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Symplectic Runge–Kutta and related methods: recent results

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Symplectic algorithms are numerical integrators for Hamiltonian systems that preserve the symplectic structure in phase space. In long time integrations these algorithms tend to perform better than their nonsymplectic counterparts. Some symplectic algorithms are derived by explicitly finding a generating function. Other symplectic algorithms are members of standard families of methods, such as Runge–Kutta methods, that just turn out to preserve the symplectic structure. Here we survey what is known about the second type of symplectic algorithms.

1. Introduction

The recent literature, both in physics and in numerical analysis, has given much attention to the numerical integration of Hamiltonian systems of differential equations by means of symplectic integrators. The list of references at the end of this paper contains more than thirty items and is far from exhaustive. For simplicity, we only consider autonomous systems with finitely many, say d, degrees of freedom:

$$\mathrm{d}p_i/\mathrm{d}t = -\partial H/\partial q_i, \quad \mathrm{d}q_i/\mathrm{d}t = \partial H/\partial p_i,$$

$$1 \le i \le d, \tag{1}$$

where $H = H(p_1, \ldots, p_d; q_1, \ldots, q_d)$ is a smooth real function defined in an open domain Ω of the (p, q) Euclidean space [1, 2]. (Extensions are possible, see e.g. refs. [3–5].) The flow ϕ_t of (1) is a canonical or symplectic transformation [1], i.e. it preserves the differential two-form $\mathrm{d}p \wedge \mathrm{d}q$. In other words, for each time t and each two-dimensional surface Σ in Ω, the sum of the oriented two-dimensional areas of the projections of Σ onto the d planes (p_i, q_i) is the same as sum of the oriented areas of the projections of $\phi_t(\Sigma)$ onto those planes. Recall that, by definition,

$\phi_t(p_0, q_0) = (p, q)$ if (p, q) is the value at time t of the solution of (1) that at time $t = 0$ takes the value (p_0, q_0). Most qualitative properties of Hamiltonian systems, including preservation of volume, absence of asymptotically stable equilibria, Poincaré recurrence, etc., can be directly derived from the symplectic character of the flow [1, 2]. If Ω possesses a trivial topology, a vector field in Ω is Hamiltonian if and only if the corresponding flow is symplectic, so that, in this respect, symplecticity provides a complete characterization of Hamiltonian systems.

Each one-step numerical method for the integration of (1) is given by a mapping ψ_t in phase space that effects the transition

$$(p_{n+1}, q_{n+1}) = \psi_h(p_n, q_n) \tag{2}$$

from the numerical approximation (p_n, q_n) at time t_n to the numerical approximation at the next time level $t_{n+1} = t_n + h$. For an rth order method ψ_t differs from ϕ_t in $\mathcal{O}(t^{r+1})$ terms. For explicit Runge–Kutta methods and many other standard methods, it turns out that the transformation ψ_t in (2) is *not* symplectic. By implication, the long-time dynamics of the numerical solutions is then,

so to speak, *non-Hamiltonian*, even if the method is of high order and provides very accurate simulations over short time intervals. It is therefore reasonable to look for numerical algorithms that result in symplectic approximations ψ_t to ϕ_t. These algorithms are called symplectic [6, 7] or canonical [8]. Numerical experiments (see e.g. refs. [9, 10]) and theoretical considerations (see e.g. ref. [11]) have revealed that, in long time integrations of Hamiltonian systems, symplectic integrators perform better than their noncanonical counterparts. This enhanced performance is felt not only in the qualitative behaviour of the numerical solution, but also quantitatively.

