

**SOME EFFICIENT IMPLEMENTATION SCHEMES  
FOR IMPLICIT RUNGE-KUTTA METHODS**

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**Abstract:** Several iteration schemes have been proposed to solve the non-linear equations arising in the implementation of implicit Runge-Kutta methods. As an alternative to the modified Newton scheme, some iteration schemes with reduced linear algebra costs have been proposed. A scheme of this type proposed in [9] avoids expensive vector transformations and is computationally more efficient. The rate of convergence of this scheme is examined in [9] when it is applied to the scalar test differential equation  $x' = qx$  and the convergence rate depends on the spectral radius of the iteration matrix  $M(z)$ , a function of  $z = hq$ , where  $h$  is the step-length. In this scheme, we require the spectral radius of  $M(z)$  to be zero at  $z = 0$  and at  $z = \infty$  in the  $z$ -plane in order to improve the rate of convergence of the scheme. New schemes with parameters are obtained for three-stage and four-stage Gauss methods. Numerical experiments are carried out to confirm the results obtained here.

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## 1. Background

Let us consider an initial value problem for stiff system of  $n(\geq 1)$  ordinary

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differential equations

$$x' = f(x(t)), \quad x(t_0) = x_0, \quad f : \mathbb{R}^n \rightarrow \mathbb{R}^n, \quad (1)$$

where  $f$  is assumed to be as smooth as necessary. An  $s$ -stage implicit Runge-Kutta method computes an approximation  $x_{r+1}$  to the solution  $x(t_{r+1})$  at grid point  $t_{r+1} = t_r + h$  by

$$x_{r+1} = x_r + h \sum_{i=1}^s b_i f(y_i)$$

where the internal approximations  $y_1, y_2, \dots, y_s$  satisfy the  $sn$  equations

$$y_i = x_r + h \sum_{j=1}^s a_{ij} f(y_j), \quad i = 1, 2, \dots, s \quad (2)$$

$A = [a_{ij}]$  is the real coefficient matrix and  $b = (b_1, b_2, \dots, b_s)^T$  is the column vector of the Runge-Kutta method. Let  $Y = y_1 \oplus y_2 \oplus \dots \oplus y_s \in \mathbb{R}^{sn}$  and let  $F(Y) = f(y_1) \oplus f(y_2) \oplus \dots \oplus f(y_s) \in \mathbb{R}^{sn}$ . Then equation (2) may be represented by the compact form

$$Y = e \otimes x_r + h(A \otimes I_n)F(Y) \quad (3)$$

where  $e = (1, 1, \dots, 1)^T$  and  $A \otimes I_n$  is the Kronecker product of the matrix  $A$  with  $n \times n$  identity matrix  $I_n$  and, in general  $A \otimes B = [a_{ij}B]$ . This article deals with methods suitable for stiff systems so that the matrix  $A$  is not strictly lower triangular and, in particular, is concerned with Gauss methods since they have highest order and good stability properties.

Equation (3) may be solved by a modified Newton iteration. Let  $J$  be the Jacobian of  $f$  evaluated at some recent point  $x_r$ , updated infrequently. The modified Newton scheme evaluates  $Y^1, Y^2, Y^3, \dots$ , to satisfy

$$(I_{sn} - hA \otimes J)(Y^m - Y^{m-1}) = D(Y^{m-1}), \quad m = 1, 2, \dots, \quad (4)$$

where  $D$  is the approximation defect,  $D(Z) = e \otimes x_r - Z + h(A \otimes I_n)F(Z)$ . In each step of this iteration, a set of  $sn$  linear equations has to be solved. Schemes have been developed, to solve equation (4), which use the fact that  $J$  is constant [1], [6], [7]. In other schemes advantage is taken of the special forms of some implicit methods [2], [4], [5], [12].

