

ORDER-4 SYMMETRIZED RUNGE-KUTTA METHODS FOR STIFF PROBLEMS

(Kaedah Runge-Kutta Tersimetri Peringkat-4 untuk Masalah Kaku)

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ABSTRACT

If a Runge-Kutta method having an asymptotic error expansion in the stepsize h is symmetric then it is characterised by an h^2 -expansion. Since elimination of the leading error terms in succession results in an increase in the order by two at a time, a symmetric method could therefore be suitable for the construction of extrapolation methods. However, when order reduction occurs for stiff problems it needs to be suppressed before an appropriate extrapolation formula can be applied. This can be achieved by a process called symmetrization which is a composition of the symmetric method with an L-stable method known as a symmetrizer. The symmetrizer is constructed so as to preserve the h^2 -asymptotic error expansion. In this paper we consider symmetrization of the 2-stage Gauss and the 3-stage Lobatto IIIA methods of order 4. We show that these methods are more efficient when used with symmetrization. Extrapolation based on the symmetrized methods is therefore expected to give greater accuracy. We also show that the method with a higher stage order is more advantageous than one with a lower stage order for solving stiff problems.

Keywords: Order reduction; symmetric methods; stiff problems; symmetrizers

ABSTRAK

Jika kaedah Runge-Kutta yang mempunyai kembangan ralat asimptot dengan saiz langkah h adalah simetri, maka ia dicirikan oleh kembangan- h^2 . Oleh sebab penghapusan sebutan ralat utama dalam hasil yang berturutan adalah dalam bentuk peningkatan dua peringkat pada suatu masa, suatu kaedah simetri adalah sesuai untuk pembinaan kaedah ekstrapolasi. Walau bagaimanapun apabila penurunan peringkat bagi masalah kaku berlaku ia perlu dikurangkan sebelum suatu rumus ekstrapolasi yang sesuai boleh digunakan. Ini boleh dicapai melalui proses pensimetrian yang merupakan komposisi di antara kaedah simetri dengan suatu kaedah yang L-stabil yang dikenali sebagai pensimetri. Pensimetri tersebut dibina agar mengekalkan kembangan ralat asimptot- h^2 . Dalam makalah ini, dipertimbangkan pensimetrian bagi kaedah Gauss tahap-2 dan Lobatto IIIA tahap-3 dengan peringkat-4. Dapat ditunjukkan bahawa kedua-dua kaedah ini adalah lebih cekap apabila digunakan dengan pensimetri. Oleh itu, ekstrapolasi yang berasaskan kaedah tersimetri diharapkan memberikan kejituan yang lebih tinggi. Turut ditunjukkan bahawa kaedah dengan peringkat tahap yang lebih tinggi mempunyai kelebihan berbanding kaedah yang berperingkat tahap lebih rendah bagi menyelesaikan masalah kaku.

Kata kunci: Penurunan peringkat; kaedah simetri; masalah kaku; pensimetri

1. Symmetric Methods

We consider a system of N initial value ordinary differential equations,

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

where $f : [x_0, x_f] \times \mathfrak{R}^N \rightarrow \mathfrak{R}^N$. The numerical solution for the n^{th} step, $x_{n-1} \mapsto x_{n-1} + h$, computed by an s -stage Runge–Kutta method is defined by

$$\begin{aligned} Y_i &= y_{n-1} + h \sum_{j=1}^s a_{ij} f(x_{n-1} + c_j h, Y_j), \quad i = 1, \dots, s, \\ y_n &= y_{n-1} + h \sum_{i=1}^s b_i f(x_{n-1} + c_i h, Y_i). \end{aligned} \quad (2)$$

Here, y_n is the update and Y_i the internal stage value for the i^{th} stage. The coefficients of the method are usually displayed in a Butcher-tableau,

$$\begin{array}{c|c} c & A \\ \hline & b^T \end{array}.$$

The stability function of the method is defined by

$$R(z) = 1 + z b^T (I - zA)^{-1} e, \quad (3)$$

where e is the $s \times 1$ vector of units. The method is said to be A -stable if $R(z)$ is bounded by 1 in the left half-plane. The method $\mathbf{R} = (A, b, c)$ is symmetric or self-adjoint if

$$-\mathbf{R}^{-1} = \mathbf{R} \quad \text{or} \quad (eb^T - A, b, e - c) = (A, b, c) = (PAP, Pb, Pc), \quad (4)$$

where P is a permutation matrix defined by $p_{ij} = \delta_{i, s+1-j}$, and equality is in terms of equivalence classes (Stetter 1973). A symmetric method is therefore characterised by coefficients that satisfy the following conditions,

$$Pb = b, \quad PAP = eb^T - A, \quad Pc = e - c, \quad (5)$$

where we have assumed the consistency condition $b^T e = 1$ and the row-sum condition $Ae = c$.

