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MODIFIED PARALLEL ROSENBROCK METHODS FOR STIFF DIFFERENTIAL EQUATIONS[*1)]

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Abstract

To raise the efficiency of Rosenbrock methods Chen Lirong and Liu Degui have constructed the parallel Rosenbrock methods in 1995, which are written as PRMs for short. In this paper we present a class of modified parallel Rosenbrock methods which possesses more free parameters to improve further the various properties of the methods and will be similarly written as MPROWs. Convergence and stability of MPROWs are discussed. Especially, by choosing free parameters appropriately, we search out the practically optimal 2-stage 3rd-order and 3-stage 4th-order MPROWs, which are all A-stable and have small error constants. Theoretical analysis and numerical experiments show that for solving stiff problems the MPROWs searched out in the present paper are much more efficient than the existing parallel and sequential methods of the same type and same order mentioned above.

Key words: Numerical analysis, Stiff ordinary differential equations, Rosenbrock methods, Parallel algorithms.

1. Introduction

In many fields of science and engineering technology, we often meet with stiff ordinary differential equations. In order to solve these systems, we have to use the implicit methods, which means that nonlinear implicit equations must be solved. In general, this nonlinear systems can be solved only by iteration. This adds to the problem of stability, that of convergence of the iterative process (cf.[5,15]). In 1963, Rosenbrock[17] first presented a class of methods, which avoids nonlinear systems by replacing them with some linear systems. Therefore at each calculating step only the Jacobian matrix has to be evaluated and linear systems have to be solved. The methods of this type are known as Rosenbrock methods and sometimes called ROW methods (cf.[1]). Since then, many methods of this type and much numerical experience with them have been obtained by Calahan[2], van der Houwen[19], Cash[3], Nϕrsett[15], Nϕrsett and Wolfbrandt[16], Kaps and Rentrop[9], Kaps and Wanner[10], Shampine[18], Kaps, Poon and Bui[8] and Kaps and Ostermann[6,7]. To raise the efficiency of sequential Rosenbrock methods, in 1995 Cheng Lirong and Liu Degui[4] presented a class of parallel Rosenbrock methods (PRMs), which also avoids nonlinear systems and is more efficient than the sequential ROW methods mentioned above. In order to improve further the convergence and stability of PRMs, in the present paper, we construct a new class of parallel Rosenbrock methods, which is called the *Modified Parallel Rosenbrock Methods* and denoted similarly by MPROWs. Since the MPROWs have more free parameters which can be appropriately chosen to improve further various properties of the

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methods, the parallel methods constructed in the present paper can achieve higher precision and better numerical stability properties. In fact, by choosing free parameters to optimize the properties of the methods, we have constructed the 2-stage MPROW of order 3 and the 3-stage MPROW of order 4, which are all A-stable and have small error constants. Theoretical analysis and numerical experiments show that for solving stiff problems with a fixed stepsize, the MPROWs are as fast as the PRMs of the same order and much faster than the ROWs of the same order, the accuracy of the computational results of the MPROWs are generally higher than that of ROWs and much higher than that of PRMs. Moreover, the number of stages of the 4th-order MPROWs is one less than that of commonly used ROWs of the same order.

The outline of the paper is as follows. Section 2 is devoted to the construction of modified parallel Rosenbrock methods. In section 3 we investigate the convergence and the stability properties of MPROWs in general. In section 4 and 5, by selecting the free parameters appropriately, we construct the 2-stage MPROW of order 3 and the 3-stage MPROW of order 4 respectively, which are demonstrated to be all A-stable and have small error constants. In the final section 6, numerical experiments are given which show that the MPROWs indeed perform better than the parallel and sequential methods of the same type.

2. Modified Parallel Rosenbrock Methods

Consider the initial value problem

$$\begin{cases} y' = f(y), & t \in [a, b], \\ y(a) = y_0, & y_0 \in \mathbf{R}^m, \end{cases} \tag{2.1}$$

where the mapping $f(y)$ is assumed to satisfy a Lipschitz condition and has all continuous derivatives used later. The exact solution of the problem (2.1) is always denoted by $y(t)$, $a \leq t \leq b$. In 1979, Nϕrsett and Wolfbrandt[16] gave the s-stage Rosenbrock methods for solving (2.1)

$$\begin{cases} (I - h\gamma_{ii}J)k_i = hf(y_n + \sum\limits_{j=1}^{i-1} \alpha_{ij}k_j) + hJ\sum\limits_{j=1}^{i-1} \beta_{ij}k_j, \quad i = 1, 2, ..., s, \\ y_{n+1} = y_n + \sum\limits_{i=1}^{s} b_i k_i, \end{cases} \tag{2.2}$$

where $h > 0$ is the integration stepsize, $t_n = a + nh$, $\gamma_{ii}, \alpha_{ij}, \beta_{ij}$ and b_i are real coefficients, I denotes the identity matrix, J denotes the Jacobian matrix $f_y(y_n)$, y_n is an approximation to $y(t_n)$, and each k_i denotes an approximation to some piece of information about the exact solution $y(t)$. In 1995, Cheng Lirong and Liu Degui[4] presented the s-stage parallel Rosenbrock methods for solving (2.1)

$$\begin{cases} (I - h\gamma J)k_{in} = hf(y_n + \sum\limits_{j=1}^{i-1} \alpha_{ij}k_{j,n-1}) + hJ\sum\limits_{j=1}^{i-1} \beta_{ij}k_{j,n-1}, \quad i = 1, 2, ..., s, \\ y_{n+1} = y_n + \sum\limits_{i=1}^{s} b_i k_{in}. \end{cases} \tag{2.3}$$