In another approach, schemes based directly on iterative procedure have been developed [3], [8], [9], [10],[13],[21]. For a singly implicit method, there is a non-singular matrix  $S$  so that  $S^{-1}AS = \lambda(I_s - L)^{-1}$ , where  $L$  is zero except

for some ones on the sub-diagonal. On applying this transformation, the scheme (4) becomes

$$\begin{aligned} [I_s \otimes (I_n - h\lambda J)]E^m &= [(I_s - L)S^{-1} \otimes I_n]D(Y^{m-1}) + (L \otimes I_n)E^m, \\ Y^m &= Y^{m-1} + (S \otimes I_n)E^m, \quad m = 1, 2, 3 \dots \end{aligned} \quad (5)$$

Cooper and Butcher [8] proposed an iterative scheme, sacrificing superlinear convergence for reduced linear algebra cost, which may be regarded as a generalization of the scheme (5) for singly implicit methods. They considered the scheme

$$\begin{aligned} [I_s \otimes (I_n - h\lambda J)]E^m &= (B_1 S^{-1} \otimes I_n)D(Y^{m-1}) + (L_1 \otimes I_n)E^m, \\ Y^m &= Y^{m-1} + (S \otimes I_n)E^m, \quad m = 1, 2, \dots, \end{aligned} \quad (6)$$

where  $B_1$  and  $S$  are real  $s \times s$  non-singular matrices and  $L_1$  is strictly lower triangular matrix of order  $s$ , and  $\lambda$  is a real constant. Cooper and Butcher [8] showed that successive over-relaxation may be applied to improve the rate of convergence for scalar test problem. Peat and Thomas [19], after extensive numerical experiments, concluded that the schemes proposed by Cooper and Butcher are, in general, the most efficient schemes for integration of stiff problems. Gladwell and Thomas [15] recommended this scheme for the two-stage Gauss method. Each step of the scheme (6) requires  $s$  function evaluations and the solution of  $s$  sets of  $n$  linear equations. These  $s$  sub-steps are performed in sequence and it is not possible to compute elements of  $Y^m = y_1^m \oplus y_2^m \oplus \dots \oplus y_s^m$  until all sub-steps are completed. Cooper and Vignesvaran [9] considered a scheme where these elements are obtained in sequence and the approximation defect is updated after each sub-step completed. Only one vector transformation is needed for each full step so that this scheme is more efficient. Another scheme was proposed by Cooper and Vignesvaran [10] in order to obtain improved rate of convergence, by adding extra sub-steps. Vigneswaran [20] obtained further improvement in the rate of convergence of the iteration scheme proposed in [10]. Gonzalez, Gonzalez and Montijano [16] proposed a scheme for Gauss methods using an iterative procedure of semi-implicit type in which the Jacobian does not appear explicitly. A scheme of this type was proposed in [17] in which convergence and stability properties of the scheme are discussed in detail.

## 2. Efficient Iteration Scheme

Cooper and Vigneswaran [9] proposed the scheme

$$\begin{aligned}
 [I_s \otimes (I_n - h\lambda J)]E^m &= (L \otimes I_n)(e \otimes x_r - Y^m) \\
 &\quad + (U \otimes I_n)(e \otimes x_r - Y^{m-1}) \\
 &\quad + h(T \otimes I_n)F(Y^m) \\
 &\quad + h(R \otimes I_n)F(Y^{m-1}) \\
 Y^m &= Y^{m-1} + E^m, m = 1, 2, \dots, \quad (7)
 \end{aligned}$$

where  $B$  is a real non-singular matrix such that  $B = L + U$  and  $BA = T + R$ ,  $L$  and  $T$  are strictly lower triangular matrices,  $U$  and  $R$  are upper triangular matrices, and  $\lambda$  is a real constant. Cooper and Vigneswaran [9] showed that  $D(Y) = 0$  if the sequence  $\{Y^m\}$  has a limit  $Y$  and  $f$  is continuous on  $\mathbb{R}^n$ . They observed that the scheme can be implemented efficiently by updating  $Y^{m-1}$  and  $F(Y^{m-1})$  as soon as each element of  $Y^m = y_1^m \oplus y_2^m \oplus \dots \oplus y_s^m$  is computed. The work involved is no more than is needed to carry out an evaluation of  $D(Y^{m-1})$  followed by a transformation to  $(B \otimes I_n)D(Y^{m-1})$ .