We also assume the global error $\Delta y_n = y_n - y(x_n)$ of a symmetric Runge-Kutta method of even order p has an asymptotic error expansion given by

$$\Delta y_n = e_p(x_n)h^p + e_{p+2}(x_n)h^{p+2} + \dots + e_{p+2m}(x_n)h_{p+2m} + O(h^{p+2m+1}), \quad h \rightarrow 0, \quad (6)$$

where the $e_i(x_n)$ are independent of h .

In this paper we consider implicit methods from the Gauss and Lobatto IIIA families. These methods are symmetric and have stability functions that satisfy $R(z)R(-z) = 1$. It follows they are A-stable. Their abscissas c_i are determined from the shifted Legendre polynomials on $[0,1]$ and the a_{ij} and b_i are then constructed using the simplifying assumptions $B(s)$ and $C(s)$ (Butcher 1963), where

$$\begin{aligned} B(p) &: & b^T c^{k-1} &= \frac{1}{k}, & k &= 1, \dots, p, \\ C(r) &: & A c^{k-1} &= \frac{1}{k} c^k, & k &= 1, \dots, r, \end{aligned} \tag{7}$$

and powers of the vector c refer to component-wise powers. We recall that the stage order of a method satisfying $B(p)$ and $C(r)$ is $\min(p, r)$. The s -stage Gauss method satisfies $C(s)$ and $B(2s)$, and is of order $2s$ and stage order s while the s -stage Lobatto IIIA method satisfies $C(s)$ and $B(2s-2)$ and is of order $2s-2$ and stage order s . In particular, we focus attention on the methods of order 4, namely, the Gauss method \mathbf{G}_2 with 2 stages and stage order 2, and the Lobatto IIIA method \mathbf{L}_3 with 3 stages and stage order 3.

$$\mathbf{G}_2 = \begin{array}{c|cc} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}, \quad \mathbf{L}_3 = \begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{5}{24} & \frac{1}{3} & -\frac{1}{24} \\ \frac{1}{2} & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \hline & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{array}.$$

Examples of order-2 methods are the implicit midpoint rule (IMR) and the implicit trapezoidal rule (ITR) with respective Butcher-tableaux,

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

We will consider these symmetric methods applied to the scalar test problem of Prothero and Robinson (1974),

$$y'(x) = q(y(x) - g(x)) + g'(x), \quad y(x_0) = g(x_0), \tag{8}$$

where q is complex with a negative real part large in magnitude, and $g(x)$ is a smooth function. The exact solution is given by $y(x) = g(x)$ and it can be shown that the global error at step n is given by

$$\varepsilon_n = y_n - y(x_n) = \sum_{i=1}^n R(x)^{n-i} \psi_i(z), \quad z=qh, \tag{9}$$

where φ_i is the local error for the i^{th} step given by

$$\psi_i(z) = \sum_{k=2}^{\infty} \frac{h^k}{k!} \left(1 - kb^T c^{k-1} + zb^T (1 - zA)^{-1} (c^k - kAc^{k-1}) \right) g^{(k)}(x_{i-1}). \quad (10)$$

The performance of a method is known to improve with increasing stage order for stiff problems. For example, the oscillatory errors shown in the plots of Figure 1 are much smaller for the ITR (stage order 2) than for the IMR (stage order 1). For the problem with $g(x) = e^{-x}$, the leading term in the global error at step n depends on $g''(x_n)$ or $g'''(x_n)$ according as to whether n is odd or even respectively. The resulting sign changes therefore explains the oscillatory error behaviour observed in Figure 1. Similar oscillatory behaviour has been observed by Gragg (1965) for the explicit midpoint rule (EMR). However, the oscillations in that case arise from the parasitic component of the numerical solution. Gragg was the first to introduce a technique known as *smoothing* to dampen the oscillations in the EMR solutions. The smoothing is achieved by simply applying the formula

$$\hat{y}_n = \frac{y_{n-1} + 2y_n + y_{n+1}}{4}.$$

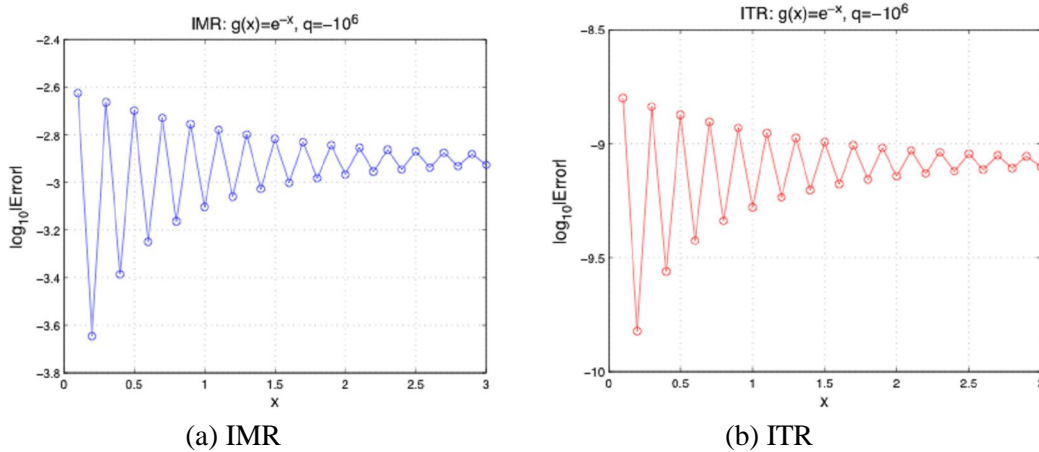


Figure 1: The error behaviour of IMR and ITR applied to the Prothero-Robinson problem for $q = -10^6$, $h = 0.1$ at $x_n = 3$

