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RESEARCH PAPER

Error Estimation by using Symmetrization and Efficient Implementation Scheme for 3-stage Gauss Method

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Abstract

This research focuses on the implementation strategies by the implicit Runge-Kutta Gauss methods in solving Robertson problem using variable stepsize setting. This research considers ideas of implementation strategies by Hairer and Wanner (HW) and Gonzalez-Pinto, Montijano and Randez (GMR) schemes that uses a certain transformation matrix T to improve the efficiency of the numerical methods. Both implementations use simplified Newton iterations to solve the nonlinear algebraic equations for the implicit methods. These implementation strategies are compared with the modified Hairer and Wanner (MHW) scheme without using any transformation matrix T. The numerical methods considered are the implicit 3-stage Gauss (G3) method of order-6. The numerical results are given for Robertson problem which is a chemical reaction stiff problem. The variable stepsize setting is adapted in Matlab code that estimates the error using symmetrization technique. Based on the numerical experiments, it is observed that GMR scheme is efficient by using the G3 method especially when the error estimation is obtained by using symmetrization technique instead of local extrapolation if compared with other schemes. In conclusion, GMR scheme is seen to be very robust in solving Robertson problem by the G3 method in terms of tolerance and computational time.

Keywords: variable stepsize setting, error estimation, local extrapolation, symmetrization.

INTRODUCTION

In numerical analysis, it is very important to choose a method that satisfy good stability properties and having higher order of convergence rate. Since Runge-Kutta (RK) methods complies with these properties, thus a method such as Gauss methods are particularly being chosen because of their advantages that suitable in solving stiff systems. This is also due to sufficiently high stage and classical orders. Even though the computational cost for Gauss methods are relatively high, however the methods provide better solution of same accuracy as the order of the implicit Runge-Kutta (IRK) methods. The study showed that the methods numerically integrate various sorts of

ODEs such as non-stiff and stiff problems, Hamiltonian systems and invertible equations.

Generally, the approximate solution obtained by an *s*-stage RK methods with stepsize h for the interval $\left[x_0, x_n\right]$ can be defined by the following equations (Butcher, 2016):

$$\begin{aligned} Y^{[n]} &= e \otimes y_{n-1} + h\left(A \otimes I_N\right) F\left(x_{n-1} + ch, Y^{[n]}\right), \\ y_n &= y_{n-1} + h\left(b^T \otimes I_N\right) F\left(x_{n-1} + ch, Y^{[n]}\right), \\ x_n &= x_0 + h, \end{aligned} \tag{1}$$

where $\otimes$ denotes the Kronecker product, $e = (1,...,1)^T$ and I_N is the $N \times N$ identity matrix and y_n is the update of the RK method. y_n will be updated until the approximate solution is obtained for each problem that being tested. Normally the numerical solution is approximated until the desired solution is obtained or until the approximate solution reached the target interval x_n.

González-Pinto et al. (1994) investigated an experiment regarding linear stability of IRK methods. In their research, they proposed a method by Cooper and Butcher (1983) in determining the most efficient method in solving IRK methods. They concluded that the implementation by using Gauss method performs much better than diagonally IRK method (simply denoted as DIRK method) even though both of the methods are categorized as *A*-stable and have the same order 4. Since the Gauss methods having the handicap of solving the implicit system as shown in Eq. 1 during the experiments, however their relatively high stages and good stability properties make them not only competitive but highly recommended to other methods like DIRK methods for the solution of nonlinear stiff problems when implemented using special iterative schemes. In few years later, Hairer and Wanner (1999) proposed an iterative scheme to solve Radau IIA method using a *T* transformation matrix.

This article focuses on the performance of 3-stage Gauss (G3) method by using the implementation schemes suggested by Hairer and Wanner (1999), González-Pinto et al. (1994) and González-Pinto et al. (1995) in solving Robertson problem.

Robertson problem is a chemical reaction problem proposed by Robertson (1966) that describes the kinetics of an autocatalytic reaction. It was known as ROBER problem and consists of a stiff system of three nonlinear ODEs (Hairer & Wanner, 1996). The problem can be written in the following form

$$\frac{dy}{dt} = f\left(y\right), \quad y\left(0\right) = y_0,$$

with

$$y \in \mathbb{R}^3, \quad t \in \left[0, T\right].$$

The function f can also be written in a system as given by

$$\begin{aligned} y_1' &= -0.04 y_1 + 10^4 y_2 y_3 & y_1\left(0\right) &= 1, \\ y_2' &= 0.04 y_1 - 10^4 y_2 y_3 - 3 \cdot 10^7 y_2^2 & y_2\left(0\right) &= 0, \\ y_3' &= 3 \cdot 10^7 y_2^2 & y_3\left(0\right) &= 0. \end{aligned} \tag{2}$$