Many symplectic integrators are now available in the literature. Broadly speaking, there are two large groups of symplectic methods. On the one hand, it is well known [1] that a canonical transformation can be expressed in terms of a (scalar) generating function S. Therefore numerical symplectic methods can be constructed [6, 7, 9, 12, 13] by identifying a suitable generating function S_t for ψ_t. Of course S_t should be an approximation to the generating function of the true flow ϕ_t, so that S_t should be an approximate solution of a Hamilton–Jacobi equation [1]. This methodology leads to algorithms that use high derivatives of H and are reminiscent of standard Taylor series methods for ordinary differential equations (ODEs). The second large group of symplectic integrators consists of algorithms that belong to conventional classes of numerical ODE methods, such as Runge–Kutta or Runge–Kutta–Nyström methods. The integrators of the second group, unlike those explicitly based on generating functions, can be applied to general (i.e. not necessarily Hamiltonian) systems of ODEs. In particular, they can be applied to small dissipative perturbations of Hamiltonian problems. Furthermore, the algorithms in the second category only require the evaluation of the vector field components $\partial H/\partial p_i$ and $\partial H/\partial q_i$, so that higher derivatives of H are not needed. Finally, in the analysis and implementation of the methods of the second group, use can be made of the vast body of available knowledge in connection with Runge–Kutta and related methods. It is our feeling that, even though algorithms of the first group may be advantageous when dealing with specific individual problems, the algorithms of the second group are more promising when it comes to designing general purpose software for Hamiltonian problems. In this paper we are only concerned with the second group of symplectic integrators. We successively consider Runge–Kutta, Runge–Kutta–Nyström and Partitioned Runge–Kutta–Nyström methods. For symplectic multistep methods see refs. [14–16].

2. Symplectic Runge–Kutta methods

Let us consider a general system of D differential equations

$$\mathrm{d}y/\mathrm{d}t = F(y),\tag{3}$$

of which (1) is of course a particular case. An s-stage Runge–Kutta (RK) method [17, 18] for the integration of (3) is specified by an $(s+1)\times s$ tableau of real constants

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1s} \\ a_{21} & a_{22} & \cdots & a_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ a_{s1} & a_{s2} & \cdots & a_{ss} \\ b_1 & b_2 & \cdots & b_s \end{pmatrix}.\tag{4}$$

The time-stepping from t_n to t_{n+1} is given by

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i F(Y_i),\tag{5}$$

where the vectors Y_i are the so-called internal stages. (The Y_i's depend, of course, on n, but this dependence is not reflected in the notation.) The

internal stages are determined by the relations

$$Y_i = y_n + h \sum_{j=1}^{s} a_{ij} F(Y_j), \quad 1 \le i \le s. \tag{6}$$

If $a_{ij} = 0$ whenever $i \le j$, eqs. (6) provide a recursion for explicitly computing each Y_i in terms of the preceding stages. The method is then called explicit. The computation of one step with an explicit RK method thus requires s evaluations of the vector field F. Explicit RK methods have of course been the most used one-step algorithms in numerical ODEs. When the method is not explicit, (6) provides a coupled system of $s \times D$ nonlinear algebraic equations that must be iteratively solved for the stages. Since the computational cost per step of an implicit RK method is definitely higher than that of an explicit RK method, implicit formulae have only been used for stiff [19] problems, where their better stability properties make up for the computational cost. In a stiff situation, simple functional iteration does not work and (6) must be solved by a Newton procedure. A common strategy is as follows [20]. If J is an approximation to the Jacobian matrix of F at y_n, then $\mathcal{J} = I - hA \otimes J$ is an approximate Jacobian for the system (6). Here A is the matrix with entries a_{ij} and $\otimes$ denotes Kronecker product [19]. When $\mathcal{J}$ is used as an approximate Jacobian for Newton's iteration, the linear systems to be solved are of the form

$$\mathcal{J} X = Z. \tag{7}$$

If A has eigenvalues λ_i, $1 \le i \le s$ and a complete set of eigenvectors, it is easy to see that (7) can be transformed into s uncoupled system of D-dimensional linear systems with matrices $I - h\lambda_i J$. If a λ_i is complex the corresponding linear system is of course complex and complex arithmetic must be used in the implementation. Alternatively the two complex systems with matrices $I - h\lambda_i J$ and $I - h\lambda_i^* J$ can be combined into a single $2D$-dimensional real system.

A particular class of implicit methods, called diagonally implicit methods, occurs when the matrix A is lower triangular ($a_{ij} = 0$ for $i < j$). Then the solution of (6) requires the successive solution of s D-dimensional nonlinear systems, which is of course far less demanding than the solution of the $s \times D$ system one would find with a general implicit method.