For the IMR and the ITR, it turns out that the use of the smoothing formula also dampens the oscillations when applied at every step (see Figure 2). Gragg was also the first to prove the existence of an asymptotic error expansion (6) for the EMR and pioneered the application of extrapolation in ordinary differential equations.

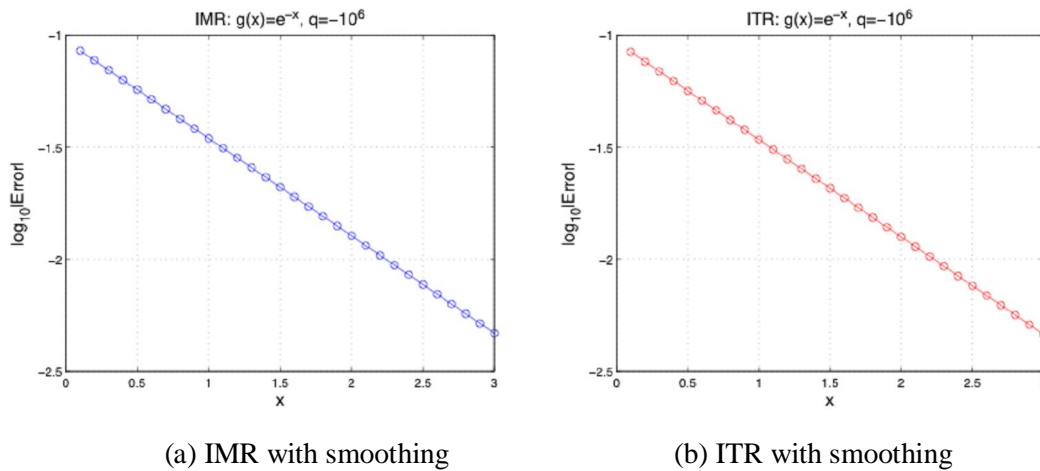


Figure 2: The error behaviour of IMR and ITR with smoothing applied to the Prothero-Robinson problem for $q = -10^6$, $h = 0.1$ at $x_n = 3$

Gragg's idea became popular and was tested by Bulirsch and Stoer (1966) for nonstiff problems. They developed an algorithm known as the "Gragg-Bulirsch-Stoer" (GBS) method using rational extrapolation and implemented with an automatic stepsize selection. This was the first code (ODEX) developed by Bulirsch and Stoer and their students in 1966. Following this success, Lindberg (1971), Bader and Deuffhard (1983) extended the application of extrapolation to the solution of stiff ordinary differential equations (ODEs). Lindberg implemented the smoothing formula of Gragg for the ITR while Bader and Deuffhard developed an extrapolation code for stiff ODEs known as METAN1 using the semi-implicit (linearly implicit) midpoint rule.

This idea of smoothing was then extended by Chan (1989) to arbitrary symmetric Runge-Kutta methods. The generalised smoothing is called *symmetrization* and is constructed by composing two symmetric Runge-Kutta methods but with different weights. The symmetrization generalises the smoothing formulas used by Dahlquist and Lindberg (1973) for the IMR and ITR. A symmetrizer is constructed with the following properties:

- (1) It preserves the h^2 -asymptotic error expansion of the symmetric method;
- (2) It is L-stable ($R(\infty) = 0$).

Symmetrization will then result in some important features such as:

- (1) The damping of the oscillatory and stiff error components in the numerical solution;
- (2) The suppression of order reduction effects that may accompany high order symmetric methods when solving stiff problems.

When an A-stable method exhibits order reduction it is not feasible to apply extrapolation. This phenomenon can be easily explained in the case of the PR test problem. Referring to

equations (7) and (10), the term $1 - kb^T c^{k-1}$ vanishes for $k = 1, \dots, p$ if $B(p)$ holds, while $c^k - kAc^{k-1}$ vanishes for $k = 1, \dots, r$ if $C(r)$ holds. Since \mathbf{G}_2 satisfies $B(4)$ and $C(2)$ we have $\varphi_i(z) = O(h^3)$ as $h \rightarrow 0$ for large $|q|$. However, $R(z) \rightarrow 1$ and the sum over the local error terms in the global error introduces a factor n which results in the global error behaving like $O(h^2)$ since $nh = x_n$. This is the phenomenon of order reduction where the error behaviour of the method for stiff problems is governed by the stage order. The situation for \mathbf{L}_3 is more complicated because its A -matrix is nonsingular. In this case, however, $C(3)$ holds and we have $\varphi_i(z) = z^{-1}O(h^4)$. Since $R(z) \rightarrow 1$ for large $|z|$, the global error therefore behaves like $z^{-1}O(h^3) = q^{-1}O(h^2)$. The features 1 and 2 above are achievable with symmetrization.

