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Symplectic integrators for Hamiltonian problems: an overview

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CONTENTS

1. Introduction

In the sciences, situations where dissipation is not significant may invariably be modelled by Hamiltonian systems of ordinary, or partial, differential equations. Symplectic integrators are numerical methods specifically aimed at advancing in time the solution of Hamiltonian systems. Roughly speaking, 'symplecticness' is a characteristic property possessed by the solutions of Hamiltonian problems. A numerical method is called symplectic if, when applied to Hamiltonian problems, it generates numerical solutions which inherit the property of symplecticness.

If the reader is expecting to find the definition of symplecticness in this introduction, I am sorry he is going to be disappointed. I have devoted Sections 2–4 to the task of explaining symplecticness in what I believe to be the simplest possible way. The fact that six pages are needed to define symplecticness should not be taken as implying that this notion is particularly difficult: for readers with a differential geometry background, symplecticness can be defined in one line. However, here and elsewhere in the article, I have tried to be understandable rather than brief. In particular I have tried hard to relate the concepts in a language accessible to numerical analysts. This has not always been easy, as the area of symplectic integration directly relates to both numerical analysis and to other branches of science, such as symplectic geometry, dynamical systems, classical mechanics and theoretical physics.

After the study of the notion of symplecticness in Sections 2–4, I define in Section 5 the concept of symplectic integrator. Symplectic integrators fall into two categories. Some of them are standard methods, such as Runge–Kutta or Runge–Kutta–Nyström methods, that just happen to achieve symplecticness through some balance in their coefficients. For a method of this kind to be symplectic it is necessary and sufficient that its coefficients satisfy some algebraic equations. This first category of symplectic methods is studied in Sections 6–8. A remarkable feature of the methods of this category is that, for them, an alternative formulation of the order conditions exists, whereby the order conditions are expressed in terms of unrooted rather than rooted trees.

The second category of symplectic methods consists of methods derived via a so-called generating function. Generating functions were introduced in the nineteenth century as a means for solving some problems in classical mechanics. They are at the root of the Hamilton–Jacobi method for integrating differential systems via the Hamilton–Jacobi partial differential equation. In Section 9 I present the necessary background on generating functions and in Section 10 I survey symplectic integrators based on generating functions. In Section 11, I return to the first category of symplectic methods (i.e. to Runge–Kutta and related symplectic methods) with the goal of seeing them in the light of the Hamilton–Jacobi theory.

In Sections 12–14, I summarize the general properties of symplectic integrators. Section 15 is devoted to the practical performance of symplectic integration and the final Section 16 contains a few indications in connection with material, such as Hamiltonian partial differential equations, not covered in the main part of the paper.

The current interest in symplectic integration started with the work of, for example, Ruth (1983), Channell (1983), Menyuk (1984), Feng (1985, 1986a,b). Since then, several dozens of papers on the subject have been written. Some of these have been published in the physics literature, while others have appeared in numerical analysis journals and others are only available as manuscripts. Under these circumstances, I cannot claim to have supplied a list of references that covers all the relevant items. However I have done my best to present a fair view of the field from a numerical analyst's point of view.

Symplectic integration is a new field. As such, much of the material reported here is likely to be superseded soon by new developments. From a theoretical point of view the field has already witnessed some interesting contributions bringing together seemingly unrelated parts of mathematics such as Hamilton–Jacobi equations and graph theory. On the other hand, little has been undertaken in the construction of practical high-order methods and the design of serious symplectic software is still waiting consideration. The area of symplectic integration is one where much scope is left for newcomers. I would be glad if this paper helped in attracting some of them to the field.

2. Hamiltonian systems

2.1. *Preliminaries*

We start by describing the class of problems with which we shall be concerned and by introducing some notation. Let Ω be a domain (i.e. a non-empty, open, connected set) in the oriented Euclidean space $\mathbb{R}^{2d}$ of the points $(\mathbf{p},\mathbf{q}) = (p_1,\ldots,p_d;q_1,\ldots,q_d)$. If H is a sufficiently smooth real function defined in Ω, then the Hamiltonian system of differential equations with Hamiltonian H is, by definition, given by

$$\frac{\mathrm{d}p_i}{\mathrm{d}t} = -\frac{\partial H}{\partial q_i}, \quad \frac{\mathrm{d}q_i}{\mathrm{d}t} = +\frac{\partial H}{\partial p_i}, \qquad 1 \le i \le d. \tag{2.1}$$

The integer d is called the *number of degrees of freedom* and Ω is the *phase space*. The exact amount of smoothness required of H will vary from place to place and will not be explicitly stated, but we throughout assume at least C^2 continuity, so that the right-hand side of the system (2.1) is C^1 and the standard existence and uniqueness theorems apply to the corresponding

initial value problem. Sometimes, the symbol S_H will be used to refer to system (2.1). A good starting point for the theory of Hamiltonian problems is the textbook by Arnold (1989). MacKay and Meiss (1987) have compiled an excellent collection of important papers in Hamiltonian dynamics. For applications to celestial mechanics see Arnold (1988). More advanced results on symplectic geometry can be found in Arnold and Novikov (1990). For the early history of the work of Hamilton and Jacobi on Hamiltonian systems, see Klein (1926).

In applications to mechanics (Arnold, 1989), the $\mathbf{q}$ variables are *generalized coordinates,* the $\mathbf{p}$ variables the conjugated *generalized momenta* and H usually corresponds to the total *mechanical energy.*

Often the Hamiltonian has the special structure

$$H(\mathbf{p},\mathbf{q}) = T(\mathbf{p}) + V(\mathbf{q}). \tag{2.2}$$

In mechanics T and V would represent the *kinetic* and *potential* energy, respectively. Hamiltonians of this form are called *separable.* A commonly occurring case has $T = \frac{1}{2}\mathbf{p}^T\mathbf{p}$, so that the Hamiltonian reads

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

Of course one may also consider *nonautonomous* (time-dependent) Hamiltonians $H = H(\mathbf{p},\mathbf{q};t)$. By using such an H in (2.1), we obtain a nonautonomous Hamiltonian system. Most of the material that follows may easily be extended to cater for the nonautonomous case. However, for simplicity, we shall assume that, unless otherwise explicitly stated, *all Hamiltonians considered are autonomous,* i.e. time-independent.

2.2. *The flow of a Hamiltonian system*

If t is a real number, we denote by $\phi_{t,H}$ the flow of the system S_H introduced in (2.1). Recall that, by definition, $\phi_{t,H}$ is a transformation mapping Ω into itself, in such a way that for $(\mathbf{p}^0,\mathbf{q}^0)$ in Ω, $(\mathbf{p},\mathbf{q}) = \phi_{t,H}(\mathbf{p}^0,\mathbf{q}^0)$ is the value at time t of the solution of (2.1) that at time $t = 0$ has the initial condition $(\mathbf{p}^0,\mathbf{q}^0)$ (see e.g. Section 1.4 of the contribution by Arnold and Ili'yashenko to the book by Anosov and Arnold (1988) or Chapter 1 in Guckenheimer and Holmes (1983)). Therefore, if in

$$(\mathbf{p},\mathbf{q}) = \phi_{t,H}(\mathbf{p}^0,\mathbf{q}^0) \tag{2.4}$$

t varies and $(\mathbf{p}^0,\mathbf{q}^0)$ is seen as fixed, then we recover the solution of (2.1) with initial condition $(\mathbf{p}^0,\mathbf{q}^0)$. The key point is that we will mainly be interested in seeing t in (2.4) as a fixed parameter and $(\mathbf{p}^0,\mathbf{q}^0)$ as a variable, so that we are defining a map of Ω into itself. In fact this is not quite true. The point $\phi_{t,H}(\mathbf{p}^0,\mathbf{q}^0)$ is defined only if the solution of (2.1) with initial condition $(\mathbf{p}^0,\mathbf{q}^0)$ exists at time t, which, for given $(\mathbf{p}^0,\mathbf{q}^0)$, is not necessarily the case if $|t|$ is large: solutions may reach the boundary of Ω in a finite time and exist only for bounded intervals of time. Thus, for given $t \neq 0$, the domain of definition of $\phi_{t,H}$ may be strictly smaller than Ω.

A simple example is provided by the the *harmonic oscillator,* the Hamiltonian system with $d = 1$, $\Omega = \mathbb{R}^2$ and $H = \frac{1}{2}p_1^2 + \frac{1}{2}q_1^2$. If we use the notation p and q for the dependent variables, and identify the point (p,q) with the column vector $[p,q]^T$, the system S_H reads

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} p \\ q \end{bmatrix} = A\begin{bmatrix} p \\ q \end{bmatrix}, \qquad A = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \tag{2.5}$$

and the t-flow is simply the mapping that rotates points in $\mathbb{R}^2$ by an angle of t radians around the origin:

$$\begin{bmatrix} p^0 \\ q^0 \end{bmatrix} \mapsto \exp(At)\begin{bmatrix} p^0 \\ q^0 \end{bmatrix} = \begin{bmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{bmatrix}\begin{bmatrix} p^0 \\ q^0 \end{bmatrix}. \tag{2.6}$$

For nonlinear Hamiltonians, in general, an explicit representation of the flow cannot be found in terms of elementary functions.

3. Area-preserving transformations

3.1. *Preservation of area by one degree of freedom Hamiltonian flows*

The idea of symplectic integration revolves around the use of symplectic transformations. In our experience, some numerical analysts find difficulties when first coming across the notion of symplecticness and tend to confuse symplectic integrators with energy-preserving integrators or with integrators whose stability function has unit modulus on the imaginary axis. It is therefore important that we devote some time to understanding symplecticness. It is best to start with the one degree of freedom case, where symplecticness is nothing but preservation of area. We then assume in this section that $d = 1$ and use the notation p and q to refer to the dependent variables p_1 and q_1 respectively.

