Journal of Computational Mathematics, Vol.20, No.1, 2002, 23–34.

MODIFIED PARALLEL ROSENBROCK METHODS FOR STIFF DIFFERENTIAL EQUATIONS*1)

Xue-nian Cao Shou-fu Li
(*Institute for Computational and Applied Mathematics, Xiangtan University, Xiangtan 411105, China*)

De-gui Liu
(*Beijing Institute of Computer Application and Simulation Technology, Beijing 100854, China*)

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

* Received December 6, 1998.
1)This project was supported by the National High-Tech ICF Committee in China.

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 $y(t),\ a \le t \le b$. 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

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