Journal of Computational Mathematics, Vol.20, No.5, 2002, 449–460.

BACKWARD ERROR ANALYSIS OF SYMPLECTIC INTEGRATORS FOR LINEAR SEPARABLE HAMILTONIAN SYSTEMS*

Peter Görtz
(*Institut für Praktische Mathematik, Universität Karlsruhe, Englerstraße 2, 76128 Karlsruhe, Germany*)

Abstract

Symplecticness, stability, and asymptotic properties of Runge–Kutta, partitioned Runge–Kutta, and Runge–Kutta–Nyström methods applied to the simple Hamiltonian system $\dot{p} = -\nu q, \dot{q} = \kappa p$ are studied. Some new results in connection with P–stability are presented. The main part is focused on backward error analysis. The numerical solution produced by a symplectic method with an appropriate stepsize is the exact solution of a perturbed Hamiltonian system at discrete points. This system is studied in detail and new results are derived. Numerical examples are presented.

Key words: Hamiltonian systems, Backward error analysis, Symplectic integrators.

1. Introduction

In the area of symplectic integration of Hamiltonian systems of the form

$$\dot{u} = -J\nabla H(u),$$

where

$$u = \begin{bmatrix} p \\ q \end{bmatrix} = \left[p^{(1)} \ \dots \ p^{(n)} \ q^{(1)} \ \dots \ q^{(n)}\right]^T, \ J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

$H \in C^{(\infty)}(\mathcal{M})$ is the Hamiltonian, $\mathcal{M} \subseteq \mathbb{R}^{2n}$ open is the phase space,

$$\nabla H = \left[\frac{\partial H}{\partial p^{(1)}} \ \dots \ \frac{\partial H}{\partial q^{(n)}}\right]^T,$$

backward error analysis plays an important role. The idea is to interprete the numerical solution produced by a symplectic one–step method as the exact solution of a perturbed Hamiltonian system. In general, this is only formally possible; the perturbed Hamiltonian system is given as a power series which is usually divergent (Feng [4], Hairer [9], Tang [15], Yoshida [17]; cf. Hairer, Nørsett, Wanner [10], Sanz–Serna, Calvo [14]). If the Hamiltonian system is linear, i.e., the Hamiltonian is a quadratic form, then the perturbed Hamiltonian system can be expressed by the logarithm of a matrix. Conditions exists which guarantee the existence of a logarithm of the relevant matrix (Wang [16]).

Often the Hamiltonian system is linear and separable as follows:

$$\left.\begin{array}{l} \begin{bmatrix} \dot{p} \\ \dot{q} \end{bmatrix} = \begin{bmatrix} 0 & -N \\ K & 0 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix}, \ K, N \in \mathbb{R}^{n\times n} \ \textit{symmetric}, \\ \textit{where a nonsingular matrix } W \in \mathbb{R}^{n\times n} \ \textit{exists with} \\ W^{-1}KW^{-T} = \operatorname{diag}(\kappa_1, \dots, \kappa_n), \ W^T N W = \operatorname{diag}(\nu_1, \dots, \nu_n). \end{array}\right\} \quad (1)$$

* Received February 23, 2000; Final revised December 31, 2000.

The Hamiltonian splits into the sum of two quadratic forms, $H(p,q) = \frac{1}{2}p^TKp + \frac{1}{2}q^TNq$. The most occuring case is that K is positive definite, then a matrix W exists with $W^{-1}KW^{-T} = I$. This is evident from the fact that with K also K^{-1} is symmetric and positive definite, and therefore by theorems about the principal axis transformation there exists a nonsingular matrix W such that $W^TK^{-1}W$ is equal to I and W^TNW is a diagonal matrix. The situation K and N positive definite arise for example in connection with small oscillation approximations for nonlinear mechanical systems near stable equilibrium points (cf. Abraham, Marsden [1], Arnold [2]).

For the numerical integration of (1) Runge–Kutta (RK) methods, partitioned Runge–Kutta (PRK) methods, and Runge–Kutta–Nyström (RKN) methods can be used (cf. Hairer, Nørsett, Wanner [10], Sanz–Serna, Calvo [14]; see also [7]), which are summarized as Runge–Kutta type (RKT) methods. After a symplectic transformation of coordinates (1) decomposes into n Hamiltonian systems of the form

$$\begin{bmatrix} \dot{p} \\ \dot{q} \end{bmatrix} = \begin{bmatrix} 0 & -\nu \\ \kappa & 0 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix}, \kappa, \nu \in \mathbb{R}, \tag{2}$$

with $H(p,q) = \frac{1}{2}\kappa p^2 + \frac{1}{2}\nu q^2$. Methods that are symplectic for all systems of type (1) are called ls–symplectic. Stability properties are studied in detail in [6] and [8]. In this paper a backward error analysis of ls–symplectic RKT methods is presented. First, in section 2 the main results concerning ls–symplecticness and stability are summarized and some new results are given. In section 3 the backward error analysis is developed. If $\kappa\nu > 0$ in (2), then the solution to given initial conditions describes an ellipse in the phase plane. The numerical solution of an ls–symplectic RKT method with an admissible step size is the exact solution of a perturbed Hamiltonian system and lies also on an ellipse; the perturbed system is formulated, the shape of the ellipse is studied. Further, the conservation of the Hamiltonian is investigated, a lower and an upper bound for the error are given. In section 4 numerical examples are presented. All the results can easily be generalized to the integration of (1).

Note that after a further symplectic transformation of coordinates system (2) reduces in the case $\kappa\nu > 0$ to $\dot{p} = -\omega q$, $\dot{q} = \omega p$ with $\omega > 0$. For only studying the stability of RKT methods this symplification reduces the amount of work, but the results are also valid for $\kappa \neq \nu$. For backward error analysis on the other side there is no real benefit from $\kappa = \nu$. So, there is no need for this further symplification here. Especially, some early investigations are not restricted to that (Feng, Qin [5]).

2. Basic results

The symplecticness and stability of RKT methods for linear separable Hamiltonian systems of type (1) are studied in detail in [6] and [8]. In this section a short summary and some new results are given which are close related to the theory of P–stability (van der Houwen, Sommeijer [11], [12]).

2.1 ls–symplecticness and stability

A one–step method is called *ls–symplectic* if it is symplectic for all systems of type (1). The basis for the investigation of ls–symplecticness of RKT methods is that such a method applied to (1) with initial condition $u(0) = u_0$ reduces to

$$u_{m+1} = G(hK, hN)u_m, \quad m = 0, 1, 2, \ldots,$$

where for square matrices X, Y of the same size

$$G(X,Y) = \begin{bmatrix} \Gamma_{11}(YX) & -Y\Gamma_{12}(XY) \\ X\Gamma_{21}(YX) & \Gamma_{22}(XY) \end{bmatrix}.$$

The $\Gamma_{ij}, i,j = 1,2$, are rational functions of the form $\frac{\Psi_{ij}}{\Psi}$, where $\Psi_{11}, \ldots, \Psi_{22}, \Psi$ are polynomials with real coefficients that are determined by the parameters of the method. For explicit methods