For each real t, the flow $\phi_{t,H}$ is an *area-preserving* transformation in Ω, in the sense that, for each bounded subdomain $\Sigma \subset \Omega$ for which $\phi_{H,t}(\Sigma)$ is defined, it holds true that Σ and $\phi_{H,t}(\Sigma)$ have the same (oriented) area. To see this, it is enough, after recalling Liouville's theorem (see e.g. Section 3.5, Chapter 1 in the article by Arnold and Il'yashenko in Anosov and Arnold (1988)), to observe that the vector field $[-\partial H/\partial q, \partial H/\partial p]^T$ that features in (2.1) is divergence free because

$$\frac{\partial}{\partial p}\left(-\frac{\partial H}{\partial q}\right) + \frac{\partial}{\partial q}\left(\frac{\partial H}{\partial p}\right) = 0.$$

In the harmonic oscillator example (2.5) the area-preserving property of the flow, i.e. of the rotation (2.6), is evident.

The area-preserving property of the flow has a marked impact on the long-time behaviour of the solutions of Hamiltonian problems. Clearly asymptotically stable equilibria or limit cycles (Guckenheimer and Holmes, 1983) cannot occur: in their neighbourhoods the area would have to shrink. The Poincaré recurrence holds (Arnold, 1989): under suitable assumptions and as t increases, each point in Ω being moved by $\phi_{t,H}$ returns repeatedly to the vicinity of its initial position.

In fact, all properties specific to the Hamiltonian dynamics can be derived from the preservation of area property. This is no surprise because the area-preserving character of the flow, which was shown earlier to hold for Hamiltonian systems, actually holds *only* for Hamiltonian systems. More precisely, assume that Ω is simply connected, i.e. it has no holes, and suppose that

$$\frac{\mathrm{d}p}{\mathrm{d}t} = f(p,q), \quad \frac{\mathrm{d}q}{\mathrm{d}t} = g(p,q), \tag{3.1}$$

is a smooth differential system whose flow is area-preserving. Then (3.1) is actually a Hamiltonian system $\mathcal{S}_H$ for a suitable H. There is nothing deep about this. By Liouville's theorem the vector field $[f,g]^T$ is divergence free, so that

$$\frac{\partial}{\partial p}(-f) = \frac{\partial}{\partial q} g.$$

But this is just the necessary and sufficient condition for the field $[g,-f]^T$ to be the gradient of a scalar function H, i.e. for (3.1) to coincide with $\mathcal{S}_H$.

If Ω is not simply connected, then systems with area-preserving flows are, in general, only locally Hamiltonian: in each ball $B \subset \Omega$ they coincide with a Hamiltonian system $\mathcal{S}_{H_B}$ but, globally, the system may not be Hamiltonian because the various H_B cannot be patched together. A typical example is given by the area-preserving system

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \frac{p}{p^2+q^2}, \quad \frac{\mathrm{d}q}{\mathrm{d}t} = \frac{q}{p^2+q^2}$$

defined in $\Omega = \mathbb{R}^2 \backslash (0,0)$. In each ball in Ω the system is Hamiltonian with H given by a branch of the argument of the point (p,q). The system is not Hamiltonian because of course the argument cannot be defined as a smooth single-valued function in $\mathbb{R}^2 \backslash (0,0)$.

3.2. Checking preservation of area: Jacobians

Let $(p^*,q^*) = \psi(p,q)$ be a $\mathcal{C}^1$ transformation defined in a domain Ω. According to the standard rule for changing variables in an integral, ψ is area-preserving if and only if the Jacobian determinant is identically 1:

$$\forall (p,q) \in \Omega, \quad \frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial q} - \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial p} = 1. \tag{3.2}$$

It is a trivial exercise in matrix multiplication to check that this relationship can be rewritten as

$$\forall (p,q) \in \Omega, \quad \psi'^T J\, \psi' = \frac{\partial (p^*,q^*)}{\partial (p,q)}^T J \frac{\partial (p^*,q^*)}{\partial (p,q)} = J, \tag{3.3}$$

where

$$J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

and $\psi' = \partial(p^*,q^*)/\partial(p,q)$ is the Jacobian matrix of the transformation. Going from (3.2) to (3.3) may appear to be just a matter of complicating things. This is not so: the matrix J is a very important character in this play. If $\mathbf{v}$ and $\mathbf{w}$ are vectors in the plane, then $\mathbf{v}^T J \mathbf{w}$ is the oriented area of the parallelogram they determine. Now, let us fix a point (p,q) in Ω and construct a parallelogram $\mathcal{P}$ having a vertex at (p,q) and having as sides two small vectors $\mathbf{v}$ and $\mathbf{w}$ (i.e. the vertices are the points (p,q), $(p,q)+\mathbf{v}$, $(p,q)+\mathbf{w}$, $(p,q)+\mathbf{v}+\mathbf{w}$). Then $\psi(\mathcal{P})$ is a parallelogram with curved sides, which can be approximated by the parallelogram $\mathcal{P}^*$ based at $\psi(p,q)$ with sides $\psi'\mathbf{v}$, $\psi'\mathbf{w}$. In fact, by the very definition of ψ', $\psi(\mathcal{P})$ and $\mathcal{P}^*$ differ in terms higher than linear in $\mathbf{v}$ and $\mathbf{w}$. Now $\mathcal{P}^*$ and $\mathcal{P}$ have the same area if and only if

$$\mathbf{v}^T \psi'^T J\, \psi' \mathbf{w} = \mathbf{v}^T J\, \mathbf{w}.$$

Clearly, the last relationship holds for all parallelograms $\mathcal{P}$ in Ω if and only if (3.3) holds. The conclusion is that (3.3) means that, at each point $(p,q) \in \Omega$, the linear transformation ψ' maps parallelograms based at (p,q) into parallelograms based at $\psi(p,q)$ without altering the oriented area.

3.3. Checking preservation of area: differential forms

Differential forms in Ω provide an alternative language with which to express the considerations made in the preceding subsection. A detailed study of the meaning and properties of differential forms is definitely outside the scope of this paper (the interested reader is referred to Arnold (1989, Chapter 7)). However the algebraic manipulations required to prove conservation of area via differential forms are as a rule easier than those required to prove conservation of area via (3.3). It is therefore advisable to comment, albeit briefly, on differential forms. Our treatment will be merely formal and we shall not explain why differential 2-forms are ways of measuring two-dimensional areas. We see a differential 1-form in Ω as a formal combination $P(p,q)\mathrm{d}p + Q(p,q)\mathrm{d}q$ where P and Q are smooth real-valued functions defined in Ω. For instance, the differentials $\mathrm{d}p^*$ and $\mathrm{d}q^*$ of the components

of the transformation ψ considered earlier are differential 1-forms

$$dp^* = \frac{\partial p^*}{\partial p}dp + \frac{\partial p^*}{\partial q}dq, \qquad dq^* = \frac{\partial q^*}{\partial p}dp + \frac{\partial q^*}{\partial q}dq.$$

Two differential 1-forms ω and ω' give rise, via the exterior product $\wedge$, to a new entity $\omega \wedge \omega'$ called a differential 2-form. The exterior product is bilinear, so that, for instance,

$$dp^* \wedge dq^* = \frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial p}dp \wedge dp + \frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial q}dp \wedge dq + \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial p}dq \wedge dp + \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial q}dq \wedge dq.$$

The exterior product is skew symmetric. In particular, it holds that

$$dp \wedge dp = dq \wedge dq = 0, \qquad dp \wedge dq = -dq \wedge dp.$$

Thus

$$dp^* \wedge dq^* = \left(\frac{\partial p^*}{\partial p}\frac{\partial q^*}{\partial q} - \frac{\partial p^*}{\partial q}\frac{\partial q^*}{\partial p}\right) dp \wedge dq$$

and from (3.2) we see that conservation of area is equivalent to

$$dp^* \wedge dq^* = dp \wedge dq.$$

This usually provides a convenient way of checking preservation of area.

4. Symplectic transformations

4.1. Hamiltonian flows and symplectic transformations

It is now time to consider the case $d > 1$. Is there something analogous to the area that is being conserved by Hamiltonian flows? The $2d$-dimensional volume in Ω appears to be a natural candidate and indeed this volume *is* conserved. However this is not what we really want. What does the trick is to consider *two-dimensional* surfaces Σ in Ω, to find the projections Σ_i, $1 \le i \le d$ onto the d two-dimensional planes of the variables (p_i, q_i) and sum the two-dimensional oriented areas of these projections. This yields a number $m(\Sigma)$. It can be proved (see e.g. Arnold (1989) Section 44) that the flow of (2.1) preserves m: $m(\phi_{t,H}(\Sigma)) = m(\Sigma)$ whenever Σ is contained in the domain of $\phi_{t,H}$. Now transformations that have this preservation property are called *symplectic* or canonical, so that we have the theorem:

Theorem 4.1 For each t, the flow $\phi_{t,H}$ of a Hamiltonian system is a symplectic transformation.

Furthermore, if Ω is simply connected (i.e. each closed curved in Ω may be shrunk down to a single point without leaving Ω), then the converse is also true: an m-preserving differential system is a Hamiltonian system, see Arnold (1989, Section 40D) (once more, if Ω fails to be simply connected then preservation of m implies that the system is locally Hamiltonian). In this respect the symplecticness of the flow is the hallmark of Hamiltonian systems and once more the dynamical features that are specific to Hamiltonian problems can be traced back to the symplectic character of the flow.

