Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Construction of symplectic (partitioned) Runge-Kutta methods with continuous stage



College of Mathematics and Statistics, Changsha University of Science and Technology, Changsha 410114, PR China

ARTICLE INFO

Keywords: Hamiltonian systems Symplectic methods Continuous-stage Runge-Kutta methods Continuous-stage partitioned Runge-Kutta methods

ABSTRACT

Hamiltonian systems, as one of the most important class of dynamical systems, are associated with a well-known geometric structure called symplecticity. Symplectic numerical algorithms, which preserve such a structure are therefore of interest. In this article, we study the construction of symplectic (partitioned) Runge–Kutta methods with continuous stage. This construction of symplectic methods mainly relies upon the expansion of orthogonal polynomials and the simplifying assumptions for (partitioned) Runge–Kutta type methods. By using suitable quadrature formulae, it also provides a new and simple way to construct symplectic (partitioned) Runge–Kutta methods in classical sense.

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1. Introduction

Geometric numerical integration is a subfield of the numerical solution of differential equations, whose main goal is the devise of efficient numerical methods for simulating the long-time dynamical behavior of those systems with special geometric structures [15]. For Hamiltonian systems, it is known that symplecticity of the flow is an important geometric property [1] and to correctly reproduce this property, well-known algorithms named symplectic methods have been proposed and extensively studied over the last few decades (see [10,15,22] and references therein), among which symplectic (partitioned) Runge–Kutta methods constitute the most important instances [21,23–25].

Runge–Kutta (RK) methods with continuous stage have been investigated and discussed by several authors recently [16,19,26,27,29], even though they were firstly presented by Butcher in 1970s [5,7]. There is no consolidated literature covering all the aspects of this kind of methods, until recently, Hairer [16] exploits them to interpret an energy-preserving variant of collocation methods. Subsequently, Tang and Sun [26] investigates time finite element methods and relates them to some continuous-stage RK methods. Moreover, it is shown in [26] that some energy-preserving RK methods including *s*-stage trapezoidal methods [17], Hamiltonian boundary value methods [2–4], average vector field methods [8,20] can also be related to such methods. The authors in [27,29] discuss the general construction of RK methods with continuous stage and present the characterizations for several geometric numerical integrators including symplectic methods, symmetric methods and energy-preserving methods. Exponentially-fitted continuous-stage RK methods with energy-preserving property for Hamiltonian systems are also presented in [19]. In this paper, we further investigate the construction of symplectic (partitioned) RK type methods. This approach naturally provides a new and simple way to construct symplectic (partitioned) RK methods in classical sense.

* Corresponding author. Tel.: +86 13875926201.

http://dx.doi.org/10.1016/j.amc.2016.04.026 0096-3003/© 2016 Elsevier Inc. All rights reserved.







E-mail addresses: tangws@lsec.cc.ac.cn (W. Tang), langguangming1984@126.com (G. Lang), luoxuqiong@163.com (X. Luo).

The outline of the paper is as follows. In Section 2, we provide some preliminaries for (partitioned) RK methods with continuous stage and review some existing results for the construction of general RK type methods with continuous stage. In Section 3, we discuss the construction of symplectic (partitioned) RK methods with continuous stage as well as the symplectic (partitioned) RK methods in classical sense. At last, we conclude this paper.

2. Construction of (partitioned) RK type methods

In this section, we first introduce the definition of (P)RK methods with continuous stage by following the formulation proposed in [16], then show some results which are useful in constructing (P)RK type methods.

2.1. Continuous-stage RK methods

Consider a first-order system of ordinary differential equations (ODEs)

$$\begin{cases} \dot{\boldsymbol{z}} = \boldsymbol{f}(t, \boldsymbol{z}), \\ \boldsymbol{z}(t_0) = \boldsymbol{z}_0 \in \mathbb{R}^d, \end{cases}$$
(2.1)

where the upper dot indicates differentiation with respect to *t* and $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a sufficiently smooth vector function.

