). In the study due to Paul and Ali (2019), it is seen that higher-order central difference MOLs can retain more accurate results for non-homogeneous BCs over the assumption made in Hicks (1967). The intention of the study is, therefore, to see the computation efficiency of higher-order finite difference MOLs in addition to the assumption made by Paul and Ali (2019). The obtained results using the technique adopted in this study, as we will see later, is found to be fairly reasonable in comparison with those of some previous studies.

The rest of the paper is organized as follows, "Materials and Method" section and its subsections deal with the materials and methodology applied for making computations. Obtained results and their discussion are presented in "Results and Discussion" section, and finally, the conclusion is presented in "Conclusion".

MATERIALS AND METHOD

Problem statement

One-dimensional heat equation with auxiliary conditions, presented in Ahmad and Yaacob (2013), can be written in the following form:

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{\partial^2 u}{\partial x^2}; 0 < x < 1; t > 0, \quad (1)$$

which is subject to the initial condition

$$u(x, t = 0) = 70^o C, \quad (2)$$

and BCs

$$u(x = 0, t) = 50^o C \quad (3)$$

$$u(x = 1, t) = 20^o C. \quad (4)$$

The above problem can be stated as a rod of unit length is heated with temperature $70^{\circ}C$, and temperatures $50^{\circ}C$ and $20^{\circ}C$ are provided at both the boundaries where the rod is covered by an insulator. In this situation, one needs to investigate the temperature profile in the rod. Here α represents the diffusivity of the substance of the rod. The state variable $u(x,t)$ stands for representing the temperature distribution of the rod at point x over time t.

Discretization of the model equation

It is stated that the interest of this study is to solve a one-dimensional heat equation with higher-order non-central difference MOLs, where the discretization of the spatial variables is made using the 5-point backward FDAM. The adopted approximation of the spatial derivative leads to

$$\frac{\partial^2 u(x,t)}{\partial x^2} \approx a_1 u(x-3h,t) + a_2 u(x-2h,t) + a_3 u(x-h,t) + a_4 u(x,t) + a_5 u(x+h,t), \quad (5)$$

where $u(x, t)$ is a state variable that depends on x and t, h indicates spatial step size and a_i $(i = 1, 2, 3, \ldots 5)$ are unknown coefficients to be determined. To compute the values of the unknown coefficients, we have solved a system of linear equations obtained by equating both sides of Eq. (5) after expanding the terms using Taylor's series at the right side of that equation. It yields $a_1 = -\frac{1}{12h^2}$, $a_2 = \frac{4}{12h^2}$, $a_3 = \frac{6}{12h^2}$, $a_4 = -\frac{20}{12h^2}$, and $a_5 = \frac{11}{12h^2}$. It is worth noting here that we have neglected fifth or higher-order terms during Taylor series expansion and the scheme has the truncation error of fourth-order. Thus, Eq. (5), by the virtue of the values of the unknown coefficients, can be put in the following form:

$$\frac{\partial^2 u(x,t)}{\partial x^2} \approx \frac{1}{12h^2}(-u(x-3h,t) + 4u(x-2h,t) + 6u(x-h,t) - 20u(x,t) + 11u(x+h,t) + O(h^4). \quad (6)$$

The finite difference approach used in Eq. (6) is the same as that used in the study of Hicks (1967) to discretize the second-order spatial derivative. This leads to the following system of ODEs:

$$\left(\frac{du}{dt}\right)_i \approx \frac{1}{12h^2}(-u_{i-3} + 4u_{i-2} + 6u_{i-1} - 20u_i + 11u_{i+1}), \quad (7)$$

where $u_i = u(x_i, t)$, $i = 1, 2, 3, \ldots, n$, represent the values of the field variables standing at $x = x_i$, i.e., at $x_i = (i-1)h$. Thus, Eq. (1) is converted into a set of ODEs specified by Eq. (7) with ICs $u_{i,0} = 70^o C$. Thus, the BCs specified by Eqs. (3)-(4) can be stated as $u_{0,j} = 50^o C$ and $u_{n,j} = 20^o C$.

Integration procedure

The system of ODEs with initial valued specified by Eq. (7) can be solved with the help of given BCs using any sophisticated ODE solvers, such as classical Runge-Kutta (RK4) method, third-order (stage) arithmetic mean Runge-Kutta (RKAM3) method, Runge-Kutta (4,5) (RK45) method, and Runge-Kutta (2,3) (RK23) method. It is pertinent to mention here that the solution can be made so easily at every grid point of the spatial domain except the first two interior points along the left boundary. For getting solutions at those points, it is required to know the values at these two exterior points. For ensuring the values, an assumption is made that every neighboring point outside the boundaries preserves the same temperature as that of the respective boundary with considerably smaller steps.