4.2. Checking symplecticness

The condition (3.3) which we used to decide whether a transformation ψ in the plane was area-preserving or was otherwise generalized to read

$$\forall (\mathbf{p}, \mathbf{q}) \in \Omega, \quad \psi'^T J \psi' = \frac{\partial(\mathbf{p}^*, \mathbf{q}^*)}{\partial(\mathbf{p}, \mathbf{q})}^T J \frac{\partial(\mathbf{p}^*, \mathbf{q}^*)}{\partial(\mathbf{p}, \mathbf{q})} = J, \tag{4.1}$$

where now

$$J = \begin{bmatrix} 0_d & I_d \\ -I_d & 0_d \end{bmatrix}, \tag{4.2}$$

with I_d and 0_d denoting the unit and zero d-dimensional matrix. Note that the matrix J has the property that, for each pair $(\mathbf{v}, \mathbf{w})$ of vectors in $\mathbb{R}^{2d}$, $\mathbf{v}^T J \mathbf{w}$ represents the sum of the two-dimensional areas of the d parallelograms that result from projecting the parallelogram determined by $\mathbf{v}$ and $\mathbf{w}$ onto the planes of the variables (p_i, q_i).

Differential forms can also be used. In the present context, 1-differential forms are formal expressions of the form $P_1 dp_1 + \cdots + P_d dp_d + Q_1 dq_1 + \cdots + Q_d dq_d$, with P_i and Q_i smooth real-valued functions defined in Ω. Again, two 1-forms give rise to a 2-form via the exterior product. The transformation ψ is symplectic if and only if

$$dp_1^* \wedge dq_1^* + \cdots + dp_d^* \wedge dq_d^* = dp_1 \wedge dq_1 + \cdots + dp_d \wedge dq_d,$$

a relationship that we can rewrite more compactly as

$$d\mathbf{p}^* \wedge d\mathbf{q}^* = d\mathbf{p} \wedge d\mathbf{q}.$$

4.3. Conservation of volume

Let $\phi_{t,H}$ play the role of ψ in (4.1) and take determinants. The result is that $\det(\phi'_{t,H})$ is either $+1$ or -1. The value -1 is excluded since, by Liouville's theorem, the flow of any differential system has a Jacobian matrix with a positive determinant. Hence $\det(\phi'_{t,H}) \equiv 1$: Hamiltonian flows preserve the oriented volume in $\mathbb{R}^{2d}$ or, in other words, points in phase-space convected by a Hamiltonian flow behave like particles of an incompressible fluid flow. Note that preservation of volume $\det(\psi') \equiv 1$ is a direct generalization to $d > 1$ of the property (3.2). However, when going from $d = 1$ to $d > 1$, the right generalization of preservation of area is symplectiness rather than preservation of volume. Symplectiness *characterizes* Hamiltonian flows; conservation of volume is a much weaker property shared by some nonHamiltonian systems.

5. Symplectic integrators

5.1. Numerical methods

Even though some attention has been given in the literature to symplectic multistep methods (see Aizu, 1985; Feng and Qin, 1987; Eirola and Sanz-Serna, 1990; Sanz-Serna and Vadillo, 1986, 1987), in this paper we restrict our interest to *one-step* integrators. If h denotes the step-length and $(\mathbf{p}^n, \mathbf{q}^n)$ denotes the numerical approximation at time $t_n = nh$, n an integer, to the value $(\mathbf{p}(t_n), (t_n))$ of a solution of (2.1), then a one-step method is specified by a smooth mapping

$$(\mathbf{p}^{n+1}, \mathbf{q}^{n+1}) = \psi_{h,H}(\mathbf{p}^n, \mathbf{q}^n). \tag{5.1}$$

The transformation $\psi_{h,H}$ itself is assumed to depend smoothly on h and H. The domain Ω_h of $\psi_{h,H}$ need not be, for each h, the whole Ω. In fact for implicit methods, where the actual computation of $(\mathbf{p}^{n+1}, \mathbf{q}^{n+1})$ involves the solution of some system of equations, it is often the case that, for fixed $(\mathbf{p}^n, \mathbf{q}^n)$, the new approximation $\psi_{h,H}(\mathbf{p}^n, \mathbf{q}^n)$ is only defined if $|h|$ is suitably small.

The method (5.1) is of order r with r an integer, if, as $h \to 0$, $\psi_{h,H}$ differs from the flow $\phi_{h,H}$ by $\mathcal{O}(h^{r+1})$ terms whenever the Hamiltonian H is suitably smooth. Consistency means order ≥ 1.

Given an initial condition $(\mathbf{p}^0, \mathbf{q}^0)$, the numerical approximation at time t_n is found by iterating the mapping $\psi_{h,H}$ n times, i.e.

$$(\mathbf{p}^n, \mathbf{q}^n) = \psi^n_{h,H}(\mathbf{p}^0, \mathbf{q}^0),$$

whereas for the true solution

$$(\mathbf{p}(t_n), \mathbf{q}(t_n)) = \phi_{t_n,H}(\mathbf{p}^0, \mathbf{q}^0) = \phi^n_{h,H}(\mathbf{p}^0, \mathbf{q}^0).$$

5.2. Symplectic numerical methods

Is it possible to construct numerical methods (5.1) that take into account the Hamiltonian nature of the problem being integrated? In other words, is there such a thing as a *Hamiltonian* numerical method? Before answering this question, let us first note that the discrete equations (5.1) do not intend to mimic the differential system (2.1). On the contrary $\psi_{h,H}$ tries to mimic the *flow* $\phi_{h,H}$. Now, we saw in Section 4 that the Hamiltonian form of the differential equations corresponds, in terms of flows, to symplecticness. Hence the right question to ask is: are there numerical methods (5.1) for which $\psi_{h,H}$ is a symplectic transformation for all Hamiltonians H and all step-lengths h? Such methods, that do exist, are called *symplectic* (or canonical) and are the subject of this paper.

Roughly speaking, there are two main groups of symplectic methods. The first group consists of formulae that belong to standard families of numerical methods, such as Runge–Kutta or Runge–Kutta–Nyström methods, and just 'happen' to be symplectic (Sanz-Serna, 1991b). These symplectic methods can be applied to general (i.e. not necessarily Hamiltonian) systems of differential equations and, when applied to a Hamiltonian system, achieve symplecticness through a suitable balance between the formula coefficients. The second main group of symplectic integrators consists of methods that are derived via a so-called *generating function*. These methods cannot be applied to general systems of differential equations, not even to small dissipative perturbations of Hamiltonian systems.

The presentation to a numerical analysis audience of the methods of the first group is easier than the presentation of the second group. We therefore consider the first group in Sections 6–8 and postpone the study of the methods of the second group until Section 10. This somehow goes against the history of the field, where methods based on generating functions came first.

5.3. Composing methods

Before we present particular examples of symplectic integrators, it is expedient to consider the issue of composition of methods, as this plays a role in later developments. If $\psi^{[1]}_{h,H}$ and $\psi^{[2]}_{h,H}$ are consistent numerical methods, then the mapping

$$\psi_{h,H} = \psi^{[2]}_{h/2,H}\psi^{[1]}_{h/2,H}$$

is clearly a new consistent numerical method. More general compositions of the form

$$\psi^{[2]}_{\theta h,H}\psi^{[1]}_{(1-\theta)h,H},$$

θ a real constant, are also possible. Since it is obvious that the composition of symplectic maps is a symplectic map, the composition of two symplectic numerical methods gives rise to a new symplectic method.

On the other hand, along with each method (5.1) we consider its *adjoint* $\hat{\psi}_{h,H}$. By definition (see e.g. Hairer *et al.* (1987, Section II.8)), this is the method such that $\hat{\psi}_{-h,H}\psi_{h,H}$ is the identity map, i.e. stepping forward with the given method is just stepping backward with its adjoint. The familiar forward and backward Euler methods are mutually adjoint. The adjoint of a symplectic method is itself a symplectic method, because the inverse of a symplectic transformation is, clearly, a symplectic transformation.

Some methods, such as the implicit midpoint rule, happen to be their own adjoints. These are called, unsurprisingly, *self-adjoint*. It is easy to see that the order of consistency r of a self-adjoint method is necessarily even.

6. Runge–Kutta and related methods: conditions for symplecticness

6.1. *Runge–Kutta methods*

The application of the Runge–Kutta (RK) method to system (2.1) with tableau

$$\begin{array}{c|ccc} a_{11} & \cdots & a_{1s} \\ \vdots & \ddots & \vdots \\ a_{s1} & \cdots & a_{ss} \\ \hline b_1 & \cdots & b_s \end{array} \tag{6.1}$$

results in the relations

$$\mathbf{P}_i = \mathbf{p}^n + h\sum_{j=1}^{s} a_{ij}\mathbf{f}(\mathbf{P}_j, \mathbf{Q}_j),\ \mathbf{Q}_i = \mathbf{q}^n + h\sum_{j=1}^{s} a_{ij}\mathbf{g}(\mathbf{P}_j, \mathbf{Q}_j),\ 1 \le i \le s, \tag{6.2}$$

$$\mathbf{p}^{n+1} = \mathbf{p}^n + h\sum_{i=1}^{s} b_i\mathbf{f}(\mathbf{P}_i, \mathbf{Q}_i), \quad \mathbf{q}^{n+1} = \mathbf{q}^n + h\sum_{i=1}^{s} b_i\mathbf{g}(\mathbf{P}_i, \mathbf{Q}_i), \tag{6.3}$$

where $\mathbf{f}$ and $\mathbf{g}$ respectively denote the d-vectors with components $-\partial H/\partial q_i$ and $\partial H/\partial p_i$ and $\mathbf{P}_i$ and $\mathbf{Q}_i$ are the internal stages corresponding to the $\mathbf{p}$ and $\mathbf{q}$ variables.

The following result was discovered independently by Lasagni (1988), Sanz-Serna (1988) and Suris (1989).

Theorem 6.1 Assume that the coefficients of the method (6.1) satisfy the relationships

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad 1 \le i, j \le s. \tag{6.4}$$

Then the method is symplectic.