Note that here the condition $\gamma_{11} = \gamma_{22} = \cdots = \gamma_{ss} = \gamma$ is imposed. However, when parallel processors are available, this condition is seems to be less desirable. Thus in order to make full use of the elements of the coefficient matrix as free parameters so as to achieve higher precision and better numerical stability properties, we relax the demand to construct a new class of methods of the form

$$\begin{cases} (I - h\gamma_{ii}J)k_{in} = hf(y_n + \sum\limits_{j=1}^{i-1} \alpha_{ij}k_{j,n-1}) + hJ\sum\limits_{j=1}^{i-1} \beta_{ij}k_{j,n-1}, \quad i = 1, 2, ..., s, \\ y_{n+1} = y_n + \sum\limits_{i=1}^{s} b_i k_{in}, \end{cases} \tag{2.4}$$

where each k_{in} denotes an approximation to certain information $k_i(t_n, h)$ about the exact solution $y(t)$, The meaning of other symbols here is the same as that in formula (2.2). In the remainder of this paper, we shall call the methods of this new class as *Modified Parallel Rosenbrock Methods*, and denote them by abbreviation MPROWs. It is easily seen that when the MPROW (2.4) is applied to the problem (2.1), for each calculating step the unknowns $k_{1n}, k_{2n}, ..., k_{sn}$ can be calculated in parallel on s processors with each processor only solving one linear system of dimension m provided that the back values $y_n, k_{1,n-1}, k_{2,n-1}, ..., k_{s,n-1}$ are known.

3. Convergence and Stability Analysis

In order to research the convergence properties, we write (2.4) as a general multivalue methods of the form (cf. [12])

$$y^{(n)} = Ay^{(n-1)} + h\varphi(y^{(n-1)}, h), \tag{3.1}$$

where

$$\begin{cases} y^{(n)} = \left(\ k_{1n}^T, k_{2n}^T, \cdots, k_{sn}^T, y_{n+1}^T \ \right)^T, \\ \\ A = \begin{pmatrix} 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}, \quad \varphi(y^{(n-1)}, h) = \begin{pmatrix} \varphi_1(y^{(n-1)}, h) \\ \vdots \\ \varphi_s(y^{(n-1)}, h) \\ \sum\limits_{i=1}^{s} b_i \varphi_i(y^{(n-1)}, h) \end{pmatrix}. \end{cases} \tag{3.2}$$

here

$$\varphi_i(y^{(n-1)}, h) = (I - h\gamma_{ii}J)^{-1}(f(y_n + \sum_{j=1}^{i-1} \alpha_{ij} k_{j,n-1}) + J \sum_{j=1}^{i-1} \beta_{ij} k_{j,n-1}), i = 1, 2, \cdots, s.$$

It is easily seen that the minimum polynomial of the matrix A satisfies the root condition, and by means of theorem 2.6.1 of [12], we conclude that

Theorem 3.1. *The method (2.4) is zero-stable and its convergence order is equal to the consistency order in the classical sense.*

To investigate the numerical stability properties, applying (2.4) with constant stepsize $h > 0$ to the test equation

$$y' = \lambda y, \qquad \lambda \in \mathbf{C},$$

we get

$$y^{(n)} = M(z) y^{(n-1)}, \qquad n = 1, 2, 3, \cdots, \tag{3.4}$$

where $z = h\lambda$,

$$M(z) = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 & m_{1,s+1} \\ m_{21} & 0 & \cdots & 0 & 0 & m_{2,s+1} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ m_{s1} & m_{s2} & \cdots & m_{s,s-1} & 0 & m_{s,s+1} \\ m_{s+1,1} & m_{s+1,2} & \cdots & m_{s+1,s-1} & 0 & m_{s+1,s+1} \end{pmatrix}, \tag{3.5}$$

where

$$\begin{cases} m_{ij} = (\alpha_{ij} + \beta_{ij}) z / (1 - \gamma_{ii} z), & 1 \le j < i \le s, \\ m_{i,s+1} = z / (1 - \gamma_{ii} z), & i = 1, 2, ..., s, \\ m_{s+1,j} = \sum\limits_{i=j+1}^{s} b_i m_{ij}, & j = 1, 2, ..., s-1, \\ m_{s+1,s+1} = 1 + \sum\limits_{i=1}^{s} b_i m_{i,s+1}. \end{cases}$$

Following definition 2.6.9 of [12], $M(z)$ is said to be the stability matrix of the method (2.4), and the absolute stability region of the method (2.4) is defined as the set

$$S = \{z \in \mathbf{C} | \text{ the spectral radius of } M(z) \text{ is less than } 1 \},$$

the generalized stability region as the set

$$S = \{z \in \mathbf{C} | \text{ the minimum polynomial of } M(z) \text{ satisfies the root condition } \}.$$

Thus we can easily use the boundary locus method and Schur criterion to draw out the stability region of the method.