Cooper and Vigneswaran [9] tested the rate of convergence of this scheme when it is applied to the scalar test problem  $x' = qx$  with rapid convergence required for all  $z \in \mathbb{C}^-$ , where  $\mathbb{C}^- = \{z \in \mathbb{C} : \text{Re} \leq 0\}$ . For this test problem, the scheme gives (7) gives

$$Y - Y^m = M(z)(Y - Y^{m-1}), \quad m = 1, 2, \dots,$$

and the rate of convergence depends on the spectral radius  $\rho[M(z)]$  of the iteration matrix

$$M(z) = I_s - [(I_s + L - z(\lambda I_s + T))^{-1}B(I_s - zA)]. \quad (8)$$

Cooper and Vigneswaran[9] imposed the condition that the iteration matrix  $M$  has only one non-zero eigenvalue  $\phi$ ,

$$\phi(z) = 1 - \beta \frac{\det(I_s - zA)}{(1 - \lambda z)^s}, \quad (9)$$

so that the spectral radius,  $\rho[M(z)]$ , given by  $\rho[M(z)] = |\phi(z)|$  and  $\lambda$  and  $\beta (= \det B)$  can be chosen to solve the problem

$$\min_{\lambda, \beta} \max_{z \in \mathbb{C}^-} \rho[M(z)]. \quad (10)$$

To solve the minimization problem (10), when  $\lambda > 0$  it follows from (9) that  $\phi$  is analytic and bounded on  $\mathbb{C}^-$  and hence  $|\phi|$  attains its maximum on the imaginary axis  $z = iy, y$  real. The polynomial  $p$ , defined by

$$p(\omega) = |\phi(iy)|^2, \quad \omega = \frac{1}{1 + (\lambda y)^2}, \tag{11}$$

is a polynomial of degree  $s$ . For a given method, the coefficients of  $p$  depends on  $\lambda$  and  $\beta$  only and Cooper and Vignesvaran[9] obtained these parameters to minimize the maximum of  $p$  on  $[0, 1]$  for the Gauss methods of order 4,6 and 8 respectively.

Consider the three-stage Gauss method with matrix of coefficients

$$A = \begin{bmatrix} \frac{5}{36} & \frac{2}{9} - \frac{\sqrt{15}}{15} & \frac{5}{36} - \frac{\sqrt{15}}{30} \\ \frac{5}{36} + \frac{\sqrt{15}}{24} & \frac{2}{9} & \frac{5}{36} - \frac{\sqrt{15}}{24} \\ \frac{5}{36} + \frac{\sqrt{15}}{30} & \frac{2}{9} + \frac{\sqrt{15}}{15} & \frac{5}{36} \end{bmatrix} \tag{12}$$

and  $\det(I - zA) = 1 - \frac{1}{2}z + \frac{1}{10}z^2 - \frac{1}{120}z^3$ .

Cooper and Vignesvaran[9]obtained the optimum values  $\lambda = 0.202740067$  and  $\beta = 1.159572736$  when solving the problem(10). For these values of  $\lambda$  and  $\beta, \rho[M(z)] < 0.1599$  for all  $z \in \mathbb{C}^-$ .

Next it remains to choose the elements of  $B = [b_{ij}]$  so that the iteration matrix  $M(z) = [m_{ij}(z)]$  is strictly upper triangular matrix except that  $m_{ss}(z) = \phi$ , a non-zero eigenvalue. For the three-stage Gauss method, the condition on  $M(z)$  gives

$$\begin{aligned} b_{11} &= 1, \\ b_{12}a_{21} + b_{13}a_{31} &= \lambda - a_{11}, \\ b_{12}(a_{22} - \lambda) + b_{13}a_{32} &= -a_{12}, \\ b_{21}b_{12} - b_{22} &= -1, \\ b_{21}(a_{12} - b_{12}a_{11}) + b_{22}(a_{22} - a_{21}b_{12}) + b_{23}(a_{32} - a_{31}b_{12}) &= \lambda, \\ b_{31}b_{12} &= 0, \\ b_{31}a_{11} + b_{32}a_{21} + b_{33}a_{31} &= 0. \end{aligned} \tag{13}$$

From (13), it happens that  $b_{31} = 0$ . Again the equations (13) together with  $\det B = \beta$  may be solved by choosing  $b_{21} = 0$  and this gives

$$B = \begin{bmatrix} 1 & 0.151290053 & 0.068750541 \\ 0 & 1 & 0.058981649 \\ 0 & -0.983175783 & 1.101583408 \end{bmatrix}. \quad (14)$$