As in the study due to Ahmad and Yaacob (2013), for four inner lines, the system of ODEs characterized by Eq. (7) considering the proposed BCs can be written as

$$\dot{U} = AU, \quad (8)$$

$$A = \frac{25}{12}\begin{pmatrix} -20 & 11 & 0 & 0 \\ 6 & -20 & 11 & 0 \\ 4 & 6 & -20 & 11 \\ -1 & 4 & 6 & -20 \end{pmatrix},$$

and $U = (u_1\, u_2\, u_3\, u_4)^T$.

The corresponding eigenvalues (computed using MATLAB R2021a) are found to be $\lambda_1 = -9.6019$, $\lambda_2 = -34.3525$, $\lambda_3 = -61.3561 + 8.3141i$ and $\lambda_4 = -61.3561 - 8.3141i$. The eigenvalues show that they have negative real parts, so the system characterized by Eq. (8) returns a stable solution with the treated BCs. Again, the stiffness ratio is computed to be $s = \frac{max|Re(\lambda_i)|}{min|Re(\lambda_i)|} = 6.39$. So, the system of equations given by Eq. (8) is mildly stiff (Ashino et al., 2000).

RESULTS AND DISCUSSION

In this study, a one-dimensional heat equation is solved using a higher-order backward finite difference MOLs along with some suitable ODE solvers, such as the RK4, RKAM3, RK45, RK23 methods considering spatial step size of $h = 0.2$ and thermal diffusivity $\alpha^2 = 0.1$. It is worth noting here that the obatained results using the solvers RK4 and RKAM3 are presented here due to space consumption and the both solvers shows relatively lower accuracy over RK45 and RK23. The computed numerical results obtained with both central and non-central FDA MOLs in coordination with only RK45 and RK23 are presented in Figs. 1-4, respectively, as these two solvers show better accuracy over the other mentioned technique for both central and non-central cases. Figures 1-2 show the 3-dimensional (3D) surface profile of the computed results using RK45 and RK23, respectively. The figures show that for both the time integrators, instabilities in initial time steps are found to be observed and they disappear soon with the evolution of time (see Figs. 1-2). In both cases (RK45 and RK23), the non-central difference approximation method was found to overcome the issue faster. The MOLs with the central difference in addition to the RK23 method takes a longer time to get stable results.

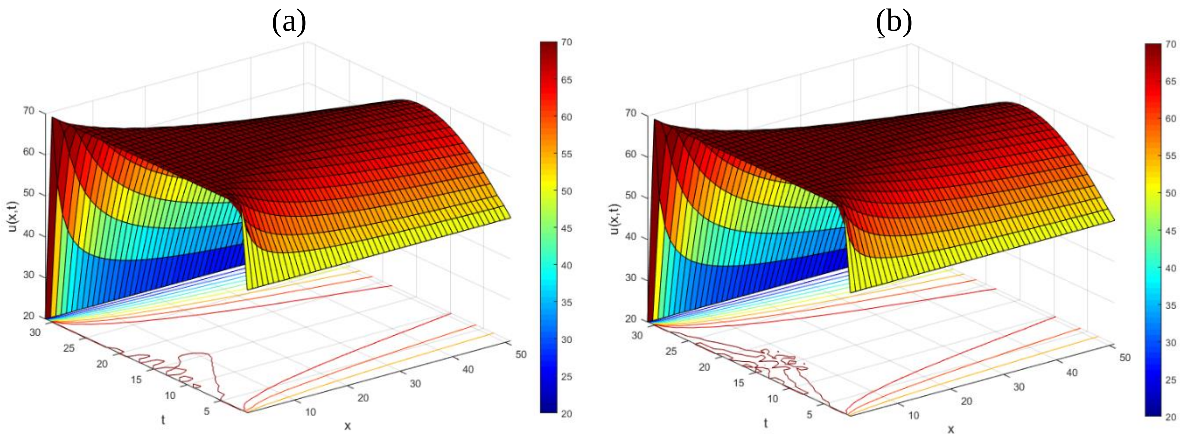

Figure 1: The 3D plots for the results obtained by using the RK45 method; (a) in respect of non-central FDAM; (b) in respect of central FDAM adopted in Paul and Ali (2019).

