On a Family of Cheap Symmetric One-Step Methods of Order Four^{*}

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Abstract. In the paper we present a new family of one-step methods. These methods are of the Runge-Kutta type. However, they have only explicit internal stages that leads to a cheap practical implementation. On the other hand, the new methods are of classical order 4 and stage order 2 or 3. They are A -stable and symmetric.

1 Introduction

When solving ordinary differential equations (ODE's) of the form

$$x'(t) = g(t, x(t)), \quad t \in [t_0, t_0 + T], \quad x(t_0) = x^0 \quad (1)$$

where $x(t) \in \mathbb{R}^n$ and $g : D \subset \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$ is a sufficiently smooth function, any one-step method reads

$$x_{k+1} = x_k + \tau_k \Phi(t_k, x_k, t_{k+1}, x_{k+1}, \tau_k), \quad k = 0, 1, \dots, K-1, \quad (2)$$

where $x_0 = x^0$, τ_k is a step size and the function $\Phi(t_k, x_k, t_{k+1}, x_{k+1}, \tau_k)$ is referred to as *an increment function* of method (2). One-step methods (2) possess many superior practical properties to solve ODE's (1) of different sorts. For instance, they can be A -stable and keep high order convergence rate that is not possible for multistep methods because of Dahlquist's second barrier [5]; they do not have any difficulties with a variable step size implementation (see, for example, [4], [5]); they are also of high importance when applied to Hamiltonian or reversible equations [6]. Unfortunately, one-step methods have some limitations in the sense of high execution time when solving large-scale ODE's (1). Usual representatives of one-step methods (2) are Runge-Kutta formulas, but only implicit of them are suitable for stiff problems. However, implicit Runge-Kutta methods of high order are very time-consuming because of the need to solve in general nonlinear systems of dimension ln where l is the number of stage

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values at each step of the numerical integration (see [4], [5]). Hopefully, serious progress was made in this area by Bickart [1] and Butcher [2].

The aim of this paper is to present a cheap family of symmetric A -stable Runge-Kutta formulas. They are of classical order 4 and of stage order 3.

2 New Family of Symmetric One-Step Methods

Further, we suppose that ODE (1) possesses a unique solution $x(t)$ on the whole interval $[t_0, t_0 + T]$. We show how to construct the methods mentioned above.

Let us fix a subinterval $[t_k, t_{k+1}] \subset [t_0, t_0 + T]$ of the length τ_k ; i.e., $\tau_k = t_{k+1} - t_k$, and consider that the exact solution of ODE (1) is known at the point t_k ; i.e., $x_k = x(t_k)$. Then, on the one hand, if two additional solutions $x(t_k + c_1\tau)$ and $x(t_k + c_2\tau)$ evaluated at internal points of the interval $[t_k, t_{k+1}]$ are known we will be able to use a two-point quadrature formula of the form

$$x_{k+1} = x(t_k) + \tau_k b_1 g(t_k + c_1\tau_k, x(t_k + c_1\tau_k)) + \tau_k b_2 g(t_k + c_2\tau_k, x(t_k + c_2\tau_k))$$

in order to find an approximation to the exact solution $x(t_{k+1})$.

On the other hand, if the exact solution $x(t_{k+1})$ is considered to be known we can try to approximate the values x_{k1} and x_{k2} of the exact solution evaluated at the points $t_k + c_1\tau_k$ and $t_k + c_2\tau_k$, respectively, by means of explicit formulas of the following form:

$$\begin{aligned} x_{k1} &= a_{11}x(t_k) + a_{12}x(t_{k+1}) + \tau_k \left(d_{11}g(t_k, x(t_k)) + d_{12}g(t_{k+1}, x(t_{k+1})) \right), \\ x_{k2} &= a_{21}x(t_k) + a_{22}x(t_{k+1}) + \tau_k \left(d_{21}g(t_k, x(t_k)) + d_{22}g(t_{k+1}, x(t_{k+1})) \right). \end{aligned}$$

Thus, our task is to search the highest order one-step methods of the form

$$x_1 = a_{11}x_k + a_{12}x_{k+1} + \tau_k (d_{11}g(t_k, x_k) + d_{12}g(t_{k+1}, x_{k+1})), \quad (3a)$$

$$x_2 = a_{21}x_k + a_{22}x_{k+1} + \tau_k (d_{21}g(t_k, x_k) + d_{22}g(t_{k+1}, x_{k+1})), \quad (3b)$$

$$x_{k+1} = x_k + \tau_k (b_1g(t_k + c_1\tau_k, x_1) + b_2g(t_k + c_2\tau_k, x_2)) \quad (3c)$$

where a_{ij} , b_i , c_i , d_{ij} , $i, j = 1, 2$, are unknown fixed coefficients.

We first remark that the Gauss quadrature formula has the highest order 4 among all formulas of the form (3c). Therefore the coefficients b_i , c_i are determined uniquely and they are: $b_1 = b_2 = 1/2$, $c_1 = (3 - \sqrt{3})/6$, $c_2 = (3 + \sqrt{3})/6$.

