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Solution of one-dimensional heat equation: An alternative approach

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ABSTRACT

We have revisited the paper of Ahmed and Yaacob [Menemui Matematik 35, 21-29, 2013] if indeed a better solution is found. In fact, in solving the heat equation by the method of lines (MOLs) with five point central difference formula, the assumption used by them at the end points in the case of inhomogeneous boundary constraints due to Hicks and Wei [Journal of the Association for Computing Machinery 14, 549-562, 1967] may invite unrealistic solutions. The problem may be rectified considering the boundaries as sinks. The system of ordinary differential equations (ODEs) having mild stiffness obtained by the mentioned MOLs approach is then solved with four sophisticated ODE solvers. The obtained results in coordination with the Dormand-Prince fourth and fifth order embedded Runge Kutta (RK45) method are found to be in good agreement with the analytical results and found to be more suitable with regard to the central processing unit time, RMSE accuracies, relative error and stability. The new approach is found to be better and efficient in solving one-dimensional heat equation subject to both homogeneous and inhomogeneous boundary conditions.

Keywords: Heat equation, Runge-Kutta method, Method of lines, Mild stiffness, Central difference approximation

INTRODUCTION

According to Tadmor (2012), partial differential equations (PDEs) provide a quantitative description for many central models in physical, biological and social sciences. Several methods have been developed for solving these PDEs analytically and numerically. Great attention has been paid to the later one due to John Von Neumann since 1940. The heat equation which governs the temperature distribution in an object at any time is a parabolic type PDE having a great importance in mathematical physics. In recent years, several tools such as finite difference method, Runge-Kutta method, finite element method, finite volume method, Laplace transform method, Fourier transform method, first recursive marching method, method of lines (MOLs) are developed to solve PDEs numerically. Now a days, in solving PDEs, the MOLs turns attention of researchers for its flexibility on discretization, greater accuracy, less computational cost and stability (see Hicks and Wei, 1967; Schiesser and Griffiths, 2009; Bakodah, 2011 and Paul et. al., 2014).

Typically, the MOLs is a semi-analytic technique, based on the finite difference approximation, to convert PDEs with auxiliary conditions into ordinary differential equations (ODEs) of initial valued discretizing all the variables leaving one continuous (see Hicks and Wei, 1967). The idea of this method was first applied by Erich Rothe in 1930 to parabolic type equations and was further developed by other investigators (see Pregla, 1987; Pregla and Pascher, 1989; Sadiku and Obiozor, 2000).

Traditionally, in the case of the MOLs, 3-point forward, central and backward finite difference approximations are used to discretize the spatial variables of the PDEs. To get an efficient result, 5, 7 and higher point finite difference approximations can be used (see Bakodah, 2011; Ahmad and Yaacob, 2013). But when discretizations are made with higher point central difference approximations, some assumptions must be imposed at some initial points. As for example, in solving heat equation by the MOLs with 5-point central difference approximation, assumption must be adopted at the initiation of first and last lines. In Ahmad and Yaacob (2013), the values were specified at the initial points of the first and last lines through the assumption proposed in Hicks (1967), but that is valid for homogeneous boundary conditions which yield symmetric heat distribution. Our main concentration is to develop a more accurate process to specify the values at the starting point for the end lines to make the solution much more realistic. With this vision, boundaries are treated as sinks, which is possible as they are maintained at the respective temperature of the boundaries. That means the points outside the boundaries will be retained at the corresponding boundary temperature. On the other hand, the ODEs obtained through the 5-point, 7-point or higher point formulae have eigenvalues with negative real parts (see Ahmad and Yaacob, 2013) that ensure the stiffness of the ODEs, which makes an importance to select ODE solvers. But in real observation of numerical procedure, we find the system of ODEs developed from the PDEs through the 5-point central difference approximation is not highly stiff (see Ahmad and Yaacob, 2013). This is also valid for 7-point, 9-point or other higher point finite difference approximations. This gives one the permission to solve the developed equations by the solvers capable of solving both the stiff and non-stiff system. Comparing the obtained results, as will see later, RK45 (Dormand-Prince embedded Runge Kutta) method can be found to work relatively well.