4. Two-Stage Third-Order Methods

Consider the two-stage modified parallel Rosenbrock method

$$\begin{cases} (I - h\gamma_{ii} J)k_{in} = hf(y_n + \sum\limits_{j=1}^{i-1} \alpha_{ij} k_{j,n-1}) + hJ \sum\limits_{j=1}^{i-1} \beta_{ij} k_{j,n-1}, \quad i = 1, 2, \\ y_{n+1} = y_n + \sum\limits_{i=1}^{2} b_i k_{in}, \end{cases} \tag{4.1}$$

where $\gamma_{ii}, \alpha_{ij}, \beta_{ij}$ and b_i are parameters to be determined, each k_{in} is an approximation to $k_i(t_n, h)$ as mentioned above and in this case we would define

$$k_i(t_n, h) := y'h + p_i y'' h^2 + (q_i f_y y'' + \frac{c_i^2}{2} f_{y^2} {y'}^2) h^3, \qquad i = 1, 2, \tag{4.2}$$

where p_i, q_i and c_i are parameters to be determined. Here and later, symbols y', y'',... are abbreviations of $y'(t_n), y''(t_n)$, $\ldots$, respectively, symbols $f_y, f_{y^2}, \ldots$ are abbreviations of $f_y(y(t_n)), f_{y^2}(y(t_n))$,..., respectively. Substituting $y(t_n)$ and $k_i(t_n, h)$ for y_n and k_{in} in (4.1) respectively, we obtain

$$\begin{cases} (I - h\gamma_{ii} f_y(y(t_n)))k_i(t_n, h) = hf(y(t_n) + \sum\limits_{j=1}^{i-1} \alpha_{ij} k_j(t_{n-1}, h)) \\ \qquad\qquad + hf_y(y(t_n)) \sum\limits_{j=1}^{i-1} \beta_{ij} k_j(t_{n-1}, h) + \delta_{in}, \ i = 1, 2, \\ y(t_{n+1}) = y(t_n) + \sum\limits_{i=1}^{2} b_i k_i(t_n, h) + \eta_n. \end{cases} \tag{4.3}$$

To guarantee the method (4.1) having consistency order at least 3, it is evidently sufficient that

$$\eta_n = O(h^4), \qquad \delta_{in} = O(h^4), \qquad i = 1, 2. \tag{4.4}$$

(4.2) with t_n replaced by t_{n-1} leads to

$$\begin{aligned} k_j(t_{n-1}, h) = {} & y'(t_{n-1})h + p_j y''(t_{n-1})h^2 + (q_j f_y(y(t_{n-1}))y''(t_{n-1}) \\ & + \tfrac{c_j^2}{2} f_{y^2}(y(t_{n-1}))(y'(t_{n-1}))^2)h^3, \qquad j = 1, 2. \end{aligned} \tag{4.5}$$

Expanding $y'(t_{n-1}), y''(t_{n-1})$ about t_n, respectively and expanding $f_y(y(t_{n-1})), f_{y^2}(y(t_{n-1}))$ about $y(t_n)$, respectively, then substituting them in (4.5), we obtain

$$\begin{aligned} k_j(t_{n-1}, h) = {} & y'h + (p_j - 1)y''h^2 + (q_j f_y y'' + \tfrac{c_j^2}{2} f_{y^2} {y'}^2 \\ & + (\tfrac{1}{2} - p_j)y''')h^3 + O(h^4), \qquad j = 1, 2. \end{aligned} \tag{4.6}$$

Using Taylor expansion together with (4.6), we get

$$
\begin{aligned}
hf(y(t_n)+\sum_{j=1}^{i-1}\alpha_{ij}k_j(t_{n-1},h)) = {} & hy'+h^2\sum_{j=1}^{i-1}\alpha_{ij}y''+h^3\{\sum_{j=1}^{i-1}\alpha_{ij}(p_j-1)f_yy'' \\
& +\tfrac{1}{2}(\sum_{j=1}^{i-1}\alpha_{ij})^2 f_{y^2}{y'}^2\}+h^4\{\sum_{j=1}^{i-1}\alpha_{ij}(q_jf_y^2y'' \\
& +\tfrac{c_j^2}{2}f_yf_{y^2}{y'}^2+(\tfrac{1}{2}-p_j)f_yy''') \\
& +\sum_{j=1}^{i-1}\alpha_{ij}\sum_{j=1}^{i-1}\alpha_{ij}(p_j-1)f_{y^2}y'y'' \\
& +\tfrac{1}{6}(\sum_{j=1}^{i-1}\alpha_{ij})^3f_{y^3}{y'}^3\}+O(h^5),
\end{aligned} \tag{4.7}
$$
$$
y(t_{n+1}) = y+y'h+\tfrac{1}{2}y''h^2+\tfrac{1}{6}y'''h^3+\tfrac{1}{24}y^{(4)}h^4+O(h^5).
$$

By substituting (4.2), (4.6), (4.7) into (4.3) and then matching the expressions in both sides of (4.3) up to and including h^3 terms we get

$$
\begin{cases}
\sum_{j=1}^{2}b_j=1, & c_i=\sum_{j=1}^{i-1}\alpha_{ij}, \\
\sum_{j=1}^{2}b_jp_j=\frac{1}{2}, & p_i=\sum_{j=1}^{i-1}(\alpha_{ij}+\beta_{ij})+\gamma_{ii}, \qquad i=1,2, \\
\sum_{j=1}^{2}b_jq_j=\frac{1}{6}, & q_i=\sum_{j=1}^{i-1}(\alpha_{ij}+\beta_{ij})(p_j-1)+\gamma_{ii}p_i, \\
\sum_{j=1}^{2}b_jc_j^2=\frac{1}{3} &
\end{cases} \tag{4.8}
$$

and

$$
\begin{cases}
\delta_{in} = -\{(\sum_{j=1}^{i-1}(\alpha_{ij}+\beta_{ij})(q_j-p_j+\frac{1}{2})+\gamma_{ii}q_i)f_y^2y'' \\
\qquad +(\sum_{j=1}^{i-1}(\alpha_{ij}+\beta_{ij})(\frac{c_j^2}{2}-p_j+\frac{1}{2})+\gamma_{ii}\frac{c_i^2}{2})f_yf_{y^2}{y'}^2 \\
\qquad +c_i\sum_{j=1}^{i-1}\alpha_{ij}(p_j-1)f_{y^2}y'y''+\frac{1}{6}c_i^3f_{y^3}{y'}^3\}h^4+O(h^5), \quad i=1,2, \\
\eta_n = \frac{1}{4!}y^{(4)}h^4+O(h^5).
\end{cases} \tag{4.9}
$$

