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Symplecticity-preserving continuous-stage Runge–Kutta–Nyström methods

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ABSTRACT

In this paper, we develop continuous-stage Runge–Kutta–Nyström (csRKN) methods for numerical integration of second-order ordinary differential equations (ODEs) written in the form $\ddot{q} = f(t, q)$. Numerous ODEs in such form can be reduced to first-order ODEs with the separable form of Hamiltonian systems and symplecticity-preserving discretizations of these systems are of interest. For the sake of designing symplectic csRKN methods, we explore the sufficient conditions for symplecticity, and we show a simple way to derive symplectic RKN-type integrators by using Legendre polynomial expansion. Numerical results show the efficiency of the presented methods.

1. Introduction

It is well-known that standard Runge–Kutta (RK) methods, partitioned Runge–Kutta (PRK) methods and Runge–Kutta–Nyström (RKN) methods play a central role in the field of numerical solution of ordinary differential equations (ODEs), and they were well-developed in the previous investigations [3,7,8].

More recently, numerical methods with infinitely many stages including continuous-stage Runge–Kutta (csRK) methods, continuous-stage partitioned Runge–Kutta (csPRK) methods have been investigated and discussed in [4,10,11,17–20]. Based on such methods, it was shown in [18,19] that simply by using quadrature formulae it offers plentiful RK and PRK methods of arbitrary-order accuracy, without resort to solving the tedious nonlinear algebraic equations that stem from the order conditions with many unknown coefficients. The construction of continuous-stage numerical methods seems easier than that of those classical methods, since the associated Butcher tableau coefficients belong to the space of continuous functions and they can be treated with orthogonal polynomial expansion techniques [18,19]. Moreover, as shown in [18,19], numerical methods serving some special purposes including symplecticity-preserving methods for Hamiltonian systems, symmetric methods for time-reversible systems, energy-preserving methods for conservative systems, conjugate-symplectic (up to a finite order) methods for Hamiltonian systems can also be constructed and investigated based on such a new framework.

It is worth mentioning that some integrators with special purposes could not possibly exist in the classical context of numerical methods but they do within the new framework. For instance, in [5] it was shown that there is no energy-preserving RK methods for general non-polynomial Hamiltonian systems, but energy-preserving methods based on csRK obviously exist [2,4,10,11,13,17,19,20]. It is also found that some Galerkin variational methods can be related to continuous-stage (P)RK

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methods, which can not be completely explained in the classical (P)RK framework [20–22]. As a consequence, continuous-stage methods provide us a new broader scope for numerical solution of ODEs and they are worth further investigating.

As is well known, second-order ODEs are commonly encountered in various fields including celestial mechanics, molecular dynamics, biological chemistry, theoretical physics and so on [7,9,14]. In this paper, we are going to develop continuous-stage RKN (csRKN) methods for solving second-order ODEs written in the form $\ddot{q} = f(t, q)$. In practical applications, there are a number of second-order ODEs which can be reduced to first-order ODEs with the form of separable Hamiltonian systems, and symplecticity-preserving discretization for such special systems is of remarkable interest [6,9,14]. For this sake, we will explore sufficient conditions for a csRKN method to be symplectic, and then show the construction of symplectic RKN-type integrators by using polynomial expansion techniques.

The outline of this paper is as follows. In the next section, we introduce the so-called csRKN methods for solving second-order ODEs. After that we present the corresponding symplectic conditions and the order conditions, then we use the orthogonal polynomial expansion technique to construct symplecticity-preserving RKN-type methods, which will be shown in Sections 3 and 4. Section 5 is devoted to discuss the construction of diagonally implicit symplectic methods. Numerical results will be shown in Section 6. At last, concluding remarks will be given.

2. Continuous-stage RKN method

Let us consider an initial value problem of second-order ODEs

$$\ddot{q} = f(t, q), \quad q(t_0) = q_0, \quad \dot{q}(t_0) = p_0, \tag{2.1}$$

where the double dots on q represent the second-order derivative with respect to t and $f : \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ is a sufficiently smooth vector-valued function.

For system (2.1), the often used treatment is to write it as a first-order differential system by introducing $p = \dot{q}$, namely

$$\begin{cases} \dot{p} = f(t, q), \quad \dot{q} = p, \\ p(t_0) = p_0, \quad q(t_0) = q_0. \end{cases} \tag{2.2}$$

As presented in [18], by using a continuous-stage partitioned Runge–Kutta (csPRK) method to solve (2.2), it gives

$$P_\tau = p_n + h\int_0^1 A_{\tau,\sigma} f(t_n + C_\sigma h, Q_\sigma)d\sigma, \quad \tau \in [0, 1], \tag{2.3a}$$

$$Q_\tau = q_n + h\int_0^1 \hat{A}_{\tau,\sigma} P_\sigma d\sigma, \quad \tau \in [0, 1], \tag{2.3b}$$

$$p_{n+1} = p_n + h\int_0^1 B_\tau f(t_n + C_\tau h, Q_\tau)d\tau, \quad n \in \mathbb{N}, \tag{2.3c}$$

$$q_{n+1} = q_n + h\int_0^1 \hat{B}_\tau P_\tau d\tau, \quad n \in \mathbb{N}, \tag{2.3d}$$

where $A_{\tau,\sigma}$, $\hat{A}_{\tau,\sigma}$ are functions of two variables $\tau, \sigma \in [0, 1]$, and B_τ, $\hat{B}_\tau$, C_τ are functions of $\tau \in [0, 1]$ satisfying [18]

$$\int_0^1 A_{\tau,\sigma} d\sigma = \int_0^1 \hat{A}_{\tau,\sigma} d\sigma = C_\tau, \quad \int_0^1 B_\tau d\tau = \int_0^1 \hat{B}_\tau d\tau = 1.$$

We call Q_τ and P_τ the internal continuous stages.

By inserting (2.3a) into (2.3b), we derive

$$Q_\tau = q_n + h\int_0^1 \hat{A}_{\tau,\sigma}\Big(p_n + h\int_0^1 A_{\sigma,\rho} f(t_n + C_\rho h, Q_\rho)d\rho\Big)d\sigma \tag{2.4}$$

$$= q_n + hC_\tau p_n + h^2\int_0^1 \bar{A}_{\tau,\sigma} f(t_n + C_\sigma h, Q_\sigma)d\sigma, \tag{2.5}$$

where we denote $\bar{A}_{\tau,\sigma} = \int_0^1 \hat{A}_{\tau,\rho} A_{\rho,\sigma} d\rho$.

Similarly, by inserting (2.3a) into (2.3d), we have

$$q_{n+1} = q_n + h\int_0^1 \hat{B}_\tau\Big(p_n + h\int_0^1 A_{\tau,\sigma} f(t_n + C_\sigma h, Q_\sigma)d\sigma\Big)d\tau \tag{2.6}$$

$$= q_n + hp_n + h^2\int_0^1 \bar{B}_\tau f(t_n + C_\tau h, Q_\tau)d\tau, \tag{2.7}$$

where we define $\bar{B}_\tau = \int_0^1 \hat{B}_\rho A_{\rho,\tau} d\rho$.