MATERIALS AND METHODS

Problem statement

The one-dimensional heat equation with auxiliary conditions presented in Ahmad and Yaacob (2013) can be put to the form:

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{\partial^2 u}{\partial x^2}; \qquad 0 < x < 1;\ t > 0, \tag{1}$$

subject to the initial condition

$$u(x,\ t=0) = 70^o C, \tag{2}$$

and with the boundary conditions

$$u(x=0,\ t) = 50^o C, \tag{3}$$

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

The above problem can be stated as - a rod composed of any material of unit length with a limiting cross sectional area having the thermal diffusivity α is heated with temperature given by Eq. (2) and the boundary conditions is set according to Eqs. (3) and (4) such that the temperatures at the end points remain fixed at the specified temperatures. The rod is then raped with an insulator except the boundaries. Here $u(x, t)$ is a function of x and t that describes the distribution of temperature in a space over time in the rod.

Discretization

In this paper, we have used the 5-point central finite difference approximation to semidiscretize Eq. (1). With this view, choosing a mesh size in the given interval to explain the domain through some node points, we introduced an integer $m > 0$ such that $x_j = jh;\ j = 0, 1, 2, 3, ..., m$ with $h = \frac{1}{m}$.

For the discretization of the equation, we have used the principle of Taylor series with central-finite difference approximation that returns the spatial derivative $\frac{\partial^2 u}{\partial x^2}$ in discretized form as Chapra and Canale (1998)

$$\frac{\partial^2 u}{\partial x^2} = \frac{-u(x_{j+2}, t) + 16u(x_{j+1}, t) - 30u(x_j, t) + 16u(x_{j-1}, t) - u(x_{j-2}, t)}{12h^2} + O(h^4); \tag{5}$$

for $j = 1, 2, ..., m-1$.

Now, invoking Eq. (5) in Eq. (1), it is simplified to the form

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{-u(x_{j+2}, t) + 16u(x_{j+1}, t) - 30u(x_j, t) + 16u(x_{j-1}, t) - u(x_{j-2}, t)}{12h^2} + O(h^4). \tag{6}$$

Introducing a notational representation, $u(x_j, t) = u_j(t)$, the 5-point central-finite difference approximation for Eq. (1) may be formulated as Chapra and Canale (1998)

$$u'(t) \approx \alpha^2 \frac{-u_{j+2}(t) + 16u_{j+1}(t) - 30u_j(t) + 16u_{j-1}(t) - u_{j-2}(t)}{12h^2}. \tag{7}$$

Also the initial and the boundary conditions can be rewritten to the forms $u_j(t=0) = 70^o C$, (initial temperature) $u_0(t) = 50^o C$ (left boundary temperature) and $u_m(t) = 20^o C$ (right boundary temperature), respectively. Then Eq. (7) can be treated as a set of first order ODEs of initial valued with t as independent variable with the set of initial conditions $u_j(t=0) = 70^o C$.

Integration procedure

The system of ODEs specified by Eq. (7) with the mentioned initial conditions can be solved using any sophisticated solvers capable of solving the equations having mildly stiffness. But the first and last ODEs of the system given by Eq. (7) involve one point (starting point) each outside the boundary. Thus some assumptions must be adopted for those points. With the view to rectifying this problem found in Ahmad and Yaacob (2013), boundaries are assumed to be sinked in that the temperatures outside the boundaries will be the same like their boundaries, i.e., if any temperatures are distributed on the points, sinking the temperatures they will be carried out to the boundary temperature. In this study, the obtained ODEs are solved by the classical Runge-Kutta (RK4) method, third order (stage) arithmetic mean Runge-Kutta (RKAM3) method (see Ahmad and Yaacob, 2013), Dormand-Prince fourth and fifth order embedded Runge Kutta method (RK45), and Bogacki-Shampine Runge-Kutta second order embedded method with third order error control(RK23) method. The choices of the methods are made due to their capabilities of solving IVPs with mildly stiffness. It is of interest to note here that the equations given by Eq. (7) are mildly stiff (see Ahmad and Yaacob, 2013). For the validation of our computed results, they are compared with the analytic results, later we will see, by the method of separation of variables through the software Maple 17. We used the Matlab solvers as well as our own codes for solving the obtained system of ODEs specified by Eq. (7). In both cases the results were found to be the same. The same problem stated in problem statement subsection is also solved in coordination with homogeneous boundary conditions with boundary temperature $20^o C$ each. All the representative results of our calculations are depicted in diagrammatic forms and sometimes in tabular form for convenience.

RESULTS AND DISCUSSION

Figures 1-4 depict our computed results for both inhomogeneous and homogeneous boundaries in coordination with the solvers mentioned above (RK4, RKAM3, RK45 and RK23). The results through the assumptions made in Ahmad and Yaacob (2013) are also presented in the figures (right panel). In our calculations no instabilities were obtained in both the cases of interest, whereas in the inhomogeneous case the results obtained by the assumption adopted in Ahmad and Yaacob (2013) are found to be inconsistent, which can be clarified from the figures (Figs. 1-4). It can be inferred from the figures that the obtained results by the present study in both the cases of interest compared well with the exact results over the results obtained through the assumption made in Ahmad and Yaacob (2013).

