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Method of Lines and Runge-Kutta Method in Solving Partial Differential Equation for Heat Equation

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Abstract: Solving the differential equation for Newton's cooling law mostly consists of several fragments formed during a long time to solve the equation. However, the stiff type problems seem cannot be solved efficiently via some of these methods. This research will try to overcome such problems and compare results from two classes of numerical methods for heat equation problems. The heat or diffusion equation, an example of parabolic equations, is classified into Partial Differential Equations. Two classes of numerical methods which are Method of Lines and Runge-Kutta will be performed and discussed. The development, analysis and implementation have been made using the Matlab language, which the graphs exhibited to highlight the accuracy and efficiency of the numerical methods. From the solution of the equations, it showed that better accuracy is achieved through the new combined method by Method of Lines and Runge-Kutta method.

Keywords: Heat equation, Partial differential equation, Runge-Kutta method, Method of Lines

1. Introduction

The numerical solution for Newton's cooling law is a long and old topic. Newton's cooling law, written in differential equation from have been devised over the years to solve such equations, and surprisingly, the old well-established methods such as the Runge-Kutta methods are still the foundation for the most effective and widely-used codes [1]. Nevertheless, there are several kinds of problems that numerical methods cannot handle effectively, which are said to be stiff. Stiff differential equations are categorized as those whose solutions or different components of a single solution evolve on very different time scales occurring simultaneously [2]. Consider, if one component of the solution has a term of the form where is a large negative value. This component, which is called the transient solution, decays to zero much more rapidly, as increases, than other slower components of the solutions. Alternatively, consider a case where a component of the solution oscillates rapidly on a time scale much shorter than that associated with the other solution components.

For a numerical method that makes use of derivative values, the fast component continues to influence the solution. As consequence, the selection of the step size in the numerical solution is problematic. This is because the required step size is governed not only by the behaviour of the solution but also by that of the rapidly varying transient which does not persist in the solution that is being monitored. The numerical values occurring in nature are frequently such as to cause stiffness [3,4]. Therefore, a realistic representation of a natural system using a differential equation is likely to encounter this phenomenon. An example is the field of chemical kinetics. Ordinary differential equations (ODEs) describe in this field is a reaction of various chemical species to form other species. The stiffness in such systems is a consequence of the fact that different reactions take place on vastly different time scales.

Another important class of stiff ODEs originates from the application of the general approach the Method of Lines (MoL) to stiff time-dependent Partial Differential Equations (PDE). In this method, the PDEs

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system is first spatially discretized, which results in a stiff coupled system of ODEs in time only. Then, any well-established numerical method is applied to achieve an accurate approximate solution to the problem [5]. Two broadly applicable techniques include Finite Difference, which is local methods and Spectral Methods, which are global methods.

For this research, the MoL is applied to approximate the parabolic type of PDE problem to reduce it to simpler ODEs. The parabolic PDE, which is a diffusion type equation, namely heat equation, produced a system of an ODE. This system of ODEs is then represented in matrix form which, eigenvalues will be calculated. Therefore, a typical purpose of this research is to propose an efficient numerical method for the numerical solution of stiff PDE in heat problem. This research is carried out such that the resulting numerical methods will not be time and cost consuming anymore.

2. Previous Works

Mechanical, chemical, economic, financial systems, even natural environment can be described at a macroscopic level by a set of PDEs governing averaged quantities such as density, temperature, concentration, velocity and so on [6]. The field of PDEs is broad and varied, as is inevitable because of the great diversity of physical phenomena that these equations model. Much of the variety is introduced by the fact that practical problems involve different geometric classifications such as hyperbolic, elliptic or parabolic; multiple space dimensions, systems of PDEs, different types of boundary conditions, varying smoothness of the initial conditions, variable coefficients and frequently, nonlinearity [7]. The earliest detection of stiffness in DEs is around 1950s, during the earlier digital computer by the two chemists, Curtiss and Hirschfelder [8]. They named the phenomenon and spotted the nature of stiffness (stability requirement dictates the choice of the step size be very small). At about this time several mathematician and physicists participated in independent research for handling and evading the problems posed by stiff DEs [9].