Let us assume that the system (3) being integrated is of Hamiltonian form. Then the present author proved [21] that the method (5), (6) would be symplectic provided that the following relations hold:

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \le i, j \le s. \tag{8}$$

This condition was discovered later and independently by Lasagni [22] and also by Suris [23]. Furthermore Lasagni showed that, except for unimportant methods with redundant stages, (8) is also necessary for (5), (6) to be symplectic. The proof of this result has not been published. However the necessity of (8) can be concluded by considering the RK method to be a particular case of partitioned Runge–Kutta method and then applying theorem 5.1 in ref. [24].

It is easy to see that condition (8) cannot be satisfied by any explicit Runge–Kutta method. On the other hand, for each s, the Gauss–Legendre method with s stages, i.e. the unique s-stage method that achieves the maximal order $2s$, is symplectic [21]. For $s = 1$ the Gauss–Legendre method is the well-known implicit midpoint rule

$$y_{n+1} = y_n + hF\left(\left(\tfrac{1}{2}\right)(y_{n+1} + y_n)\right), \tag{9}$$

which has traditionally been much used in the time-integration of Hamiltonian systems that arise from the space discretization of Hamiltonian partial differential equations. The two-stage, fourth order Gauss method has been successfully used by Pullin and Saffman [25] for the integration of the four-vortex motion. Much work remains to be done in the practical implementation of

the Gauss–Legendre methods, particularly in studying how to get good initial guesses for the solution of the nonlinear equations and which iterative procedure to use. Work in this direction is being done by J.M. Hyman. Since the problems of interest are not necessarily stiff, current strategies [26], designed for the stiff case, may well be far from optimal. At any rate, it is most likely that the cost per step of a Gauss–Legendre method, even when efficiently implemented, will turn out to be higher than that of an explicit RK method of the same order. In long time integrations of Hamiltonian systems, the symplecticness of the Gauss–Legendre is expected to make up for the extra cost. Furthermore, if (1) happens to be stiff, then explicit RK methods are out of the question, while Gauss–Legendre methods have excellent nonlinear stability properties and can use long time steps.

Diagonally implicit symplectic RK methods do exist. These have tableaux

$$\begin{pmatrix} b_1/2 & 0 & \cdots & 0 \\ b_1 & b_2/2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ b_1 & b_2 & \cdots & b_s/2 \\ b_1 & b_2 & \cdots & b_s \end{pmatrix}. \qquad (10)$$

and hence with s stages provide s free parameters. When $s = 1$ the requirement that the method has at least order $r = 1$ leads to $b_1 = 1$ and we recover once more the implicit midpoint rule (9). More generally, a step of length h with (10) is simply a concatenation of s implicit midpoint steps with lengths $b_i h$. Hence the family (10) is very easily implementable and is particularly appealing for the time integration of space-discretizations of partial differential equations and other large stiff systems. A method of the family (10) with $s = 3$ and order $r = 4$ was constructed in ref. [27]. This method has been tested in ref. [28] in the time integration of the Korteweg-de Vries equation. Furthermore, by using concatenations similar to those in ref. [29], it is not difficult to

prove that the family (10) includes methods of arbitrarily high order.

Iserles [30] has constructed a three-stage, fourth-order, fully implicit symplectic RK method for which the matrix A has real eigenvalues and a complete set of eigenvectors. As explained above, for such a method the linear algebra to be carried out in the Newton iteration consists of the solution of D-dimensional systems. This method has not been tested in practice.