Since past decade, the ROBER problem became very popular among mathematicians for the numerical studies and is favorable to be used as a test problem for the solution of stiff systems. Originally, the problem was posed on the time interval $0 \le t \le 40$, but it is reasonable to integrate on much longer intervals in determining their stability and efficiency. However, Hindmarsh (1980) discovered that many codes fail if the problem is integrated at a longer computational time t. Since Robertson problem is a nonlinear stiff problem, thus a variable stepsize setting is a crucial components that need to be catered in improving the convergence rate and satisfying the efficiency properties. Many researchers such as Xu et al. (2015), Wang et al. (2017) and Yang et al. (2020) implemented the variable stepsize setting in their research and it has been proven to give a robust implementation, thus suitable in solving higher order methods. Since variable stepsize are very useful in getting excellent performance for IRK methods, thus it is favorable to solve the Robertson problem in this research.

MATERIALS AND METHODS/ METHODOLOGY

The IRK methods are expensive and difficult to implement due to the nonlinear equations involved when finding the internal stage derivatives $Y^{[n]}$ and need to be replaced by an iterative computation which is known as Newton-Raphson iteration. The Newton-Raphson iteration for $f(x) = 0$ where $f(x): \mathbb{R}^n \to \mathbb{R}^n$ is given by

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \; f'(x_n) \neq 0. \tag{3}$$

There are two ways to implement Newton-Raphson iterations such as full Newton and simplified Newton. Full Newton iteration is preferred for nonstiff problems as investigated by Muhammad and Gorgey (2018). Since Robertson problem is a stiff problem, thus only simplified Newton is considered throughout the investigation where the variable stepsize setting is used to investigate the performances of G3 method for three different implementation strategies.

As we concern, the variable stepsize setting is very important to be implemented as many researchers are still finding the best way that suitable to solve certain problems either in mathematical, biological, chemical, physical, engineering or in any related fields. Many researchers have used variable stepsize to obtain efficient numerical results. Among them are Gorgey (2016), Wang et al. (2017) and González-Pinto et al. (2020). This shows that the variable stepsize is a crutial component that need to be implemented in order to achieve convergence and satisfy the efficiency behaviour.

Implementation schemes by González-Pinto et al. (1994, 1995) and Hairer and Wanner (1999)

For this research, three different implementation strategies have been investigated. The implementation scheme by González-Pinto et al. (1994, 1995) is denoted by GMR scheme, Hairer and Wanner (1999) is denoted by HW scheme and the last one is denoted by MHW scheme which refers to modified HW scheme. The difference between HW and MHW scheme is that no transformation such that

$(hA)^{-1} \otimes I_N$, $S = T^{-1}A^{-1}T$ and $W^{[n]} = \left(T^{-1} \otimes I_N\right)Z^{[n]}$ is applied to MHW scheme. The HW scheme is specially designed for the 3-stage Radau method and this scheme has been proven to give a robust implementation. The reason for multiplying the stage derivatives by $(hA)^{-1} \otimes I_N$ is to transform matrix T so that $S = T^{-1}A^{-1}T$ and $W^{[n]} = \left(T^{-1} \otimes I_N\right)Z^{[n]}$ can be introduced where S is the Jordan canonical form of A that has the same diagonal elements.

The stage equation of HW scheme is given by

$$G\left(W^{[n]}\right) = h^{-1}\left(S \otimes I_N\right)W^{[n]} - \left(T^{-1} \otimes I_N\right)F\left(x_{n-1} + ch, \left(T \otimes I_N\right)W^{[n]} + e \otimes y_{n-1}\right), \tag{4}$$

with block diagonal matrix of the Jacobian such that

$$D_G\left(W^{[n]}\right) = h^{-1}\left(S \otimes I_N\right) - \left(T^{-1} \otimes I_N\right)J\left(x_{n-1} + ch, \left(T \otimes I_N\right)W^{[n]} + e \otimes y_{n-1}\right). \tag{5}$$

