A symplectic Runge–Kutta–Nyström method with minimal phase-lag

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Abstract

In this Letter we introduce a symplectic explicit RKN method for Hamiltonian systems with periodical solutions. The method has algebraic order three and phase-lag order six at a cost of three function evaluations per step. Numerical experiments show the relevance of the developed algorithm. It is found that the new method is much more efficient than the standard symplectic fourth-order method [M.P. Calvo, J.M. Sanz-Serna, SIAM J. Sci. Comput. 14 (1993) 936].

1. Introduction

Hamiltonian systems are systems of first-order ordinary differential equations that can be expressed as

$$p' = -\frac{\partial H}{\partial q}(p, q), \qquad q' = \frac{\partial H}{\partial p}(p, q), \tag{1.1}$$

where $p, q \in \mathbb{R}^d$ and H is a twice continuously differentiable function $H : U \to \mathbb{R}$ ($U \subset \mathbb{R}^{2d}$ is an open set). Hamiltonian systems appear frequently in the area of classical mechanics, physics, chemistry and elsewhere. A numerical method is called symplectic if, when applied to Hamiltonian problems, it preserves the symplectic structure in phase space, thus reproducing the main qualitative property of solutions of Hamiltonian systems. This leads to an excellent long-time behaviour. The past decades a lot of attention has been paid to symplectic integrators for the numerical solution of (1.1). Excellent reviews can be found in [1,2].

Quite often the solution of (1.1) exhibits a pronounced oscillatory character. Oscillatory problems are usually considered as difficult. One way to obtain a more efficient integration process is constructing numerical methods with an increased algebraic order. On the other hand, the construction and implementation of high algebraic order (symplectic) methods is not evident. An alternative way is considering methods which take into account the nature of the problem. The resulting methods can be divided in two main categories. The first category are methods with coefficients depending on the problem. If a good estimate of the period, or of the dominant frequency, is known in advance, then some important classes of numerical methods, such as *exponentially-fitted* [3] (in short: EF) or *phase-fitted* methods are available. The second category are methods with constant coefficients. A large number of methods selected for specific properties, such as *P-stability* or *minimal phase-lag*, have appeared in the literature. Note that these methods can be applied to every oscillatory problem, even if the frequency is not initially known. We mention the pioneering paper of Brusa and Nigro [4], in which the *phase-lag* (or *dispersion*) property was introduced. This is actually a different type of truncation error, namely the angle between the analytical solution and the numerical solution. This theory was extended to RK(N) methods by

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van der Houwen and Sommeijer [5]. They have derived the so-called *phase-lag relations* for RK(N) methods and presented several RK(N) methods with phase-lag order up to ten whereas the algebraic order of accuracy is only two or three. Since then, many authors have constructed RK(N) methods with high phase-lag order, see for example [6–8].

Very recently, several authors have devoted much attention to the combination of exponential fitting and symplecticity [9–17]. The highest order of a symplectic EF method achieved until now, is four [9,16]. The structure preservation of these methods is investigated in [9]. To our knowledge, the investigation of symplectic RK(N) methods with increased phase-lag order is not performed so far. The purpose of this Letter is to start this study with a lower order example: we investigate the construction of a third-order symplectic explicit RKN method with phase-lag order six.

2. General theory

We restrict our attention to systems of the special form

$$p' = f(q), \qquad q' = p, \tag{2.2}$$

i.e., to second-order systems $q'' = f(q)$. If f is the gradient of a scalar function $-V(q)$, then (2.2) is a Hamiltonian system with

$$H(p,q) = T(p) + V(q), \quad T(p) = \frac{1}{2}p^T p. \tag{2.3}$$

In mechanics, the q variables represent Lagrangian coordinates, the p variables the corresponding momenta, f the forces, T the kinetic energy, V the potential energy, and H the total energy. For the numerical solution of (2.2) we consider the s-stage *Runge–Kutta–Nyström* (*RKN*) method

$$Q_i = q_n + hc_i p_n + h^2 \sum_{j=1}^{s} a_{ij} f(Q_j),$$

$$q_{n+1} = q_n + hp_n + h^2 \sum_{i=1}^{s} \bar{b}_i f(Q_i),$$

$$p_{n+1} = p_n + h \sum_{i=1}^{s} b_i f(Q_i), \tag{2.4}$$

where we assume that the following well-known *simplifying condition* holds [18]

$$\bar{b}_i = b_i(1 - c_i), \quad i = 1, \dots, s. \tag{2.5}$$

The RKN method is completely determined by means of its Butcher tableau

$$
\begin{array}{c|cccc}
c_1 & a_{11} & a_{12} & \dots & a_{1s} \\
c_2 & a_{21} & a_{22} & \dots & a_{2s} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
c_s & a_{s1} & a_{s2} & \dots & a_{ss} \\
\hline
 & \bar{b}_1 & \bar{b}_2 & \dots & \bar{b}_s \\
\hline
 & b_1 & b_2 & \dots & b_s
\end{array}
\quad = \quad
\begin{array}{c|c}
c & A \\
\hline
 & \bar{b}^T \\
\hline
 & b^T
\end{array}.
$$

The method is said to be *explicit* when A is strictly lower triangular.

2.1. RKN methods and symplecticity

Definition 1. A differentiable map $g : U \to \mathbb{R}^{2d}$ is called symplectic if the Jacobian matrix $g'(p, q)$ is everywhere symplectic

$$g'(p,q)^T J g'(p,q) = J \quad \text{with } J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

There is a geometric interpretation: in the case that $d = 1$ it means that a symplectic transformation preserves the area. We associate with the Hamiltonian system (1.1) the following flow

$$\psi_t : U \to \mathbb{R}^{2d} : (p_0, q_0) \to \big(p(t, p_0, q_0), q(t, p_0, q_0)\big), \tag{2.6}$$

where $(p(t, p_0, q_0), q(t, p_0, q_0))$ is the solution of the system (1.1) corresponding to initial values $p(0) = p_0, q(0) = q_0$. Symplecticity is a characteristic property of Hamiltonian systems. Therefore it is natural to search for numerical methods that share this property. We denote a one-step method for (1.1) as $y_{n+1} = \Phi_h(y_n)$, with $y_n = (p_n, q_n)^T$.