Second, we require the defect (or the local error) of method (3) to be $O(\tau_k^5)$ for any ODE (1) with a sufficiently smooth right-hand side. The latter condition admits the following one-parametric family of the coefficients to provide the fourth order convergence for method (3):

$$a_{11} = \theta, \quad a_{12} = 1 - \theta, \quad a_{21} = 1 - \theta, \quad a_{22} = \theta, \quad (4a)$$

$$d_{11} = \frac{6\theta - 2 - \sqrt{3}}{12}, \quad d_{12} = \frac{6\theta - 4 - \sqrt{3}}{12}, \quad (4b)$$

$$d_{21} = \frac{4 + \sqrt{3} - 6\theta}{12}, \quad d_{22} = \frac{2 + \sqrt{3} - 6\theta}{12}. \quad (4c)$$

Below, we consider that methods (3) are based on the Gauss quadrature formula of order 4 and their coefficients satisfy conditions (4). So, it is not difficult to check that all these methods are symmetric. We refer the reader to [4] for the necessary theory. It is also quite evident that the stability functions of all the constructed methods are $R_{22}(z)$, which means the $(2, 2)$ -Padé approximation to the exponential function e^z (see, for example, [5]). The latter implies that our methods are A -stable. Thus, the family of methods (3) can be useful to integrate both nonstiff and stiff ODE's (including reversible problems).

3 Practical Implementation

For nonstiff ODE's, we recommend to use fixed-point iterations with both trivial predictor and nontrivial one. Particulars on implementation of this iteration in iterative Runge-Kutta methods and estimation of a sufficient number for iteration steps to provide the maximum order convergence can be found in [7].

When solving stiff ODE's we are constrained with Newton-type iterations only and have to implement the iteration in the form that does not ruin A -stability of the underlying method (see, for example, [3], [5]). From this point of view, the modified Newton iteration is a proper one. Unfortunately, the high execution cost, which is about $4n^3/3$ arithmetical operations per evaluation of the Jacobi matrix and its LU decomposition, makes it pretty unpractical for large n . Hopefully, the number of operations can be reduced with a factor of 4 by replacement of the full Jacobian of method (3) with a simplified one, as follows:

$$(I - \tau_k J/4)^2 (x_{k+1}^\ell - x_{k+1}^{\ell-1}) = -x_{k+1}^{\ell-1} + \bar{x}_k + \tau_k (b_1 g(t_k + c_1 \tau_k, x_{k1}^{\ell-1}) + b_2 g(t_k + c_2 \tau_k, x_{k2}^{\ell-1})), \quad (5)$$

where $\ell = 1, 2, \dots, N$ and $\bar{x}_k$ is the numerical solution derived by method (3) with N Newton iteration steps per grid point; i.e., $\bar{x}_k \stackrel{\text{def}}{=} x_k^N$, $k = 1, 2, \dots, K$. Here, $J \stackrel{\text{def}}{=} \partial_x g(t_{k+1}, x_{k+1}^0)$ be the partial derivative of the right-hand side of ODE (1) with respect to the second variable evaluated at the point (t_{k+1}, x_{k+1}^0) . Note that iteration (5) implies a single LU decomposition of the matrix $I - \tau_k J/4$ and successive solutions of two linear systems with the same decomposed coefficient matrix. This feature makes methods (3) comparable to SDIRK, which are very efficient to solve stiff ODE's (see [3], [5]).

At the end, we exhibit nice practical properties of iteration (5). First, the Jacobian replacement made above does not influence the sufficient number of iteration steps with both trivial predictor and nontrivial one to provide the fourth order convergence. It follows from Theorem 3 in [8]. Second, iteration (5) is A -stable. To see this, we apply one step of iteration (5) to the Dahlquist test equation $x' = \lambda x$ where λ is a fixed complex number with a nonpositive real

part and consider that $x_{k+1}^0 = x_k$. Simple calculations give the stability function of method (5) in the form $R(z) = (1 + z/4)^2/(1 - z/4)^2$, which is evidently A -stable.

4 Numerical Experiments

To test our methods, we apply the method (3) when $\theta = 1/2 + 2\sqrt{3}/9$ and with iteration (5) to the two dimensional Brusselator with diffusion and the periodic boundary conditions (see [5, p. 151–152] for full detail). We take the number of the grid points in each dimension to be equal 50. It leads to a system of ODE of dimension 5000. We solve this problem on the interval $[0, 6]$ by the method (3) and by the Gauss method of order 4 (termed also Hammer and Hollingsworth's method). Both methods are based on the same quadrature formula and they are of the same classical order. However, the stage order of our method is 3 and of the Gauss one is 2.

We use the same variable step size implementation of these two methods with modified Newton iterations and with the same step size selection mechanism based on the local error estimate evaluated by the Richardson extrapolation. We apply the modified Newton iteration in the form of algorithm (5) in method (3) and do the conventional implementation for the Gauss method. We also want to emphasize that the correct step size control requires two iteration steps per grid point in algorithm (5) and three iteration steps in the modified Newton iteration applied to the Gauss method (see, for example, [8]). The local error tolerance is chosen to be 10^{-01} .

Statistics of both integrations is presented in form of the following table and clearly displays the better performance of the method (3), at least for this test problem:

Statistics	method (3)	Gauss method
execution time (in sec.)	843.985	2456.656
number of rejected steps	6	1
number of accepted steps	44	24

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