

RUNGE-KUTTA SCHEMES FOR HAMILTONIAN SYSTEMS

J. M. SANZ-SERNA

Departamento de Matemática Aplicada y Computación, Facultad de Ciencias, Universidad de Valladolid, Valladolid, Spain

Abstract.

We study the application of Runge-Kutta schemes to Hamiltonian systems of ordinary differential equations. We investigate which schemes possess the canonical property of the Hamiltonian flow. We also consider the issue of exact conservation in the time-discretization of the continuous invariants of motion.

Classification: AMS 65 L, 70H.

Keywords: Runge-Kutta methods, Hamiltonian systems, symplectic geometry, conservation of energy.

1. Introduction.

Physical systems from mechanics, optics, etc. are often described through a set of Hamilton equations with g degrees of freedom

$$(1.1) \quad d\mathbf{p}/dt = \mathbf{f}(\mathbf{p}, \mathbf{q}), \quad d\mathbf{q}/dt = \mathbf{g}(\mathbf{p}, \mathbf{q}).$$

Here \mathbf{p} and \mathbf{q} are g -dimensional real vectors and the components $f^{(n)}, g^{(n)}$ of the vector-valued functions \mathbf{f} and \mathbf{g} satisfy

$$(1.2) \quad f^{(n)} = D_{g+n}H(\mathbf{p}, \mathbf{q}), \quad g^{(n)} = -D_nH(\mathbf{p}, \mathbf{q}), \quad 1 \leq n \leq g,$$

where H is a real function of $2g$ real variables (the Hamiltonian function) and D_n denotes partial differentiation with respect to the n -th argument, $1 \leq n \leq 2g$. The system (1.1) may arise either directly in the modelling of a physical system with a finite number of degrees of freedom or as a spatial discretization of an infinite-dimensional Hamiltonian system. Throughout this note we assume that the vector of coordinates \mathbf{q} takes values in an open subset Ω of R^g , that the vector of momenta \mathbf{p} takes values in the whole of R^g and that H is a C^2 function defined in the phase space $R^g \times \Omega$.

A fundamental property of (1.1) is that, for each fixed value of t , the corresponding t -flow F_t is a *canonical mapping* (see e.g. [1]). Recall that, by definition, $F_t(\mathbf{p}_0, \mathbf{q}_0) = (\mathbf{p}, \mathbf{q})$ if (\mathbf{p}, \mathbf{q}) is the value at time t of the solution of (1.1) which at time 0 takes the value $(\mathbf{p}_0, \mathbf{q}_0)$. A mapping is said to be canonical [1] if it preserves the differential form

$$\omega = d\mathbf{p} \wedge d\mathbf{q} = dp^{(1)} \wedge dq^{(1)} + dp^{(2)} \wedge dq^{(2)} + \dots + dp^{(g)} \wedge dq^{(g)},$$

which defines the *symplectic structure* of the phase space. In plain terms, the canonical character of the flow means that if we choose an open subset W of the phase space, project it onto the g two-dimensional planes of the variables $(p^{(n)}, q^{(n)})$, $1 \leq n \leq g$ and sum the two-dimensional areas of the resulting projections, then such a sum remains invariant as W evolves in time within the phase space according to the dynamics of (1.1). The conservation of ω clearly entails the conservation of its exterior powers $\omega^2, \dots, \omega^g$, which can be interpreted as conservation of higher-dimensional volumes. In particular the conservation of ω^g is the conservation of the $2g$ -dimensional volume in the phase space, a fact which implies the existence of the important phenomenon of the Poincaré recurrence [1]. More generally, many interesting qualitative properties of (1.1) derive from the canonical character of its flow [1].

When the system (1.1) is numerically integrated by means of a standard one-step method, the mapping which advances in time the solution by an amount Δt is not, in general, canonical. Thus, generally speaking, numerical approximations to the solutions of (1.1) obtained by a standard method will typically not have many of the relevant qualitative properties of their exact counterparts. It is then natural to look for canonical numerical discretizations of Hamiltonian systems, as suggested by Feng [5]. Feng [7] says that a one-step numerical scheme for (1.1) is symplectic if, except for roundoff errors, the mapping that advances the discrete solution is canonical. The implicit midpoint rule is easily seen to be symplectic [5]. For *linear* Hamiltonian systems the approximations based on diagonal Padé approximations to the exponential function are also symplectic [6]. For the *nonlinear* case, Feng and his coworkers [6] have used the theory of generating functions to construct symplectic schemes of arbitrarily high orders; these schemes are implicit and use high order partial derivatives of the Hamiltonian function H . In the linear case they generate diagonal Padé approximations.