Consider the four-stage Gauss method with matrix of coefficients  $A = [a_{ij}]$  obtained by solving the sets of equations

$$\sum_{j=1}^4 a_{ij} c_j^{r-1} = \frac{c_i^r}{r}, \quad r = 1, 2, 3, 4,$$

for each  $i = 1, 2, 3, 4$ , where  $c_1, c_2, c_3, c_4$  are the zeros of  $P_4(2x - 1)$ , the transformed legendre polynomial of degree 4. For this method,

$$\det(I - zA) = 1 - \frac{1}{2}z + \frac{3}{28}z^2 - \frac{1}{84}z^3 + \frac{1}{1680}z^4.$$

The condition on  $M(z)$  with the choices  $b_{31} = 0$  and  $b_{41} = b_{42} = 0$  give a system of equations which may be ordered as a sequence of sets of linear equations given below:

$$\begin{aligned} b_{11} &= 1, \\ b_{12}a_{21} + b_{13}a_{31} + b_{14}a_{41} &= (\lambda - a_{11}), \\ b_{12}(a_{22} - \lambda) + b_{13}a_{32} + b_{14}a_{42} &= -a_{12}, \\ b_{12}a_{23} + b_{13}(a_{33} - \lambda) + b_{14}a_{43} &= -a_{13}, \end{aligned} \quad (15)$$

$$\begin{aligned} b_{12}b_{21} - b_{22} &= -1, \\ b_{13}b_{21} - b_{23} &= 0, \\ (b_{12}a_{11} - a_{12})b_{21} + (b_{12}a_{21} - a_{22})b_{22} \\ + (b_{12}a_{31} - a_{32})b_{23} + (b_{12}a_{41} - a_{42})b_{24} &= -\lambda, \\ (a_{13} - b_{13}a_{11})b_{21} + (a_{23} - b_{13}a_{21})b_{22} \\ + (a_{33} - b_{13}a_{31})b_{23} + (a_{43} - b_{13}a_{41})b_{24} &= 0, \end{aligned} \quad (16)$$

$$\begin{aligned}
 b_{33} &= 1, \\
 b_{32}a_{21} + b_{34}a_{41} &= -a_{31}, \\
 b_{32}a_{23} + b_{34}a_{43} &= \lambda - a_{33},
 \end{aligned} \tag{17}$$

$$b_{43}a_{31} + b_{44}a_{41} = 0. \tag{18}$$

Cooper and Vignesvaran[9] showed that these equations can be solved only for one positive value of  $\lambda$ ,  $\lambda = 0.146840443$  and they obtained the optimum value  $\beta = 1.034$  to solve the problem (10). In this case,  $\rho[M(z)] < 0.3467$  for  $\text{Re}(z) \leq 0$ . With these values of  $\lambda$  and  $\beta$ , the set of equations (15),(16),(17),(18) and the equation  $\det B = \beta$  give

$$B = \begin{bmatrix} 1 & 0.265166833 & 0.079402432 & -0.018488567 \\ 0.124164683 & 1.032924356 & 0.009858978 & 0.124164683 \\ 0 & -0.786754443 & 1 & -0.108118541 \\ 0 & 0 & -1.109340683 & 1.045019753 \end{bmatrix}. \tag{19}$$

### 3. Schemes with Improving Rates of Convergence

In this section, additional constraints, which require super-linear convergence at the origin and infinity, are imposed on the spectral radius of the iteration matrix  $M(z)$  in addition to the condition that  $M(z)$  has only one non-zero eigenvalue. The results were obtained for the two-stage Gauss method in [22]. In this paper, new schemes corresponding to the iteration scheme (7) for three-stage and four-stage Gauss methods are obtained respectively.

#### 3.1. The Case $\rho[M(z)] = 0$ at $z = 0$

For the three-stage Gauss method, the additional constraint  $\rho[M(z)] = 0$  at  $z = 0$  gives  $\beta = 1$ . Therefore, the other parameter  $\lambda$  has to be chosen to solve

the problem(10). It follows from (11) that the polynomial  $p$  is given by

$$p(\omega) = a_0\omega(1 - \omega)^2 + (1 - \omega)[a_1\omega - a_2(1 - \omega)]^2,$$

where  $a_0 = 3 - \frac{1}{10\lambda^2}$ ,  $a_1 = 3 - \frac{1}{2\lambda}$ ,  $a_2 = 1 - \frac{1}{120\lambda^3}$ .