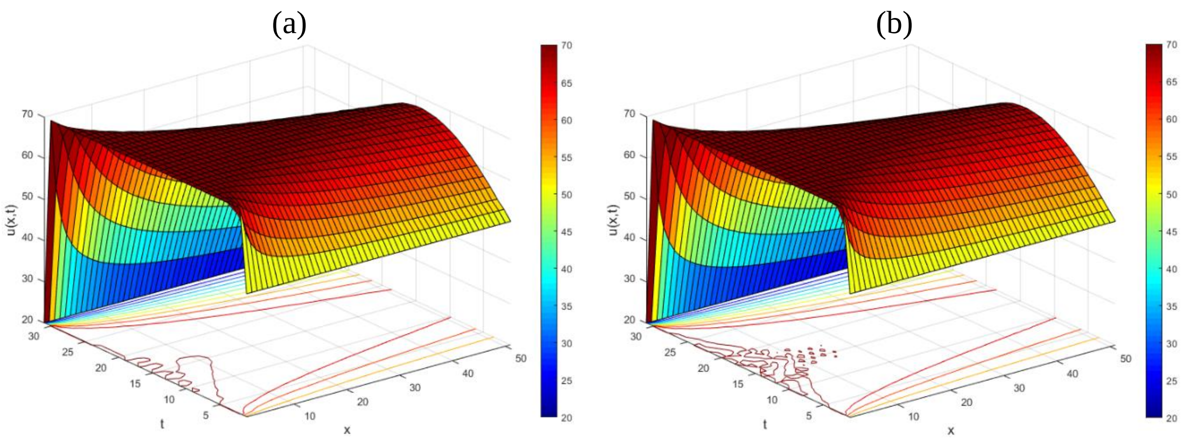

Figure 2: The 3D plots for the results attained by the RK23 method; (a) in respect of non-central FDAM; (b) in respect of central FDAM adopted in Paul and Ali (2019).

The obtained numerical results at time $t = 1$ are also compared with the analytic solution and are illustrated in Figs. 3-4, whereas the analytic results were computed by using advanced analytical mathematical software Maple 17. It is found that the results agree fairly well with the analytic solution.

It can also be inferred from Figs. 3 and 4 that the results obtained with higher-order non-central FDAM retain a more accurate result relative to the use of central FDAM. It can also be seen from the figures that the results nearer to the right boundary is more accurate relative to the results nearer to the left boundary (see Figs. 3-4 and Table 1). The reason behind this may be the use of a higher-order non-central backward FDAM.

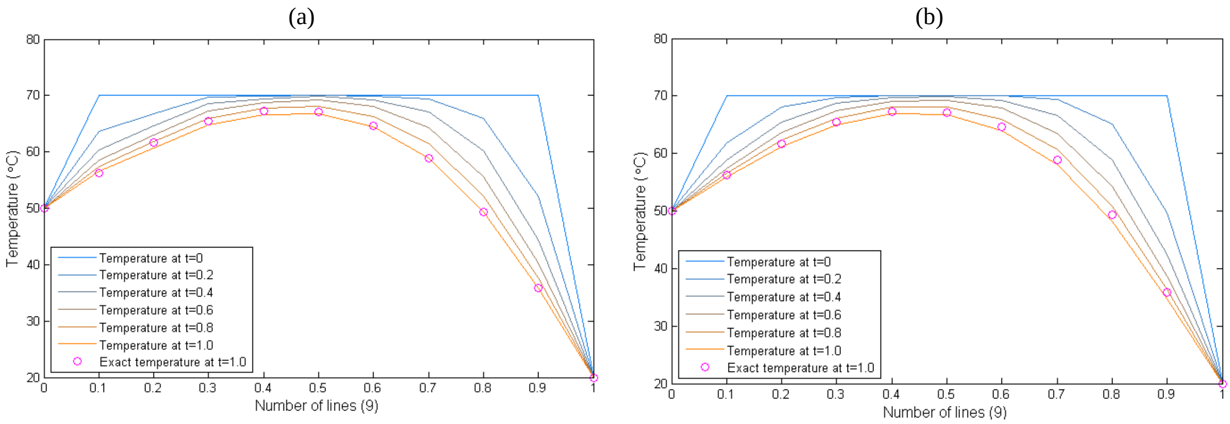

Figure 3: The graphical outputs of the results obtained by the RK45 method; (a) in respect of non-central FDAM; (b) in respect of central FDAM adopted in Paul and Ali (2019).