It is to be noted down here that in the depicted results, the programs were run for 99 lines with the time step $\Delta t = \frac{0.3}{25000}$ and the temperature distribution only for some times are displayed for the sake of brevity and the final result ($t = 0.3$) and a result prior to it ($t = 0.15$) are compared with the analytic result obtained from solving the problem with the method of separation of variables through the Maple 17 software. For better understanding of the superiority of our results, the graphical outputs of relative errors with the mentioned methods are presented in Fig. 5 as well as the relative errors obtained through the RK45 and RKAM3 methods for equally spaced 19 lines out of 99 along with analytic solution at time $t = 0.3$ are presented in Table 1. It can be observed from Fig. 5 and Table 1 that the results that came out through our calculation by both the methods (RK45 and RKAM3) have less relative error in comparison with the results obtained with the assumption made in Ahmad and Yaacob (2013). The table for other solvers is omitted due to save space consumption. But they also bear the similar results. It is of interest to note here that we used some other sophisticated ODE solvers for solving the problem, but the used solvers in the study yielded better solutions.

To test the performance of our computed results, the root mean square error (RMSE) analysis was made in both the homogeneous and inhomogeneous fixed boundaries which are presented in Table 2. In both the cases, our results show better performance over the ones obtained through the assumptions made in Ahmad and Yaacob (2013). The performance of the approach adopted in the present study and the one adopted in Ahmad and Yaacob (2013) were also analyzed with reference to the RMSE values for several number of lines in the case of the inhomogeneous boundaries in coordination with the solvers mentioned above. Due to the shake of brevity the results through the RK45 method are presented only in Table 3. It is to be noted here that the outputs through the use of the other solvers bear about the same meaning. It can be inferred from Table 3 that the performance of the approach adopted in the present study increases with the increase in number of lines, which is conflicted by the approach adopted in Ahmad and Yaacob (2013) and in each case of the considered number of lines, the present study can be found to perform well over the approach of the revisited paper.

To test computational efficiency, the results were calculated on the same computer for the same number of lines with the same time step using all the assumed methods in the case of inhomogeneous boundaries and are presented in Table 4. It is seen from Table 4 that the present study needs less computing time. The same result bears for the problem with homogeneous boundaries and is not shown for the similar reason mentioned above.

We also computed our results solving the equation by the MOLs using the 3-point central difference approximation in coordination with the used solvers. Due to avoiding the space consumption, RMSE values obtained by the RK45 solver are only presented in Table 5. Comparison of these RMSE values show that the present study has a better performance with the increase of the number of lines as it is to be expected whereas that of the results using the 3-point central difference approximation method fluctuate with the increase in number of lines.

The problem with inhomogeneous boundaries applying initial temperature distribution to the rod through space dependent initial condition $\sin(x)$ was also solved by the solvers of interest. Again, due to a similar reason mentioned above, the graphical outputs by only the solvers, RK45 and RKAM3 in comparison with the results obtained through the assumption adopted in Ahmad and Yaacob (2013) are presented in Fig. 6, whereas all of the remaining methods bear about the same results. The figure clearly shows that the approach adopted in the study is better over the one adopted in Ahmad and Yaacob (2013).

We have also examined the performance of all the four solvers in solving our problems with regard to the RMSE values. In all the cases RK45 showed better performance [see Tables 2, 4]. It is to be noted down here that all of the results presented above are taken considering same lines except the two boundary lines as the temperature at them are always retained at the boundary temperature. Thus the present study in coordination with the RK45 seems to yield more effective solutions in all the regards, namely computational stability, relative error, computational cost and efficiency in solving heat equation in both the inhomogeneous and homogeneous boundaries with the assumptions proposed in the present study.

The absolute stability regions (ASR) for the methods (RK4, RKAM3, RK23 and RK45) are also estimated and presented in Fig. 7 (see Ashino et al. 2000; Butcher, 2016). It is known that ASR helps to choose step size for which the method will converge. From Fig. 7, one can make understand easily that ASR obtained from RK45 (ode45 in MATLAB suit) is more flexible over the mentioned solvers in choosing step size in the case of the present study. With a large step size, the method returns a good results and if error is generated due to the use of large step size, it will be automatically controlled by comparing higher order method (see Ashino et al., 2000). It is also to be mentioned in this juncture that our computed ASR for RK45 agrees well with that presented in Ashino et al. (2000). As Ahmad and Yaacob (2013), the obtained system of ODEs represented by Eq. 7 is mildly stiff. RK45 embedded scheme can be found to mitigate the stiffness properly. Therefore, the use of the RK45 method may be a good choice for solving the system of mentioned ODEs. Table 2 also reflects the same meaning.