2. Symmetrization

The technique of symmetrization is given by Chan (1990) as follows:

- (1) Apply $n-1$ steps of the symmetric method \mathbf{R} with stepsize $h = H/n$ over a total length of $H - h$.
- (2) Replace the last step of length h by the symmetrizer $\tilde{\mathbf{R}}$.

The main reason for applying a symmetrizer at the last step is to improve the accuracy of the solution because the symmetrizer dampens the influence of the stiff components.

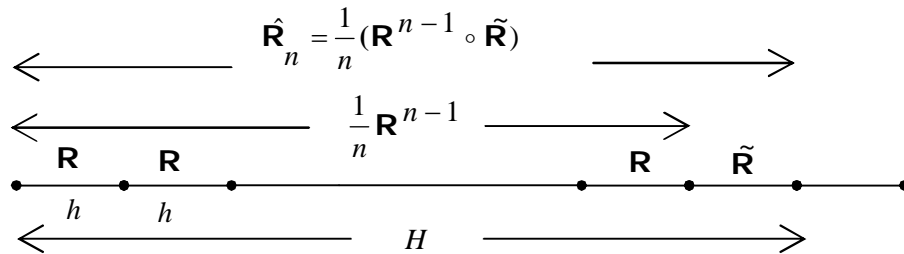


Figure 3: Symmetrization technique

This effect of the smoothing technique for strongly stiff problems was observed by Lindberg (1971) for the ITR and by Auzinger and Frank (1989) for the IMR.

3. Construction of Symmetrizers

Symmetrizers are constructed so as to satisfy the damping property, $\tilde{R}(\infty) = 0$, and as many order conditions as possible. A symmetrizer $\tilde{\mathbf{R}}$ for the symmetric method $\mathbf{R} = (A, b, c)$ with s stages is generated by

$$\tilde{\mathbf{R}} = \frac{c}{e+c} \left| \begin{array}{cc|cc} & & A & O \\ & & eb^T & A \\ \hline & & b^T - u^T P & u^T \end{array} \right., \quad (11)$$

where P is the permutation matrix that interchanges the first component with the last, second with the second last, etc.

The symmetrizer itself is a method consisting of the composition of two steps of \mathbf{R} but with different weights for the final update. The weight vector u carries s parameters to be determined. The internal stages at the n^{th} and $(n+1)^{\text{st}}$ steps are computed and then combined to give the update at the n^{th} step using the weights as given in (11). Moreover, the symmetrizer can be applied in different ways:

- In the *passive* mode we compute many steps with the symmetric method, storing the values of the update as well as the internal stage values, and apply symmetrization whenever required.
- In the *active* mode we use the symmetrized value to propagate the numerical solution. In this way symmetrization can be applied at every step, or at every two or more steps. Although this involves additional computational cost compared to the passive mode, the greater accuracy obtained could result in greater efficiency.

The construction of symmetrizers for higher order methods is more complicated than the smoothing formula of Gragg which involves the update values only. It requires additional storage of the internal stage values as well as the update values.

Let $(\tilde{A}, \tilde{b}, \tilde{c})$ denote the triple for the symmetrizer, where

$$\tilde{A} = \begin{bmatrix} A & O \\ eb^T & A \end{bmatrix}, \quad \tilde{c} = \begin{bmatrix} c \\ e+c \end{bmatrix}, \quad \tilde{b} = \begin{bmatrix} b - Pu \\ u \end{bmatrix}, \quad \tilde{I} = \begin{bmatrix} I & 0 \\ 0 & I \end{bmatrix}, \quad \tilde{e} = \begin{bmatrix} e \\ e \end{bmatrix}. \quad (12)$$

The stability function of the symmetrizer is given by

$$\tilde{R}(z) = 1 + z\tilde{b}^T (\tilde{I} - z\tilde{A})^{-1} \tilde{e} = R(z)(1 + 2z^2 u^T (I - z^2 A^2)^{-1} c). \quad (13)$$