In [12] and [13] F. Vadillo and the present author have proved that the standard leap-frog (explicit midpoint rule) for (1.1), when rewritten as a one-step recursion, is symplectic. Furthermore the papers [12] and [13] show how the canonical character of the discretization can be used, in conjunction with the Kolmogorov-Arnold-Moser (KAM) theory [1], to derive useful stability results.

The main purpose of this note is to study which Runge-Kutta schemes are symplectic. We show that all Gauss-Legendre methods are indeed canonical. Therefore there exist symplectic Runge-Kutta (RK) schemes of arbitrarily high

order. Note that RK schemes, unlike those constructed by applying the theory of generating functions, only require the evaluation of the right hand side functions f and g in (1.1).

We also include a section on energy-conserving RK schemes. It turns out that, for linear problems, the condition for an RK scheme to be symplectic also guarantees exact conservation of energy.

2. Symplectic Runge-Kutta schemes.

With each s -stage RK method with Butcher's tableau

$$(2.1) \quad \begin{array}{c} c \\ A \\ b^T \end{array}$$

we associated the $s \times s$ matrix M with entries

$$(2.2) \quad m_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j, \quad i, j = 1, 2, \dots, s.$$

The matrix M is of course well known from the definition of algebraic stability of RK methods introduced by Burrage and Butcher [2] (see [4] for more references).

Our main result is as follows.

THEOREM 1. *If the condition $M = 0$ holds, where M is the matrix defined in (2.2), then the RK method (2.1) is symplectic.*

PROOF. The RK method, as applied to the system (1.1), results in the equations

$$(2.3) \quad Y_i = p + \tau \sum_{j=1}^s a_{ij} f(Y_j, Z_j), \quad Z_i = q + \tau \sum_{j=1}^s a_{ij} g(Y_j, Z_j), \quad 1 \leq i \leq s,$$

$$(2.4) \quad P = p + \tau \sum_{i=1}^s b_i f(Y_i, Z_i), \quad Q = q + \tau \sum_{i=1}^s b_i g(Y_i, Z_i).$$

Here $P, Q, Y_i, Z_i, 1 \leq i \leq s$, are functions of p, q and τ , defined at least for τ sufficiently small. (How small τ must be may depend on p, q .) We use the notation

$$k_i = f(Y_i, Z_i), \quad l_i = g(Y_i, Z_i), \quad 1 \leq i \leq s,$$

for the "slopes" at the interval vectors.

Differentiate (2.4) and take external products to arrive at

$$(2.5) \quad dP \wedge dQ = dp \wedge dq + \tau \sum_{i=1}^s b_i dk_i \wedge dq + \tau \sum_{j=1}^s b_j dp \wedge dl_j + \\ + \tau^2 \sum_{i,j=1}^s b_i b_j dk_i \wedge dl_j.$$

Now differentiate (2.3) and take the exterior product of the result with dk_i, dl_j to obtain a set of relations for $dk_i \wedge dq, dp \wedge dl_j, 1 \leq i, j \leq s$. Next, eliminate $dk_i \wedge dq, dp \wedge dl_j$ between the obtained relations and (2.5). These manipulations yield, on taking (2.2) into account:

$$(2.6) \quad dP \wedge dQ - dp \wedge dq = \tau \sum_{i=1}^s b_i [dk_i \wedge dZ_i + dY_i \wedge dl_i] - \tau^2 \sum_{i,j=1}^s m_{ij} dk_i \wedge dl_j.$$

So far the Hamiltonian character of (1.1), as given by (1.2), has not been resorted to. We now use (1.2) to show that the expression in brackets in (2.6) vanishes for each $i, 1 \leq i \leq s$. In fact, omitting the subscript i , we can write (with super-indices denoting component)

$$\begin{aligned} dk \wedge dZ + dY \wedge dl &= \sum_{m=1}^g [dk^{(m)} \wedge dZ^{(m)} + dY^{(m)} \wedge dl^{(m)}] \\ &= \sum_{m,n=1}^g [D_n f^{(m)} dY^{(n)} \wedge dZ^{(m)} + D_{g+n} f^{(m)} dZ^{(n)} \wedge dZ^{(m)} + \\ &\quad + D_n g^{(m)} dY^{(m)} \wedge dY^{(n)} + D_{g+n} g^{(m)} dY^{(m)} \wedge dZ^{(n)}]. \end{aligned}$$

