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Efficiency of Extrapolated Runge-Kutta Methods in Solving Linear and Nonlinear Problems

Kecekapan Extrapolasi Kaedah Runge-Kutta dalam Menyelesaikan Masalah Linear dan Tak Linear

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Abstract

Extrapolation involves taking a certain linear combination of the numerical solutions of a base method applied with different stepsizes to obtain greater accuracy. This linear combination is done to eliminate the leading error term. The technique of extrapolation (passive and active) in accelerating convergence has been used successfully in numerical solution of ordinary differential equations. In this study, symmetric Runge-Kutta methods for solving linear and nonlinear stiff problem are considered. Symmetric methods admit asymptotic error expansion in even powers of the stepsize and are therefore of special interest because successive extrapolations can increase the order by two at time. Two ways of applying extrapolation are considered such as the active and the passive. It is interesting to know which modes of applying extrapolation are the most efficient when applied with symmetric methods. Results of numerical experiments are given which show the efficiency of the rational and polynomial extrapolated Implicit Midpoint Rule (IMR) and the Implicit Trapezoidal Rule (ITR) in solving Chemistry and Chemical Reaction problems. Numerical results show that in both types of extrapolation, the passive mode is considered to be the most efficient. The results also show that extrapolation with smoothing gives better results than without smoothing.

Keywords Runge-Kutta methods, symmetric methods, smoothing, rational and polynomial extrapolation

Abstrak

Extrapolasi melibatkan pengambilan beberapa gabungan linear daripada penyelesaian berangka bagi kaedah asas yang diaplikasikan dengan jarak langkauan yang berbeza untuk mendapatkan kejituan yang tinggi. Gabungan linear ini dilakukan untuk menghapuskan sebutan ralat yang tinggal. Teknik extrapolasi (pasif dan aktif) dalam mempercepatkan penumpuan telah berjaya dalam penyelesaian berangka bagi persamaan pembezaan biasa. Dalam kajian ini, kaedah Runga-Kutta yang simetrik telah dipilih untuk menyelesaikan masalah linear dan tak linear. Kaedah simetrik membenarkan pengembangan ralat asimtotik dalam kuasa dua genap bagi jarak langkauan. Dengan itu menjadikannya tarikan yang istimewa kerana extrapolasi yang berjaya boleh ditingkatkan sebanyak dua peringkat pada satu-satu masa. Terdapat dua cara mengaplikasi extrapolasi iaitu secara aktif dan pasif. Adalah menarik untuk mengetahui mod aplikasi extrapolasi yang paling efisyen apabila diaplikasikan dengan kaedah simetri. Hasil eksperimen berangka telah diberi dan menunjukkan kecekapan extrapolasi rasional dan polinomial bagi Kaedah Titik Tengah Pepenjuru Tersirat (IMR) dan Kaedah Trapezoid Tersirat (ITR) dalam menyelesaikan masalah Kimia dan Tindak Balas Kimia. Keputusan berangka menunjukkan antara kedua-dua jenis extrapolasi, mod pasif adalah lebih cekap. Hasil kajian juga menunjukkan bahawa extrapolasi dengan teknik pelicinan memberikan hasil yang lebih baik berbanding tanpa pelicinan.

Kata kunci Kaedah Runge-Kutta, kaedah simetri, pelicinan, extrapolasi rasional dan polinomial

INTRODUCTION

Extrapolation technique has been used successfully by the Runge-Kutta methods in solving physical, chemical and biological problems. Extrapolation involves taking a certain linear combination of the numerical solutions of a base method applied with different stepsizes to obtain greater accuracy. Several methods can be combined with extrapolation to increase the accuracy of the solutions whether in solving ordinary differential equations (ODEs), boundary value problems (BVPs) or partial differential equations (PDEs). These methods are fitted operator finite difference (Munyakazi & Patidar, 2008), General Linear Methods (Cardone, Jackiewicz, Sandu & Zhangx, 2014), iterated discrete projection (Zhongying, Guoqiang & Gnaneshwar, 2009), Runge-Kutta methods (Gorgey, 2012) and Crank-Nicolson method (Gorgey, 2014).