If the matrix A is nonsingular, the requirement $\tilde{R}(\infty) = 0$ then leads to the damping condition

$$u^T A^{-1} e = \frac{1}{2}, \quad (14)$$

and the symmetrized update is given by

$$\tilde{y}_n = u^T A^{-1} (PY^n + Y^{n+1}).$$

The condition for the symmetrizer to be of order 3 is

$$u^T c = 0. \quad (15)$$

Solving (14) and (15) for \mathbf{G}_2 then yields $u_1 = \frac{1}{24} + \frac{\sqrt{3}}{24}$, $u_2 = \frac{1}{24} - \frac{\sqrt{3}}{24}$ and hence

$$\tilde{y}_n = \left(\frac{1}{4} + \frac{\sqrt{3}}{6} \right) (Y_1^{n+1} + Y_2^n) + \left(\frac{1}{4} - \frac{\sqrt{3}}{6} \right) (Y_1^n + Y_2^{n+1}), \quad (16)$$

that is, the symmetrized update at the n^{th} step is obtained by taking the linear combination of the internal stage values at the n^{th} and the $(n+1)^{\text{st}}$ steps of the method \mathbf{G}_2 . The stability function of the symmetrizer is given by

$$\tilde{R}(z) = \frac{1 - \frac{1}{12}z^2}{\left(1 - \frac{1}{2}z + \frac{1}{12}z^2\right)^2}. \quad (17)$$

If A is singular, we use an invertible submatrix to construct the symmetrizer. We consider the special case of the s -stage Lobatto IIIA method where the first row of A is a row of zeros and the last row of A is equal to the weights. We define

$$A = \begin{bmatrix} 0 & 0 \\ \bar{a} & \bar{A} \end{bmatrix}, \quad c = \begin{bmatrix} 0 \\ \bar{c} \end{bmatrix}, \quad b = \begin{bmatrix} b_1 \\ \bar{b} \end{bmatrix}, \quad I = \begin{bmatrix} 1 & 0 \\ 0 & \bar{I} \end{bmatrix}, \quad e = \begin{bmatrix} 1 \\ \bar{e} \end{bmatrix}. \quad (18)$$

where $\bar{a}, \bar{b}, \bar{c}$ and \bar{e} are $(s-1) \times 1$ subvectors and \bar{A}, \bar{I} are the $(s-1) \times (s-1)$ reduced submatrices. In this case, (11) is reducible by one stage and therefore the symmetrizer carries only $(s-1)$ parameters.

From (13) the stability function in this case is given by

$$\tilde{R}(z) = R(z) \left(1 + 2z^2 \bar{u}^T (\bar{I} - z^2 \bar{A}^2)^{-1} \bar{c} \right). \quad (19)$$

As $z \rightarrow \infty$, we have

$$\tilde{R}(\infty) = R(\infty) (1 - 2\bar{u}^T \bar{A}^{-2} \bar{c}), \quad (20)$$

which gives the damping condition $\bar{u}^T \bar{A}^{-2} \bar{c} = \frac{1}{2}$. Using a similar approach to that for \mathbf{G}_2 reducibility gives only two parameters u_1 and u_2 that need to be solved. Solving for u_1 and u_2

using the order condition $\bar{u}^T \bar{c} = 0$ and the damping condition then gives the symmetrized update for \mathbf{L}_3 as

$$\tilde{y}_n = \frac{1}{2} \left(-y_{n-1} + 4Y^{(n)} + 6y_n + 4Y^{(n+1)} - y_{n+1} \right), \quad (21)$$

where $Y^{(\bullet)}$ refers to the stage value at the midpoint of the step. The stability function is also given by (17).

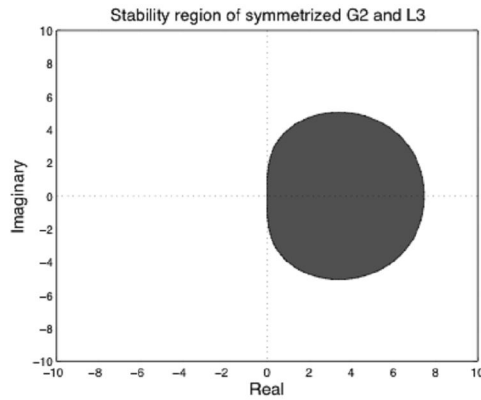


Figure 4: The unshaded region is the stability region which includes the left half-plane

4. Numerical Experiments

In this section we present numerical results for \mathbf{G}_2 and \mathbf{L}_3 with active and passive symmetrization. We will show that the methods are more efficient when used with symmetrization in either mode. The numerical results are given for some linear and nonlinear test problems. Efficiency has been measured in terms of CPU time. In all the graphs the symmetric methods are denoted by G2 and L3, while passive and active modes are denoted by PS and AS respectively.

Problem 1

$$y' = qy + e^{-x}, \quad y(0) = -\frac{1}{1+q}, \quad q \in (-\infty, -2], \quad y(x) = -\frac{1}{1+q} e^{-x}.$$

We integrated to $x_n = 10$ with stepsize $h = 0.5$ and $q = -10^6$.

Problem 2: Kaps

$$\begin{aligned} y_1'(x) &= (q-1)y_1 - qy_2^2, & y_1(0) &= 1, & y_1(x) &= e^{-2x}, \\ y_2'(x) &= y_1 - y_2(1+y_2), & y_2(0) &= 1, & y_2(x) &= e^{-x}. \end{aligned}$$

We integrated to $x_n = 10$ with $h = 0.5$.