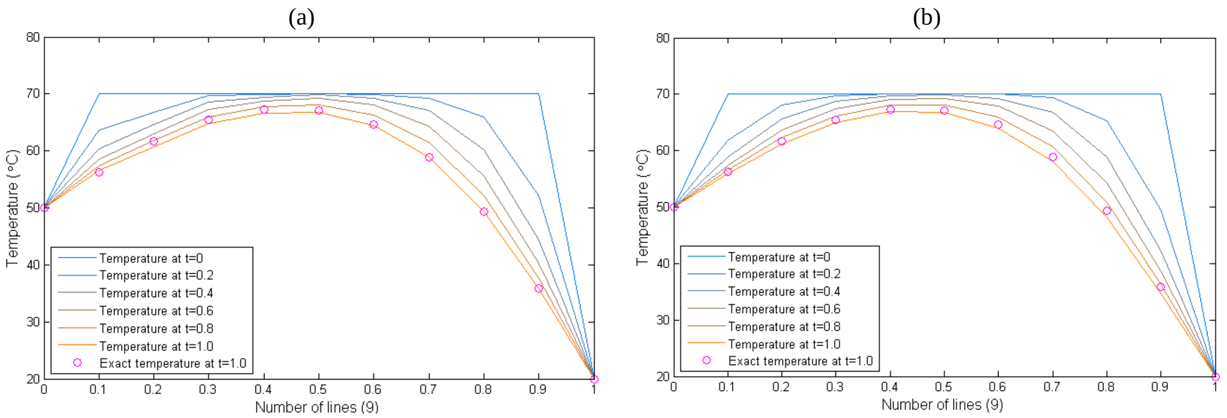

Figure 4: The graphical illustration of the outputs obtained by the RK23; (a) in respect of non-central FDAM; (b) in respect of central FDAM adopted in Paul and Ali (2019).

The relative errors for both cases (central and non-central finite difference method) are calculated and the results for nine grid points are presented in Table 1. From the table based on the relative errors, it is found that the results due to the use of the non-central backward FDAM are in good agreement over the central FDAM for both the ODE solvers, RK23 and RK45. It can also be observed from Table 1 that the RK23 returns more accurate results over the RK45 for the non-central FDAM. On the other hand, the RK45 works well when the discretization is made using central difference approximation method. This may be the result of the moderately stiff computing ability of RK23, which is seen previously that the obtained system of ODEs is mildly stiff with a stiffness ratio of about 6.

Table 1: Analytic results (obtained by using analytic mathematical software MAPLE 17) at different grid points and relative errors.

Grid points	Analytic result	Relative errors			
		Non-central difference method		Central difference method adopted in Paul and Ali (2019)	
		RK45	RK23	RK45	RK23
$x = 0.10$	56.3266	0.0049	0.0049	0.0080	0.0080
$x = 0.20$	61.6612	0.0150	0.0150	0.0069	0.0070
$x = 0.30$	65.3733	0.0084	0.0084	0.0054	0.0054
$x = 0.40$	67.2353	0.0084	0.0084	0.0047	0.0047

$x = 0.50$	67.1142	0.0047	0.0047	0.0056	0.0056
$x = 0.60$	64.5904	0.0024	0.0024	0.0085	0.0084
$x = 0.70$	58.8812	0.0005	0.0005	0.0135	0.0135
$x = 0.80$	49.2675	0.0021	0.0020	0.0212	0.0213
$x = 0.90$	35.8409	0.0019	0.0017	0.0313	0.0314

We have estimated RMSE (Root Mean Square Error) values for testing the performances of the solvers RK45 and RK23 based on the RMSE values for both the cases of interest when discretizing the spatial derivatives of our equation of interest using the central and non-central FDAMs. The RMSE values are presented in Table 2. The results show that the RK23 works well when discretization is made by using the higher-order non-central FDAM while the RK45 shows better performance when the discretization is made using the higher-order central finite difference method. It is pertinent to note here that the used time integrator, RK23, is a four-stage Bogacki Shampine embedded system of order 2 and 3 with error control, whereas the RK45 is an embedded method of orders 4 and 5 with error control introduced by Dormand and Prince (Ashino et al., 2000). Thus, the RK23 method with the 5-point backward scheme presented in this study may have a local truncation error of order $O(\Delta t^2) + O(h^4)$ or $O(\Delta t^3) + O(h^4)$ ($\Delta t =$ step size in time) for any grid points. Similarly, for the RK45 technique, we may obtain local truncation error of order $O(\Delta t^4) + O(h^4)$ or $O(\Delta t^5) + O(h^4)$ for every grid point. But the RK23 is capable of handling moderate stiff differential equations that may invite much changes in RMSE values.