Consider a system of N initial value ordinary differential equations

$$y' = f(x, y), \quad y(x_0) = y_0 \tag{1}$$

In solving the problem (1), Runge-Kutta methods is applied. Runge-Kutta methods can be defined as

$$Y_i = y_{n-1} + h\sum_{i=1}^{S} a_{ij} f(x_{n-1} + c_j h, Y_j), \tag{2a}$$

$$Y_n = y_{n-1} + h\sum_{i=1}^{S} b_{ij} f(x_{n-1} + c_j h, Y_j), \tag{2b}$$

where Y_i represent the internal stage values and y_n represent the update of y at the n^{th}step (Butcher, 2005). This research is only focus on the implicit midpoint rule (IMR) and the implicit trapezoidal rule (ITR). The Butcher tableau for IMR and ITR are defined as given in Table 1 and Table 2.

$$\begin{array}{c|c} \frac{1}{2} & \frac{1}{2} \\ \hline & 1 \end{array}$$

Table 1 The Butcher tableau for IMR

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & \frac{1}{2} & \frac{1}{2} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}.$$

Table 2 The Butcher tableau for ITR

IMR and ITR methods are lower order implicit methods of order-2. Although these two popular methods have been used widely, there are limitations due to the lower order. These methods are restricted in solving linear and nonlinear problems. However, due to the symmetric properties (Chan, 1993; Chan & Gorgey, 2013) with extrapolation, the order of the method increases by two at a time. This is due to the asymptotic error expansions that are in even powers. Therefore it is interesting to observe how well these methods with extrapolation can solve linear and nonlinear stiff problems.

For symmetric methods, the asymptotic error expansion is in even powers

$$Y_n = y(x) + \sigma_1(x)h^p + \sigma_2(x)h^{p+2} + \ldots + \sigma_{p+k}(x)h^{p+2k} + O(h^{(p+2k)}), \quad k = 1,2,\ldots,$$

where $\sigma_1, \sigma_2, \ldots, \sigma_k$ are any smooth functions.

For example, consider applying IMR and ITR to the Prothero and Robinson (1974) problem

$$y' = \lambda(y - g(x)) + g'(x),$$

with $g(x) = e^{-x}$ and $y(0) = 1$.

The asymptotic error expansion for IMR is given by

$$\overbrace{y_n}^{IMR} = \left(R^n - e^{-nh}\right)\left(\frac{1}{12}\left(\frac{1+3\lambda}{1+\lambda}\right)h^2 + \frac{7}{2880}\left(\frac{1+6\lambda+\frac{75}{7}\lambda^2}{(1+\lambda)^2}\right)h^4 + O\left(h^6\right) + \ldots\right),$$

and for ITR the asymptotic error expansion is given by

$$\overbrace{y_n}^{IMR} = -\left(R^n - e^{-nh}\right)\left(\frac{1}{6}\left(\frac{1}{1+\lambda}\right)h^2 - \frac{1}{360}\left(\frac{1+6\lambda}{(1+\lambda)^2}\right)h^4 + O\left(h^6\right) + \ldots\right),$$

Where R is the stability function given by,

$$R(h\lambda) = \frac{1+\frac{1}{2}h\lambda}{1-\frac{1}{2}h\lambda}$$

of IMR and ITR. Both IMR and ITR have asymptotic error expansions in h^2, h^4 which are even powers. If the error expansion satisfies up to h^2 then the method is said to have order h^4+O.

PRELIMINARIES

Smoothing Technique

In the context of ODEs, the idea of extrapolation was first extended by Gragg (1965) when he studied the behaviour of explicit midpoint rule (EMR) in solving Kepler problem. Gragg observed that the numerical solutions of the EMR give oscillatory solutions hence with extrapolation the solutions, failed. Therefore, Gragg introduced the smoothing technique to dampen the oscillations in the EMR solutions. The smoothing is achieved by simply applying the formula

$$\overline{y}_n = \frac{y_{n-1} + 2y_n + y_{n+1}}{4} \tag{3}$$

For IMR and ITR methods, it turned out that the smoothing formula can also be used to dampen the oscillatory behaviour arise by the global errors due to the stability (Chan & Gorgey, 2011). The extension of smoothing known as symmetrizer is possible for higher order symmetric methods (Chan, 1993; Gorgey, 2012).

In this paper, the experiments on the IMR and ITR with smoothing and extrapolation are given for Chemistry Problem 1 and Chemistry Reaction Problem 2 in results and discussion section.