3. Symplectic Runge–Kutta–Nyström methods

A second family of conventional ODE methods that includes symplectic scheme is provided by Runge–Kutta–Nyström (RKN) methods [18]. These are methods for systems of the special form

$$\mathrm{d}p/\mathrm{d}t = f(q), \quad \mathrm{d}q/\mathrm{d}t = p, \qquad (11)$$

with p and q d-dimensional vectors, or, equivalently, for second order systems $\mathrm{d}^2q/\mathrm{d}t^2 = f(q)$. Note that (11) is a Hamiltonian system if f is the gradient of a scalar function $-V$ and then

$$H = (\tfrac{1}{2})p^\mathrm{T}p + V(q). \qquad (12)$$

Each RKN method is specified by a tableau of real constants of the form

$$\begin{pmatrix} \gamma_1 & \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1s} \\ \gamma_2 & \alpha_{21} & \alpha_{22} & \cdots & \alpha_{2s} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \gamma_s & \alpha_{s1} & \alpha_{s2} & \cdots & \alpha_{ss} \\ & b_1 & b_2 & \cdots & b_s \\ & \beta_1 & \beta_2 & \cdots & \beta_s \end{pmatrix}. \qquad (13)$$

The time-stepping is effected by the formulae

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

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

where now the internal stages Q_i are defined by

$$Q_i = q_n + h\gamma_i p_n + h^2 \sum_{j=1}^{s} \alpha_{ij} f(Q_j).$$

The method is explicit if $\alpha_{ij} = 0$ for $i \le j$. Explicit RKN formulae are state of the art methods for the integration of systems of the form (11).

When (11) is Hamiltonian, Suris [23] has shown that the conditions

$$\beta_i = b_i(1 - \gamma_i), \quad 1 \le i \le s, \tag{14}$$

and

$$b_i(\beta_j - \alpha_{ij}) = b_j(\beta_i - \alpha_{ji}), \quad 1 \le i, j \le s, \tag{15}$$

ensure symplecticness. An alternative proof can be seen in ref. [31]. Furthermore for methods without redundant stages (14), (15) are also necessary for symplecticity [32].

There are explicit RKN methods that are symplectic. These have the tableau

$$\begin{pmatrix} \gamma_1 & 0 & 0 & \cdots & 0 \\ \gamma_2 & b_1(\gamma_2 - \gamma_1) & 0 & \ddots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \gamma_s & b_1(\gamma_s - \gamma_1) & b_2(\gamma_s - \gamma_2) & \cdots & 0 \\ & b_1 & b_2 & \cdots & b_s \\ & b_1(1 - \gamma_1) & b_2(1 - \gamma_2) & \cdots & b_s(1 - \gamma_s) \end{pmatrix}. \tag{16}$$

and hence, with s stages include $2s$ free parameters. Okunbor and Skeel [33] have noticed that the method (16) can be implemented with the minimal conceivable storage, namely with only two d-dimensional vectors. The idea is to reformulate (16) as a partitioned Runge–Kutta method (see below).

In ref. [34] M.P. Calvo and the present author have considered the family of fourth-order, five-stage methods of the form (16) that effectively require four evaluations of f per step due to the fact that the last evaluation in the current step provides the first evaluation for the next step. An

optimal method within this family has been obtained by minimizing the error constants. Numerical comparisons with an optimized nonsymplectic formula due to Dormand et al. are given. Similar work for higher order methods is under way.

Okunbor and Skeel [31] show that an explicit RKN method is canonical if and only if its adjoint method is explicit. Recall that the adjoint of a one-step numerical method (2) is, by definition the method $\tilde{\psi}_t$ such that $\psi_t^{-1} = \tilde{\psi}_{-t}$. In other words, a step of length $-h < 0$ with the adjoint method undoes a step of length h with the given method. The result by Okunbor and Skeel could be employed, in conjunction with an idea used in ref. [10], as follows. Suppose that, for n even, the step $t_n \mapsto t_{n+1}$ is taken with an explicit symplectic RKN method ψ_t, while for n odd the step is taken with the adjoint method. The overall algorithm is explicit and symplectic. However each step cancels all the coefficients of the even powers of h in the expansion of the local error at the preceding time step. If ψ_t has odd order r, then the leading $\mathcal{O}(t^{r+1})$ term in the truncation error is annihilated by the next step, so that the algorithm just defined has global order of accuracy $r + 1$ at all grid points. In this way one may have, say, sixth-order integrations while employing fifth-order formulae for each step.