We have also conducted the study with higher order finite difference approximations, namely 7-point and 11-point and the results were found to be consistent with the ones presented in the case of the 5-point central difference approximation. In this study we do not use time dependent boundary but it may be a future study.

CONCLUSION

In this paper, we have solved one-dimensional heat equation with a new approach, the MOLs in addition with some suitable RK methods, where discretization is made with higher point central difference approximation. As a test case the 5-point central difference approximation is used. New assumptions are made to remove the boundary constraints arising when discretizing the equation by the 5-point central difference approximation, which is valid for other higher point central difference approximations. The obtained results in coordination with the RK45 solver are found to be in good agreement with the analytical results and found to be more suitable with regard to the central processing unit time, RMSE accuracies, relative error and stability. The outcome of the study can be expanded in the study of fluid dynamics, electrodynamics, heat conduction system, etc.

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Table 1: The analytic result and relative errors.

Domain	Analytic result	Relative errors			
		Results with the present study		Results by the method adopted in Ahmad and Yaacob (2013)	
		RK45	RKAM3	RK45	RKAM3
$x = 0.05$	56.32660678	0.00092599	0.00048054	0.13129487	0.13150430
$x = 0.10$	59.16830556	0.00084422	0.00002044	0.10095766	0.10155624
$x = 0.15$	61.66119839	0.00070639	0.00034074	0.07628174	0.07675606
$x = 0.20$	63.74137018	0.0006268	0.0005976	0.05583074	0.05676340
$x = 0.25$	65.37326488	0.00047818	0.00076258	0.04054282	0.04108319
$x = 0.30$	66.54101634	0.00043546	0.00086132	0.02806579	0.02915496
$x = 0.35$	66.54101634	0.0003141	0.00092681	0.01986006	0.02041474
$x = 0.40$	67.23532910	0.00033508	0.00099294	0.01306919	0.01433803
$x = 0.45$	67.43895153	0.00027136	0.00108794	0.00973681	0.01047043
$x = 0.50$	67.11416494	0.00037748	0.00122849	0.00678086	0.00845039
$x = 0.55$	66.19552904	0.00039907	0.00141504	0.00679778	0.00802668
$x = 0.60$	64.59042211	0.00061085	0.00162902	0.00671944	0.00907360
$x = 0.65$	62.18870917	0.00074753	0.00183206	0.00960865	0.01160978
$x = 0.70$	58.88118426	0.00109026	0.00196647	0.01267476	0.01583108
$x = 0.75$	54.58440226	0.00138299	0.00195552	0.01941325	0.02217783
$x = 0.80$	49.26750138	0.00190442	0.00170036	0.02781413	0.03147681
$x = 0.85$	42.9751957	0.00244343	0.00106796	0.04224974	0.04525206
$x = 0.90$	35.84092088	0.0032905	0.00014457	0.06328147	0.06645897
$x = 0.95$	28.08555431	0.00440216	0.00231401	0.09963727	0.10146443

Table 2: The RMSE values by the RK45 solver for different number of lines in the case of the inhomogeneous and homogeneous boundaries

Inhomogeneous boundary		
Solver	Result by the present study	Result by the method adopted in Ahmad and Yaacob (2013)
RK4	0.072082699	2.985070416
RKAM3	0.072075371	2.985067105
RK45	0.063602016	2.943050056
RK23	0.069912257	2.943050056
Homogeneous boundary		
RK4	0.098542723	1.640816879
RKAM3	0.098532711	1.640809389
RK45	0.083905329	1.546338837
RK23	0.094474273	1.546115966

Table 3: The RMSE values obtained by the RK45 solver for the inhomogeneous boundary condition in both cases of interest

Number of lines	Result by the present study	Result by the method adopted in Ahmad and Yaacob (2013)
N=49	0.126551992	2.842503488
N=99	0.063602016	2.943050056
N=199	0.031960961	2.993426858
N=499	0.013592306	3.023711283
N=799	0.008204899	3.031293953
N=999	0.007245730	3.033814169

Table 4: Computational costs (in second) for solving the problem with the inhomogeneous boundaries obtained by the adopted solvers along with the method adopted in Ahmad and Yaacob (2013)

