Comparison of One-Step and Two-Step Symmetrization in the Variable Stepsize Setting
(Perbandingan Satu dan Dua Langkah Pensimetrian dalam Persekitaran Saiz Langkah Berubah-Ubah)

N. Razali*, Z.M. Nopiah & H. Othman

ABSTRACT

In this paper, we study the effects of symmetrization by the implicit midpoint rule (IMR) and the implicit trapezoidal rule (ITR) on the numerical solution of ordinary differential equations. We extend the study of the well-known formula of Gragg to a two-step symmetrizer and compare the efficiency of their use with the IMR and ITR. We present the experimental results on nonlinear problem using variable stepsize setting and the results show greater efficiency of the two-step symmetrizers over the one-step symmetrizers of IMR and ITR.

Keywords: Implicit midpoint rule; implicit trapezoidal rule; symmetrizers

ABSTRAK

Dalam kertas ini, kami mengkaji kesan pensimetrian kaedah titik tengah tersirat (IMR) dan kaedah trapezium tersirat (ITR) ke atas penyelesaian berangka persamaan pembezaan biasa. Kami melanjutkan kajian terkenal oleh Gragg kepada pensimetri dua langkah dan membandingkan kecekapan penggunaannya dengan IMR dan ITR. Keputusan uji kaji pada masalah tidak linear menggunakan saiz langkah yang berubah-ubah menunjukkan bahawa pensimetri dua langkah adalah lebih cekap berbanding pensimetri satu langkah.

Kata kunci: Kaedah titik tengah tersirat; kaedah trapezium tersirat; pensimetri

INTRODUCTION

The study of numerical methods for initial value problems including stiff problems has introduced several new ideas on stability and error propagation. Stiff ordinary differential equation systems arise in many different application areas where the components of the solution have widely different rates of change. These problems involving rapidly decaying transient components as well as steady-state ones occur naturally in many different situations including the damped spring system, control systems and chemical kinetics. Some studies on stiff problems have been reported in Auzinger and Macsek (1990), Bjurel et al. (1970), Burrage (1978), Enright et al. (1975), Liniger and Willoughby (1970) and Mazzia et al. (2012).

We are interested in solving ordinary differential equations, especially stiff problems. Symmetric Runge-Kutta methods are considered because their numerical solution possesses an asymptotic error expansion in even powers of the stepsize h. When applied with Richardson extrapolation the order can potentially increase by two at each level of extrapolation. Gragg (1965) first proved the existence of an asymptotic error expansion for the explicit midpoint rule which laid the foundation for the application of Richardson extrapolation. He also introduced the concept of smoothing to suppress the effects of the parasitic oscillatory component in the numerical solution. Since then, the concept of extrapolation and smoothing has been applied in nonstiff and stiff problems by many researchers. Following the idea of Gragg, Chan (1989) generalized the smoothing technique for arbitrary symmetric Runge-Kutta methods. He called the process symmetrization and showed how it can be achieved by an *L*-stable method known as the symmetrizer that is constructed so as to preserve the asymptotic error expansion in even powers of stepsize and to provide the necessary damping for stiff problems. In 2012, Gorgey extended Chan's theoretical study of extrapolation and symmetrization by means of practical implementation and experimental study. She investigated the two modes of symmetrization, that are, active and passive symmetrizations of one-step symmetrizers for Gauss and Lobatto IIIA methods of order 4 and 6 in the constant and variable stepsize settings. She analyzed the most efficient way of implementing symmetrization with and without extrapolation on order-4 and order-6 methods, providing evidence that the one-step symmetrizers can restore the classical order especially the order-4 Gauss and Lobatto IIIA methods (Chan & Gorgey 2013, 2011).

Symmetrization can be applied in different ways. In a constant stepsize setting, the possibilities are:

Active Symmetrization: Each time a symmetrized value is computed it is then used to propagate the numerical solution. Symmetrization can be performed at every step, every two steps or every three steps.

Passive Symmetrization: The implementation in the passive mode involves computing many steps with the symmetric method, storing at each step the update as well as the internal stage values and then applying symmetrization where required using the stored values.