4. Symplectic partitioned Runge–Kutta methods

The third and final class of standard methods considered here is not as widely known as those of RK and RKN methods. Partitioned Runge–Kutta (PRK) methods are methods for the integration of systems of ODEs where the dependent variables have been divided into two groups and different RK tableaux are used for the two groups. PRK methods are of interest, for instance, when the given system includes a group of stiff equations and a group of nonstiff equations. For the purposes of this paper, it is enough to consider

systems of ODEs of the form

$$dp/dt = f(q), \quad dq/dt = g(p), \tag{17}$$

with p and q d-dimensional vectors. The system (17) is Hamiltonian if f and g are gradients of scalar functions $-V$ and T respectively and then the Hamiltonian is given by

$$H = T(p) + V(q). \tag{18}$$

Hamiltonians of this form are called separable.

A PRK method is specified by two tableaux of real constants

$$
\begin{pmatrix}
a_{11} & a_{12} & \cdots & a_{1s} \\
a_{21} & a_{22} & \cdots & a_{2s} \\
\vdots & \vdots & \ddots & \vdots \\
a_{s1} & a_{s2} & \cdots & a_{ss} \\
b_1 & b_2 & \cdots & b_s
\end{pmatrix},
$$

$$
\begin{pmatrix}
A_{11} & A_{12} & \cdots & A_{1s} \\
A_{21} & A_{22} & \cdots & A_{2s} \\
\vdots & \vdots & \ddots & \vdots \\
A_{s1} & A_{s2} & \cdots & A_{ss} \\
B_1 & B_2 & \cdots & B_s
\end{pmatrix}. \tag{19}
$$

The formulae for the computation of a step are

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

$$q_{n+1} = q_n + h \sum_{i=1}^{s} B_i g(P_i),$$

with the stages P_i and Q_i defined by

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

$$Q_i = q_n + h \sum_{j=1}^{s} A_{ij} g(P_j), \quad 1 \le i \le s.$$

The method (19) is symplectic for all separable

Hamiltonians (18) if

$$b_i A_{ij} + B_j a_{ji} - b_i B_j = 0, \quad 1 \le i, j \le s. \tag{20}$$

This result was announced by the present author at the 1989 London Numerical ODE conference and was independently discovered by Suris [35]. Furthermore (20) is also necessary for symplecticness if the method has no redundant stages [24].

While (20) is similar to (8), we have now two tableaux instead of one and it is possible to achieve symplecticity with an explicit algorithm. Namely the methods with

$$
\begin{pmatrix}
b_1 & 0 & \cdots & 0 \\
b_1 & b_2 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
b_1 & b_2 & \cdots & b_s \\
b_1 & b_2 & \cdots & b_s
\end{pmatrix},
\begin{pmatrix}
0 & 0 & \cdots & 0 \\
B_1 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
B_1 & B_2 & \cdots & 0 \\
B_1 & B_2 & \cdots & B_s
\end{pmatrix}. \tag{21}
$$

satisfy (20) and are effectively explicit. (It is clearly possible to change the roles of p and q and use the strictly lower triangular coefficient matrix for the p equations and the matrix with nontrivial diagonal for the q equations.) The method with array (21) can be implemented while only storing two d-dimensional vectors: Q_1 is nothing but q_n, P_1 can be overwritten on p_n, Q_2 can be overwritten on Q_1, etc.... Note that the number $2s$ of free parameters in (21) is the same as the number of free parameters for an explicit s-stage RKN method (16). On the other hand, (21) is symplectic for all separable Hamiltonians (18), whilst (16) only caters for the case where the kinetic energy T is a sum of squares. At first, it may be concluded that explicit PRK methods should be preferred to RKN method. However this is not necessarily the case: since PRK methods can integrate systems of ODE of the form (17), while RKN methods only accommodate systems of the simple form (11), the number of equations that must be imposed on the method coefficients for a PRK formula to have order $\ge r$

is higher than the corresponding number for an RKN formula. Hence RKN formulae make up for their more limited applicability by requiring less stages to achieve a given order (see section 6 below). Since most separable Hamiltonians that arise in applications are in fact of the form (12), it seems that the class (21) is of limited interest. However symplectic PRK formulae have so far received more attention than symplectic RKN formulae.