Extrapolation

Richardson Extrapolation (Richardson, 1911) is a technique to increase the accuracy of the method. There are two ways of applying extrapolation which is active and passive. Active extrapolation occurs when the extrapolated value is used in the next computations and if the extrapolated value is not being used in any subsequent computations then the extrapolation is called passive. Although the idea of extrapolation is old, many researchers are still trying to find out which mode of extrapolations is the most efficient and to avoid uncertainties many prefer to use both modes of extrapolation. For example, Faragó, Havasi and Zlatev (2010) investigated the computing time for both active and passive extrapolations compared with the Backward Euler. Their results showed that the computing done by the extrapolation for both active and passive is ten times smaller than the corresponding computing time for the Backward Euler. Hence, they concluded that regardless of active or passive modes, both modes of extrapolation are still powerful to increase the accuracy. On the other hand, Zlatev, Georgiev and Dimov (2014) studied on the absolute stability properties of the Richardson Extrapolation by the explicit Runge–Kutta methods of order-1– order-4. They mentioned that the passive extrapolation may fail when the method is not stable for large stepsize in solving certain problems but active extrapolation works fine for larger stepsize although the method is not stable. Besides that, Faragó, Havasi and Zlatev (2013) also studied the convergence of the diagonally implicit Runge–Kutta method with active extrapolation. The extrapolation results in a convergent numerical method if the initial value problem satisfied the Lipschitz condition.

In this paper, the studies of extrapolation focuses on two ways of extrapolation which is rational and polynomial and also two modes of extrapolation which are active and passive by the IMR and ITR methods in solving linear and nonlinear problems.

The extrapolation formula used is defined in equation (4)

$$y(x) = \frac{2^p y\left(\frac{h}{2}\right) - y(h)}{2^p - 1} \tag{4}$$

where p stand for order, h is stepsize of the method. This formula is used especially when the base methods are symmetric.

RESULTS AND DISCUSSION

Numerical experiments are given for linear and nonlinear stiff problems. The first problem is the chemistry problem by Shieh, Chang and Carmichael (1988) while the second problem is the nonlinear chemistry reaction taken in DeTEST problems (Hull, Enright, Fellen & Sedgwick, 1972). Each problem will be tested based on the efficiencies (CPU time) of the rational and polynomial extrapolations with active and passive modes. Smoothing technique is also applied together with extrapolation.

The numerical results for IMR and ITR are given with rational and polynomial active and passive extrapolations. Results are also given for extrapolation with smoothing. IMRs stand for implicit midpoint rule with smoothing and ITRs means implicit trapezoidal rule with smoothing. AX is the abbreviation for active extrapolation while PX is the abbreviation for passive extrapolation. Rat and Poly stands for rational and polynomial extrapolations respectively. The numerical results for Problem 1 are given in Figure 1- 4 while the numerical results for Problem 2 are given in Figure 5 and Figure 6.

Problem 1: Chemistry problem

$$
\begin{aligned}
y_1' &= -10y_1 + \alpha y_2, \\
y_2' &= -\alpha y_1 - 10y_2, \\
y_3' &= -4y_3, \\
y_4' &= -y_4, \\
y_5' &= -0.5y_5, \\
y_6' &= -0.1y_6,
\end{aligned}
$$

with $y_1(0) = 1, y_2(0) = 1, y_3(0) = 1$, $y_4(0) = 1, y_5(0) = 1, y_6(0) = 1$.

Figures 1 - 4 show the efficiencies diagrams for Problem 1. Figure 1 and Figure 3 are the results for the IMR while Figure 2 and Figure 4 are the results for the ITR. For, it is shown that for both methods, passive mode of rational and polynomial extrapolations is more efficient than the active mode.

On the other hand, interesting results obtained for $\alpha = 10^6$. The base methods with active and passive rational and polynomial extrapolations failed for Problem 1 but works when smoothing is applied with active and passive rational and polynomial extrapolations. For both methods, passive mode of rational and polynomial extrapolations is shown to be more efficient than the active mode of either type of extrapolations. It is also interesting to see the behaviour of the polynomial and rational extrapolations are almost the same. Hence, smoothing is important for certain types of problem when extrapolation fails with the base method.