A simple grid search procedure shows that good approximation to the optimum value of  $\lambda$  to minimize the maximum of  $p$  on  $[0, 1]$  is given by  $\lambda = 0.191729022$ . Again the condition on  $M(z)$  gives the set of equations (13) and these equations together with  $\det B = \beta$  may be solved by choosing  $b_{21} = 0$ . This gives

$$B = \begin{bmatrix} 1 & 0.115697224 & 0.067542178 & 0 \\ 0 & 1 & 0.009448755 & 0 \\ 0 & -0.885047715 & 0.991637400 & 0 \end{bmatrix}. \quad (20)$$

In this case  $\rho[M(z)] < 0.2326$  for all  $z \in \mathbb{C}^-$ .

For the four-stage Gauss method, the additional constraint  $\rho[M(z)] = 0$  at  $z = 0$  gives  $\beta = 1$ . Again from (11), the polynomial  $p$  is given by

$$p(\omega) = (1 - \omega)^2[a_4(1 - \omega) - a_2\omega]^2 + \omega(1 - \omega)[a_1\omega - a_3(1 - \omega)]^2,$$

where  $a_1 = 4 - \frac{1}{2\lambda}$ ,  $a_2 = 6 - \frac{3}{28\lambda^2}$ ,  $a_3 = 4 - \frac{1}{84\lambda^3}$ ,  $a_4 = 1 - \frac{1}{1680\lambda^4}$ . Again the system of equations (15),(16),(17) and (18) can be solved only for  $\lambda = 0.146840443$  and for these fixed values of  $\lambda$  and  $\beta$ , the equations (15), (16), (17), (18)and  $\det B = \beta$  gives

$$B = \begin{bmatrix} 1 & 0.265166833 & 0.079402432 & -0.018488567 \\ 0.124164683 & 1.032924356 & 0.009858978 & 0.124164683 \\ 0 & -0.786754443 & 1 & -0.108118541 \\ 0 & 0 & -1.072863330 & 1.010657402 \end{bmatrix}. \quad (21)$$

In this case  $\rho[M(z)] < 0.3542$  for all  $z \in \mathbb{C}^-$ .

The equation  $|\phi(z)| = c$  describes a closed curve in the  $z$ -plane. Typical curves are plotted for different values of  $c$  and sketched in Figures 1 and 2 for three-stage and four-stage Gauss methods respectively. In this case,  $\rho[M(z)] \leq c$  on and interior to the curve. Since  $\rho[M(0)] = 0$ , these schemes are expected to perform well as typical stiff problems have Jacobian with some eigenvalues of small modulus.



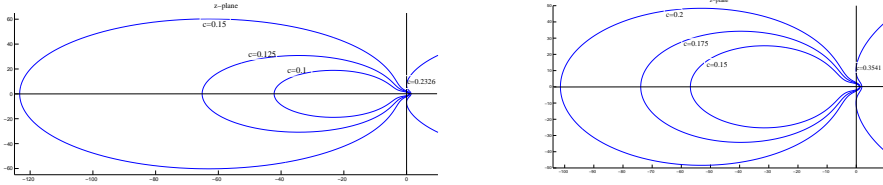


Figure 1: Curves  $\rho[M(z)] = c$  for  $s = 3$       Figure 2: Curves  $\rho[M(z)] = c$  for  $s = 4$

**3.2. The Case  $\rho[M(z)] = 0$  at  $z = \infty$**

The constraint  $\rho[M(\infty)] = 0$  for the three-stage Gauss method gives  $\lambda = \sqrt[3]{\frac{\beta}{120}}$  and the polynomial  $p$ , given by (11), is

$$p(\omega) = \omega[a_0\omega - a_2(1 - \omega)]^2 + a_1^2\omega^2(1 - \omega),$$

where  $a_0 = 1 - \beta$ ,  $a_1 = 3 - \frac{\beta}{2\lambda}$ ,  $a_2 = 3 - \frac{\beta}{10\lambda^2}$ . By search procedure, a good approximation to the optimum value of  $\beta$  is obtained by  $\beta = 1.181387098$  and the corresponding  $\lambda$  is given by  $\lambda = 0.214323763$ . In this case  $\rho[M(z)] < 0.2359$  for all  $z \in \mathbb{C}^-$ . With these values of  $\lambda$  and  $\beta$ , the equations (13) with  $\det B = \beta$  may be solved by choosing  $b_{21} = 0$ . This gives

$$B = \begin{bmatrix} 1 & 0.187138824 & 0.071808998 \\ 0 & 1 & 0.112237507 \\ 0 & -0.958395854 & 1.073819136 \end{bmatrix}. \tag{22}$$