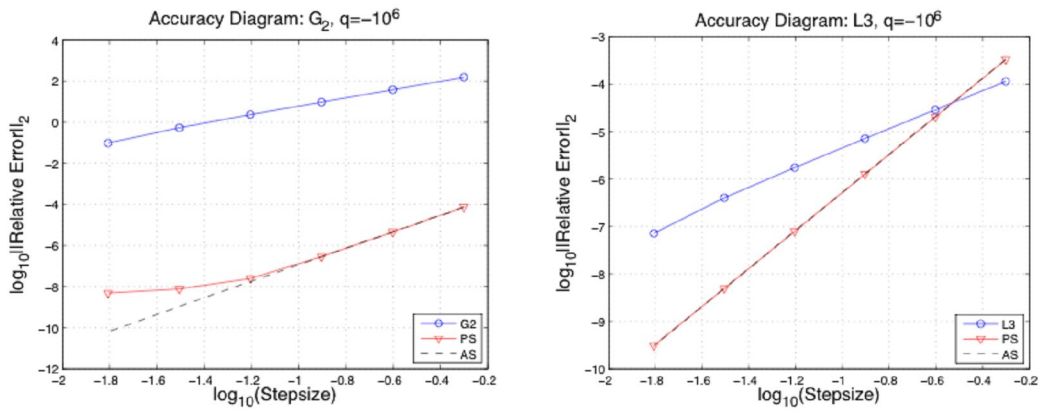


Figure 5: Accuracy diagram G_2 and L_3 with active and passive symmetrization applied to Problem 1

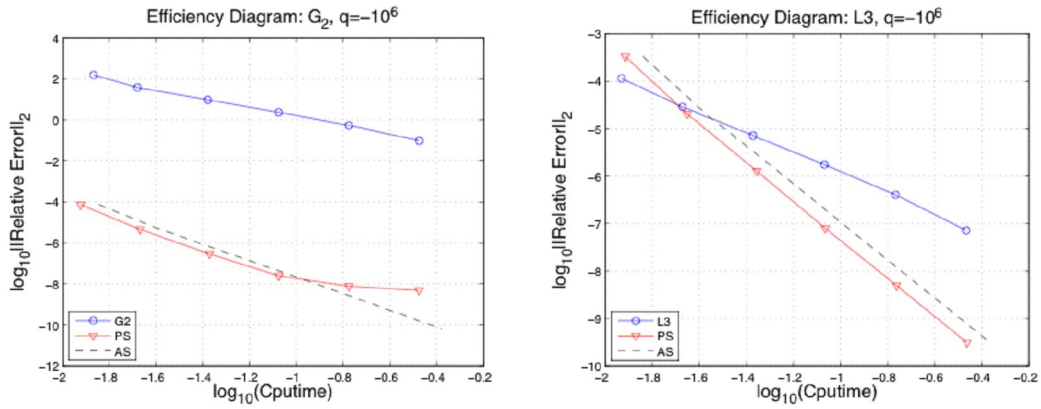


Figure 6: Efficiency diagram of G_2 and L_3 with active and passive symmetrization applied to Problem 1

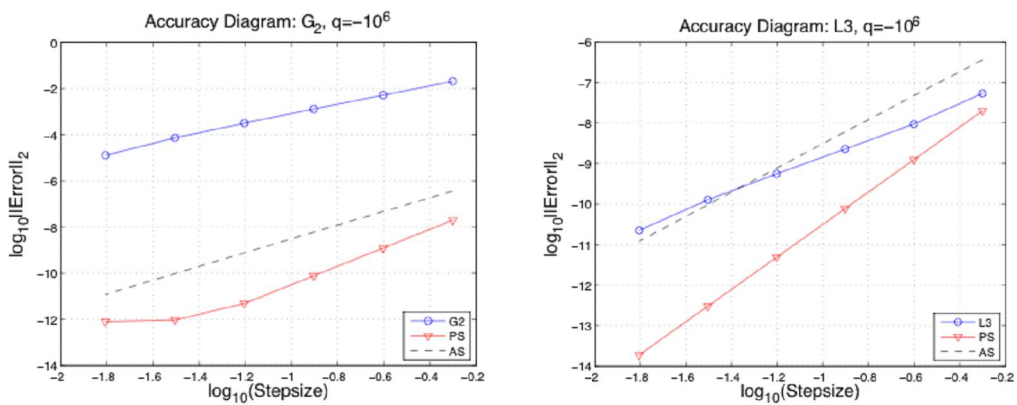


Figure 7: Accuracy diagram of G_2 and L_3 with active and passive symmetrization applied to Problem 2