The family of methods (21) was first introduced by Ruth [8], in one of the very first papers on symplectic integrators. Ruth considered methods with $s = r = 1, 2, 3$. Later a method with $s = r = 4$ has been independently constructed by several authors [36–38]. Yoshida [29] has shown that the family (21) includes methods of arbitrarily high order. Furthermore he has constructed several high-order methods.

5. Generating functions

Even though the symplectic methods considered so far are not derived from a generating function, they must possess generating functions, as any other canonical transformation in phase space. Here we consider generating function of the second kind $S(p_n, q_{n+1}; h)$ that define canonical transformations via

$$p_{n+1(i)} = \partial S / \partial p_{n+1(i)}, \quad q_{n(i)} = \partial S / \partial p_{n(i)},$$

$$1 \leq i \leq d. \tag{22}$$

(Subscripts in brackets denote components.) Lasagni showed (cf. ref. [27]) that for an RK method subject to the simplecticness condition (8), the generating function is given by

$$S(p_n, q_{n+1}; h) = p_n^T q_{n+1} - h \sum_i b_i H(Y_i)$$

$$- h^2 \sum_{ij} b_i a_{ij} H_p(Y_i) H_q(Y_j)^T. \tag{23}$$

In (23), $Y_i = (P_i^T, Q_i^T)^T$ are the stages defined in (5) and H_p, H_p are gradients, row vectors of partial derivatives. Of course here the Y_i should be seen as functions of p_n, q_{n+1} and h defined implicitly by the relations (5), (6). The implicit function theorem shows that this interpretation is possible at least for h sufficiently small. On the other hand note that S exists globally in phase space.

For symplectic RKN and PRK methods the expressions for the generating function can be seen in refs. [39] and [24], respectively.

6. Order conditions

Let us first consider the, not necessarily symplectic, RK method (4). The conditions that ensure that (4) has order $\geq r$ are well known. For instance, for order ≥ 1 we impose

$$\sum_i b_i = 1, \tag{24}$$

for order ≥ 2 we impose (24) and

$$\sum_{ij} b_i a_{ij} = \tfrac{1}{2}, \tag{25}$$

for order ≥ 3 we further add

$$\sum_{ijk} b_i a_{ij} a_{ik} = \tfrac{1}{3}, \quad \sum_{ijk} b_i a_{ij} a_{jk} = \tfrac{1}{6}. \tag{26}$$

It is important to emphasize that these order conditions can be easily written in a systematic way [17, 18] by using some simple graph theory. The second column in table 1 gives the number of order conditions that must be imposed to ensure order $\geq r$, $r = 1, \dots, 8$.

It is in principle conceivable that the order r^* of (4) when applied to the restricted class of Hamiltonian problems (1) would be higher than its standard order r, which refers to systems (3) with arbitrary F. However this is not the case, because each differential system with D equa-

Table 1
Number of order conditions for order $\geq r$

r	General RK	Symplectic RK	RKN subject to (14)	Symplectic RKN	General PRK	Symplectic PRK
1	1	1	1	1	2	2
2	2	1	2	2	4	3
3	4	2	4	4	8	5
4	8	3	7	6	16	8
5	17	6	13	10	34	14
6	37	10	23	15	74	24
7	85	21	43	25	170	46
8	200	40	79	39	400	88

tions can be embedded in a Hamiltonian system with $2D$ equations. Hence $r = r^*$ and when referring to order it does not matter whether the underlying system is Hamiltonian or otherwise.

The order conditions are independent if the coefficients in the tableau (4) are seen as independent variables. For instance, in (24)–(26) no equation is implied by the others. However, if the method (4) under consideration satisfies the symplecticity condition (8) the coefficients b_i and a_{ij} are no longer independent and it is conceivable that some of the order equations may be redundant. This is actually the case. For instance, it is not difficult to see that, when (8) holds, (25) is a consequence of (24) and that, when (8) and (24), hold the two equations in (26) are mutually equivalent. In ref. [27] a procedure is given to systematically eliminate the redundant order conditions for symplectic RK methods. Equivalently, ref. [27] shows how to systematically write a subset of the standard order conditions that, together with (8), ensure order $\geq r$. The third column in table 1 provides the number of order conditions that must be imposed when the symplecticness condition (8) holds true.