Proof. We follow the technique used by Sanz-Serna (1988). Suris (1989) resorts to Jacobians rather than to differential forms. No proof is presented in Lasagni (1988). We employ the notation

$$\mathbf{k}_i = \mathbf{f}(\mathbf{P}_i, \mathbf{Q}_i), \qquad \mathbf{l}_i = \mathbf{g}(\mathbf{P}_i, \mathbf{Q}_i)$$

for the 'slopes' at the stages. Differentiate (6.3) and form the exterior product to arrive at

$$\begin{aligned} \mathrm{d}\mathbf{p}^{n+1} \wedge \mathrm{d}\mathbf{q}^{n+1} &= \mathrm{d}\mathbf{p}^n \wedge \mathrm{d}\mathbf{q}^n + h\sum_{i=1}^{s} b_i \mathrm{d}\mathbf{k}_i \wedge \mathrm{d}\mathbf{q}^n \\ &\quad + h\sum_{j=1}^{s} b_j \mathrm{d}\mathbf{p}^n \wedge \mathrm{d}\mathbf{l}_j + h^2 \sum_{i,j=1}^{s} b_i b_j \mathrm{d}\mathbf{k}_i \wedge \mathrm{d}\mathbf{l}_j. \end{aligned}$$

Our next step is to eliminate $\mathrm{d}\mathbf{k}_i \wedge \mathrm{d}\mathbf{q}^n$ and $\mathrm{d}\mathbf{p}^n \wedge \mathrm{d}\mathbf{l}_j$ from this expression. This is easily achieved by differentiating (6.2) and taking the exterior product of the result with $\mathbf{dk}_i$, $\mathbf{dl}_j$. The outcome of the elimination is

$$\begin{aligned} \mathrm{d}\mathbf{p}^{n+1} \wedge \mathrm{d}\mathbf{q}^{n+1} - \mathrm{d}\mathbf{p}^n \wedge \mathrm{d}\mathbf{q}^n &= h\sum_{i=1}^{s} b_i \left[\mathrm{d}\mathbf{k}_i \wedge \mathrm{d}\mathbf{Q}_i + \mathrm{d}\mathbf{P}_i \wedge \mathrm{d}\mathbf{l}_i\right] \\ &\quad - h^2 \sum_{i,j=1}^{s} (b_i a_{ij} + b_j a_{ji} - b_i b_j)\, \mathrm{d}\mathbf{k}_i \wedge \mathrm{d}\mathbf{l}_j. \end{aligned}$$

The second term on the right-hand side vanishes in view of (6.4). To finish the proof is then sufficient to show that, for each i, $d\mathbf{k}_i \wedge d\mathbf{Q}_i + d\mathbf{P}_i \wedge d\mathbf{l}_i$ is 0. In fact, dropping the subscript i that numbers the stages, we can write

$$\begin{aligned} d\mathbf{k} \wedge d\mathbf{Q} + d\mathbf{P} \wedge d\mathbf{l} &= \sum_{\mu=1}^{d} \left[dk_\mu \wedge dQ_\mu + dP_\mu \wedge dl_\mu\right] \\ &= \sum_{\mu,\nu=1}^{d} \left[\frac{\partial f_\mu}{\partial p_\nu} dP_\nu \wedge dQ_\mu + \frac{\partial f_\mu}{\partial q_\nu} dQ_\nu \wedge dQ_\mu \right. \\ &\quad \left. + \frac{\partial g_\mu}{\partial p_\nu} dP_\mu \wedge dP_\nu + \frac{\partial g_\mu}{\partial q_\nu} dP_\mu \wedge dQ_\nu \right]. \end{aligned}$$

To see that this expression vanishes express f_μ and g_μ as derivatives of H and recall the skew-symmetry of the exterior product. □

The symplecticness of the method must be understood in the following sense. Assume that, for a given h, $(\mathbf{p}^{n+1}, \mathbf{q}^{n+1}) = \psi_{h,H}(\mathbf{p}^n, \mathbf{q}^n)$ is a smooth function defined in a subdomain Ω_h of Ω and satisfying the RK equations (6.2)–(6.3), then $\psi_{h,H}$ is a symplectic transformation. In general, for a given h there can be several such functions (nonuniqueness of solutions of the RK scheme). Of course, for $h \to 0$ there is a *unique* RK solution that approximates the true solution and the corresponding domain of definition Ω_h tends to Ω. However spurious RK solutions may also exist and they are also symplectic. For material on the existence and uniqueness of RK solutions see e.g. Dekker and Verwer (1984, Chapter 5) and Sanz-Serna and Griffiths (1991). For spurious solutions see Iserles (1990a) and Hairer *et al.* (1990).

Lasagni (1988, 1990) has shown that, for RK methods without redundant stages, (6.4) is actually necessary for the method to be symplectic. A direct proof of this result is not available in the published literature. However the result is a corollary of Theorem 5.1 in Abia and Sanz-Serna (1990).

6.2. *Partitioned Runge–Kutta methods*

In the integration of systems of differential equations it is perfectly possible to integrate some components of the unknown vector with a numerical method and the remaining components with a different numerical method. For instance, one may wish to do this if the system includes both stiff and nonstiff components. In our setting, we may wish to 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 and is specified by two tableaux

$$\begin{array}{c|ccc} a_{11} & \cdots & a_{1s} \\ \vdots & \ddots & \vdots \\ a_{s1} & \cdots & a_{ss} \\ \hline b_1 & \cdots & b_s \end{array}, \qquad \begin{array}{c|ccc} A_{11} & \cdots & A_{1s} \\ \vdots & \ddots & \vdots \\ A_{s1} & \cdots & A_{ss} \\ \hline B_1 & \cdots & B_s \end{array}. \tag{6.5}$$

The application of (6.5) to system (2.1) results in the relationships (cf. (6.2)–(6.3))

$$\mathbf{P}_i = \mathbf{p}^n + h\sum_{j=1}^{s} a_{ij}\mathbf{f}(\mathbf{P}_j, \mathbf{Q}_j),$$

$$\mathbf{Q}_i = \mathbf{q}^n + h\sum_{j=1}^{s} A_{ij}\mathbf{g}(\mathbf{P}_j, \mathbf{Q}_j),\ 1 \le i \le s.$$

$$\mathbf{p}^{n+1} = \mathbf{p}^n + h\sum_{i=1}^{s} b_i\mathbf{f}(\mathbf{P}_i, \mathbf{Q}_i), \quad \mathbf{q}^{n+1} = \mathbf{q}^n + h\sum_{i=1}^{s} B_i\mathbf{g}(\mathbf{P}_i, \mathbf{Q}_i).$$

Of course an RK method is a particular instance of (6.5) where both tableaux just happen to have the same entries. The following result was first given by the present author at the London 1989 ODE meeting (Sanz-Serna, 1989) and discovered independently by Suris (1990). The proof is analogous to that of Theorem 6.1.

Theorem 6.2 Assume that the coefficients of the method (6.5) satisfy the relationships

$$b_iA_{ij} + B_ja_{ji} - b_iB_j = 0, \quad 1 \le i, j \le s. \tag{6.6}$$

then the method is symplectic when applied to separable Hamiltonian problems (2.1), (2.2).

Symplecticness must again be understood as in Theorem 6.1 and, once more, (6.6) is necessary for symplectiness, provided that the method has no redundant stages, see Abia and Sanz-Serna (1990).

6.3. *Runge–Kutta–Nyström methods*

Systems of differential equations of the special form

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \mathbf{f}(\mathbf{q}), \qquad \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = \mathbf{p}, \tag{6.7}$$

or, equivalently, second-order systems $\mathrm{d}^2\mathbf{q}/\mathrm{d}t^2 = \mathbf{f}(\mathbf{q})$ can be efficiently integrated by means of Runge–Kutta–Nyström (RKN) methods (see e.g. Hairer *et al.* (1987, Section II.13)). For the RKN procedure with array

$$\begin{array}{c|ccc} \gamma_1 & \alpha_{11} & \cdots & \alpha_{1s} \\ \vdots & \vdots & \ddots & \vdots \\ \gamma_s & \alpha_{s1} & \cdots & \alpha_{ss} \\ \hline & \beta_1 & \cdots & \beta_s \\ \hline & b_1 & \cdots & b_s \end{array} \tag{6.8}$$

the intermediate stages $\mathbf{Q}_i$ are defined by

$$\mathbf{Q}_i = \mathbf{q}^n + h\gamma_i\mathbf{p}^n + h^2\sum_{j=1}^{s} \alpha_{ij}\mathbf{f}(\mathbf{Q}_j),$$

and the approximation at the next time level is

$$\mathbf{p}^{n+1} = \mathbf{p}^n + h\sum_{i=1}^{s} b_i\mathbf{f}(\mathbf{Q}_j), \quad \mathbf{q}^{n+1} = \mathbf{q}^n + h\mathbf{p}^n + h^2\sum_{i=1}^{s} \beta_i\mathbf{f}(\mathbf{Q}_i).$$

The system (6.7) is Hamiltonian if and only if **f** (the 'force') is the gradient of a scalar function $-V$. When this condition is satisfied the Hamiltonian is given by (2.3). The following result is due to Suris (1989), who used Jacobians in the proof. A proof based on differential forms, similar to that of Theorem 6.1 is easily given, and can be seen in Okunbor and Skeel (1990).

Theorem 6.3 Assume that the coefficients of the method (6.8) satisfy the conditions

$$\beta_i = b_i(1 - \gamma_i), \quad 1 \le i \le s, \tag{6.9}$$

$$b_i(\beta_j - \alpha_{ij}) = b_j(\beta_i - \alpha_{ji}), \quad 1 \le i, j \le s. \tag{6.10}$$

Then the method is symplectic when applied to Hamiltonian problems (2.1), (2.3).

The conditions (6.9) and (6.10) are also necessary for methods without redundant stages to be symplectic, see Calvo (1991).

7. Runge–Kutta and related methods: order conditions for symplectic methods

Before we construct specific formulae within the classes of symplectic methods we have identified in the previous section, it is clearly appropriate to discuss the corresponding order conditions, i.e. the sets of relationships that the method coefficients must satisfy to ensure that a prescribed order of consistency r is reached.