Considerable efforts have gone into developing numerical integration for stiff problems, and hence, the problem of stiffness was brought to the attention of the mathematical and computer science community. The idea of using spectral representations for numerical solutions of ODEs goes back at least to Lanczos in 1938 [10]. Spectral methods are a class of techniques used in applied mathematics and scientific computing to numerically solve certain PDEs, often involve the use of Fast Fourier Transform (FFT) [11]. The spectral methods have been widely used for spatial discretization in the context of solving time dependent PDEs since the early 1970s [12-14].

Given that stiffness has extensive practical applications and arises in many physical situations, the demand for special techniques that permit the use of a step size governed by the rate of change of the overall solution is very great [15]. However, even though numerical integrations of stiff systems with constant coefficients have been considered in detail, a stiff DE does not lend itself readily to numerical solution by classical methods. In principle, the stability region of the integration method must include the eigenvalues of the discrete linear operator of a stiff PDE to be stable [16].

However, discretization of a nonlinear PDE leads to a large nonlinear system of equations that must be solved at each time step. This renders implicit schemes costly to implement. Various methods have been proposed to avoid the difficulties that appear when trying to solve nonlinear equations with an implicit method [17]. A popular strategy is to combine pairs of an explicit multistep formula to advance the nonlinear part of the problem and an implicit method to advance the linear part. This strategy forms the basis of the so-called Implicit-Explicit (I-E) schemes. These schemes were proposed to solve stiff PDEs late 1970’s. Other more complicated forms of the I-E schemes such as the Runge-Kutta method [18].

Most of the research focuses on the accuracy and stability of the numerical methods. The system of ODEs obtained from the semi-discretization of PDEs is usually stiff and expensive to solve. Thus, the MOL has been proposed to fulfil the needs, which is so far the most flexible method in spatial discretization to approximate the PDEs into a system of ODEs.

3. Method of Solution

Differential equations are the most common and important mathematical models in science and engineering. Many phenomena in nature may be described mathematically by independent variables and parameters. Given by a function of position and time, typical PDEs arises if one studies the flow quantities like density, concentration, heat and so on.

3.1 Heat Equation

The study of heat problems started in the 18th century. Many researchers have been published numerical methods for heat problems. However, the comparison of these methods is usually restricted to the analysis of the stability of the schemes used. The parabolic type of PDEs, which is a diffusion equation and known as the heat equation, is used as an example of stiff problems in this research. Parabolic problems describe evolutionary phenomena that lead to a steady state described by an elliptic equation. In this research, we will solve the following PDEs, which known as one dimensional heat equation.

$$\frac{\partial u}{\partial t} = \alpha^2 \frac{\partial^2 u}{\partial x^2} \quad \text{for} \quad 0 < x < 1 \tag{1}$$

3.2 Method of Lines

The Method of Lines (MoL) is a technique that enables the conversion of PDEs into sets of ODEs that are equivalent to the former PDEs. The basic idea behind the MoL methodology is discretized along with the spatial coordinates only, this approximation is what we called semi-discretization. If discretize in space and leave time continuous, a system of ODEs obtained. The focus of the MoL is the calculation of accurate numerical solutions. Thus, one of the salient features of the MoL is the use of existing and generally well-established numerical methods for ODEs. The derivative of the PDEs heat problem is approximated by a linear combination of function values at the structured grid points. Arbitrary order approximations can be derived from a Taylor series expansion.

$$u(x)=\sum_{n=0}^{\infty}\frac{(x-x_i)^n}{n!}\left(\frac{\partial^n u}{\partial x^n}\right) \tag{2}$$

A geometric interpretation of the different equations is shown in Fig. 1. The derivative for the function of x can be approximated in many ways. The most common are called the forward, backward and central approximation, all of which are drawn and indicated on Fig. 1.

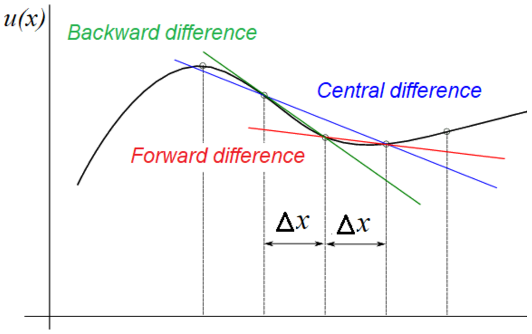

Fig. 1 – Geometric interpretations of the first-order finite difference approximation related to central difference approximation

It is important to use the same order of approximation accuracy for the discretization in space as for the discretization in time achieved by the numerical integration algorithm. Thus, to integrate the set of ODEs with a 4th order method, 4th order accurate discretization formula is needed in the discretization of u_{xx}.