An s-stage Runge-Kutta method with stepsize h for the step $(x_{n-1}, y_{n-1}) \mapsto (x_n, y_n)$ is a one-step method defined by,

$$Y_i = y_{n-1} + h \sum_{j=1}^{n} a_{ij} f\left(x_{n-1} + c_j h, Y_j\right), \quad i = 1,...,s,$$

$$y_n = y_{n-1} + h \sum_{i=1}^{s} b_i f\left(x_{n-1} + c_i h, Y_i\right), \tag{1}$$

where A is an $s \times s$ Runge-Kutta matrix, b and c are $s \times 1$ vectors of weights and abscissas, respectively. The Butcher tableau for the method is given by,

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \cdots & a_{1s} \\
c_2 & a_{21} & a_{22} & \cdots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & \cdots & a_{ss} \\
\hline
& b_1 & b_2 & \cdots & b_s
\end{array}
\quad \text{or} \quad
\begin{array}{c|c}
c & A \\
\hline
& b^T
\end{array}.
$$

The method $\mathscr{R}$ is symmetric if $-\mathscr{R}^{-1} = \mathscr{R}$, where $-\mathscr{R}^{-1}$ is the adjoint of $\mathscr{R}$. If $\mathscr{R}$ is generated by (A,b,c), the algebraic characterization of symmetry is given by,

$$PA + AP = eb^T, Pb = b, Pc = e - c. \tag{2}$$

Here e is the $s \times 1$ vector of units, and P is the $s \times s$ permutation matrix that reverses the order of the stages with (i, j)-th element given by the Kronecker $\delta_{i,s+1-j}$. These conditions assumes that $b^T e = 1$ and $Ae = c$ hold.

The stability function of a Runge-Kutta method with coefficients (A, b, c) is defined by

$$R(z) = 1 + zb^T (I - zA)^{-1} e. \tag{3}$$

A method is said to be A-stable if it is bounded by 1 in the left half-plane, that is, when $|R(z)| \leq 1$ for $z \in \mathbb{C}$ with $\mathrm{Re}(z) \leq 0$.

The one-step symmetrizer is generated by

$$\left(\tilde{A}, \tilde{b}, \tilde{c}\right) = \left(\begin{bmatrix} A & 0 \\ eb^T & A \end{bmatrix}, \begin{bmatrix} b - Pu \\ u \end{bmatrix}, \begin{bmatrix} c \\ e + c \end{bmatrix} \right), \tag{4}$$

where the vector u is chosen to satisfy damping and order conditions (Chan & Razali 2014). While the two-step symmetrizer is a composition of four symmetric steps and is generated by,

$$\left(\tilde{A}, \tilde{b}, \tilde{c}\right) = \left(\begin{bmatrix} A & 0 & 0 & 0 \\ eb^T & A & 0 & 0 \\ eb^T & eb^T & A & 0 \\ eb^T & eb^T & eb^T & A \end{bmatrix}, \begin{bmatrix} b - Pv \\ b - Pu \\ u \\ v \end{bmatrix}, \begin{bmatrix} c \\ e + c \\ 2e + c \\ 3e + c \end{bmatrix} \right) \tag{5}$$

Two-step symmetrizers carry twice the number of parameters (u and v) compared to one-step symmetrizers (u). This gives flexibility especially for higher order methods in satisfying the order and other desirable conditions. The stability function for one-step and two-step symmetrizers are the same with equation (3) except that the coefficients (A, b, c) are now denoted as $\left(\tilde{A}, \tilde{b}, \tilde{c}\right)$ as given in (4) and (5), respectively.

In 2014, Chan and Razali have investigated the efficiency and accuracy of one-step and two-step symmetrizations for Implicit Midpoint Rule (IMR) and Implicit Trapezoidal Rule (ITR) in a constant stepsize setting. The Butcher tableau for the one-step IMR and ITR are,

$$
\begin{array}{c|cc}
\frac{1}{2} & \frac{1}{2} & 0 \\
\frac{3}{2} & 1 & \frac{1}{2} \\
\hline
& \frac{3}{4} & \frac{1}{4}
\end{array}
$$

$$
\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
1 & \frac{1}{2} & \frac{1}{2} & 0 \\
2 & \frac{1}{2} & 1 & \frac{1}{2} \\
\hline
& \frac{3}{8} & \frac{1}{2} & \frac{1}{8}
\end{array}
$$

with the stability function (3) for both methods turn out to be the same which is,

$$\tilde{R}(z) = \frac{1}{\left(1 - \frac{1}{2}z\right)^2} \tag{6}$$

In the nonstiff case, the summation leads to the global error losing one power of h compared to the local error and behaves like an order-1 method. In the stiff case the symmetrizer possesses the damping property since $\tilde{R}(z) \to \frac{4}{z^2}$ as $z \to \infty$. As a result, the order-2 behaviour is retained because the local errors for all steps except the last are damped by $\tilde{R}(z)$ so that the global error is essentially determined by the local error of the last step.