Similar considerations apply for RKN methods. Once more there is no difference between the standard order r and the order for Hamiltonian problems r^*. Furthermore the symplecticness conditions (14) and (15) induce some redundancy amongst the standard order conditions. The fourth column in table 1 gives the number of

order conditions for a general RKN formula subject to (14) (RKN methods that do not obey (14) are seldom used in practice). The fifth column of the table corresponds to symplectic methods satisfying both (14) and (15). The prescriptions for the systematic construction of the order conditions for symplectic and nonsymplectic RKN methods can be seen in ref. [39].

For PRK methods once again $r = r^*$ and the symplecticness condition makes it possible not to consider some of the standard order conditions. The number of order conditions for the general and symplectic cases can be seen in the last two columns of table 1. The prescriptions for the systematic construction of the order conditions for symplectic and nonsymplectic PRK methods can be seen in ref. [24].

7. Canonical theory of the order

In the special case where a sympectic RK, RKN or PRK method is used to integrate a Hamiltonian system, it is possible to derive the conditions for order $\geq r$ not by looking at the Taylor expansion of the local error, but rather [27] by Taylor expanding a scalar function Γ derived from the generating function S considered in section 5 above. Essentially, this approach measures by how much the generating function of the numerical algorithm fails to be a solution of the Hamilton–Jacobi equation [1]. For RK, RKN

and PRK methods the computation of the Taylor expansion of Γ can be systematized by using graph theory. When using this approach the order conditions appear in a form somewhat more complicated than that found in the standard derivation discussed in the previous section. On the other hand, this approach results in a set of order conditions where the redundancies due to symplecticity are automatically filtered out. For instance, in the RK case and for order ≥ 3, the canonical approach yields eqs. (24) and

$$3 \sum_{ijk} b_i a_{ij} a_{ik} - 6 \sum_{ijk} b_i a_{ij} a_{jk} = 0. \tag{27}$$

The superfluous condition (25) does not turn up here and rather than having the two equivalent equations in (26) we get the single one (27), which is clearly equivalent to (26). Further details can be seen in refs. [27, 24, 32].

One of the referees has pointed out that a connection between graph theory and Hamilton–Jacobi equations, vaguely reminiscent of that mentioned in this section, has been considered in ref. [40].

8. Variable steps

Standard numerical ODE methods were first derived and analyzed in a constant step-size mode, but nevertheless should be used in the far more efficient variable step-size implementations. In a similar vein the development of symplectic algorithms has started with constant step-size implementations and the numerical tests available in the literature involve the comparison, for Hamiltonian problems, of symplectic, constant step-size formulae against standard constant step-size algorithms. The results of these comparisons clearly favour symplecticity. However, two questions arise: (1) Can the constant step-size symplectic algorithms now available in the literature improve on a modern standard variable step-size code? (2) Can symplectic algorithms be imple-

mented in a code with error estimation/variable step-size facilities? These questions have been addressed in ref. [34]. The answer to (1) is positive (of course with some qualifications). This implies that there is something to be gained by further exploring the idea of symplectic integrators. On the other hand, the experiments in ref. [34] unambiguously show that when a symplectic formula is implemented with variable step-sizes, its performance is that of a nonsymplectic (variable step-size) algorithm. In other words, the benefits of symplecticity and variable step-sizes cannot be combined.

It thus seems that the key feature in symplectic integration is to find iterates ψ_h^n of a single symplectic transformation ψ_h approximating the true flow ϕ_h. In a variable step-size environment, the initial condition is advanced by a symplectic composition $\psi_{h_n} \psi_{h_{n-1}} \ldots \psi_{h_1}$. The long-time dynamics of such compositions appear to differ substantially from the long times of iterates ψ_h^n of a single symplectic map. A more detailed discussion can be seen in ref. [41].

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