To see that the last expression vanishes, it is enough to notice the antisymmetry of the exterior product and that (1.2) and the assumed smoothness of H imply $D_n f^{(m)} = -D_{g+m} g^{(n)}, D_{g+n} f^{(m)} = D_{g+m} f^{(n)}, D_n g^{(m)} = D_m g^{(n)}, 1 \leq m, n \leq g$. Thus (2.6) leads to

$$dP \wedge dQ - dp \wedge dq = -\tau^2 \sum_{i,j=1}^s m_{ij} dk_i \wedge dl_j,$$

a relation valid for all s -stage RK schemes which shows that the condition $M = 0$ implies the conservation of the symplectic structure. ■

Since it is well known that for Gauss-Legendre methods $M = 0$ (see e.g. Theorem 4.6 of [4]), the following result holds true.

COROLLARY. *The Gauss-Legendre RK methods are symplectic.*

On the other hand, Cooper [3] points out that no explicit RK method has $M = 0$. This author also investigates the existence of singly-implicit methods with $M = 0$.

The (consistent) method with a given set of positive weights $b_j, 1 \leq j \leq s$, can easily be generated. Denote by B the diagonal $s \times s$ matrix whose diagonal elements are the weights, let W be an $s \times s$ matrix with $W^T B W = I$ (the identity matrix), and set $X = W^{-1} A W$. Then a simple computation (see [4], page 123) shows that $W^T M W = X + X^T - e_1 e_1^T$, where e_1 represents the first coordinate vector. Therefore $M = 0$ is equivalent to $X = \frac{1}{2} e_1 e_1^T + N$, with N a skew-

symmetric matrix, or

$$A = W(\mathbf{e}_1 \mathbf{e}_1^T + N)W^{-1}.$$

Each choice of a skew-symmetric matrix N yields, via the previous formula, a consistent method with $M = 0$. The theory of the W -transformation of Hairer and Wanner (see e.g. [4], Theorem 4.6.16) can be applied to characterize the choices for N which lead to high-order RK schemes.

3. Conservation of energy and other invariants of motion.

It is well known that H is a first integral for the system (1.1)-(1.2), i.e. if $(\mathbf{p}(t), \mathbf{q}(t))$ is a solution of (1.1)-(1.2) then $H(\mathbf{p}(t), \mathbf{q}(t))$ does not depend on t , a fact which in physical terms often corresponds to conservation of energy. In this section we investigate whether the RK scheme (2.1) also conserves H , i.e. whether, with the notations in (2.4), $H(\mathbf{P}, \mathbf{Q}) \equiv H(\mathbf{p}, \mathbf{q})$. More generally, we are interested in knowing which first integrals or invariants of motion of (1.1) are also conserved by the RK scheme. It is convenient to consider, instead of (1.1), a general system of ODEs

$$(3.1) \quad d\mathbf{y}/dt = \mathbf{G}(\mathbf{y}),$$

where \mathbf{y} takes values in R^d and \mathbf{G} is a C_1 function defined in an open subset of R^d . We first study the conservation of quadratic functions, i.e. functions of the form $\mathbf{y}^T P \mathbf{y}$, with P a symmetric constant $d \times d$ matrix.

THEOREM 2. *If, for the matrix M defined in (2.2), $M = 0$, then the RK method (2.1) conserves all quadratic first integrals of (3.1).*

PROOF. The result is given by Cooper [3] for P non-singular, and his proof is valid in the general case. When P is the identity matrix, the same proof had essentially been given in [4], Example 10.3.8. See also the Appendix of [14]. ■

COROLLARY. *The Gauss-Legendre RK methods conserve all quadratic first integrals of (3.1)*

REMARK 1. It is clear that all (continuous) functions $K(\mathbf{y})$ conserved by a convergent numerical scheme for (3.1) must also be conserved by (3.1) itself.