Solver	Result by the present study	Result by the method adopted in Ahmad and Yaacob (2013)
RK4	172.9319	173.7571
RKAM3	164.5327	164.9230
RK45	10.31987	10.52753
RK23	10.38126	10.54278

Table 5: Comparison of the RMSE values in the case of the inhomogeneous problem between the results through the 3-point and 5-point formulae using the RK45 solver

Number of lines	3-point formula	5-point formula
N=49	0.019992	0.126552
N=99	0.023333	0.063602
N=499	0.014744	0.013592
N=699	0.002316	0.009247
N=799	0.006751	0.008205
N=999	0.011508	0.007246

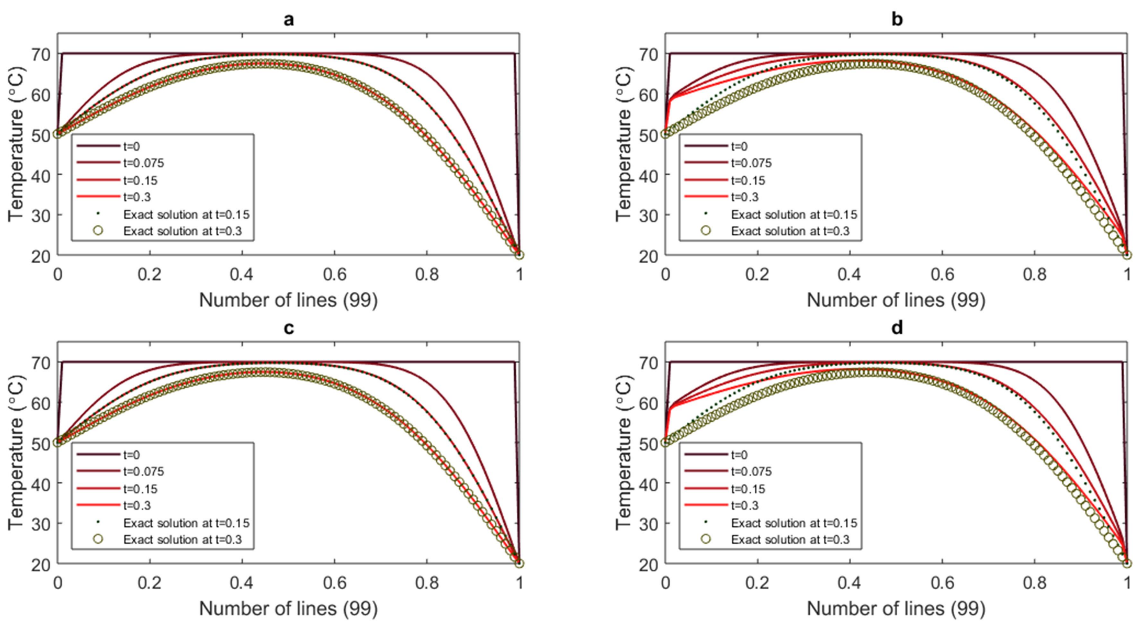

Figure 1: The graphical outputs for the inhomogeneous boundaries with the RK4 and RKAM3 solvers; (a) representation due to the present study using RK4; (b) representation due to the assumption made in Ahmad and Yaacob (2013) using RK4; (c) representation due to the present study using RKAM3; (d) representation due to the assumption made in Ahmad and Yaacob (2013) using RKAM3

