Journal of Computational Mathematics, Vol.11, No.3, 1993, 250–260.

CONSTRUCTION OF HIGH ORDER SYMPLECTIC RUNGE-KUTTA METHODS*1)

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Abstract

Characterizations of symmetric and symplectic Runge-Kutta methods, which are based on the W-transformation of Hairer and Wanner, are presented. Using these characterizations we construct two classes of high order symplectic (symmetric and algebraically stable or algebraically stable) Runge-Kutta methods. They include and extend known classes of high order implicit Runge-Kutta methods.

§1. Introduction

In this paper we construct high order implicit Runge-Kutta methods which are based on certain combinations of the normalized shifted Legendre polynomials . Of particular interest is the symplectic property of these methods as well as their order, symmetry and stability properties. The construction of such methods heavily relies on the following simplifying assumptions of order conditions introduced by Butcher[2]:

$$B(p): b^T c^{k-1} = \frac{1}{k}, \qquad k = 1(1)p,$$

$$C(\eta): Ac^{k-1} = \frac{1}{k}c^k, \qquad k = 1(1)\eta,$$

$$D(\zeta): (bc^{k-1})^T A = \frac{1}{k}(b^T - (bc^k)^T), \qquad k = 1(1)\zeta$$

where A is an $s\times s$ matrix, and b, c are $s\times 1$ vectors of weights and abscissae, respectively. Butcher proved the following fundamental theorem:

Theorem 1.1. *If the coefficients A, b, c of an RK method satisfy $B(p), C(\eta), D(\zeta)$ with $p \le \eta + \zeta + 1$ and $p \le 2\eta + 2$, then the RK method is of order p.*

On the other hand it will be seen that the construction also relies heavily on the W-transformation proposed by Hairer and Wanner[6],[8]. In particular , the W-transformation facilitates more the construction of high order symplectic RK methods. Recently[4,5] the research of symplectic methods is very active. The symplecticness,

* Received December 21, 1991 .

1) The Project Supported by Swiss National Science Foundation and by National Natural Science Foundation of China.

roughly speaking, is a characteristic property of geometry possessed by the solution of Hamiltonian problems. A numerical method is called symplectic if, when applied to Hamiltonian problems, it generates numerical solutions that inherit the property of symplecticness. Sanz-Serna[11] obtained the following result : if the coefficients of an RK method satisfy

$$M = BA + A^T B - bb^T = 0,$$

where

$$B = \operatorname{diag}(b_1, \cdots, b_s),$$

then the method is symplectic. In fact , for an irreducible RK method this condition also is necessary[9]. Up to now it was only found out that symmetric and algebraically stable Gauss, Lobatto III E[10,3], and Lobatto III S[3] methods are symplectic in the class of high order RK methods.

In Section 2 we recall the W-transformation of Hairer and Wanner and present characterizations of symmetric and symplectic methods based on the W-transformation. The properties of known high order RK methods are immediately obtained from these characterizations. In Section 3 we first construct a two-parameter family of symmetric and symplectic methods based on the combination

$$M(x) = P_s(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-3}}\alpha P_{s-2}(x),$$

where $P_s(x), P_{s-2}(x)$ are the Legendre polynomials of degrees s and $s-2$ respectively , and give , with special choice of parameters, known symmetric and algebraically stable methods and examples of these new methods for 2 and 3 stages , particularly diagonally implicit methods for 2 and 3 stages. Then, we construct a one-parameter family of symplectic and algebraically stable methods based on the combination

$$M(x) = P_s(x) + \frac{\sqrt{2s+1}}{\sqrt{2s-1}}\alpha P_{s-1}(x),$$

and obtain , with special choice of the parameter , two kinds of new methods which are called Radau I B and Radau II B respectively as new members of the Radau family. Finally, examples of new methods for 2 and 3 stages are given.

§2. Characterization of Symmetric and Symplectic Methods

Hairer and Wanner, in their study of algebraic stability of high order implicit RK methods, introduced a generalized Vandermonde matrix W defined by

$$W = (P_0(c), P_1(c), \cdots, P_{s-1}(c)) \tag{2.1}$$

where the normalized shifted Legendre polynomials are defined by

$$P_k(x) = \sqrt{2k+1}\sum_{i=0}^{k}(-1)^{k+i}\binom{k}{i}\binom{k+i}{i}x^i, \qquad k = 0, 1, \cdots.$$