3.3 Runge-Kutta Method

System of ODEs can be obtained by discretize the equation in space and leave time continuously. The system can be solved by a standard method, Runge-Kutta method. Currently, there are two general ways to solve stiff PDEs numerically. The first approach is based on implicit methods and the second uses explicit stabilized Runge-Kutta methods. Implicit methods are great for very stiff problems of not very large dimensions, while stabilized explicit methods are efficient for very big systems of not very large stiffness and real spectrum.

The Runge-Kutta method is single-step methods, however with multiple stages per step. They are motivated by the dependence of the Taylor methods on the specific initial value problem. These new methods do not require derivatives of the right-hand side function and are therefore general-purpose initial value problem solvers. For this research, the 3rd order Runge-Kutta method was used to solve the ODEs system for heat equation. The new 3rd order Runge-Kutta method is developed to pair with the MoL in the attempt to solve the stiff problems that arises in heat problem.

$$\begin{aligned}
k_1 &= f(x, y_n)\\
k_2 &= f(x+c_1h, y_n+a_1hk_1)\\
k_3 &= f(x+c_2h, y_n+a_2hk_1+a_3hk_2)\\
y_{n+1} &= y_n+\frac{h}{4}(b_1k_1+\ldots+b_nk_n)
\end{aligned} \tag{3}$$

where,

$$a_1=\frac{2-\sqrt{2}}{3},\quad a_2=a_3=\frac{1}{6}$$
$$b_1=4+3\sqrt{2},\quad b_2=-3\left(4+3\sqrt{2}\right),\quad b_3=6\left(2+\sqrt{2}\right)$$
$$c_1=\frac{2-\sqrt{2}}{3},\quad c_2=\frac{1}{3}$$

The equation (3) are known as the stages of the Runge-Kutta method, correspond to the different estimates for the slope of the solution.

4. Results and Discussion

Numerical methods used to solve mathematical models should be robust. It should be reliable and give accurate values for a large range of parameter values. Sometimes, however, a method may fail and give unexpected results. Then it is important to know how to investigate why an erroneous result has occurred and how it can be remedied. In this section, the results and discussion on the stability analysis of the model will be presented.

4.1 Stability Analysis

The stability analysis of the MoL for PDEs represents the most important factor for their solutions and at the same time is a critical factor that should be handled carefully. The importance lies in its unique ability to judge acceptable solution for the given equation, of being critical is due to its dependence on the nature of the eigenvalues of the matrix representation connection with their number. The stability analysis constitutes the essential study of the numerical solution of PDEs, in general, this is because such study provides the means by which the step size and the numerical integration scheme for the given DEs could be selected so as to secure manageable numerical solution. Regarding the MoL for parabolic PDE in two variables, it can be classified according to the nature of the resulting system in connection with the direction of discretization as shown in Table 1.

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Table 1 – Nature of system in connection with the direction of discretization

Discretization direction	Nature of the resulting system
x - direction	Boundary type in ODEs
t - direction	Initial types in ODEs

To analyze the stability of equation (1), the spatial derivative should be replaced. By choose five-point difference approximations for the second derivative, submit these derivatives into equation (1) will give the ODEs that must be integrated numerically at the spatial grid points. Note that all negative eigenvalues given by equation (1) have negative real parts, which mean that the system of first-order ODEs is stable.

4.2 Testing Case

The Finite Different, MoL and Explicit Runge-Kutta schemes was implemented for solving the heat equation by using Matlab. By simulation of the Matlab code gave the results as shown in Fig. 2 to Fig 5., which shows the behaviour of the numerical solutions for the heat problems from the collaboration of MoL and Explicit Runge-Kutta schemes.