Solving for $W^{[n]}$ by using Newton-Raphson iteration yields

$$\Delta W^{[n]} = \left(-G\left(W^{[n]}\right)\right)\left(D_G\left(W^{[n]}\right)\right)^{-1}, \tag{6}$$

where

$$\Delta W^{[n]} = W^{[n+1]} - W^{[n]}.$$

The update y_n as given in Eq. 1 is therefore given by

$$y_n = y_{n-1} + b^T A^{-1}\left(T \otimes I_N\right)W^{[n]} . \tag{7}$$

As mentioned previously, GMR scheme is a modification from Cooper and Butcher (1983) implementation scheme. Their scheme is proven to give a convergent behaviour for linear and constant coefficient problems and also very efficient for general problems. Since the nonlinear stiff problems has been not investigated in details, thus the GMR scheme is implemented in solving the nonlinear stiff problem which is Robertson problem for G3 method. The general equation of the iterative scheme given by González-Pinto et al. (1994, 1995) are modified based on Eq. 1. The derivation of the iterative scheme can be found in González-Pinto et al. (1994) and the general equation are given as follows:

$$\begin{gathered}\left[I_N - h\left(T \otimes J\right)\right]E^{[n]} = Y^{[n]} - e \otimes y_{n-1} + h\left(A \otimes I_N\right)F\left(Y^{[n]}\right), \\ Y^{[n+1]} = Y^{[n]} + E^{[n]},\end{gathered} \tag{8}$$

where $n = 1, 2, \ldots, s$. In González-Pinto et al. (1994, 1995), the coefficient k is used instead of n. In this research, we changed into coefficient n because we want to use the same coefficient as the general equations of Runge-Kutta methods introduced by

Butcher (2016). Smaller quantities $Z^{[n]} = Y^{[n]} - e \otimes y_{n-1}$ is applied to Eq. 8 and the new equation of the iteration are given by

$$\begin{gathered}\left[I_N - h(T \otimes J)\right]E^{[n]} = Z^{[n]} + h(A \otimes I_N)F\left(Z^{[n]} + e \otimes y_{n-1}\right), \\ Z^{[n+1]} = Z^{[n]} + E^{[n]},\end{gathered} \tag{9}$$

There exists matrix T such that T is a real nonsingular constant matrix of dimension s and it contained a unique eigenvalue $\lambda > 0$. This matrix T could be advantages in reducing the additional cost that was involved in the implementation.

In addition to this error estimation, the authors have also used the error estimation suggested by Gorgey (2016) that uses symmetrization approach. The implementation of symmetrizer does not involve much cost as symmetrization is only applied at the end of the step by the update which is given by

$$\tilde{y} = u^T A^{-1}\left(PY^{[n]} + Y^{[n+1]}\right) \tag{10}$$

where *Y* refers to the internal stage values and the weight vector *u* is chosen to satisfy the damping and order conditions by the G3 method (Chan & Gorgey, 2013). For G3 method, *u* is given by $u = \left[\frac{13+3\sqrt{15}}{360}, -\frac{1}{45}, \frac{13-3\sqrt{15}}{360}\right]T$.

For example, the order-5 symmetrizers for G3 method by referring to Eq. 10 is therefore given by

$$\tilde{y}_n = \left(\frac{1}{4} + \frac{\sqrt{15}}{15}\right)\left(Y_1^{[n+1]} + Y_3^{[n]}\right) + \left(\frac{1}{4} - \frac{\sqrt{15}}{15}\right)\left(Y_1^{[n]} + Y_3^{[n+1]}\right). \tag{11}$$

In solving stiff ODEs problems of IRK methods, extrapolation technique has been introduced as an alternative for local error estimation and is applied together with G3 method. The general equation of extrapolation is given by

$$\bar{y} = \frac{2^p\left(y_2\right) - y_1}{2^p - 1}, \tag{12}$$

where p is the order of the RK methods and y_2 and y_1 are the solutions attained by using stepsizes, h and $h/2$ respectively. The difference between y_1 and y_2 gives the local error estimation. Extrapolation can be found in two difference modes such as active and passive modes. Active extrapolation happened when the value of extrapolation is used to capture the next computation while passive extrapolation occurs when there is no need in using the extrapolated value for any subsequent computations (Ismail & Gorgey, 2015). Therefore, there is only one mode that can be applied in the variable stepsize setting which is the active mode. In Ismail and Gorgey (2013), they mentioned that the passive mode of rational and polynomial failed to perform when the stiff ratio is high. This is clearly explained that the passive mode is not suitable for stiff problems. Since Robertson problem is a stiff problem, thus the passive mode is not recommended to be used.

The error estimation by the symmetrization is also used as an embedded pair. For instant, if G3 is the base method y_n as defined in Eq. 1 and the symmetizer of G3 is $\tilde{y}_n$ as given in Eq. 11, the error estimation is obtained by taking the difference between y_n and $\tilde{y}_n$. Detailed explanation about this approach is given by Gorgey (2016).

RESULTS AND DISCUSSION

In the numerical experiments, the Robertson problem as given in Eq. 2 is integrated to $x_n = 10$ with stepsize $h = 0.01$. The numerical result for G3 method are given in Figure 1, Figure 2 and Figure 3 respectively. The Butcher tableau of G3 method can be found in Butcher (2016). Figure 1 and Figure 2 showed two plots which are the loglog error versus loglog tolerance plot and loglog error versus CPU time plot for Robertson problem using three different implementation strategies as mentioned previously. In Figure 1, it is observed that GMR scheme gives the smallest error among the others as the tolerances get stringent.