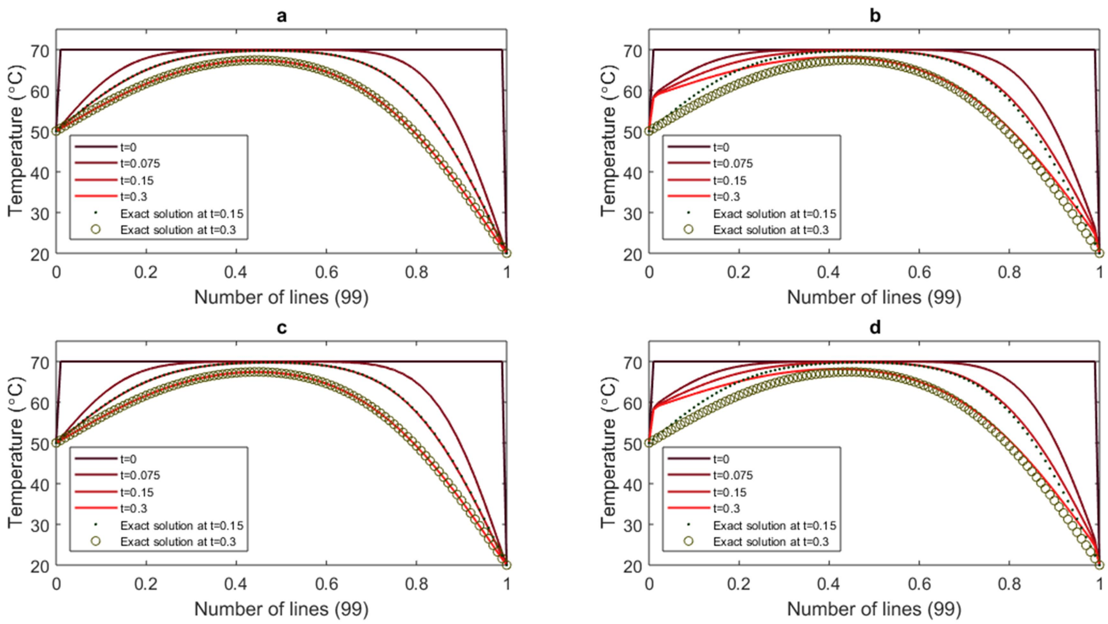

Figure 2: The graphical outputs for the inhomogeneous boundaries with the RK45 and RK23 solvers; (a) representation due to the present study using RK45; (b) representation due to the assumption made in Ahmad and Yaacob (2013) using RK45; (c) representation due to the present study using RK23; (d) representation due to the assumption made in Ahmad and Yaacob (2013) using RK23

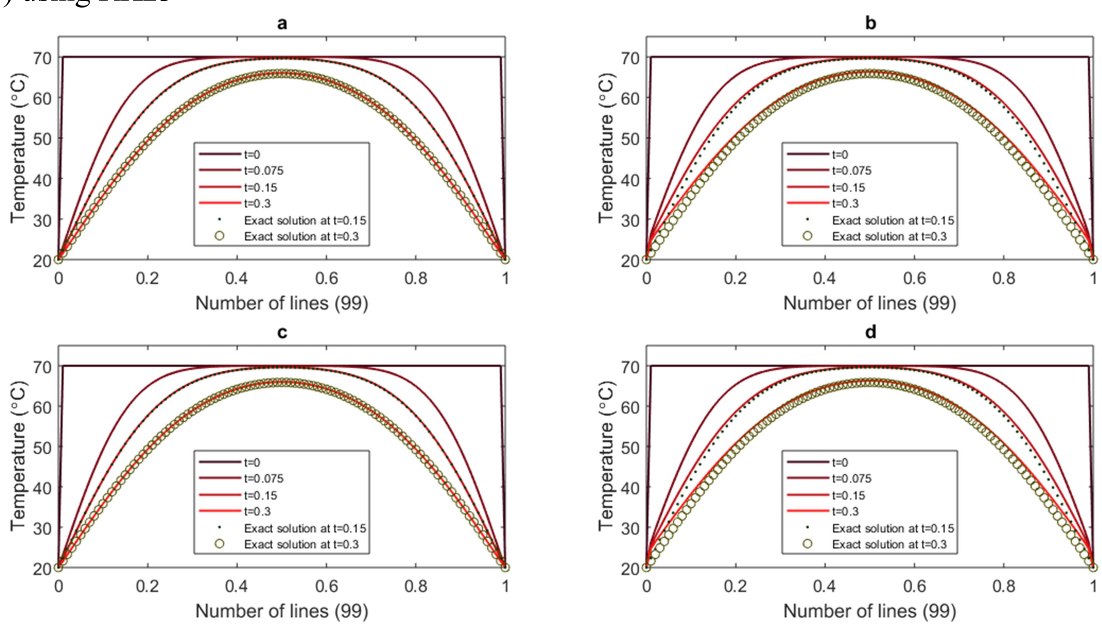

Figure 3: The graphical outputs for the homogeneous boundaries with the RK4 and RKAM3 solvers; (a) representation due to the present study using RK4; (b) representation due to the assumption made in Ahmad and Yaacob (2013) using RK4; (c) representation due to the present study using RKAM3; (d) representation due to the assumption made in Ahmad and Yaacob (2013) using RKAM3