REMARK 2. Along with quadratic invariants of (3.1, we could have considered *bilinear* invariants, i.e. functions $\mathbf{w}^T P \mathbf{y}$ of two vector variables (P a constant, not necessarily symmetric $d \times d$ matrix) such that, if $\mathbf{w}(t), \mathbf{y}(t)$ are any two solutions of (3.1), then $\mathbf{w}(t)^T P \mathbf{y}(t)$ does not vary in time. With a proof almost identical

to that of Theorem 2, it is possible to show that the condition $M = 0$, guarantees that the RK method conserves all bilinear invariants of (3.1).

We now leave the general system (3.1) and return to the Hamilton equations (1.1). From the previous theorem it is clear that if the Hamiltonian function H is quadratic (which entails that (1.1) is linear), then RK schemes with $M = 0$ lead to exact conservation of the Hamiltonian. Therefore, *linear* Hamiltonian systems can be integrated numerically by means of RK methods in such a way that *both* the energy and the symplectic structure can be conserved exactly. For the *nonlinear* case we have seen that it is still possible to conserve the symplectic structure. However, the energy is *not* conserved, even if $M = 0$.

It has often been argued in the literature that exact conservation of the energy is a desirable feature for numerical schemes to possess. Claims in that direction by the present author were made in [8], [9], [11]. When the energy is not quadratic, standard numerical methods usually fail to conserve energy, and it is then possible to suggest *ad hoc* modifications of the schemes to make them energy-conserving [8], [9], [11] (see also [7]). However, numerical experimentation [10], [14] has now convinced the author that energy-conserving schemes do not necessarily capture all relevant qualitative features of the continuous model. In a similar vein, *ad hoc* modifications introduced to conserve energy exactly may easily lead to a degradation of the practical performance of a numerical scheme [10]. In the context of the present note, it is perhaps useful to point out that such modifications often destroy the symplectic property of the scheme.

REFERENCES

1. V. I. Arnold, *Mathematical Methods of Classical Mechanics*, Springer, New York (1978).
2. K. Burrage and J. C. Butcher, *Stability criteria for implicit Runge-Kutta methods*, SIAM J. Numer. Anal. 16 (1979), 46–57.
3. G. J. Cooper, *Stability of Runge-Kutta methods for trajectory problems*, IMA J. Numer. Anal. 7 (1987), 1–13.
4. K. Dekker and J. G. Verwer, *Stability of Runge-Kutta Methods for Stiff Nonlinear Differential Equations*, North-Holland, Amsterdam (1984).
5. K. Feng, *On difference schemes and symplectic geometry*, in Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations, Chief Editor K. Feng, Science Press, Beijing (1985), 42–58.
6. K. Feng, *Difference schemes for Hamiltonian formalism and symplectic geometry*, J. Comput. Maths. 4 (1986), 279–289.
7. K. Feng and M. Qin, *The symplectic methods for the computation of Hamiltonian equations*, to appear.
8. J. M. Sanz-Serna, *An explicit finite-difference scheme with exact conservation properties*, J. Comput. Phys. 47 (1982), 199–210.
9. J. M. Sanz-Serna, *Methods for the numerical solution of the nonlinear Schroedinger equation*, Math. Comput. 43 (1984), 21–27.
10. J. M. Sanz-Serna and I. Christie, *Finite elements for nonlinear integro-differential equations and their integration in time*, in *The Mathematics of Finite Elements and Applications V*, MAFELAP 84, J. R. Whiteman editor, Academic Press, London, 415–420.
11. J. M. Sanz-Serna and V. S. Manoranjan, *A method for the integration in time of certain partial differential equations*, J. Comput. Phys. 52 (1983), 273–289.

12. J. M. Sanz-Serna and F. Vaddillo, *Nonlinear instability, the dynamic approach*, in *Numerical Analysis*, D. F. Griffiths and G. A. Watson editors, Pitman Research Notes in Mathematics 140, Longman Scientific and Technical (1986), 187–199.
13. J. M. Sanz-Serna and F. Vaddillo, *Studies in numerical nonlinear instability. III: Augmented Hamiltonian systems*, SIAM J. Appl. Math. 47 (1987), 92–108.
14. M. Sanz-Serna and J. G. Verwer, *Conservative and nonconservative schemes for the solution of the nonlinear Schroedinger equation*, IMA J. Numer. Anal. 6 (1986), 25–42.