7.1. Runge–Kutta methods

Since Hamiltonian problems are only a subclass of the family of all differential problems, it is *a priori* conceivable that the order of consistency r^* that an RK method achieves for Hamiltonian problems is higher than the classical order of consistency r, i.e. the order of consistency for the most general problem. This is not the case. By considering Hamiltonians of the form $H = \mathbf{p}^T\mathbf{g}(\mathbf{q})$, we see that any d-dimensional differential system $\mathrm{d}\mathbf{q}/\mathrm{d}t = \mathbf{g}(\mathbf{q})$ can be thought of as being the $\mathbf{q}$ equations of a Hamiltonian system with d-degrees of freedom. Hence $r = r^*$ and therefore the material in this subsection applies even if the system being integrated is not Hamiltonian.

The conditions that (6.1) should satisfy to achieve order $\geq r$ are well known (Butcher, 1987, Theorem 306A; Hairer *et al.*, 1987, Theorem 2.13). Each *rooted* tree $\rho\tau$ with r or fewer vertices gives rise to a condition

$$\Phi(\rho\tau) = 1/\gamma(\rho\tau). \tag{7.1}$$

Here the *density* $\gamma(\rho\tau)$ is an (easily computable) integer associated with $\rho\tau$ and the *elementary weight* $\Phi(\rho\tau)$ is a polynomial in the method coefficients a_{ij}, b_i. Figure 1 contains the rooted trees with four vertices or less; we have highlighted the roots by means of a cross.

As an illustration, let us recall that for consistency $r \geq 1$ we require, in connection with $\rho\tau_{1,1}$,

$$\sum_{i=1}^{s} b_i = 1.$$

For order $r \geq 2$ we further impose, in connection with $\rho\tau_{2,1}$,

$$\sum_{i,j=1}^{s} b_i a_{ij} = \tfrac{1}{2}.$$

For order $r \geq 3$ we add further, in view of $\rho\tau_{3,1}$,

$$\sum_{i,j,k=1}^{s} b_i a_{ij} a_{jk} = \tfrac{1}{6}, \tag{7.2}$$

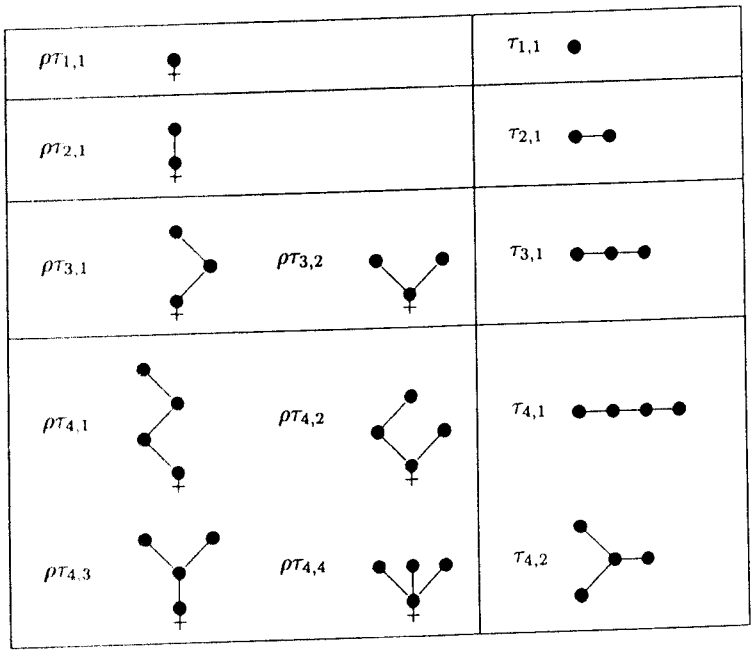

Fig. 1. Rooted n-trees and n-trees, $n = 1, 2, 3, 4$.

and, in view of $\rho\tau_{3,2}$,

$$\sum_{i,j,k=1}^{s} b_i a_{ij} a_{ik} = \tfrac{1}{3}. \tag{7.3}$$

Butcher (1987, Theorem 306A) proves that, if the number of stages s and the coefficients a_{ij}, b_i are regarded as free parameters, then each equation of the form (7.1) is independent of the others. However, when the symplecticness conditions (6.4) are imposed, the method coefficients are no longer free parameters and it turns out that some redundancies appear amongst the classical order conditions (7.1) arising from the various $\rho\tau$. As a result, in order to achieve order $\geq r$ it is not necessary to write down an equation for *every* rooted tree of order $\leq r$. This point has been studied by Sanz-Serna and Abia (1991), whose treatment we follow closely.

Assume that two rooted trees are identified if they only differ in the location of the root, but otherwise consist of the same vertices and edges. (In Figure 1, this is the case for the rooted trees $\rho_{3,1}$ and $\rho_{3,2}$, or for the rooted trees $\rho_{4,1}$ and $\rho_{4,2}$.) Each equivalence class under this equivalence relation is called a *tree*. Thus, in Figure 1, the eight rooted trees of order ≤ 4 give rise to only five trees.

Some trees are called *superfluous*. These are the trees that result when

Table 1. *Number of order conditions.*

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

two copies of the same rooted tree with N vertices are joined by their roots to give rise to a graph with $2N$ vertices. For instance, in Figure 1, the tree $\tau_{2,1}$ is superfluous because it is the juxtaposition of two copies of $\rho\tau_{1,1}$. In a similar manner, $\tau_{4,1}$ is superfluous as it is the juxtaposition of two copies of $\rho\tau_{2,1}$. There is an alternative way of thinking of superfluous trees. Assume that trees are *coloured* in such a way that each vertex is painted either black or white with adjacent vertices receiving distinct colours. Most trees can be coloured in two different ways: in $\tau_{3,1}$ we could have either a black vertex between two white vertices or a white vertex between two black vertices. However some trees can be coloured in only one way: in $\tau_{2,1}$ we can only have a black vertex shaking hands with a white vertex. These trees are precisely the superfluous trees.

After these preliminaries we are ready for the main result.

Theorem 7.1 Assume that the RK method (6.1) satisfies the symplecticness requirement (6.4) and has order of consistency $\geq r \geq 1$. Then it has order of consistency $\geq r+1$ if and only if for each *nonsuperfluous* tree τ with $r+1$ or fewer vertices there is a rooted tree $\rho\tau \in \tau$ for which (7.1) holds.

For instance, since only the tree with two vertices is superfluous, each consistent symplectic RK method actually possesses an order of at least 2. To ensure order ≥ 3, it is sufficient to impose *either* (7.2) or (7.3). In other words (7.2) and (7.3) have become equivalent, as coming from the same tree. In general, for symplectic RK methods, the number of order conditions for order $\geq r$ equals the number of nonsuperfluous trees with r or fewer nodes, as distinct from the situation for general RK methods, where there is an order condition for each rooted tree with r or fewer vertices. The reduction in the number of order conditions is borne out in Table 1.

7.2. *Partitioned Runge–Kutta methods*

A similar theory exists for PRK methods (Abia and Sanz-Serna, 1990) applied to *separable* Hamiltonian systems. Again, there is no distinction between the order r of the method (6.5) for separable Hamiltonian systems and the classical order when applied to systems of the form

$$\frac{d\mathbf{p}}{dt} = \mathbf{f}(\mathbf{q}), \qquad \frac{d\mathbf{q}}{dt} = \mathbf{g}(\mathbf{p}),$$

where $\mathbf{f}$ and $\mathbf{g}$ are any smooth functions, rather than gradients of scalar functions $-V$ and T as they would be in the Hamiltonian case.

It is well known that graph theory can again be used to systematize the writing of the standard order conditions (e.g. Hairer *et al.* 1987, Section II.14). We now need *bicolour* rooted trees $\beta\rho\tau$, i.e. rooted trees with vertices coloured black or white as previously described. Clearly each rooted tree gives rise to two bicolour rooted trees: the root can be coloured either black or white and the colour of the root recursively determines the colour of all vertices (cf. Figure 2). There is an order condition for each $\beta\rho\tau$. The first of these are as follows. For the two bicolour rooted trees with one vertex we get

$$\sum_{i=1}^{s} b_i = 1, \qquad \sum_{i=1}^{s} B_i = 1.$$

Vertices of one colour bring in lower case letters and the vertices of the other colour bring in upper case letters. In connection with the two bicolour rooted trees with two vertices, we have

$$\sum_{i,j=1}^{s} b_i A_{ij} = \tfrac{1}{2}, \qquad \sum_{i,j=1}^{s} B_i a_{ij} = \tfrac{1}{2}, \tag{7.4}$$

etc. The symplecticness conditions (6.6) bring about some redundancies among the standard order conditions we have just presented (Abia and Sanz-Serna, 1990). Again the key point is to disregard the location of the root: bicolour rooted trees which only differ in the location of the root make an equivalence class called a bicolour tree $\beta\rho$ (see Figure 2). Then for symplectic methods, it is enough to consider an order condition for *a particular* bicolour rooted tree in each bicolour tree. For instance for a consistent symplectic method to have order 2 we impose *one* of the two conditions in (7.4). It should perhaps be emphasized that now bicolour trees arising from colouring a superfluous tree must also be considered. The difference between superfluous and nonsuperfluous trees is that a nonsuperfluous tree gives rise to *two* bicolour trees (two order conditions), while a superfluous tree only generates *one* bicolour tree (only one order condition).

The reduction in the number of order conditions is borne out in Table 1.