For any given c_2,γ_{11} with $c_2\neq 0$ and $\gamma_{11}\neq\frac{1}{2}+\frac{1}{3c_2^2}$, we can uniquely solve the set of equations (4.8) for all other parameters. Thus we get

$$
\begin{cases}
\alpha_{21}=c_2, \\
b_2=1/(3c_2^2), \\
b_1=1-b_2, \\
p_1=\gamma_{11}, \\
q_1=\gamma_{11}^2, \\
p_2=(0.5-b_1p_1)/b_2, \\
q_2=(1/6-b_1q_1)/b_2, \\
\beta_{21}=(p_2(p_2-\alpha_{21})-(q_2-\alpha_{21}(p_1-1)))/(p_2-p_1+1), \\
\gamma_{22}=p_2-\alpha_{21}-\beta_{21}.
\end{cases} \tag{4.10}
$$

(4.1)-(4.10) can be regarded as a class of two-stage third-order modified parallel Rosenbrock methods with two free parameters c_2 and γ_{11}. Using the software OSR of Li Shoufu (cf.[13,14]) to optimize the convergence and stability properties of the methods, we get the practically optimal values of the free parameters

$$
c_2=\frac{1}{2}, \qquad \gamma_{11}=1
$$

and get correspondingly a special 2-stage 3rd-order MPROW of the form

$$\left\{\begin{array}{l} (I-hJ)k_{1n}=hf(y_n), \\ (I-\frac{3}{5}hJ)k_{2n}=hf(y_n+\frac{1}{2}k_{1,n-1})-\frac{19}{40}hJk_{1,n-1}, \\ y_{n+1}=y_n-\frac{1}{3}k_{1n}+\frac{4}{3}k_{2n}. \end{array}\right. \tag{4.11}$$

The residual errors of the method (4.11) are

$$\left\{\begin{array}{l} \delta_{1n}=-f_y^2y''h^4+O(h^5), \\ \delta_{2n}=-\{\frac{19}{80}f_y^2y''+\frac{1}{16}f_yf_{y^2}{y'}^2+\frac{1}{48}f_{y^3}{y'}^3\}h^4+O(h^5), \\ \eta_n=\frac{1}{24}y^{(4)}h^4+O(h^5). \end{array}\right. \tag{4.12}$$

By using the boundary locus method and Schur criterion, the absolute stability region of the method (4.11) is drawn out in Fig1., which demonstrates that the method is A-stable.

5. Three-Stage Fourth-Order Methods

In order to increase the consistency order of the method, we will consider the three-stage modified parallel Rosenbrock method

$$\left\{\begin{array}{l} (I-h\gamma_{ii}J)k_{in}=hf(y_n+\sum\limits_{j=1}^{i-1}\alpha_{ij}k_{j,n-1})+hJ\sum\limits_{j=1}^{i-1}\beta_{ij}k_{j,n-1}, \quad i=1,2,3, \\ y_{n+1}=y_n+\sum\limits_{i=1}^{3}b_ik_{in}, \end{array}\right. \tag{5.1}$$

where $\gamma_{ii},\alpha_{ij},\beta_{ij}$ and b_i are parameters to be determined, each k_{in} is an approximation to $k_i(t_n,h)$ as mentioned above, but in this case we would define

$$\begin{array}{r} k_i(t_n,h):=y'h+p_iy''h^2+(q_if_yy''+\frac{c_i^2}{2}f_{y^2}{y'}^2)h^3 \\ +(u_if_y^2y''+v_if_yf_{y^2}{y'}^2+w_if_{y^2}y'y''+\frac{1}{6}c_i^3f_{y^3}{y'}^3)h^4, \end{array} \tag{5.2}$$

where p_i,q_i,c_i,u_i,v_i and w_i are parameters to be determined. Substituting $y(t_n)$ and $k_i(t_n,h)$ for y_n and k_{in} in (5.1), respectively, we obtain

$$\left\{\begin{array}{l} (I-h\gamma_{ii}f_y(y(t_n)))k_i(t_n,h)=hf(y(t_n)+\sum\limits_{j=1}^{i-1}\alpha_{ij}k_j(t_{n-1},h)) \\ \qquad\qquad +hf_y(y(t_n))\sum\limits_{j=1}^{i-1}\beta_{ij}k_j(t_{n-1},h)+\delta_{in}, \quad i=1,2,3, \\ y(t_{n+1})=y(t_n)+\sum\limits_{i=1}^{3}b_ik_i(t_n,h)+\eta_n. \end{array}\right. \tag{5.3}$$