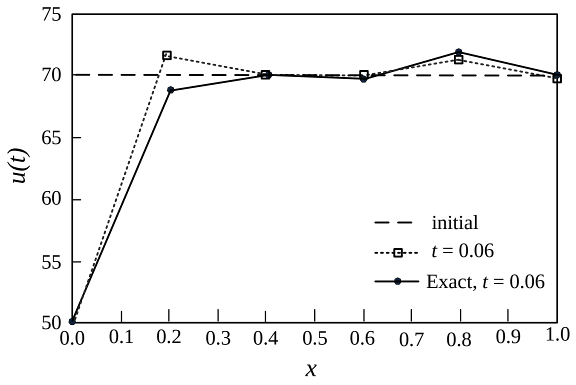

Fig. 2 – The graph of the MoL + Explicit Runge-Kutta method at *Δx*=0.2 and *Δt*=0.06

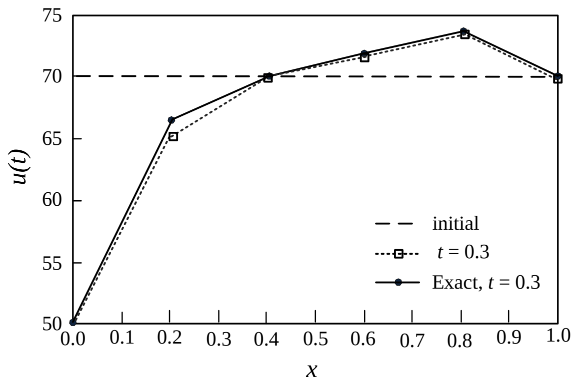

Fig. 3 – The graph of the MoL + Explicit Runge-Kutta method at *Δx*=0.2 and *Δt*=0.3

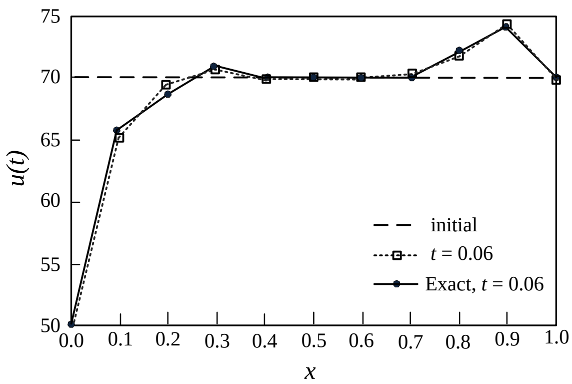

Fig. 4 – The graph of the MoL + Explicit Runge-Kutta method at *Δx*=0.1 and *Δt*=0.06

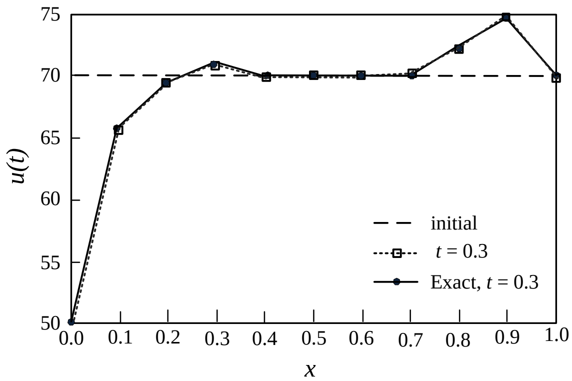

Fig. 5 – The graph of the MoL + Explicit Runge-Kutta method at *Δx*=0.1 and *Δt*=0.3

From the figures, it shows that the combination of the MoL and Explicit Runge-Kutta method loses a few points at $\Delta x = 0.2$ but gains back the accuracy at the other points. Showing that finer mesh typically results in a more accurate solution. So, we can say that, as we decrease the space mesh size and time step size, the solution converges to the exact solution.

5. Conclusion

This research deals with two methods which are combined to combat stiffness occurred in the PDEs. The first method is the MoL, which are used to transform the PDEs into a system of ODEs through semidiscretization on the spatial variable. The second method is the explicit Runge-Kutta method of order three, which is applied in the final step in completing the task to crack the stiff problem. Theoretical analysis by earlier research showing that the mathematical model been solved using finite difference method. The result obtained showed that a better accuracy is achieved through the new combined method, MoL and explicit Runge-Kutta. The development, analysis and implementation have been made using the Matlab language, which the graphs exhibited to highlight the accuracy and efficiency of the numerical methods.

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Even though the combination of the five-point MoLs and explicit Runge-Kutta of order three shows some loses at the but gains back the accuracy within the rest points along the spatial coordinates. In the previous chapter, we showed that the MoL and explicit Runge-Kutta method has significant advantages to solve PDEs. The combination of five-point MoL and the explicit Runge-Kutta method brings a new finding that it works better if to be compared to the finite difference method.

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