Order-4 symmetrized Runge-Kutta methods for stiff problems

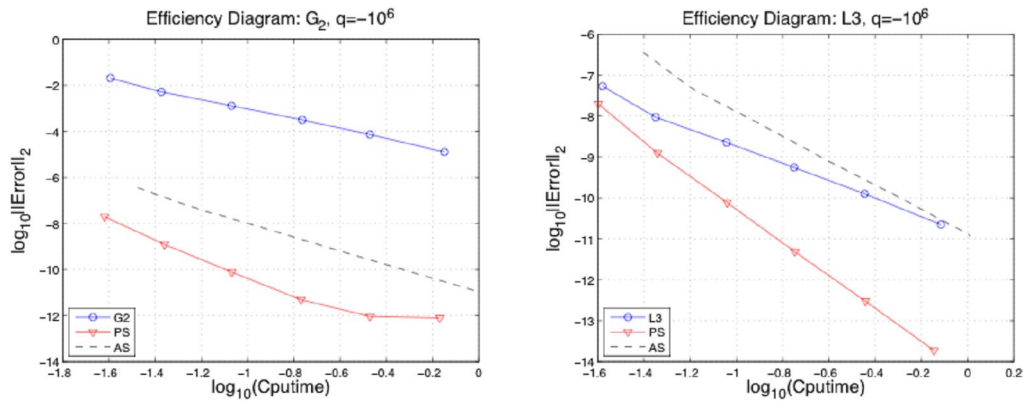


Figure 8: Efficiency diagram of G_2 and L_3 with active and passive symmetrization applied to Problem 2

Problem 3

$$\begin{aligned}
 y_1'(x) &= qy_1 + y_2^2, & y_1(0) &= -\frac{1}{q+2}, & y_1(x) &= -\frac{e^{-2x}}{q+2}, \\
 y_2'(x) &= -y_2, & y_2(0) &= 1, & y_2(x) &= e^{-x}.
 \end{aligned}$$

We integrated to $x_n = 10$ with $h = 0.5$.

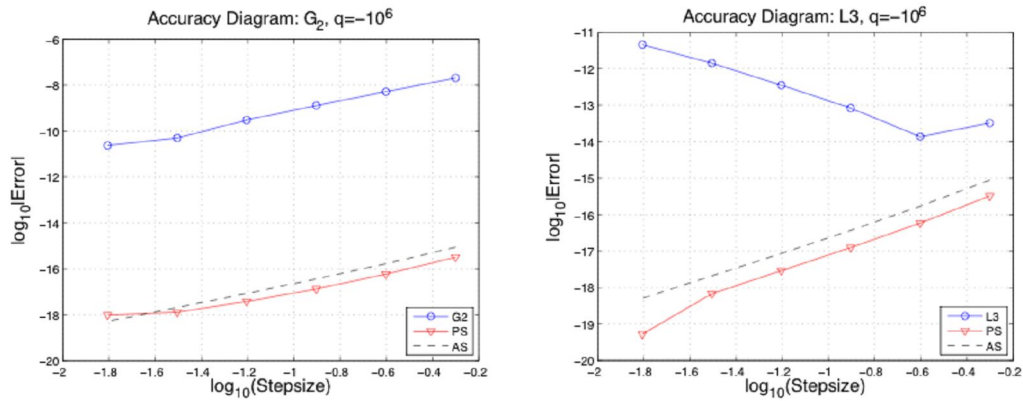


Figure 9: Accuracy diagram of G_2 and L_3 with active and passive symmetrization applied to Problem 3 for the first component of y_1

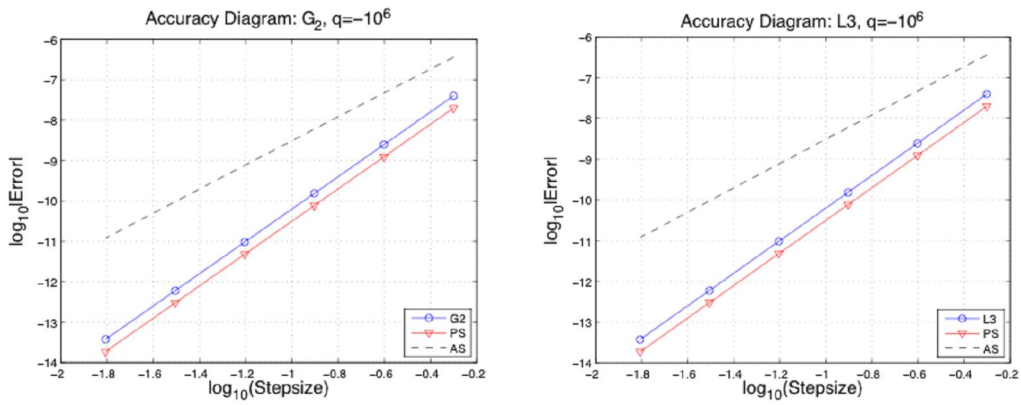


Figure 10: Accuracy diagram of \mathbf{G}_2 and \mathbf{L}_3 with active and passive symmetrization applied to Problem 3 for the second component of y_2