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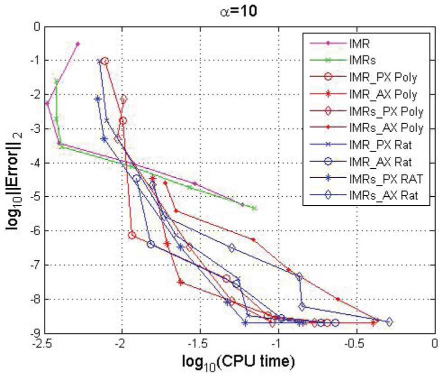

Figure 1 Problem 1 by the IMR for α = 10

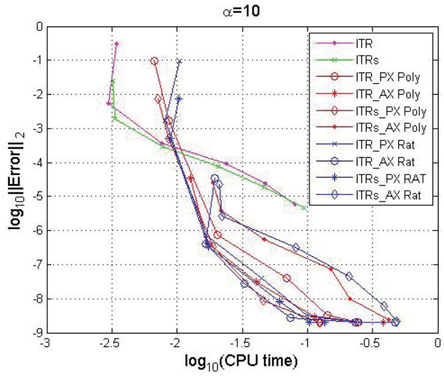

Figure 2 Problem 1 by the ITR for α = 10

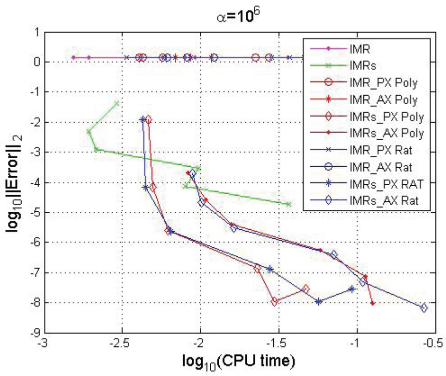

Figure 3 Problem 1 by the IMR for $\alpha = 10^6$

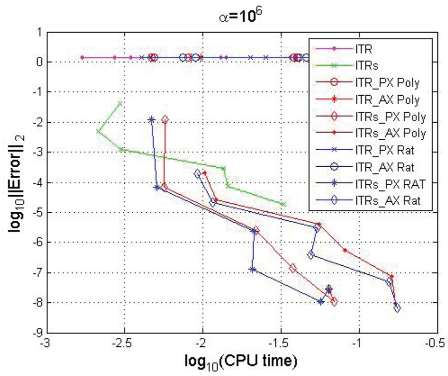

Figure 4 Problem 1 by the ITR for $\alpha = 10^6$

Problem 2: Nonlinear Chemistry Reaction

$$y_1' = y_1,$$
$$y_2' = y_1 - y_2^2,$$
$$y_3' = y_2^2,$$

with $y_1(0) = 1, y_2(0) = 0, y_3(0) = 0.$

For Problem 2, the numerical results are given in Figure 5 and Figure 6. It is shown that for both IMR and ITR, passive mode of polynomial is the most efficient. Almost similar observation is observed in Problem 1 that passive mode is the most efficient.

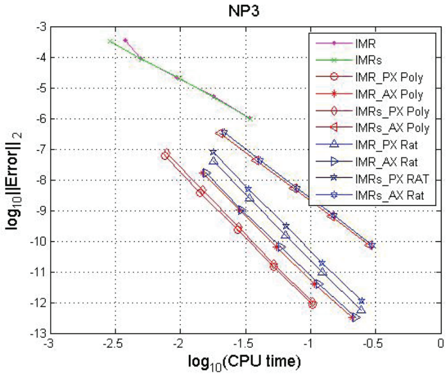

Figure 5 Problem 2 by the IMR

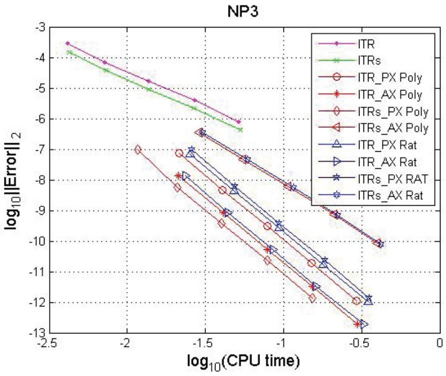

Figure 6 Problem 2 by the ITR

CONCLUSIONS

Although the numerical experiments are only given for two types of problem, however for the future research, the numerical results for other types of problems will be explored. From the numerical experiments, it is observed that the passive mode of rational and polynomial extrapolation is the most efficient in solving Chemistry problems and only passive mode of polynomial in solving Chemistry Reaction problems. In addition to this, when the stiff ratio is high, both methods (passive mode of rational and polynomial) failed to perform with extrapolation but with smoothing, extrapolation works well. It is therefore interesting to continue researching on what types of problems extrapolation works well.