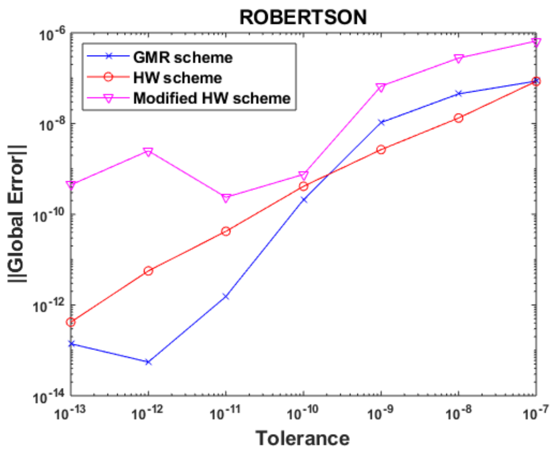

Figure 1. Global error versus tolerance graph of 3-stage (G3) Gauss method for Robertson problem

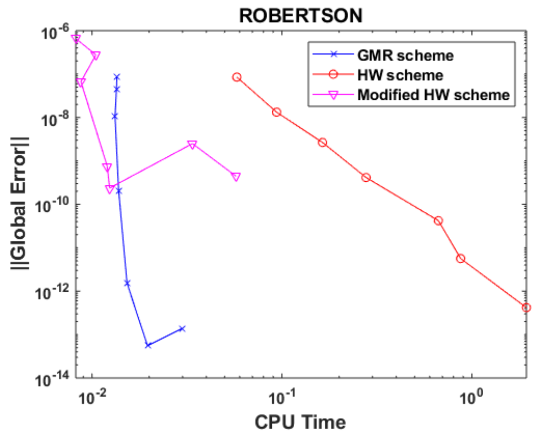

Figure 2. Global error versus CPU time graphs of 3-stage (G3) Gauss method for Robertson problem

However, for longer computational time the GMR scheme got destroyed by the round-off error as given in Figure 2 and decay much faster than the others even though the solution gives the least error. HW scheme requires more computational time if compared with GMR and modified HW (MHW) schemes. Based on Figure 2, for the next numerical results which is to compare the error estimation by the symmetrization and local extrapolation, the comparison are only given for GMR and MHW schemes. In Figure 3, there are four graphs obtained. The first two graphs which denoted by MHW and GMR schemes refer to the numerical results by using symmetrization technique, while the last two graphs which denoted by MHW and GMR scheme xtrap refer to the numerical results by using local extrapolation technique. The term 'xtrap' stands for extrapolation.

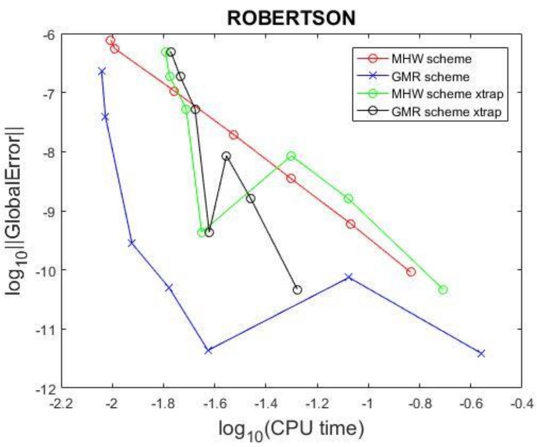

Figure 3. Global error versus CPU time graphs of 3-stage (G3) Gauss method for Robertson problem by using symmetrization technique and local extrapolation

Figure 3 shows the error estimation by using symmetrization and local extrapolation for G3 methods with GMR and MHW schemes. GMR scheme is observed to give the smallest error for the longer computational time compared to the others. MHW on the other hand although gives a straight line for the plot, the scheme is not as efficient as GMR scheme. Both schemes show the error estimation using local extrapolation is not as efficient as error estimation using symmetrization technique.

CONCLUSION

The main objectives of this research is to study the behaviour of variable stepsize setting which implemented using implementation schemes by González-Pinto et al. (1994, 1995) and Hairer and Wanner (1999) by the 3-stage (G3) Gauss method.

Generally, the GMR scheme is constructed for the families of Gauss methods while HW scheme is constructed for Radau IIA method. However, based on this research, it is shown that the standard implementation scheme with some tuning using HW scheme known as modified HW (MHW) scheme that does not involve any transformation matrix T can be as efficient as the HW and GMR schemes. GMR scheme also shown to give greater accuracy for error estimation using symmetrization technique if compared with local extrapolation.

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