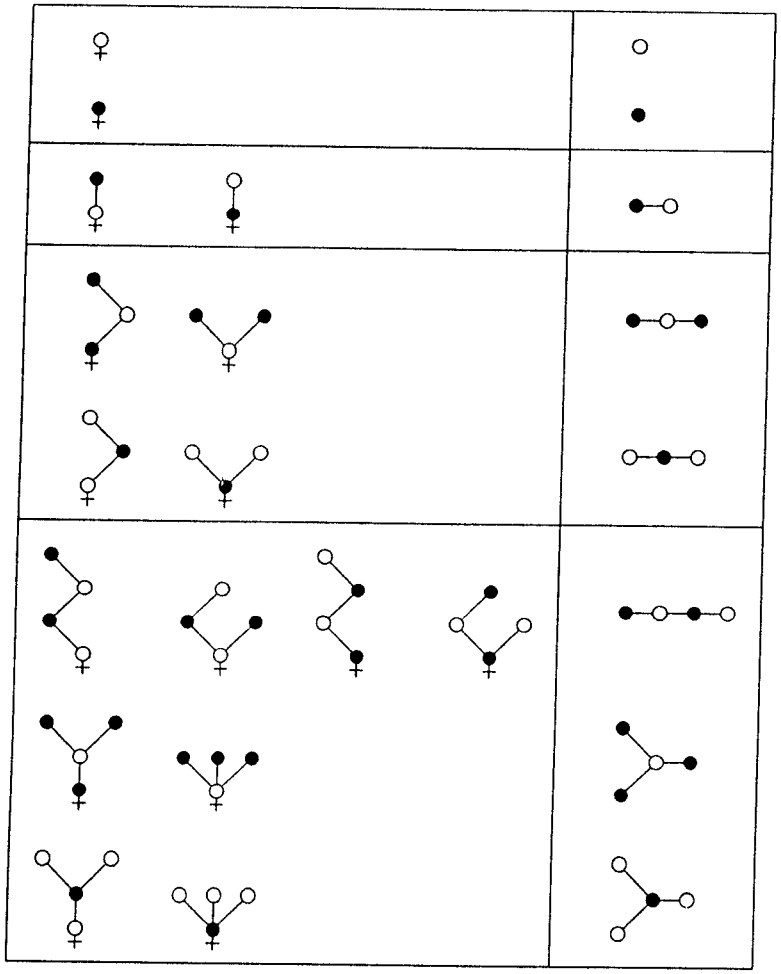

Fig. 2. Rooted bicolour n-trees and bicolour n-trees, $n = 1, 2, 3, 4$.

7.3. *Runge–Kutta–Nyström methods*

Similar considerations hold for RKN methods. In the interest of brevity we omit the corresponding results and the interested reader is referred to Calvo and Sanz-Serna (1991a). The reduction in the number of order conditions is apparent in Table 1. A word of warning: in the table, a general RKN method means a method satisfying (6.9); practical methods as a rule satisfy this condition.

7.4. *The homogeneous form of the order conditions for symplectic methods*

Let us return to the RK case. The fact that, in order to write the order conditions for symplectic methods, we are free to choose any rooted tree within each nonsuperfluous tree introduces some asymmetry among the various rooted trees. For instance, at the $r = 3$ stage, we are free to disregard $\rho\tau_{3,1}$ or $\rho\tau_{3,2}$, i.e. to omit (7.2) or (7.3). Sanz-Serna and Abia (1991) provide an alternative way of writing the order conditions, where all rooted trees belonging to a nonsuperfluous tree play a symmetric role. For a consistent method to have order $r \geq 4$, Sanz-Serna and Abia (1991) put

$$6 \sum_{ijk=1}^{s} b_i a_{ij} a_{jk} - 3 \sum_{ijk=1}^{s} b_i a_{ij} a_{ik} = 0, \tag{7.5}$$

$$12 \sum_{ijkl=1}^{s} b_i a_{ij} a_{jk} a_{jl} - 4 \sum_{ijkl=1}^{s} b_i a_{ij} a_{ik} a_{il} = 0. \tag{7.6}$$

It may be observed that in (7.5) we find the elemetary weights associated with (7.2) *and* (7.3), while in (7.6) we find the elementary weights arising from both rooted trees in the nonsuperfluous tree with four vertices $\tau_{4,2}$. This alternative form of the order conditions is called *homogeneous*. Full details concerning the systematic writing of the homogeneous order conditions and a proof of the equivalence between the homogeneous and standard forms can be found in Sanz-Serna and Abia (1991).

Homogeneous forms for PRK and RKN methods exist and can be seen in Abia and Sanz-Serna (1990) and Calvo (1991) respectively.

8. Runge–Kutta and related methods: available symplectic methods

8.1. *Runge–Kutta methods*

We start by noticing that, for methods satisfying the symplecticness condition (6.4), it may be assumed that all the weights b_i are not equal to 0. In fact, if $b_j = 0$, then (6.4) implies that $b_i a_{ij} = 0$ for all i and therefore neither does the jth stage, which does not contribute to the final quadrature (6.3), contribute to any other stage with nontrivial b_i: thus the method is equivalent to a method with fewer stages. Under the assumption of nonzero weights, (6.4) with $i = j$ reveals that a symplectic Runge–Kutta method *cannot be explicit*.

A second observation is that the left-hand side of (6.4) provides the entries of the M matrix that features in the definition of algebraic stability introduced by Burrage and Butcher (1979) and Crouzeix (1979) (see also Dekker and Verwer (1984)). The condition $M = 0$ was investigated by Cooper (1987) in a different context. It is well known that the Gauss–Legendre

methods satisfy this condition (see e.g. Dekker and Verwer 1984, Theorem 4.6) and hence we have the following result (cf. Sanz-Serna, 1988).

Theorem 8.1 The Gauss–Legendre Runge–Kutta methods are symplectic.

We recall that with s stages the Gauss–Legendre method is the unique RK method that achieves order $2s$. It is also A- and B-stable. There is a price to be paid: the high computational cost deriving from implicitness. The efficient implementation of the Gauss–Legendre methods for Hamiltonian problems is an area where much work is needed. Current strategies for choosing the iterative method and initial guess for the solution of the nonlinear algebraic equations in RK processes are based on the assumption that the underlying system is stiff. This is reasonable: stiffness has been until now the main motivation for switching from explicit to implicit methods. However the problems with which we are concerned are not necessarily stiff and fresh ideas are required when dealing with the implementation. For references on the implementation of implicit RK methods see the references in Cooper and Vignesvaran (1990).

The two-stage, order 4 method has been successfully tested by Pullin and Saffman (1991) in a difficult Hamiltonian problem arising in fluid mechanics.

Of course, when the system being integrated is linear, the Gauss–Legendre methods generate diagonal Padé approximants to the exponential. The symplecticness of these rational approximants was shown by Feng (1986a), see also Feng *et al.* (1990).

A way of bringing down the implementation costs associated with implicitness is to resort to *diagonally implicit* methods. These satisfy (6.4) if and only if they have the tableau

$$\begin{array}{c|ccccc} b_1/2 & 0 & 0 & \cdots & 0 \\ b_1 & b_2/2 & 0 & \cdots & 0 \\ b_1 & b_2 & b_3/2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_1 & b_2 & b_3 & \cdots & b_s/2 \\ \hline b_1 & b_2 & b_3 & \cdots & b_s. \end{array} \tag{8.1}$$

A step of length h with the method (8.1) is just a concatenation of an implicit midpoint step of length $b_1 h$, an implicit midpoint step of length $b_2 h$, etc. Hence diagonally implicit symplectic methods are as easy to implement as the implicit midpoint rule. This sort of method is appealing when the number of degrees of freedom d is high, as would be the case if the system being integrated in time was the result of the space discretization of a partial differential equation.

Sanz-Serna and Abia (1991) show that the self-adjoint three-stage method (8.1) with

$$b_1 = b_3 = \frac{1+\omega+\omega^{-1}}{3}, \quad \omega = 2^{1/3}, \quad b_2 = 1 - 2b_1$$

has order 4. This method has been applied to the time-integration of some partial differential equations by de Frutos and Sanz-Serna (1991). If $\psi_{h,H}^{[\mathrm{MP}]}$ represents the midpoint rule, the fourth-order method is given by

$$\psi_{h,H}^{[4]} = \psi_{b_1 h,H}^{[\mathrm{MP}]}\, \psi_{(b_2 h,H}^{[\mathrm{MP}]}\, \psi_{b_1 h,H}^{[\mathrm{MP}]}.$$

Following ideas in Yoshida (1990), this construction can be taken further. Consider the method

$$\psi_{\alpha h,H}^{[4]} \psi_{\beta h,H}^{[4]} \psi_{\alpha h,H}^{[4]}, \tag{8.2}$$

with α and β chosen in such a way that $2\alpha + \beta = 1$ (consistency) and $2\alpha^5 + \beta^5 = 0$ (the leading h^5 term in the truncation error of the composition vanishes). Then (8.2) has order ≥ 5, but being self-adjoint the order must actually be ≥ 6. In turn, a sixth-order self-adjoint method can be composed to give rise to an eighth-order method etc. The conclusion is that there are diagonally implicit symplectic RK methods of arbitrarily high order. Of course it is an open question to decide whether high order methods constructed in this way have some *practical* interest.

Diagonally implicit methods are not the only 'easily implementable' implicit RK methods. It is well known that, following Butcher (1976), the RK methods with a matrix $A = (a_{ij})$ can be subjected to a transformation $A \mapsto T^{-1}AT$ with a view to simplifying the linear algebra. For symplectic methods this idea has been explored by Iserles (1990b) (see also Iserles and Nørsett, 1991, Section 3.7).