The computational costs are also computed (in second) for both solvers in both cases and are displayed in Table 3. It can be observed from Table 3 that the RK23 method works faster in both cases and it works better for using a higher-order non-central finite difference method as stated in the study due to Hicks (1967). This is the reason for computing numbers of functions for a single step. In RK23, five functions are computed while in RK45, 7 functions are computed in every single step. It is to be noted here that the computed numerical results due to RK4 are relatively better on the basis of relative errors and RMSE value (0.1662) with a very small step size (with steps>900) but have a high computational cost. On the other hand, the number of steps is being used for the RK45 and RK23 methods is only 25 for displaying the computed results.

Table 2: The RMSE values obtained by using different RK solvers for both central and non-central FDAMs

Solvers	Non-central difference	Central difference adopted in Paul and Ali (2019)
RK45	0.3912	0.6059
RK23	0.3910	0.6069

Table 3: Computational cost for both central and non-central differences (in second).

Solvers	Non-central difference	Central difference adopted in Paul and Ali (2019)
RK45	0.640240	0.613762
RK23	0.541899	0.606201

From the above discussion, it may be said that the MOLs along with the RK23 solver works well when the discretization is made using a higher-order (5-point) non-central (backward) FDAM in coordination with sink type assumptions for exterior points.

However, the absolute stability regions (ASR) for the two methods, namely RK23 and RK45 are also presented in Fig. 5 (Ashino et al., 2000; Butcher, 2016). It is known that the ASR helps to choose step size for with the method will converge. From Fig. 5, one can make understand easily that the ASR obtained from RK45 (actually RK45 in MATLAB suit) have more flexibility on step size. With a large step size, the method returns a good result and if due to the large step size, errors are generated, it is automatically controlled by comparing higher-order methods (Ashino et al., 2000). On the other hand, BoShaRK23 has a relatively smaller ASR, but it can return a relatively good solution for moderately stiff differential equations. It is also to be noted here that our computed ASR for RK45 agrees well with the result presented in the study due to Ashino et al. (2000).

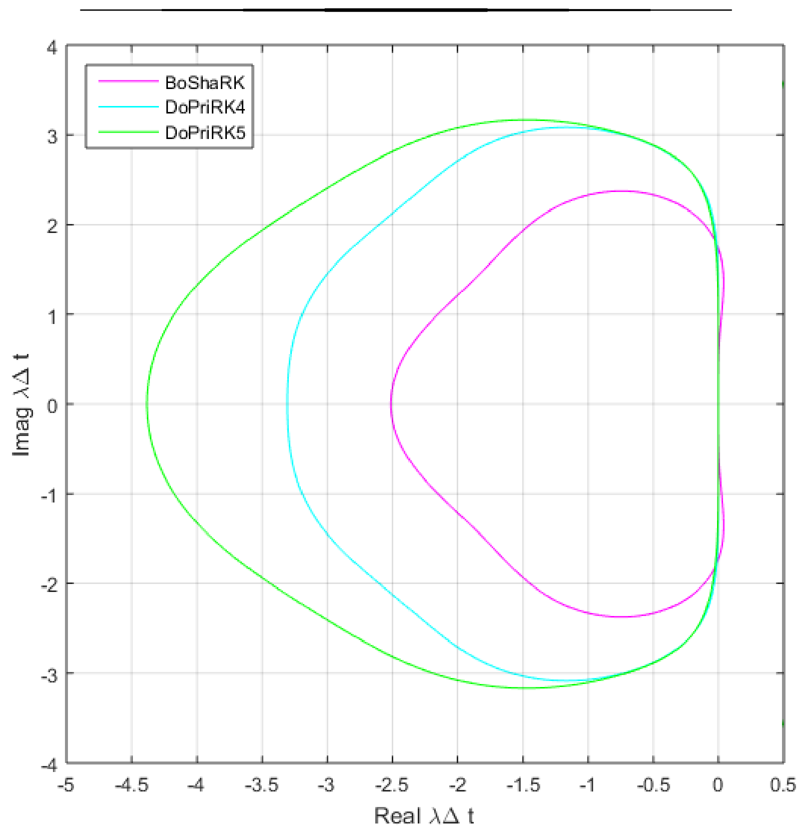

Figure 5: The absolute stability region in the complex xy-plane of two solvers RK23, and RK45.

CONCLUSION

In this study, a one-dimensional heat equation is solved using a higher-order backward finite difference MOLs along with some suitable ODE tools considering a new assumption in the case of exterior points. The computed numerical results obtained are fairly reasonable on the basis of the RMSE values and the computed relative errors. The higher-order backward finite difference MOLs can retain a better result over the higher-order central finite difference MOLs in solving the heat equation and the use of RK23 make the results more finer. This study may help the researchers in getting a more accurate solution of the parabolic equation and thus, the approach can be a suitable alternative in such computation.

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