For the four-stage Gauss method, the additional constraint  $\rho[M(\infty)] = 0$  gives  $\beta = 1680\lambda^4$ . It follows from (11) that the polynomial  $p$  is given by

$$p(\omega) = [a_0\omega^2 - a_2\omega(1 - \omega)]^2 + \omega(1 - \omega)[a_1\omega - a_3(1 - \omega)]^2,$$

where  $a_0 = 1 - \beta$ ,  $a_1 = 4 - \frac{\beta}{2\lambda}$ ,  $a_2 = 6 - \frac{3\beta}{28\lambda^2}$ ,  $a_3 = 4 - \frac{\beta}{84\lambda^3}$ . With the value  $\lambda = 0.146840443$ , which solves the sets of equations 15),(16),(17),(18), and the corresponding value of  $\beta$ , those sets of equations and  $\det B = \beta$  give

$$B = \begin{bmatrix} 1 & 0.265166833 & 0.079402432 & -0.018488567 \\ 0.124164683 & 1.032924356 & 0.009858978 & 0.124164683 \\ 0 & -0.786754443 & 1 & -0.108118541 \\ 0 & 0 & -0.837985352 & 0.789397936 \end{bmatrix}. \quad (23)$$

In this case  $\rho[M(z)] < 0.2189$  for all  $z \in \mathbb{C}^-$ .

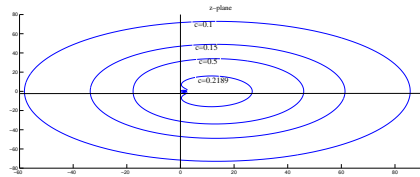
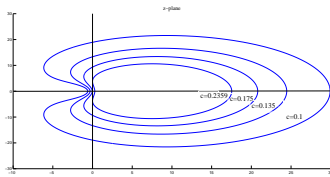


Figure 3: Curves  $\rho[M(z)] = c$  for  $s = 3$       Figure 4: Curves  $\rho[M(z)] = c$  for  $s = 4$

As per the plotted curves for  $\rho[M(z)] = c$  for different values of  $c$  in in Figures 3 and 4 for three-stage and four-stage Gauss methods, these schemes are expected to perform well as typical stiff problems have Jacobian with some eigenvalues of large negative real parts and  $\rho[M(\infty)] = 0$ .

### 4. Numerical Results

To evaluate the efficiency of the schemes obtained here, a range of numerical experiments was carried out. For each experiment, a single step was carried out, in each case, using the Jacobian evaluated at the initial point. For each scheme tested, the initial iterate  $Y^0$  is chosen as  $Y^0 = e \otimes x$ , where  $x$  is the true solution at the initial point.

**Problem 1** denotes the non-linear system given by [14]

$$\begin{aligned} x'_1 &= -0.013x_1 + 1000x_1x_3, & x_1(0) &= 1, \\ x'_2 &= 2500x_2x_3, & x_2(0) &= 1, \\ x'_3 &= 0.013x_1 - 1000x_1x_3 - 2500x_2x_3, & x_3(0) &= 0, \end{aligned}$$

where the eigenvalues of the Jacobian at the initial point are 0,  $-0.0093$  and  $-3500$ .

**Problem 2** is the elliptic two-body problem, with eccentricity 0.6,

$$\begin{aligned}x'_1 &= x_3, & x_1(0) &= 0.4, \\x'_2 &= x_4, & x_2(0) &= 0, \\x'_3 &= -x_1(x_1^2 + x_2^2)^{-3/2}, & x_3(0) &= 0, \\x'_4 &= -x_2(x_1^2 + x_2^2)^{-3/2}, & x_4(0) &= 2.\end{aligned}$$

The eigenvalues at the initial point are  $\pm 5.5902$  and  $\pm 3.9528i$ .