To guarantee the method (5.1) having consistency order at least 4, it is evidently sufficient that

$$\eta_n=O(h^5), \qquad \delta_{in}=O(h^5), \qquad i=1,2,3. \tag{5.4}$$

Similarly, expand $k_j(t_{n-1},h)$, $f(y(t_n)+\sum\limits_{j=1}^{i-1}\alpha_{ij}k_j(t_{n-1},h))$ and $y(t_{n+1})$ about t_n, $y(t_n)$ and t_n, respectively, substitute them into (5.3), and then match the expressions in both sides of (5.3) up to and including h^4 terms. We thus get the following order conditions

$$\left\{\begin{array}{ll}
\sum_{j=1}^{3} b_j = 1, & c_i = \sum_{j=1}^{i-1} \alpha_{ij}, \\
\sum_{j=1}^{3} b_j p_j = \frac{1}{2}, & p_i = \sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij}) + \gamma_{ii}, \\
\sum_{j=1}^{3} b_j q_j = \frac{1}{6}, & q_i = \sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij})(p_j - 1) + \gamma_{ii} p_i, \\
\sum_{j=1}^{3} b_j u_j = \frac{1}{24}, & u_i = \sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij})(q_j - p_j + \frac{1}{2}) + \gamma_{ii} q_i, \quad i = 1, 2, 3, \\
\sum_{j=1}^{3} b_j v_j = \frac{1}{24}, & v_i = \sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij})(\frac{c_j^2}{2} - p_j + \frac{1}{2}) + \gamma_{ii} \frac{c_i^2}{2}, \\
\sum_{j=1}^{3} b_j w_j = \frac{1}{8}, & w_i = c_i \sum_{j=1}^{i-1} \alpha_{ij} (p_j - 1), \\
\sum_{j=2}^{3} b_j c_j^2 = \frac{1}{3}, & \sum_{j=2}^{3} b_j c_j^3 = \frac{1}{4}
\end{array}\right. \tag{5.5}$$

and the residual errors

$$\left\{\begin{array}{l}
\delta_{in} = -\{(\sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij})(u_j - q_j + \frac{p_j}{2} - \frac{1}{6}) + \gamma_{ii} u_i) f_y^3 y'' \\
\qquad + (\sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij})(v_j - q_j + \frac{p_j}{2} - \frac{1}{6}) + \gamma_{ii} v_i) f_y^2 f_{y^2} {y'}^2 \\
\qquad + (\sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij})(w_j - q_j - c_j^2 + \frac{3p_j}{2} - \frac{1}{2}) + \gamma_{ii} w_i) f_y f_{y^2} y' y'' \\
\qquad + (\sum_{j=1}^{i-1} (\alpha_{ij} + \beta_{ij})(\frac{c_j^3}{6} - \frac{c_j^2}{2} + \frac{p_j}{2} - \frac{1}{6}) + \gamma_{ii} \frac{c_i^3}{6}) f_y f_{y^3} {y'}^3 \\
\qquad + \frac{1}{2} (\sum_{j=1}^{i-1} \alpha_{ij} (p_j - 1))^2 f_{y^2} {y''}^2 + c_i \sum_{j=1}^{i-1} \alpha_{ij} (q_j - p_j + \frac{1}{2}) f_{y^2} y' f_y y'' \\
\qquad + c_i \sum_{j=1}^{i-1} \alpha_{ij} (\frac{c_j^2}{2} - p_j + \frac{1}{2}) f_{y^2} y' f_{y^2} {y'}^2) \\
\qquad + \frac{1}{2} c_i^2 \sum_{j=1}^{i-1} \alpha_{ij} (p_j - 1) f_{y^3} {y'}^2 y'' + \frac{1}{24} c_i^4 f_{y^4} {y'}^4 \} h^5 + O(h^6), \qquad i = 1, 2, 3, \\
\eta_n = \frac{1}{5!} y^{(5)} h^5 + O(h^6).
\end{array}\right. \tag{5.6}$$

For any given c_2, c_3, γ_{11} and p_2, all other parameters can be determined by the set of equations (5.5). Thus (5.1)-(5.5) can be regarded as a class of three-stage fourth-order modified parallel Rosenbrock methods with four free parameters c_2, c_3, γ_{11} and p_2. Using the software OSR of Li Shoufu to optimize the convergence and stability properties of the methods, we get the practically optimal values of the free parameters

$$\left\{\begin{array}{ll}
\gamma_{11} = 6.04093114026981e-1, & c_2 = 3.39701870165151e-1, \\
c_3 = -2.76943875477869e-1, & p_2 = 4.51188434532367e-1,
\end{array}\right. \tag{5.7}$$

this leads to a special 3-stage 4th-order MPROW (5.1)-(5.5)-(5.7), which can be approximately written as

$$\left\{\begin{array}{ll}
(I - 0.604093114027hJ)k_{1n} & = hf(y_n), \\
(I - 0.398820192518hJ)k_{2n} & = hf(y_n + 0.3397018701652k_{1,n-1}) \\
& \qquad -0.2873336281504hJk_{1,n-1}, \\
(I - 0.320748354582hJ)k_{3n} & = hf(y_n + 1.82155681102k_{1,n-1} - 2.09850068650k_{2,n-1} \\
& \qquad +hJ(-1.800580150078k_{1,n-1} + 2.142501534643k_{2,n-1}), \\
y_{n+1} = y_n - 0.9188016315798k_{1n} & + 4.810540100875k_{2n} - 2.891738469296k_{3n}
\end{array}\right. \tag{5.8}$$