The Butcher tableau for two-step symmetrization of IMR and ITR is given by,

$\frac{1}{2}$	$\frac{1}{2}$	0	0	0
$\frac{3}{2}$	1	$\frac{1}{2}$	0	0
$\frac{5}{2}$	1	1	$\frac{1}{2}$	0
$\frac{7}{2}$	1	1	1	$\frac{1}{2}$
	$\frac{17}{16}$	$\frac{13}{16}$	$\frac{3}{16}$	$-\frac{1}{16}$

0	0	0	0	0	0
1	$\frac{1}{2}$	$\frac{1}{2}$	0	0	0
2	$\frac{1}{2}$	1	$\frac{1}{2}$	0	0
3	$\frac{1}{2}$	1	1	$\frac{1}{2}$	0
4	$\frac{1}{2}$	1	1	1	$\frac{1}{2}$
	$\frac{17}{32}$	$\frac{15}{16}$	$\frac{1}{2}$	$\frac{1}{16}$	$-\frac{1}{32}$

The stability function (3) for both methods turn out to be,

$$\tilde{R}(z) = \frac{1 - \dfrac{z^2}{2}}{\left(1 - \dfrac{z}{2}\right)^4} \tag{7}$$

We note that $\tilde{R}(z) \rightarrow -8/z^2$ as $z \rightarrow \infty$ compared $\tilde{R}(z) \rightarrow 4/h^2$ to for the one-step symmetrizer.

We have investigated two-step symmetrization in a constant stepsize setting (Chan & Razali 2014). However, it is unrealistic to use a constant stepsize in nearly all applications. Thus, a practical implementation of varying the step as the integration proceeds is necessary. To achieve a specified accuracy, we have to choose a stepsize small enough so that the approximate solution is close to the exact solution. In order to achieve this, a tolerance is specified and a method is designed so that at each step of the computation the estimated error lies within the given tolerance and the stepsize for the next step can be predicted which gives an error within the tolerance. We have seen in Chan and Razali (2014) that the two-step symmetrization in the active mode can be more accurate than the one-step symmetrization. Hence, we focus our attention on applying variable stepsize code in the active mode.

APPLICATION

Error estimation is a practical tool for choosing the right stepsize and ensure efficient implementation although there is a cost associated with it. Some techniques for estimating the error, for example, by local extrapolation, embedding technique and quadrature formula have been discussed in Ceschino and Kuntzmann (1963), Enright and Hull (1976), González-Pinto et al. (2004), Merson (1957) and Shampine (1985). We follow the suggestion by Gorgey (2012) to use symmetrization to estimate the local error because the results show that symmetrization give good error estimates. In our case, two-step symmetrization is implemented. The error at the n-th step is obtained by evaluating the difference between the update y_n of the symmetric method and that of the symmetrizer $\hat{y}_n$. Examples 1 and 2 show the error estimation of the implicit midpoint and trapezoidal rules, respectively.

Example 1 Implicit Midpoint Rule

The update for the IMR is

$$yn = 2Y^{[n]} - y_{n-1}, \tag{8}$$

where $Y^{[n]}$ is the internal stage value at the n-th step. The update for two-step symmetrization of IMR is given by,

$$\hat{y}_n = \frac{5}{8}\left(Y^{[n]} + Y^{[n+1]}\right) - \frac{1}{8}\left(Y^{[n-1]} + Y^{[n+2]}\right). \tag{9}$$

The error is then given by

$$\hat{\varepsilon}_n = \hat{y}_n - y_n. \tag{10}$$

Example 2 Implicit Trapezoidal Rule

The update for the ITR is

$$y_n = Y^{[n]}, \tag{11}$$

where $Y^{[n]}$ is the internal stage value at the n-th step. The update for two-step symmetrization of ITR is given by,

$$\hat{y}_n = \frac{1}{16}\left(-Y^{[n+2]} + 4Y^{[n-1]} + 10Y^{[n]} + 4Y^{[n+1]} - Y^{[n+2]}\right) \tag{12}$$

The error is given by (10).