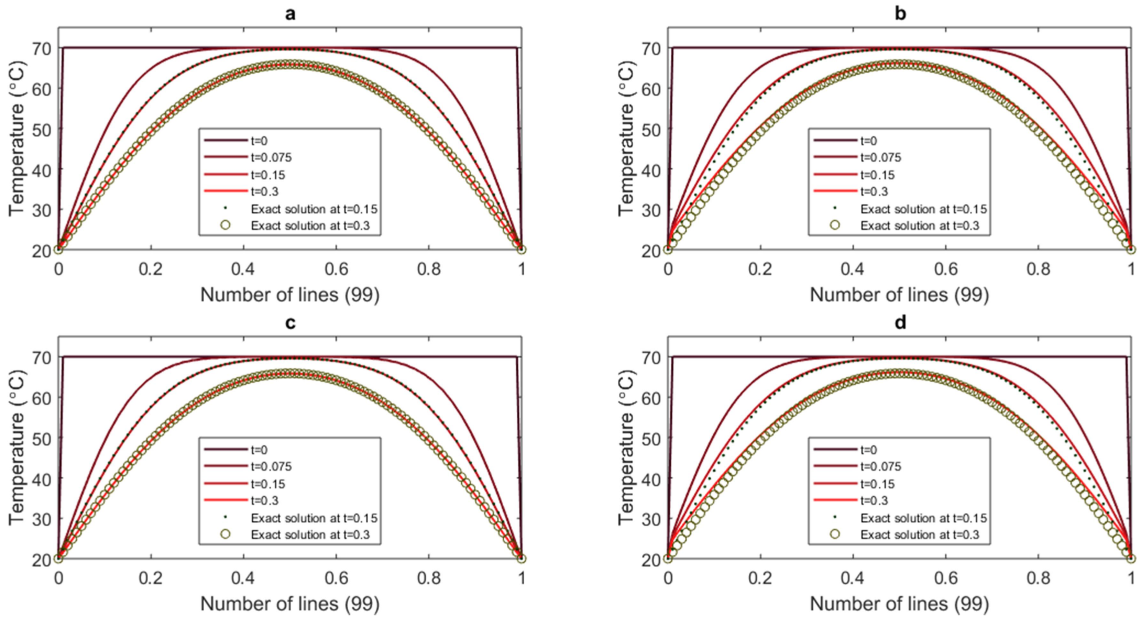

Figure 4: The graphical outputs for the homogeneous boundaries with the RK4 and RKAM3 solvers; (a) representation due to the present study using RK45; (b) representation due to the assumption made in Ahmad and Yaacob (2013) using RK45; (c) representation due to the present study using RK23; (d) representation due to the assumption made in Ahmad and Yaacob (2013) using RK23

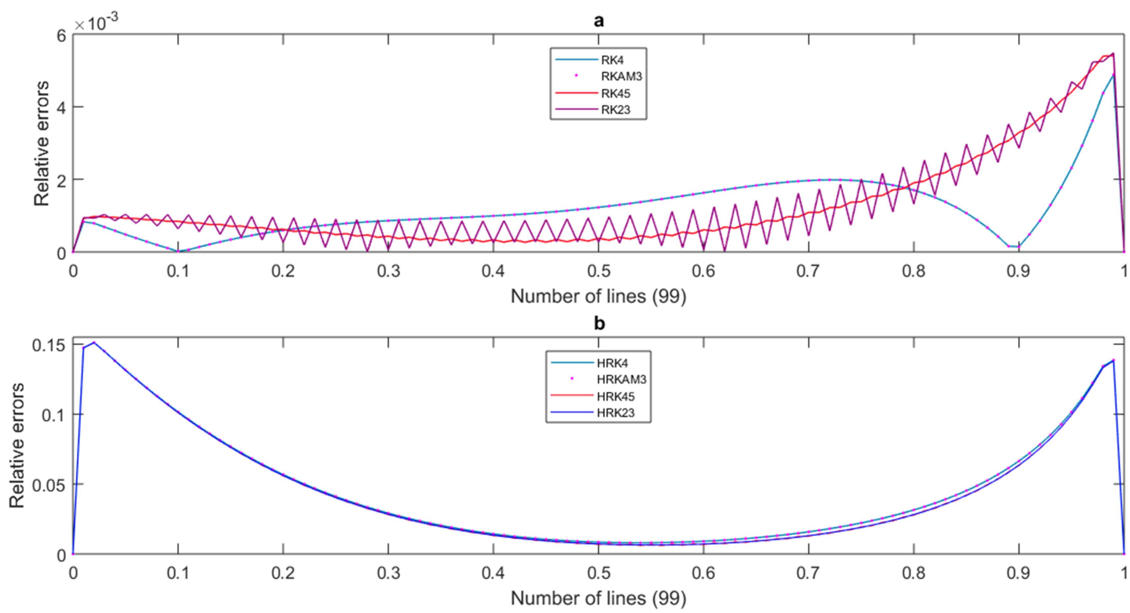

Figure 5: The graphical outputs of relative errors for the inhomogeneous boundaries for the used solvers; (a) due to the present study; (b) representation due to the results through the assumption made in Ahmad and Yaacob (2013)