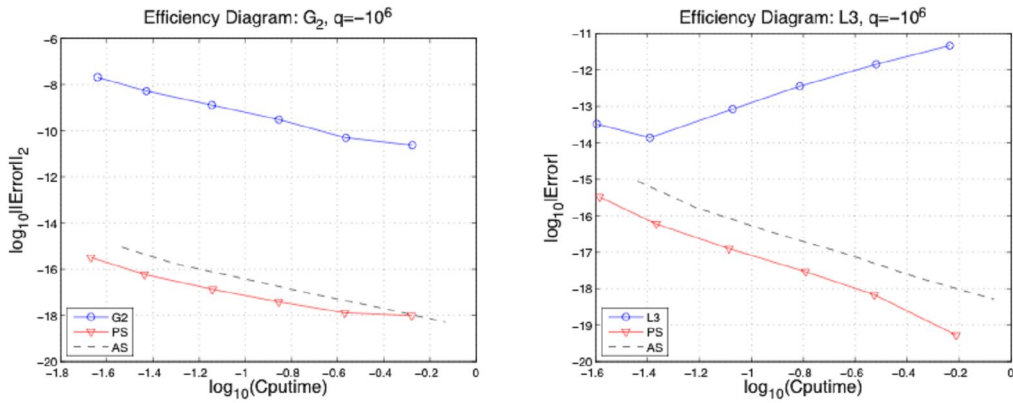


Figure 11: Efficiency diagram of \mathbf{G}_2 and \mathbf{L}_3 with active and passive symmetrization applied to Problem 3 for the first component of y_1

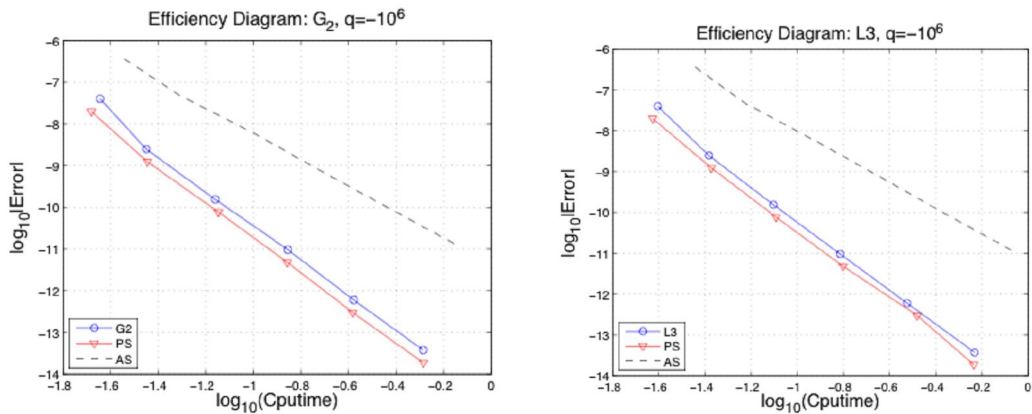


Figure 12: Efficiency diagram of \mathbf{G}_2 and \mathbf{L}_3 with active and passive symmetrization applied to Problem 3 for the second component of y_2

Problem 3 is different from Problem 2. It is a coupling from nonstiff to stiff where the exact solution is now dependent on the stiff parameter and the solution becomes smaller as $|q|$ increases. Therefore we present the graphs of the base methods as well as the active and passive symmetrization on each component y_1 and y_2 . In this plot, we observe an interesting result on the stiff component. The summary of the results for each problem is discussed in the following section.

Discussion

The numerical results obtained for the three test problems suggest the following:

- (1) In all cases symmetric methods are more efficient when applied with symmetrization, and that the passive mode is more efficient than the active mode.
- (2) In Problems 1 and 2 symmetrization increases the order of G2 and L3. In the passive mode the classical order is restored; in the active mode, the classical order is restored for Problem 1 whereas the order is one less for Problem 2.
- (3) We note that in Problem 3 the error in the stiff component of L3 increases with decreasing stepsize. This is in contrast to its behaviour in Problems 1 and 2. However, it is interesting that symmetrization in both modes gives much greater efficiency (see Figure 11). On the other hand we observed that the nonstiff component of L3 gives greater accuracy since the method does not suffer from order reduction. Nevertheless, passive symmetrization is marginally more efficient than the base method (see Figure 12).

We are not in the position to decide which of G2 or L3 is more efficient on the basis of our experimental results. It is necessary to perform further experiments on a wider variety of problems.

5. Conclusion

This study provides some evidence to suggest that symmetrization is essential in order to increase the efficacy of using symmetric methods for solving strongly stiff problems. This is particularly important for higher order symmetric methods in underpinning the use of extrapolation. Further experiments are being conducted using a variable stepsize algorithm on nonlinear, stiff and mildly stiff problems of higher dimensions and will be reported in a future publication.

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