8.2. *Partitioned Runge–Kutta methods*

Unlike the class of RK methods, the class of PRK methods includes formulae that are both explicit and symplectic. However it should be emphasized that these properties only hold when dealing with separable Hamiltonians (2.2). In fact the methods of the form

$$\begin{array}{c|ccccc} b_1 & 0 & 0 & \cdots & 0 \\ b_1 & b_2 & 0 & \cdots & 0 \\ b_1 & b_2 & b_3 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b_1 & b_2 & b_3 & \cdots & b_s \\ \hline b_1 & b_2 & b_3 & \cdots & b_s \end{array} \qquad \begin{array}{c|ccccc} 0 & 0 & 0 & \cdots & 0 \\ B_1 & 0 & 0 & \cdots & 0 \\ B_1 & B_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_1 & B_2 & B_3 & \cdots & 0 \\ \hline B_1 & B_2 & B_3 & \cdots & B_s \end{array} \tag{8.3}$$

are explicit, symplectic and have the further favourable property that they can be implemented while only storing two d-dimensional vectors: $\mathbf{Q}_1$ is nothing but $\mathbf{q}^n$, $\mathbf{P}_1$ can be overwritten on $\mathbf{q}^n$, $\mathbf{Q}_2$ can be overwritten on $\mathbf{Q}_1$, etc.

The family of methods (8.3) was introduced by Ruth (1983) in one of the very first papers on symplectic integration. Ruth constructed methods with $s = r = 1, 2, 3$. In the case $s = r = 3$, there is a one-parameter family of methods and Ruth has chosen the parameter so as to obtain simple coefficients b_i, B_i. Sanz-Serna (1989) suggested a different choice for the parameter. Furthermore by composing the third-order, three-stage method $\psi_{h,H}$ with its adjoint $\widehat{\psi}_{h,H}$, he constructed an explicit symplectic method $\widehat{\psi}_{h/2,H}\psi_{h/2,H}$ that requires five evaluations per step, but produces fourth-order results both at the grid points $t_n = nh$ and at the points $t_{(n+1/2)} = (n+1/2)h$. A method with $s = r = 4$ has been constructed by Neri (1987), Forest and Ruth (1990) and Candy and Rozmus (1991). Yoshida (1990), by using a construction similar to that discussed earlier for diagonally implicit RK methods, has proved that there are methods of the form (8.3) possessing arbitrarily high orders. He furthermore derives sixth-order methods that use seven function evaluations per step and eighth-order methods requiring sixteen function evaluations per step.

8.3. *Runge–Kutta–Nyström methods*

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

$$\begin{array}{c|cccc} \gamma_1 & 0 & 0 & \cdots & 0 \\ \gamma_2 & b_1(\gamma_2-\gamma_1) & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \gamma_s & b_1(\gamma_s-\gamma_1) & b_2(\gamma_s-\gamma_2) & \cdots & 0 \\ \hline & b_1(1-\gamma_1) & b_2(1-\gamma_2) & \cdots & b_s(1-\gamma_s) \\ \hline & b_1 & b_2 & \cdots & b_s \end{array} \tag{8.4}$$

and hence with s stages provide $2s$ free parameters. Okunbor and Skeel (1991) have pointed out that, for implementation purposes, (8.4) can be rewritten as an explicit PRK method, and hence only requires the storage of two d-dimensional vectors. Okunbor and Skeel (1990) prove that an explicit RKN method is symplectic if and only if its adjoint method is also explicit. This idea can be used to compose a method with its adjoint as shown earlier for the PRK case. Calvo and Sanz-Serna (1991b) have considered the family of fourth-order, five-stage methods of the form (8.4) that effectively require four function evaluations per step due to the fact that the last evaluation in the current step provides the first evaluation in the next step. An optimal method within this class has been obtained by minimizing the error constants. Similar work is under way for higher order methods.

Given a number of stages s and an order r, the tableaux (8.4) and (8.3) have the same number $2s$ of free parameters, while Table 1 makes it clear that the number of order conditions for the RKN case is substantially smaller than the number of order conditions for PRK methods. This is due to the fact that in the PRK case we are catering for all separable Hamiltonians (2.2) where RKN methods can only cope with the special case (2.3). However case (2.3) is very common in the applications and this should make the construction of explicit symplectic RKN methods an important practical issue.

9. Generating functions

We cannot make any further progress with the topic of symplectic integrators without first reviewing some basic facts about the generating functions of a symplectic transformation.

It is a remarkable feature of Hamiltonian problems that each system of the form (2.1) is fully determined by the choice of a *scalar* function H, whereas a general system $\mathbf{dy}/\mathrm{d}t = \mathbf{f}(\mathbf{y})$ is determined by a *vector field* $\mathbf{f}$. In a similar vein, a symplectic transformation $(\mathbf{p}^*, \mathbf{q}^*) = \psi(\mathbf{p}, \mathbf{q})$ can be expressed in terms of a single real-valued function S, rather than in terms of the $2d$ components of ψ. The function S is called the *generating function* of ψ.

9.1. *Generating functions of the first kind*

Let $(\mathbf{p}^*, \mathbf{q}^*) = \psi(\mathbf{p}, \mathbf{q})$ be a symplectic transformation defined in a simply connected domain Ω. For each closed path γ in Ω

$$\int_\gamma \mathbf{p}\,\mathrm{d}\mathbf{q} - \int_\gamma \mathbf{p}^*\,\mathrm{d}\mathbf{q}^* = 0, \tag{9.1}$$

where $\mathbf{p}\,\mathrm{d}\mathbf{q}$ is the differential form $p_1\,\mathrm{d}q_1 + \cdots + p_d\,\mathrm{d}q_d$, etc. In fact, by Stokes theorem, the first integral is the quantity $m(\Sigma)$, where m is the sum of two-dimensional areas considered in Section 4 and Σ is any two-dimensional surface bounded by γ. The second integral is $m(\psi(\Sigma))$ and hence (9.1) is just a way of saying that ψ is symplectic. The key observation is that (9.1) is the condition for $\mathbf{p}\,\mathrm{d}\mathbf{q} - \mathbf{p}^*\,\mathrm{d}\mathbf{q}^*$ to be the differential of a function S defined in Ω:

$$\mathrm{d}S = \mathbf{p}\,\mathrm{d}\mathbf{q} - \mathbf{p}^*\,\mathrm{d}\mathbf{q}^*. \tag{9.2}$$

Now let us further assume that $\mathbf{q}$ and $\mathbf{q}^*$ are *independent* functions in Ω, i.e. each point in Ω may be uniquely specified by the corresponding values of $\mathbf{q}$ and $\mathbf{q}^*$. Then we can express $S(\mathbf{p}, \mathbf{q})$ in (9.2) as a function S^1 of $\mathbf{q}$ and

$\mathbf{q}^*$. It is evident from (9.2) that

$$\mathbf{p} = \frac{\partial S^1}{\partial \mathbf{q}}, \qquad \mathbf{p}^* = -\frac{\partial S^1}{\partial \mathbf{q}^*}. \tag{9.3}$$

These formulae implicitly define ψ by providing $2d$ relationships among the $4d$ components of $\mathbf{q}$, $\mathbf{p}$, $\mathbf{p}^*$, $\mathbf{q}^*$. The function $S^1(\mathbf{q}, \mathbf{q}^*)$ is called the generating function (of the first kind) of ψ. The reader may wish to check that for the rotation in (2.6)

$$S^1(q, q^*) = \frac{\cot t}{2}\left(q^2 + q^{*2}\right) - \underset{t}{\operatorname{cosec}}\, qq^*. \tag{9.4}$$

Conversely, if we choose any smooth function $S^1(\mathbf{q}, \mathbf{q}^*)$ satisfying the condition that the Hessian determinant $\det \partial^2 S^1/\partial \mathbf{q} \partial \mathbf{q}^*$ does not vanish at a point $(\mathbf{q}_0, \mathbf{q}_0^*)$, then the formulae (9.3) implicitly define, in the neighbourhood of $(\mathbf{q}_0, \mathbf{q}_0^*)$, a *symplectic* transformation (see e.g. Arnold (1989, Section 47A)).

9.2. *Generating functions of the third kind*

For a symplectic transformation ψ to have a generating function of the first kind, it is clearly necessary that $\mathbf{q}$ and $\mathbf{q}^*$ are *independent*, a condition not fulfilled by the identity transformation. (Note that (9.4) has a singularity at $t = 0$, where the rotation (2.6) is just the identity.) Since we are interested in generating consistent numerical methods $\psi_{h,H}$, which, at $h = 0$, give the identity transformation, generating functions of the first kind are not really what we want.

Let us proceed as follows. Note that from (9.2)

$$\mathrm{d}(\mathbf{p}^T\mathbf{q} - S) = \mathbf{q}\,\mathrm{d}\mathbf{p} + \mathbf{p}^*\,\mathrm{d}\mathbf{q}^* \tag{9.5}$$

and now assume that $\mathbf{p}$ and $\mathbf{q}^*$ are *independent* functions (which they are for the identity transformation). Then we can express the function in brackets in (9.5) in terms of the independent variables $\mathbf{p}$ and $\mathbf{q}^*$. The result $S^3(\mathbf{p}, \mathbf{q}^*)$ is called the generating function of the third kind of ψ and, from (9.5) we conclude that the formulae that now implicitly define ψ when S^3 is known are

$$\mathbf{p}^* = \frac{\partial S^3}{\partial \mathbf{q}^*}, \qquad \mathbf{q} = \frac{\partial S^3}{\partial \mathbf{p}}. \tag{9.6}$$

The generating function of the identity is $\mathbf{p}^T\mathbf{q}^*$. For the rotation (2.6) we find

$$S^3(p, q^*) = -\frac{\tan t}{2}\left(p^2 + q^{*2}\right) + \underset{t}{\sec}\, pq^*;$$

this is regular near $t = 0$, but breaks down when t approaches $\pm 2\pi$: at these values $p = q^*$ and p and q^* cannot be taken as independent coordinates.

Conversely given a function $S^3(\mathbf{p}, \mathbf{q}^*)$ with a locally nonvanishing Hessian $\det \partial^2 S^3/\partial \mathbf{p} \partial \mathbf{q}^*$, the formulae (9.6) locally define a symplectic transformation.