**Problem 3** is the HIRES problem given by [18],

$$\begin{aligned}x'_1 &= -1.71x_1 + 0.43x_2 + 8.32x_3 + 0.0007, & x_1(0) &= 1, \\x'_2 &= 1.71x_1 - 8.75x_2, & x_2(0) &= 0, \\x'_3 &= -10.03x_3 + 0.43x_4 + 0.035x_5, & x_3(0) &= 0, \\x'_4 &= 8.32x_2 + 1.71x_3 - 1.12x_4, & x_4(0) &= 0, \\x'_5 &= -1.745x_5 + 0.43x_6 + 0.43x_7, & x_5(0) &= 0, \\x'_6 &= -280x_6x_8 + 0.69x_4 + 1.71x_5) - 0.43x_6 + 0.69x_7, & x_6(0) &= 0, \\x'_7 &= 280x_6x_8 - 1.81x_7, & x_7(0) &= 0, \\x'_8 &= -x'_7, & x_8(0) &= 0.0057.\end{aligned}$$

The eigenvalues of the Jacobian at the initial point are  $0, -10.4841, -8.278, -0.2595, -0.5058, -2.3147$  and  $-2.6745 \pm 0.1499i$ .

**Problem 4** denotes the system

$$\begin{aligned}x'_1 &= x_2, & x_1(0) &= 2, \\x'_2 &= 10^6((1 - x_1^2)x_2) - x_1, & x_2(0) &= 0,\end{aligned}$$

derived from the Van der Pol's equation and given by [11]. The eigenvalues of the Jacobian at the initial point are close to 0 and  $-3000000$ .

**Problem 5** denotes the system, with non-linear coupling between smooth and transient components,

$$\begin{aligned}x'_1 &= -10^5x_1 + 2, & x_1(0) &= 1, \\x'_2 &= -10^6x_2 + 0.1x_1^2, & x_2(0) &= 1, \\x'_3 &= -40 \times 10^5x_3 + 0.4(x_1^2 + x_2^2), & x_3(0) &= 1, \\x'_4 &= -10^7x_4 + x_1^2 + x_2^2 + x_3^2, & x_4(0) &= 1,\end{aligned}$$

where the Jacobian has constant eigenvalues  $-10^5, -10^6, -40 \times 10^5$  and  $-10^7$ .

For each problem, a single step was carried out, in each case, using the Jacobian evaluated at the initial point. For each scheme tested, the initial iterate  $Y^0$  is chosen as  $Y^0 = e \otimes x$ , where  $x$  is the true solution at the initial point.

$e_m$	Method 1	Method 1*	Method 2	Method 2*
$e_1$	0.000956220	0.000824833	0.000895782	0.000866327
$e_2$	0.000152341	0.000110398	0.000142783	0.000143328
$e_3$	0.000024273	0.000000910	0.000028768	0.000028367
$e_4$	0.000003867	0.000000031	0.000001011	0.000000127
$e_5$	0.000000616	0.000000005	0.000000054	0.000000033
$e_6$	0.000000098	0.000000001	0.000000016	0.000000008
$e_7$	0.000000016	0.000000000	0.000000005	0.000000002
$e_8$	0.000000002		0.000000001	0.000000001
$e_9$	0.000000000		0.000000000	

Table 1: Values of  $e_m$  for Problem 1 with  $h = 0.1$ 

**Method 1** denotes the three-stage Gauss method implemented according to the iteration scheme(7) with  $\lambda = 0.202740067$  and the matrix  $B$  given by (14). **Method 1\*** is the same method implemented using the scheme (7) with  $\lambda = 0.191729022$  and  $B$  given by (20) for the case  $\rho[M(z)] = 0$  at  $z = 0$ . **Method 1\*\*** is also the same method implemented using the scheme (7) with  $\lambda = 0.214323763$ ,  $B$  given by (22) for the case  $\rho[M(z)] = 0$  at  $z = \infty$ . **Method 2** denotes the four-stage Gauss method implemented according to the scheme (7) with  $\lambda = 0.146840443$  and  $B$  given by (19). **Method 2\*** is the same method implemented using the scheme (7) with  $\lambda = 0.146840443$  and  $B$  given by (21) for  $\rho[M(0)] = 0$ . **Method 2\*\*** is also the same method implemented using the scheme (7) with the same value of  $\lambda$  and  $B$  given by (23) for  $\rho[M(\infty)] = 0$ .