Definition 2.1 [16,29]. Let $A_{\tau,\sigma}$ be a function of two variables $\tau, \sigma \in [0, 1]$, B_{τ} be a function of $\tau \in [0, 1]$ and define $C_{\tau} = \int_{0}^{1} A_{\tau,\sigma} d\sigma$. The one-step method $\Phi_h: \mathbf{z}_0 \mapsto \mathbf{z}_1$ given by

$$\boldsymbol{Z}_{\tau} = \boldsymbol{z}_{0} + h \int_{0}^{1} A_{\tau,\sigma} \boldsymbol{f}(t_{0} + C_{\sigma}h, \boldsymbol{Z}_{\sigma}) \, \mathrm{d}\sigma, \quad \tau \in [0, 1],$$

$$\boldsymbol{z}_{1} = \boldsymbol{z}_{0} + h \int_{0}^{1} B_{\tau} \boldsymbol{f}(t_{0} + C_{\tau}h, \boldsymbol{Z}_{\tau}) \, \mathrm{d}\tau, \qquad (2.2)$$

is called a continuous-stage Runge–Kutta (csRK) method, where $\mathbf{Z}_{\tau} \approx \mathbf{z}(t_0 + C_{\tau}h), \mathbf{z}_1 \approx \mathbf{z}(t_0 + h)$.

In this paper, the construction of csRK methods mainly relies upon the following simplifying assumptions of order conditions [16]

$$\begin{split} \bar{B}(\xi) &: \int_0^1 B_\tau C_\tau^{\kappa-1} \, \mathrm{d}\tau = \frac{1}{\kappa}, \quad \kappa = 1, \dots, \xi, \\ \bar{C}(\eta) &: \int_0^1 A_{\tau,\sigma} C_\sigma^{\kappa-1} \, \mathrm{d}\sigma = \frac{1}{\kappa} C_\tau^{\kappa}, \quad \kappa = 1, \dots, \eta, \\ \bar{D}(\zeta) &: \int_0^1 B_\tau C_\tau^{\kappa-1} A_{\tau,\sigma} \, \mathrm{d}\tau = \frac{1}{\kappa} B_\sigma \left(1 - C_\sigma^{\kappa}\right), \quad \kappa = 1, \dots, \zeta. \end{split}$$

Analogously to the classical result [6] given by Butcher in 1964, we can obtain a useful theorem and determine the order of a csRK method with it.

Theorem 2.1 [29]. If a csRK method (2.2) with coefficients $(A_{\tau,\sigma}, B_{\tau}, C_{\tau})$ satisfies $\bar{B}(\rho)$, $\bar{C}(\alpha)$ and $\bar{D}(\beta)$, then it is of order at least

$$\min(\rho, 2\alpha + 2, \alpha + \beta + 1)$$

Proof. This statement can be proved by using a similar idea to the one used in Theorem 7.4 [13]. \Box

According to Proposition 2.1 shown in [29], we assume $B_{\tau} = 1$ in the current paper and to proceed conveniently, hereafter we also assume $C_{\tau} = \tau$. In such a case, $\tilde{B}(\xi)$ is reduced to

$$\int_0^1 \tau^{\kappa-1} \, \mathrm{d}\tau = \frac{1}{\kappa}, \quad \kappa = 1, \dots, \xi$$

which implies $\bar{B}(\xi)$ holds with $\xi = \infty$. Now we introduce the *i*-degree normalized shifted Legendre polynomial $P_i(x)$, which can be explicitly computed by the Rodrigues formula

$$P_0(x) = 1, P_{\iota}(x) = \frac{\sqrt{2\iota + 1}}{\iota!} \frac{d^{\iota}}{dx^{\iota}} (x^{\iota}(x-1)^{\iota}), \quad \iota = 1, 2, 3, \cdots$$

A well-known property of such Legendre polynomials is that they are orthogonal to each other with respect to the L^2 inner product in [0, 1]

$$\int_0^1 P_\iota(t) P_\kappa(t) \,\mathrm{d}t = \delta_{\iota\kappa}, \quad \iota, \, \kappa = 0, \, 1, \, 2, \, \ldots,$$

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