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SOME EFFICIENT IMPLEMENTATION SCHEMES FOR IMPLICIT RUNGE-KUTTA METHODS

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Abstract: Several iteration schemes have been proposed to solve the nonlinear 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. Backround

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

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differential equations

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

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 $y_1, y_2, \cdots, y_s$ satisfy the sn equations

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

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

$$Y = e \otimes x_r + h(A \otimes I_n)F(Y) \tag{3}$$

where $e = (1, 1, \cdots, 1)^T$ 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 $Y^1, Y^2, Y^3, \cdots$, to satisfy

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

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

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

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

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

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 λ 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 $Y^m = y_1^m \oplus y_2^m \oplus \cdots \oplus y_s^m$ 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 Vignesvaran [9] proposed the scheme

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

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 λ is a real constant. Cooper and Vignesvaran [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 $Y^m = y_1^m \oplus y_2^m \oplus \cdots \oplus y_s^m$ 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 Vignesvaran [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 $\mathbb{C}^- = \{z \in \mathbb{C} : \mathrm{Re} \leq 0\}$. For this test problem, the scheme gives (7) gives

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

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

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

Cooper and Vignesvaran[9] imposed the condition that the iteration matrix M has only one non-zero eigenvalue ϕ,

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

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

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

To solve the minimization problem (10),when $\lambda > 0$ it follows from (9) that ϕ 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 polynimial of degree s. For a given method, the coefficients of p depends on λ and β 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 λ and β, $\rho[M(z)] < 0.1599$ 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

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

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

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

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 lnear equations given below:

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

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

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

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

Cooper and Vignesvaran[9] showed that these equations can be solved only for one positive value of λ, $\lambda = 0.146840443$ and they obtained the optimum value $\beta = 1.034$ to solve the problem (10). In this case, $\rho[M(z)] < 0.3467$ for $\mathrm{Re}(z) \leq 0$. With these values of λ and β, 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 λ 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 $a_0 = 3 - \frac{1}{10\ \lambda^2},\quad a_1 = 3 - \frac{1}{2\ \lambda},\quad ,\quad a_2 = 1 - \frac{1}{120\ \lambda^3}.$

A simple grid search procedure shows that good approximation to the optimum value of λ 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 togethger with $\det B = \beta$ may be solved by choosing $b_{21} = 0$. This gives

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

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

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

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.

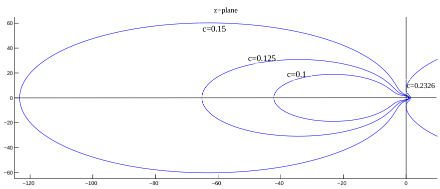

Figure 1: Curves $\rho[M(z)] = c$ for $s = 3$

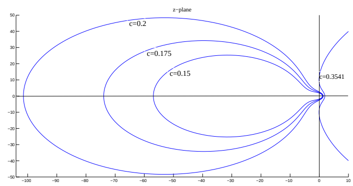

Figure 2: Curves $\rho[M(z)] = c$ for $s = 4$

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

The constraint $\rho[M(\infty)] = 0$ for the three-stage Gauss method gives $\lambda = \sqrt[3]{\dfrac{\beta}{120}}$ 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 $a_0 = 1 - \beta$, $a_1 = 3 - \dfrac{\beta}{2\lambda}$, $a_2 = 3 - \dfrac{\beta}{10\lambda^2}$. By search procedure, a good approximation to the optimum value of β is obtained by $\beta = 1.181387098$ and the corresponding λ is given by $\lambda = 0.214323763$. In this case $\rho[M(z)] < 0.2359$ for all $z \in \mathbb{C}^-$. With these values of λ and β, the equations (13) with $\det B = \beta$ may be solved by choosing $b_{21} = 0$. This gives

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

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 $a_0 = 1 - \beta$, $a_1 = 4 - \dfrac{\beta}{2\lambda}$, $a_2 = 6 - \dfrac{3\beta}{28\lambda^2}$, $a_3 = 4 - \dfrac{\beta}{84\lambda^3}$. With the value $\lambda = 0.146840443$, which solves the sets of equations 15),(16),(17),(18), and the corresponding value of β, 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 $z \in \mathbb{C}^-$.

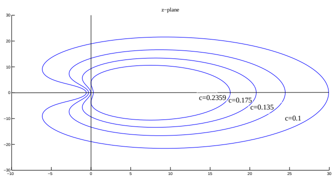

Figure 3: Curves $\rho[M(z)] = c$ for $s = 3$

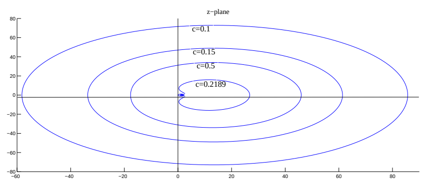

Figure 4: Curves $\rho[M(z)] = c$ for $s = 4$

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,

$$\begin{aligned} x_1' &= x_3, & x_1(0) &= 0.4,\\ x_2' &= x_4, & x_2(0) &= 0,\\ x_3' &= -x_1\left(x_1^2+x_2^2\right)^{-3/2}, & x_3(0) &= 0,\\ x_4' &= -x_2\left(x_1^2+x_2^2\right)^{-3/2}, & x_4(0) &= 2. \end{aligned}$$

The eigenvalues at the initial point are ± 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,

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

where the Jacobian has constant eigenvalues -10^5, -10^6, -40×10^5 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 λ and B given by (23) for $\rho[M(\infty)] = 0$.

For each method and problem, the quantities

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

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 peform well.

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