with the residual errors

$$\left\{\begin{array}{l} \delta_{1n} = -0.133172803116436 f_y^3 y'' h^5 + O(h^6), \\ \delta_{2n} = -\{0.030294813563091 f_y^3 y'' - 0.005017684169195 f_y^2 f_{y^2} {y'}^2 \\ \qquad -0.016062585388198 f_y f_{y^2} y' y'' + 0.009695278595627 f_y f_{y^3} {y'}^3 \\ \qquad +0.009043821684964 f_{y^2} {y''}^2 + 0.030099713984621 f_{y^2} y' f_y y'' \\ \qquad -0.012012070614693 f_{y^2} y' f_{y^2} {y'}^2 + 0.000521816576062 f_{y^3} {y'}^2 y'' \\ \qquad +0.000554856284666 f_{y^4} {y'}^4\} h^5 + O(h^6), \\ \delta_{3n} = -\{0.012871970854685 f_y^3 y'' - 0.003706856444963 f_y^2 f_{y^2} {y'}^2 \\ \qquad -0.043692455557190 f_y f_{y^2} y' y'' + 0.002045863214505 f_y f_{y^3} {y'}^3 \\ \qquad +0.092671394140650 f_{y^2} {y''}^2 - 0.010688046843972 f_{y^2} y' f_y y'' \\ \qquad +0.114411980129195 f_{y^2} y' f_{y^2} {y'}^2 + 0.003553851131319 f_{y^3} {y'}^2 y'' \\ \qquad +0.000245107059318 f_{y^4} {y'}^4\} h^5 + O(h^6), \\ \eta_n = 0.008333333333333 y^{(5)} h^5 + O(h^6). \end{array}\right. \tag{5.9}$$

Similarly, by using the boundary locus method and Schur criterion, we draw out the absolute stability region of the method (5.1)-(5.5)-(5.7) in Fig2. and come to the conclusion that the method is also A-stable.

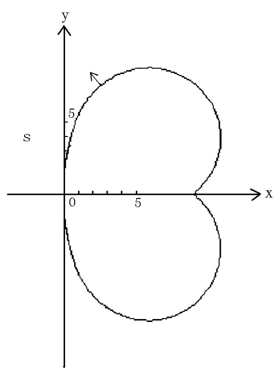

Figure 4.1 Stability region for the 2-stage MPROW (4.11) of order 3

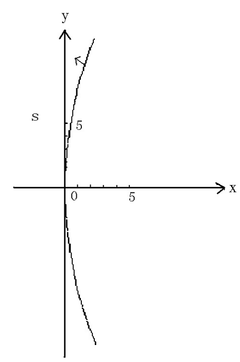

Figure 5.1 Stability region for the 3-stage MPROW (5.1)-(5.5)-(5.7) of order 4

6. Numerical Experiments

In this section the 2-stage 3rd-order MPROW (4.11) and the 3-stage 4th-order MPROW (5.1)-(5.5)-(5.7) are tested on the following examples of stiff problems.

Example 1. Stiff nonlinear ordinary differential equations

$$\left\{\begin{array}{l} y_1' = -(\epsilon^{-1}+2)y_1 + \epsilon^{-1} y_2^2, \\ y_2' = y_1 - y_2 - y_2^2, \\ y_1(0) = 1, \quad y_2(0) = 1, \end{array}\right. \qquad 0 \le t \le 1,$$

where $\epsilon = 10^{-8}$. The exact solution of the system is

$$y_1(t) = e^{-2t}, \qquad y_2(t) = e^{-t}.$$

Example 2. System of linear differential equations with eigenvalues of the coefficient matrix lying near or on the imaginary axis

$$\left\{\begin{array}{l} y_1' = -\alpha y_1 - \beta y_2 + (\alpha+\beta-1)e^{-t} + (\alpha+\beta) sint + cost, \\ y_2' = \beta y_1 - \alpha y_2 + (\alpha-\beta-1)e^{-t} + (\alpha-\beta) sint + cost, \\ y_1(0) = 1, \quad y_2(0) = 1. \end{array}\right. \qquad 0 \le t \le 50,$$

The eigenvalues of the the coefficient matrix are $\lambda_{1,2} = -\alpha \pm \beta i$, the exact solution of the system is

$$\begin{cases} y_1(t) = e^{-t} + sint, \\ y_2(t) = e^{-t} + sint. \end{cases}$$

The parameters α and β are chosen as

$$(1)\ \alpha = 1, \beta = 100; \qquad (2)\ \alpha = 0, \beta = 100.$$

Example 3. Stiff non-autonomous linear ordinary differential equations

$$\begin{cases} y'(t) = E(t)\begin{bmatrix} -\frac{1}{\epsilon} & 0 \\ 0 & -1 \end{bmatrix} E^{-1}(t)y(t) + \begin{bmatrix} -3sint + (\frac{2}{\epsilon}-1)cost \\ 3cost + (\frac{2}{\epsilon}-1)sint \end{bmatrix}, \ 0 \le t \le 2\pi, \\ y(0) = \begin{bmatrix} 2+\epsilon \\ 2+\epsilon\lambda \end{bmatrix}, \end{cases}$$

where $\epsilon = 10^{-6}$, $E(t) = \begin{bmatrix} cost, & -sint \\ sint, & cost \end{bmatrix}$, $\lambda = \frac{-1}{2\epsilon}(1+\epsilon-\sqrt{1-2\epsilon-3\epsilon^2})$. The exact solution of the system is

$$y(t) = E(t)\begin{bmatrix} \epsilon e^{\lambda t} \\ (1+\epsilon\lambda)e^{\lambda t} \end{bmatrix} + \begin{bmatrix} 2cost - sint \\ 2sint + cost \end{bmatrix}.$$

Example 4. Weakly damped oscillatory differential equations

$$\begin{cases} y' = Ay, \\ y(0) = y_0, \end{cases} \qquad 0 \le t \le 10,$$

where

$$A = \begin{pmatrix} -0.01 & -1 & -1 \\ 2 & -100.005 & 99.995 \\ 2 & 99.995 & -100.005 \end{pmatrix}, y_0 = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}.$$