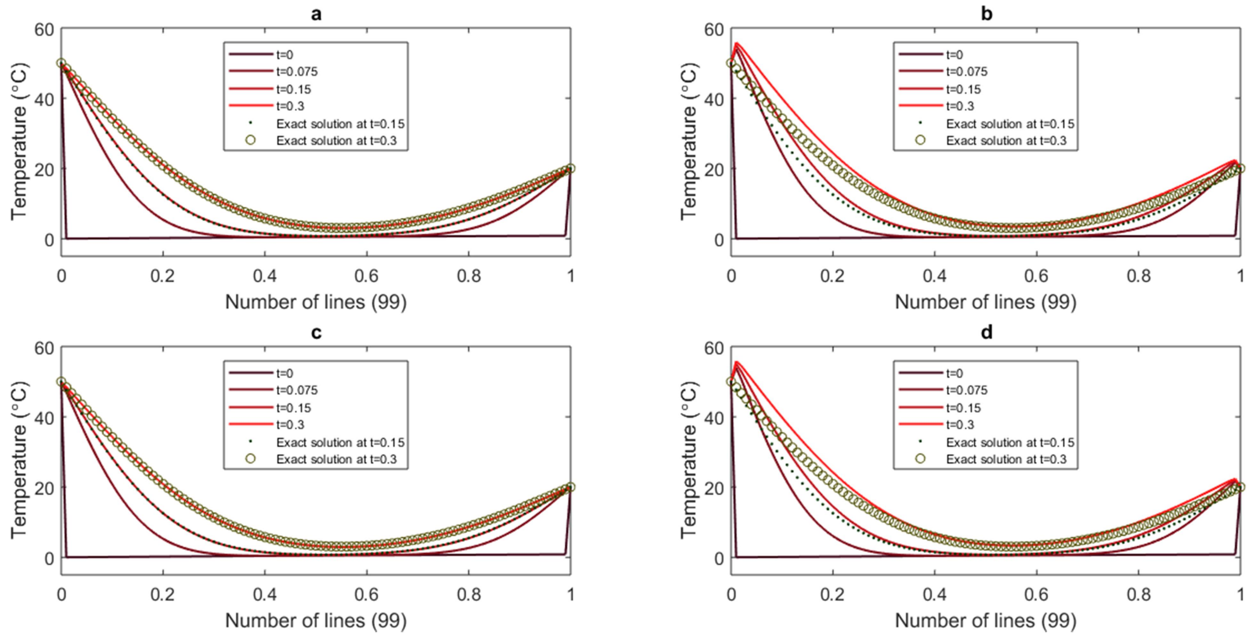

Figure 6: The graphical outputs for the inhomogeneous boundaries treating variable initial condition with the RK45 and RKAM3 solvers; (a) representation due to the present study using the RK45 solver; (b) representation due to the assumption made in Ahmad and Yaacob (2013) using the RK45 solver; (c) representation due to present study using the RKAM3 solver; (d) representation due to the assumption made in Ahmad and Yaacob (2013) using the RKAM3 solver

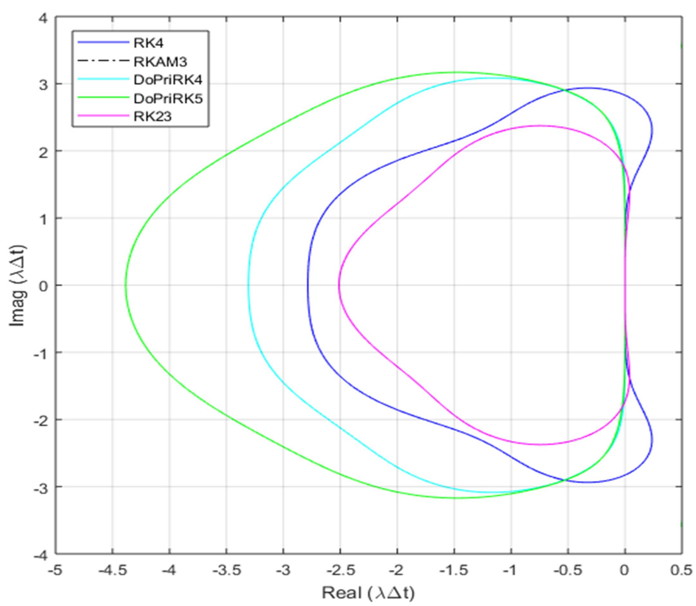

Figure 7: The absolute stability region in complex xy-plane of ODE solvers