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REFERENCES

Butcher, J. C. (2005). *Runge-Kutta methods for ordinary differential equations*. New Zealand: Springer.

Cardone, A., Jackiewicz, Z., Sandu, A., & Zhangx, H. (2014). Extrapolation based implicit-explicit general linear methods. *NumerAlgor*, *65*, 377-399. doi: 10.1007/s11075-013-9759-y

Chan, R. P. K., & Gorgey, A. (2011). Order-4 symmetrized Runge-Kutta methods for stiff problems. *Journal of Quality Measurement and Analysis, 7*(1), 53-66.

Chan, R. P. K. (1993). Generalized symmetric Runge-Kutta methods. *Computing, 50*(1), 31-49.

Chan, R. P. K., & Gorgey, A. (2013). Active and passive symmetrization of Runge-Kutta Gauss methods. *Applied Numerical Mathematics*, *67*, 64-77. doi:10.1016/j.apnum.2011.06.013

Faragó, I., Havasi, **Á.**, & Zlatev, Z. (2010). Efficient implementation of stable Richardson Extrapolation algorithms. *Computers and Mathematics with Applications*, *60*, 2309–2325. doi:10.1016/j.camwa.2010.08.025

Faragó, I., Havasi, **Á.**, & Zlatev, Z. (2013). The convergence of diagonally implicit Runge–Kutta methods combined with Richardson Extrapolation. *Computers and Mathematics with Applications*, *65*, 395–401. doi:10.1016/j.camwa.2012.04.016

ISSN 2462-2052

Gorgey, A. (2012). Extrapolation of symmetrized Runge-Kutta methods (unpublished PhD Thesis). University of Auckland, New Zealand.

Gorgey, A. (2014). Extrapolation of Boundary Value Problems. *Australian Journal of Basic and Applied Sciences*, *8*(11), 23-29.

Gragg, W. B. (1965). On extrapolation algorithm for ordinary initial value problems. *SIAM J. Numer. Anal*., *2*, 384 –403.

Han, G., & Wang, R. (2002). Richardson extrapolation of iterated discrete Galerkin solution for two-dimensional Fredholm integral equations. *Journal of Computational and Applied Mathematics*, *139*, 49-63. doi:10.1016/S0377-0427(01)00390-9

Hull, T. E., Enright, W. H., Fellen, B. M., & Sedgwick, A. E. (1972). Comparing numerical methods for ordinary differential equations. *SIAM Journal of Numerical Analysis*, *9*(4), 603 – 637.

Muyakazi, J. B., & Patidar, K.C. (2008). On Richardson extrapolation for fitted operator finite difference. *Applied Mathematics and computation, 201,* 465-480. doi: 10.1016/j.amc.2007.12.035

Prothero, A., & Robinson, A. (1974). On the stability and accuracy of one-step methods for solving stiff systems of ordinary differential equations. *Math. Comp*., *28*, 145 – 162.

Richardson, L. F. (1911). The approximate arithmetical solution by finite differences of physical problems involving differential equation, with an application to the stresses in amasonry dam. *Philos. Trans. Roy. Soc. London, ser.A*, *210*, 307- 857.

Shieh, D. S. S., Chang, Y., & Carmichael, G. R. (1988). The evaluation of numerical techniques for solution of stiff ordinary differential equations arising from chemical kinetic problems. *Enviromental Software*, *3* (1), 28 – 38. doi:10.1016/0266-9838(88)90006-8

Zlatev, Z., Georgiev, K., & Dimov, I. (2014). Studying absolute stability properties of the Richardson Extrapolation combined with explicit Runge–Kutta methods. *Computers and Mathematics with Applications*, *67*, 2294–2307. doi:10.1016/j.camwa.2014.02.025

Zhongying, C., Guaoqiang, L., & Gnaneshwar, N. (2009). Richardson extrapolation of iterated discrete projection methods for eigenvalue approximation. *Journal of Computational and Applied Mathematics, 223,* 48-61. doi:10.1016/j.cam.2007.12.019