In our variable stepsize code, the error estimates that we use are by symmetrization and the error is given by (10), while the starting values for the Newton iterations, the stopping criterion and the stepsize selection are based on the approach given in Hairer and Wanner (1991). Shampine et al. (1985) suggested that the first step is critical because the justification of the algorithms for the adjustment of the stepsize on subsequent steps depends on making small changes. Thus, we follow Shampine's idea on the automatic selection of the initial stepsize. An experiment is carried out to show the efficiency of the symmetrization approach to error estimation for variable stepsize. We set $x = x_0$ and p is the order of the method. The value of h_{max} and h_{min} are chosen based on the information from literature and the stepsize h is estimated using the automatic selection. The algorithm for variable stepsize setting is as shown:

while $(x < x_n)$ and $(h \geq h_{min})$

if $(x + h > x_n)$

$\{h \leftarrow x_n - x$

Compute one step of y and $\hat{y}$

Obtain h_{out}

if TRACE $h = h_{out}$

Estimate the error $\hat{\varepsilon} = \hat{y} - y$ as given in (10)

$\delta \leftarrow \|\hat{\varepsilon}\|_\infty$

$\tau \leftarrow \text{Tol.max}(\|y\|_\infty, 1.0)$

if $(\delta \leq \tau)$

$x \leftarrow x + h$

$y \leftarrow \hat{y}$

if $(\delta = \tau)$

$h \leftarrow \min([h_{max}, 4.h, 0.9.h.(\tau/\delta)^{p+1}])$

Accept h.

else if

Reject h

$h \leftarrow h.\max([0.25, 0.9.h.(\tau/\delta)^{p+1}])$

VAN DER POL

The Van der Pol (VDP) problem is a two-dimensional system of ODEs. This problem describes the behaviour of nonlinear vacuum tube circuits and was proposed by B. Van der Pol (Hairer & Wanner 1991). The parameter ε is a stiffness parameter. The stiffness of the problem increases with ε. The problem is represented by,

$$y_1' = y_2$$
$$y_2' = \frac{1}{\varepsilon}\left((1 - y_1^2)y_2 - y_1\right),$$

(13)

with $y_1(0) = 2$ and $y_2 = (0) = 0$ and integrated to $X = 5$ and $\varepsilon = 10^{-2}$.

CH

The problem by Curtiss and Hirschfelder (CH)) (1952) is a moderately stiff problem defined by,

$$y' = -50(y - \cos(x)),$$

(14)

with $y(0) = 1$ and integrated to $X = 15$.

Exact solution: $y(x) = \frac{2500}{2501}\cos(x) + \frac{50}{2501}\sin(x) + \frac{1}{2501}e^{-50x}$, $x \geq 0$.

RESULTS AND DISCUSSION

The two-step symmetrized IMR and ITR are compared with the one-step symmetrization of the same method in active mode. The efficiency is measured in CPU time. In variable stepsize setting, the local errors for both IMR and ITR are estimated using the differences between the approximations for the base method and the symmetrizer as shown in Examples 1 and 2. Each method is plotted in a different colour and the abbreviation used to explain the graph is given in Table 1.

Figure 1 shows two pictures of the stepsizes for solving VDP problem. The picture at the top shows the solution of one-step and two-step active symmetrization of the implicit midpoint and trapezoidal rules with all accepted integration steps for y_1. In the picture at the bottom, the stepsize obtained by both methods are plotted as functions of x. We observe that for this problem, the two-step active symmetrization of IMR and ITR (2ASIMR and 2ASITR) have larger stepsizes than the 1AS of both methods. Larger stepsizes result in a reduction of computation time. For this particular problem, the stiffness $\varepsilon = 10^{-2}$ is mild since the method does not converge when solving a strongly stiff case due to the lower order of the method. Figure 2 is the efficiency graphs which is a log-log plot of absolute error versus CPU time. In this figure, 2ASIMR and 2ASITR lie at the bottom of the graph indicating that it is the most efficient and confirm the previous statement. Figures 3 and 4 show the solution of active symmetrization and the stepsizes obtained by the IMR, the ITR and the symmetrizers for the CH problem, respectively. We observe that the stepsizes of 2ASITR are larger than other methods and achieved a stable stepsize 0.5 followed by the 2ASIMR. This is due to the local errors for 2ASITR that have leading coefficients that are smaller in magnitude compared to one-step symmetrizer and restores the very accurate behaviour of the basic ITR method itself. The result partly reflected in the efficiency plots shown in Figure 4 which indicate the greater efficiency of two-step over one-step symmetrization.