The exact solution of the system is

$$\begin{cases} y_1(t) = e^{-0.01t}(cos2t - sin2t), \\ y_2(t) = e^{-0.01t}(cos2t + sin2t) + e^{-200t}, \\ y_3(t) = e^{-0.01t}(cos2t + sin2t) - e^{-200t}. \end{cases}$$

For comparison purposes, we have also included in our tests the 2-stage 3rd-order and the 4-stage 4th-order ROWs (cf.[2,16]) as well as the 2-stage 3rd-order and the 3-stage 4th-order PRMs (cf.[4]). The systems have been integrated with fixed stepsize h. Numerical results for these problems are shown in Tables 1-4, in which s denotes the number of stages of the method, p the consistency order of the method, T the execution time for the parallel or sequential computation, and

$$e_i := \begin{cases} |\frac{y_i(b) - y_{hi}(b)}{y_{hi}(b)}| & |y_{hi}(b)| > 1, \\ |y_i(b) - y_{hi}(b)| & |y_{hi}(b)| \le 1, \end{cases}$$

the i-th component of the global error at the endpoint of the integration interval, where $y_i(b)$, $y_{hi}(b)$ are the i-th component of the exact solution and the numerical solution at the endpoint of the integration interval respectively, i=1,2,...,m. From Tables 1-4, we see that the 2-stage MPROW of order 3 is performed as fast as the PRM of the same order and almost twice as fast as the ROW of the same order and that the 3-stage MPROW of order 4 is also performed as fast as the PRM of the same order and close to 4 times as fast as the ROW of the same order if the CPU-time needed to exchange information on different processors is ignored. The accuracy of the computational results of the 2-stage 3rd-order and the 3-stage 4th-order MPROWs are generally higher than that of ROWs of the same order and much higher than that of PRMs of the same order. Furthermore, for problems whose Jacobian matrix has eigenvalues near or on the imaginary axis, the computational results obtained by using the 3-stage PRM of order 4 and the 4-stage ROW of order 4 seem to be quite undesirable whereas in this case the 3-stage MPROW of order 4 is still performed efficiently. Thus we can conclude that for solving stiff problems, MPROWs are generally superior to PRMs and ROWs.

Table 1 Results of MPROW, PRM and ROW with p=3,s=2 for examples 1,2,3

	$Method$	h	e_1	e_2	T (second)
Example 1	MPROW	0.01	2.349e-06	2.072e-08	0.01
		0.001	2.457e-08	1.966e-11	0.17
	PRM	0.01	2.784e-05	4.579e-07	0.03
		0.001	2.738e-07	4.699e-10	0.17
	ROW	0.01	4.560e-06	3.209e-08	0.05
		0.001	4.517e-08	3.984e-11	0.33
Example 2 (case 1)	MPROW	0.1	2.259e-04	1.944e-04	0.19
		0.01	2.447e-06	1.650e-07	1.95
		0.001	2.931e-09	2.226e-09	19.47
	PRM	0.1	3.427e-03	3.265e-03	0.22
		0.01	3.240e-05	1.538e-05	1.95
		0.001	8.445e-08	4.603e-08	19.47
	ROW	0.1	4.283e-04	3.512e-04	0.38
		0.01	4.455e-06	1.656e-07	3.73
		0.001	5.174e-09	4.112e-09	37.46
Example 2 (case 2)	MPROW	0.1	2.261e-04	1.945e-04	0.19
		0.01	2.460e-06	1.546e-07	1.95
		0.001	9.296e-09	6.101e-09	19.50
	PRM	0.1	3.428e-03	3.265e-03	0.20
		0.01	3.252e-05	1.539e-05	1.98
		0.001	8.499e-08	4.713e-08	19.50
	ROW	0.1	4.288e-04	3.515e-04	0.38
		0.01	4.478e-06	1.455e-07	3.73
		0.001	1.521e-08	8.469e-09	37.46
Example 3	MPROW	0.001	4.371e-07	8.492e-04	2.97
		0.0001	9.050e-10	8.458e-07	29.55
	PRM	0.001	1.576e-06	1.396e-03	2.97
		0.0001	1.005e-08	1.408e-06	29.58
	ROW	0.001	2.255e-08	3.522e-04	5.71
		0.0001	1.646e-09	3.552e-07	57.29

Table 2 Results of MPROW, PRM and ROW with p=3,s=2 for example 4

$Method$	h	e_1	e_2	e_3	T (second)
MPROW	0.01	4.785e-06	9.130e-06	9.130e-06	0.18
	0.001	4.512e-09	9.240e-09	9.240e-09	1.68
PRM	0.01	1.104e-04	2.015e-04	2.015e-04	0.18
	0.001	1.009e-07	2.055e-07	2.055e-07	1.71
ROW	0.01	7.265e-06	1.410e-05	1.410e-05	0.38
	0.001	6.935e-09	1.423e-08	1.423e-08	3.13

