

SYMPLECTIC PARTITIONED RUNGE-KUTTA METHODS*¹⁾

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Abstract

For partitioned Runge-Kutta methods, in the integration of Hamiltonian systems, a condition for symplecticness and its characterization which is based on the W -transformation of Hairer and Wanner are presented. Examples for partitioned Runge-Kutta methods which satisfy the symplecticness condition are given. A special class of symplectic partitioned Runge-Kutta methods is constructed.

1. Introduction

Let Ω be a domain (i.e. a non-empty, open, simply connected set) in the oriented Euclidean space \mathbb{R}^{2d} of the point $(p, q) = (p_1, \dots, p_d; q_1, \dots, q_d)$. If H is a sufficiently smooth real function defined in Ω , then the Hamiltonian system of differential equations with Hamiltonian H is given by

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} =: f_i(p, q), \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} =: g_i(p, q), \quad 1 \leq i \leq d. \quad (1.1)$$

The integer d is called the number of degrees of freedom and Ω is the phase space. Here we assume that all Hamiltonians considered are autonomous, i.e. time-independent.

A smooth transformation $(p, q) = \psi(p^*, q^*)$ defined in Ω is said to be symplectic (with respect to symplectic matrix J) if the Jacobian $\psi' = \frac{\partial(p, q)}{\partial(p^*, q^*)}$ satisfies

$$\psi'^T J \psi' = \frac{\partial(p, q)^T}{\partial(p^*, q^*)} J \frac{\partial(p, q)}{\partial(p^*, q^*)} = J, \quad \forall (p^*, q^*) \in \Omega,$$

where $J = \begin{pmatrix} 0 & I_d \\ -I_d & 0 \end{pmatrix}$ is the standard symplectic matrix. This property is the hallmark of Hamiltonian systems.

In this paper we restrict our interest to one-step methods. If h denotes the step-length and (p^n, q^n) denotes the numerical approximations at time $t_n = nh$ to the value $(p(t_n), q(t_n))$ of a solution of (1.1), the one-step method is specified by a smooth mapping

$$(p^{n+1}, q^{n+1}) = \psi_{h,H}(p^n, q^n)$$

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and $\psi_{h,H}$ is assumed to depend only smoothly on h and H . In numerically solving the Hamiltonian systems of differential equations (1.1), it is natural to require that numerical solutions should preserve the property of symplecticness. Then the numerical method

$$(p^{n+1}, q^{n+1}) = \psi_{h,H}(p^n, q^n)$$

should be a symplectic transformation. Consequently we may give the following definitions.

Definition 1.1. *A one-step method is called symplectic if, as applied to the Hamiltonian system (1.1), the underlying formula generating numerical solutions $(p^{n+1}, q^{n+1}) = \psi_{h,H}(p^n, q^n)$ is a symplectic transformation, that is ,*

$$\psi_{h,H}'^T J \psi_{h,H}' = \frac{\partial(p^{n+1}, q^{n+1})^T}{\partial(p^n, q^n)} J \frac{\partial(p^{n+1}, q^{n+1})}{\partial(p^n, q^n)} = J, \quad \forall (p^n, q^n) \in \Omega, \quad (1.2)$$

where $\psi_{h,H}' = \frac{\partial(p^{n+1}, q^{n+1})^T}{\partial(p^n, q^n)}$ is the Jacobian matrix of the transformation.

At least three authors ([5],[6]and [9]) discovered independently the fact that the Runge-Kutta method with tableau

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ c_2 & a_{21} & \dots & a_{2s} \\ \vdots & \vdots & \dots & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array} \quad (1.3)$$

applied to the Hamiltonian system (1.1), if its coefficients (1.3) satisfy the relation

$$M = BA + A^T B - bb^T = 0 \text{ or } m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \leq i, j \leq s, \quad (1.4)$$

where $B = \text{diag}(b_1, b_2, \dots, b_s)$, then the Runge-Kutta method is symplectic.

In the integration of systems of differential equations it is possible to integrate some components of an unknown vector with a numerical method and the remaining components with an other one, as in dealing with some stiff systems including both stiff and nonstiff components. In Section 2, for Hamiltonian systems we shall integrate the p equations with an RK formula and the q equations with a different RK formula. The overall scheme is called a partitioned Runge-Kutta (PRK) scheme. For PRK scheme we shall give the conditions for symplecticness and its characterization which is based on the W -transformation of Hairer and Wanner^{[3],[4]}. Besides, some examples are presented. In Section 3, a special class of symplectic PRK methods is constructed.

2. Conditions for symplecticness and its Characterization

In this section first of all we derive the conditions of symplecticness for PRK methods. For notational simplicity we shall assume $d = 1$ in the following.