CONCLUSION

The result in this paper proves that the two-step symmetrization is shown to be cost effective. The VDP and CH are mildly stiff low dimensional problems and the results show greater efficiency for two-step over one-step

TABLE 1. Notation for numerical experiments

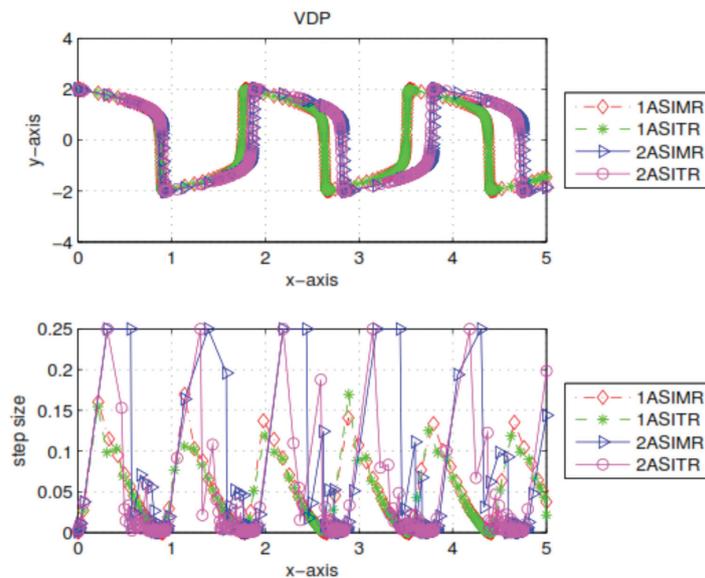| Abbreviation	Definition	Implementation
1ASIMR	One-step symmetrization of IMR	Active
1ASITR	One-step symmetrization of ITR	Active
2ASIMR	Two-step symmetrization of IMR	Active
2ASITR	Two-step symmetrization of IMR	Active

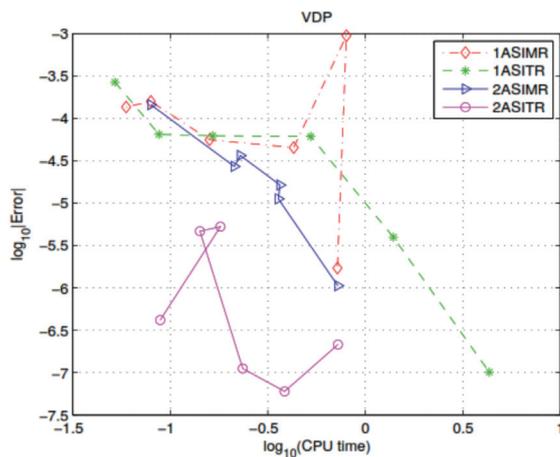FIGURE 1. Stepsizes for solving VDP problem
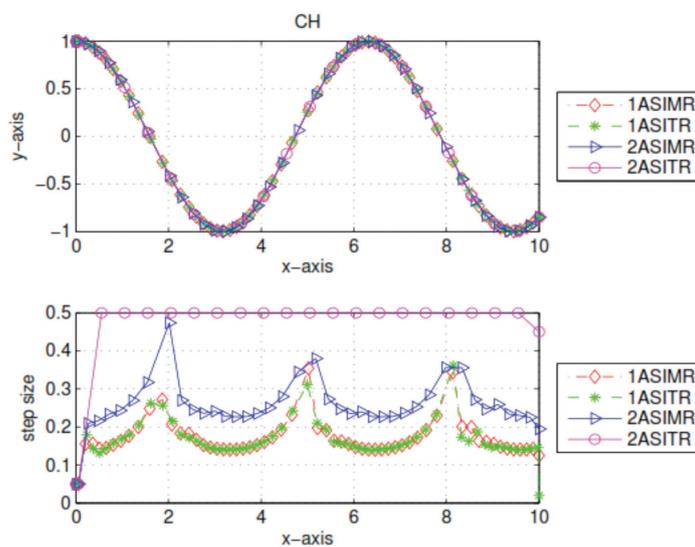

FIGURE 2. Efficiency plots for VDP problem

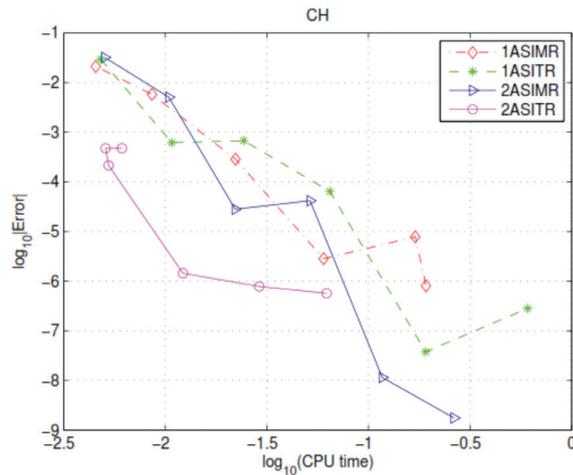FIGURE 3. Stepsizes for solving CH problem