For each method and problem, the quantities

$$e_m = \|E^m\|, \quad m = 1, 2, 3, \dots$$

were computed using the maximum norm on  $\mathbb{R}^{ns}$ . The values  $e_m$  for which  $e_m \leq \text{TOL} = 10^{-9}$  are tabulated for each problem and method. Similar results are obtained for different values of TOL. The results are given below for each problem for three-stage and four-stage Gauss methods.

$e_m$	Method 1	Method 1*	Method 2	Method 2*
$e_1$	0.064323263	0.055470109	0.060234720	0.058254081
$e_2$	0.010337141	0.007429666	0.009595467	0.009632142
$e_3$	0.001670882	0.000067048	0.001945151	0.001918104
$e_4$	0.000270379	0.000000270	0.000072013	0.000008450
$e_5$	0.000043831	0.000000002	0.000002754	0.000000149
$e_6$	0.000007117	0.000000000	0.000000106	0.000000000
$e_7$	0.000001157		0.000000004	
$e_8$	0.000000189		0.000000000	
$e_9$	0.000000031			
$e_{10}$	0.000000005			
$e_{11}$	0.000000001			

Table 2: Values of  $e_m$  for Problem 2 with  $h = 0.01$ 

$e_m$	Method 1	Method 1*	Method 2	Method 2*
$e_1$	0.017382122	0.015000547	0.016278083	0.015742827
$e_2$	0.002728084	0.002012693	0.002608108	0.002618024
$e_3$	0.000428244	0.000013213	0.000523517	0.000516215
$e_4$	0.000067235	0.000000021	0.000017567	0.000003710
$e_5$	0.000010557	0.000000000	0.000000591	0.000000025
$e_6$	0.000001658		0.000000020	0.000000000
$e_7$	0.000000260		0.000000001	
$e_8$	0.000000041			
$e_9$	0.000000006			
$e_{10}$	0.000000001			
$e_{11}$	0.000000000			

Table 3: Values of  $e_m$  for Problem 3 with  $h = 0.01$ 

## 5. Concluding Remarks

According to the numerical results, for three-stage Gauss method, the method 1\* performs better than method 1 for the problems whose Jacobian matrices have small eigenvalues and the method 1\*\* performs better than method 1 for the problems whose Jacobian matrices have eigenvalues with large negative real part. For four-stage Gauss method, Method 2\* is better than Method 2 for

$e_m$	Method 1	Method 1**	Method 2	Method 2**
$e_1$	0.000000820	0.000000840	0.000000884	0.000000876
$e_2$	0.000000149	0.000000155	0.000000364	0.000000275
$e_3$	0.000000024	0.000000018	0.000000119	0.000000007
$e_4$	0.000000004	0.000000000	0.000000039	0.000000001
$e_5$	0.000000001		0.000000013	0.000000000
$e_6$			0.000000004	
$e_7$			0.000000001	
$e_8$			0.000000001	

Table 4: Values of  $e_m$  for Problem 4 with  $h = 0.1$ 

$e_m$	Method 1	Method 1**	Method 2	Method 2**
$e_1$	1.229888995	1.259710539	1.325937141	1.313889816
$e_2$	0.223847832	0.232791462	0.546093036	0.412513120
$e_3$	0.035719849	0.026955933	0.177844840	0.010989760
$e_4$	0.005699876	0.000005372	0.057918610	0.000015235
$e_5$	0.000909531	0.000000009	0.018862359	0.000000018
$e_6$	0.000145134	0.000000001	0.006142907	0.000000000
$e_7$	0.000023159	0.000000000	0.002000561	
$e_8$	0.000003696		0.000651523	
$e_9$	0.000000590		0.000212182	
$e_{10}$	0.000000094		0.000069101	
$e_{11}$	0.000000015		0.000022504	
$e_{12}$	0.000000002		0.000007329	
$e_{13}$	0.000000000		0.000002387	
$e_{14}$			0.000000777	
$e_{15}$			0.000000253	

Table 5: Values of  $e_m$  for Problem 5 with  $h = 0.1$ 

problems with small eigenvalues and Method 2\*\* is better than Method 2 for problems with eigenvalues which have large negative real parts. In overall, the numerical experiments confirm that the new schemes obtained for the Gauss methods perform well.

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