Table 3 Results of MPROW, PRM and ROW with p=4 for examples 1,2,3

	Method	h	e_1	e_2	T (second)
Example 1	MPROW	0.01	1.326e-07	2.554e-10	0.02
	(s=3)	0.001	9.584e-10	1.772e-11	0.17
	PRM	0.01	5.457e-05	8.400e-08	0.02
	(s=3)	0.001	5.377e-07	1.104e-11	0.17
	ROW	0.01	6.863e-06	4.636e-11	0.06
	(s=4)	0.001	6.775e-08	2.571e-13	0.66
Example 2	MPROW	0.1	1.460e-04	7.845e-05	0.18
(case 1)	(s=3)	0.01	6.135e-08	3.288e-08	1.80
		0.001	4.566e-12	6.151e-12	17.93
	PRM	0.1	7.545e-03	7.147e-03	0.16
	(s=3)	0.01	6.750e-05	2.993e-05	1.81
		0.001	1.771e-08	1.435e-07	17.93
	ROW	0.1	1.338e-02	3.182e-03	0.66
	(s=4)	0.01	5.445e-04	4.983e-04	6.70
		0.001	5.579e-05	5.579e-05	66.63
Example 2	MPROW	0.1	1.465e-04	7.848e-05	0.18
(case 2)	(s=3)	0.01	6.087e-08	3.405e-08	1.80
		0.001	1.978e-11	5.302e-13	17.94
	PRM	0.1	7.547e-03	7.149e-03	0.18
	(s=3)	0.01	6.776e-05	2.999e-05	1.79
		0.001	1.552e-08	1.447e-07	17.94
	ROW	0.1	1.341e-02	3.116e-03	0.66
	(s=4)	0.01	5.433e-04	4.982e-04	6.64
		0.001	5.571e-05	5.588e-05	66.63
Example 3	MPROW	0.001	7.329e-07	1.808e-03	2.44
	(s=3)	0.0001	1.837e-11	1.781e-06	24.28
	PRM	0.001	2.929e-06	2.337e-03	2.43
	(s=3)	0.0001	1.974e-08	2.352e-06	24.28
	ROW	0.001	6.366e-05	4.516e-02	8.35
	(s=4)	0.0001	7.924e-06	3.868e-04	83.15

Table 4 Results of MPROW, PRM and ROW with p=4 for example 4

Method	h	e_1	e_2	e_3	T (second)
MPROW	0.01	8.375e-08	2.880e-08	2.880e-08	0.17
(s=3)	0.001	8.439e-12	2.901e-12	2.901e-12	1.70
PRM	0.01	8.779e-05	4.599e-05	4.599e-05	0.18
(s=3)	0.001	9.650e-09	3.371e-09	3.371e-09	1.72
ROW	0.01	4.663e-08	1.732e-08	1.732e-08	0.82
(s=4)	0.001	4.723e-12	1.637e-12	1.637e-12	8.07

References

[1] K. Burrage, Parallel and Sequential Methods for Ordinary Differential Equations, Clarendon Press, Oxford, 1995.

[2] D.A. Calahan, A-Stable, Accurate Method of Numerical Integration for Nonlinear Systems, *Proc. IEEE,* **56** (1968), 944.

[3] J.R. Cash, Semi-implicit Runge-Kutta procedures with error estimates for the numerical integration of stiff systems of ordinary differential equations, *JACM*, **23** (1976), 455-460.

[4] L.R. Chen, D.G. Liu, A Class of Parallel Rosenbrock Formulas, Proceedings of 3rd BICSC'95, 89-92, Beijing, 1995.

[5] E. Hairer, G. Wanner, Solving Ordinary Differential equations II: Stiff and Differential-Algebraic Problems, Berlin, Heidelberg, New York, Tokyo: Springer 1991.

[6] P. Kaps, A. Ostermann, Rosenbrock methods using few LU-decompositions, *IMA J. Numer. Anal.,* **9** (1989), 15-27.

[7] P. Kaps, A. Ostermann, $L(\alpha)$-stable variable order Rosenbrock-methods, Proceedings of the Halle Seminar 1989, Teubner Texte zur Mathematics, 1990.

[8] P. Kaps, S.W.H. Poon, T.D. Bui, Rosenbrock methods for stiff ODEs: a comparison of Richardson extrapolation and embedding technique, *Computing*, **34** (1985), 17-40.

[9] P. Kaps, P. Rentrop, Generalized Runge-Kutta methods of order four with stepsize control for stiff ordinary differential equations, *Numer. Math.*, **33** (1979), 55-68.

[10] P. Kaps, G. Wanner, A study of Rosenbrock-type methods of high order, *Numer. Math.*, **38** (1981), 279-298.

[11] J.D. Lambert, Computational Methods in Ordinary Differential Equations. John Wiley and Sons, 1973.

[12] S.F. Li, Theory of Computational Methods for Stiff Differential Equations, Hunan Science and Technology Press, 1997.

[13] S.F. Li, M. Qiu, A Class of Parallel Adams predictor-corrector algorithms, Proceedings of the fifth National Conference on Parallel Computation, 99-102, Shanxi Science and Technology Press, 1997.

[14] S.F. Li, K. Su, A Class of Parallel Multistep Hybrid Methods, Proceedings of the fifth National Conference on Parallel Computation, 96-98, Shanxi Science and Technology Press, 1997.

[15] S.P. Nϕrsett, Runge-Kutta methods with coefficients depending on the Jacobian, Report No. 1/75, Dept. of Math., Univ. of Trondheim, Norway, 1975.

[16] S.P. Nϕrsett, A. Wolfbrandt, Order conditions for Rosenbrock types methods, *Numer. Math.*, **32** (1979), 1-15.

[17] H.H. Rosenbrock, Some general implicit processes for the numerical solution of differential equations. *Comput. J.*, **5** (1963), 329-331.

[18] L.F. Shampine, Implementation of Rosenbrock methods. *ACM, Trans. on Math. Soft.*, **8** (1982), 93-113.

[19] P.J. Van der Houwen, One-step methods with adaptive stability functions for the integration of differential equations. Lecture Notes in Mathematics No. 333, Springer-Verlag, Berlin, (1973), 164-174.