FIGURE 4. Efficiency plots for CH problem

active symmetrization, although preliminary, nevertheless provide an incentive to pursue two-step symmetrization. When a very small stepsize is used, a roundoff error might dominate whereas with large stepsizes, the accumulated truncation errors that will dominate. Hence, it is of interest to improve the algorithm by applying compensated summation to capture the round-off error in each individual step and minimize the effect of round-off error. We also wish to apply the two-step symmetrization with extrapolation either in active or passive modes to observe the behaviour of this method when solving other stiff problems.

REFERENCES

Auzinger, R.F.W. & Macsek, F. 1990. Asymptotic error expansions for stiff equations: The implicit euler scheme. *SIAM Journal on Numerical Analysis* 27(1): 67-104.

Bjurel, B.L.S.L.G., Dahlquist, G. & Oden, L. 1970. *Survey of Stiff Ordinary Differential Equations*. Report NA 70.11, Dept. of Information Processing, RocalInst. of Tech., Stockholm.

Burrage, K. 1978. A special family of Runge-Kutta methods for solving stiff differential equations. *BIT Numerical Mathematics* 18: 22-41.

Ceschino, F. & Kuntzmann, J. 1963. *Numerical Solution of Initial Value Problems*. Dunod, Paris: Prentice Hall Inc.

Curtiss, C.F. & Hirschfelder, J.O. 1952. Integration of stiff equations. *Proc. Nat. Acad. Sci.* 38(3): 235-243.

Chan, R.P.K. 1989. Extrapolation of Runge-Kutta methods for stiff initial value problems. PhD Thesis, University of Auckland (Unpublished).

Chan, R.P.K. & Razali, N. 2014. Smoothing effects on the IMR and ITR. *Numerical Algorithms* 65(3): 401-420.

Chan, R.P.K. & Gorgey, A. 2013. Active and passive symmetrization of Runge-Kutta Gauss methods. *Applied Numerical Mathematics* 67: 64-77.

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.

Enright, W.H. & Hull, T.E. 1976. Test results on initial value methods for non-stiff ordinary differential equations. *SIAM Journal on Numerical Analysis* 13(6): 944-961.

Enright, W.H., Hull, T.E. & Lindberg, B. 1975. Comparing numerical methods for stiff systems of O.D.E:s. *BIT Numerical Mathematics* 15(1): 10-48.

Gladwell, L.F.S.I. & Brankin, R.W. 1987. Automatic selection of the initial step size for an ODE solver. *Journal of Computational and Applied Mathematics* 18(2): 175-192.

González-Pinto, S., Montijano, J.I. & Rodríguez, S.P. 2004. Two-step error estimators for implicit Runge-Kutta methods applied to stiff systems. *ACM Trans. Math. Softw.* 30(1): 1-18.

Gorgey, A. 2012. Extrapolation of Symmetrized Runge-Kutta Methods. PhD Thesis, University of Auckland (Unpublished).

Gragg, W.B. 1965. On extrapolation algorithms for ordinary initial value problems. *Journal of the Society for Industrial and Applied Mathematics: Series B, Numerical Analysis* 2(3): 384-403.

Hairer, S.N.E. & Wanner, G. 1991. *Solving Ordinary Differential Equations II (Stiff and Differential-Algebraic Problems)*. Springer-Verlag Berlin Heidelberg.

Liniger, W. & Willoughby, R.A. 1970. Efficient integration methods for stiff systems of ordinary differential equations. *SIAM Journal on Numerical Analysis* 7(1): 47-66.

Mazzia, F., Cash, J.R. & Soetaert, K. 2012. A test set for stiff initial value problem solvers in the open source software R: Package deTestSet. *Journal of Computational and Applied Mathematics* 236(16): 4119-4131.

Merson, R.H. 1957. An operational Method for the Study of Integration Processes. *Proc. Symposium Data Processing*.

Shampine, L.F. 1985. Local error estimation by doubling. *Computing* 34(2): 179-190.

Centre of Research in Engineering Education and Built Environment
Program of Fundamental Engineering Studies
Faculty of Engineering and Built Environment
Universiti Kebangsaan Malaysia
43600 UKM Bangi, Selangor Darul Ehsan
Malaysia

*Corresponding author; email: helyna@ukm.edu.my