9.3. *Generating functions of all kinds*

Some classical books on Hamiltonian mechanics considered four kinds of generating functions. Arnold (1989) has 2^n kinds. And in fact there are many more. According to Feng (1986a), Feng and Qin (1987), Feng *et al.* (1989), Wu (1988) the general idea is as follows. Collect in a ($2d$-dimensional) vector $\mathbf{y}$ the components of $(\mathbf{p}, \mathbf{q})$ and in a vector $\mathbf{y}^*$ the components of $(\mathbf{p}^*, \mathbf{q}^*)$. Introduce new $2d$-dimensional variables $\mathbf{w}$ and $\mathbf{w}^*$, such that $\mathbf{w}$ and $\mathbf{w}^*$ are linear functions of $\mathbf{y}$ and $\mathbf{y}^*$ (i.e. $\mathbf{w} = A\mathbf{y} + B\mathbf{y}^*$ and $\mathbf{w} = C\mathbf{y} + D\mathbf{y}^*$ for fixed $2d \times 2d$ matrices A, B, C, D). Under suitable hypotheses, the symplectic transformation $(\mathbf{p}^*, \mathbf{q}^*) = \psi(\mathbf{p}, \mathbf{q})$ reads, in terms of $\mathbf{w}$ and $\mathbf{w}^*$, $\mathbf{w}^* = \chi(\mathbf{w})$, where χ is the gradient of a scalar generating function σ. In the case of the generating functions of the first kind, A is the matrix that extracts the $\mathbf{q}$ variables of $\mathbf{y}$, B is the matrix that extracts the $\mathbf{q}^*$ variables of $\mathbf{y}^*$ etc.

A useful generating function is the so-called *Poincaré* generating function. Here $\mathbf{w}$ is taken to be the average of $\mathbf{y}$ and $\mathbf{y}^*$. The formulae for the transformation are (cf. MacKay, 1991)

$$\mathbf{p}^* = \mathbf{p} - \partial_2 S^P\left(\frac{\mathbf{p}^* + \mathbf{p}}{2}, \frac{\mathbf{q}^* + \mathbf{q}}{2}\right), \qquad \mathbf{q}^* = \mathbf{q} + \partial_1 S^P\left(\frac{\mathbf{p}^* + \mathbf{p}}{2}, \frac{\mathbf{q}^* + \mathbf{q}}{2}\right),$$

where ∂_1 and ∂_2 respectively represent differentiation with respect to the first and second groups of arguments in S^P. The Poincaré generating function of the identity is the 0 function.

9.4. *Hamilton–Jacobi equations*

Let us now complicate things and consider symplectic transformations ψ_t that depend on t. We assume that ψ_t has a generating function of the third kind S^3, which depends on t. Let us further consider a Hamiltonian system (2.1) in the variables $\mathbf{p}$, $\mathbf{q}$. If we change variables in this system we obtain a new differential system for the new unknowns $\mathbf{p}^*$, $\mathbf{q}^*$. Then the following holds true (Arnold, 1989, Section 45A).

Theorem 9.1 In the situation earlier, the transformed system is also a Hamiltonian system, with the nonautonomous Hamiltonian function

$$H^*(\mathbf{p}^*, \mathbf{q}^*; t) = H - \frac{\partial S^3}{\partial t}. \tag{9.7}$$

In (9.7) it is understood that once S^3 has been differentiated with respect to t with $\mathbf{p}$ and $\mathbf{q}^*$ constant, the formulae (9.6) that define the transformation

are used to express the right-hand side in terms of the new variables $\mathbf{p}^*$ and $\mathbf{q}^*$.

A first corollary of this result refers to the case where the transformation is actually independent of t: then in the new variables the Hamiltonian system is still an autonomous Hamiltonian system and the new Hamiltonian is obtained by changing variables in the old Hamiltonian.

Another remarkable application arises when ψ_t is the t-flow of (2.1) and we see the old variables evolving under the Hamiltonian system with Hamiltonian $-H(\mathbf{p},\mathbf{q})$, i.e. under the flow $\phi_{t,-H} = \phi_{t,H}^{-1}$. Then, the symplectic transformation ψ_t just undoes what the Hamiltonian evolution under $-H$ does; in the new variables, the solutions of the differential equations are $\mathbf{p}^* = \textit{constant}$ and $\mathbf{q}^* = \textit{constant}$ and the new Hamiltonian $H^* = -H - \partial S^3/\partial t$ must be 0 (or a constant: Hamiltonians are only defined up to an additive constant). We have proved that the generating function S^3 of the flow of the Hamiltonian system with Hamiltonian H satisfies

$$\frac{\partial S^3}{\partial t}(\mathbf{p},\mathbf{q}^*;t) + H(\mathbf{p},\mathbf{q}) = 0. \tag{9.8}$$

This is the celebrated *Hamilton–Jacobi* equation. Upon replacing $\mathbf{q}$ by $\partial S^3/\partial \mathbf{p}$ (cf. (9.6)), the relationship (9.8) is a partial differential equation of the first order for a function S^3 of the variables $\mathbf{p}$ and t (the $\mathbf{q}^*$ act just as parameters). If this equation can be solved explicitly, we find the generating function of the flow and hence the solution of the system (2.1). This is Jacobi's approach to the solution of Hamilton's equation. Jacobi and others used this technique explicitly to integrate problems of mechanics that had proved intractable by other techniques (see e.g. Arnold (1989, Section 47)). On the other hand, if we want to solve (9.8) by the method of characteristics, we find that the system of ordinary differential equations that defines the characteristics is none other than system (2.1)! The equivalence between the solution of a Hamiltonian ordinary differential system and the solution of a first-order partial differential equation with Hamilton–Jacobi structure is thus complete.

These ideas are not confined to generating functions of the third kind; they do work for all kinds of generating functions. The details of the construction of the new Hamiltonian H^* (and hence the form of the Hamilton–Jacobi equation) vary with the kind of generating function being used. The interested reader is referred to Feng (1986a), Feng and Qin (1987), Feng *et al.* (1989) and Wu (1988).

10. Symplectic integrators based on generating functions

Theorem 9.1 is the key to the construction of symplectic integrators via Hamiltonian functions (Channell, 1983; Menyuk, 1984; Feng, 1986a; Feng and Qin, 1987; Wu, 1988; Feng *et al.*, 1989; Channell and Scovel, 1990; Miesbach and Pesch, 1990). Let $\psi_{t,H}$ be a symplectic numerical method consistent of order r with generating function S^3. An argument similar to that leading to the Hamilton–Jacobi equation, proves that $H^* = -H - \partial S^3/\partial t$ is $\mathcal{O}(t^r)$ as $t \to 0$; now the transformation $\psi_{t,H}$ undoes the effect of the evolution $\phi_{t,-H}$ except for terms of order $\mathcal{O}(t^r)$. Conversely, any function S^3 that makes $H^* = \mathcal{O}(t^r)$ generates a symplectic, rth-order numerical method, see Sanz-Serna and Abia (1991, Theorem 6.1).

Feng and his coworkers take the following approach (Feng, 1986a; Feng and Qin, 1987; Feng *et al.*, 1989; Wu, 1988). They begin by expanding S^3 in (9.8) in powers of t. On substituting this power series in (9.8), expanding H and collecting similar powers of t, the generating function S^3 can be expressed in terms of derivatives of H. When the series for S^3 is truncated, an approximate solution of the Hamilton–Jacobi equation is obtained, which is then used to generate the numerical method via (9.6).

Of course, similar approaches can be taken for generating functions other than generating functions of the third kind. The use of the Poincaré format is appealing, because it easily leads to self-adjoint schemes, with only odd powers of h in the Taylor expansion of the truncation error. The second-order method derived from the Poincaré generating funtion is none other than the familiar midpoint rule, with generating function $S^P = hH$.

The expression for the fourth-order method turns out to be

$$\begin{aligned} p_i^{n+1} = p_i^n - hH_{q_i} - \frac{h^3}{24}\Big[& H_{p_jp_kq_i}H_{q_j}H_{q_k} + 2H_{p_jp_k}H_{q_jq_i}H_{q_k} \\ & - 2H_{p_jq_kq_i}H_{p_j}H_{q_k} - 2H_{p_jq_k}H_{p_jq_i}H_{q_k} - 2H_{p_jq_k}H_{p_j}H_{q_kq_i} \\ & + 2H_{q_jq_k}H_{p_jq_i}H_{p_k} + H_{q_jq_kq_i}H_{p_j}H_{p_k}\Big], \\ q_i^{n+1} = q_i^n + hH_{p_i} + \frac{h^3}{24}\Big[& H_{p_jp_kp_i}H_{q_j}H_{q_k} + 2H_{p_jp_k}H_{q_jp_i}H_{q_k} \\ & - 2H_{p_jq_kp_i}H_{p_j}H_{q_k} - 2H_{p_jq_k}H_{p_jp_i}H_{q_k} - 2H_{p_jq_k}H_{p_j}H_{q_kp_i} \\ & + 2H_{q_jq_k}H_{p_jp_i}H_{p_k} + H_{q_jq_kp_i}H_{p_j}H_{p_k}\Big]. \end{aligned}$$

Here summation in repeated indices must be understood and the functions featuring in the right-hand sides are evaluated at the averages

$$[\tfrac{1}{2}(\mathbf{p}^* + \mathbf{p}), \tfrac{1}{2}(\mathbf{q}^* + \mathbf{q})],$$

so that the scheme is implicit. We have reported these formulae to emphasize the Taylor-series character of Feng's methods. As with any other Taylor-series method, these schemes would only be feasible if applied in conjunction with some automatic procedure for the computation of the higher derivatives.

Miesbach and Pesch (1990) note that, in Runge–Kutta methods for $\mathrm{d}\mathbf{y}/\mathrm{d}t = \mathbf{f}(\mathbf{y})$, one obtains high-order schemes without resorting to higher deriva-

tives of $\mathbf{f}$ by using as increment $\mathbf{y}^{n+1} - \mathbf{y}^n$ a weighted sum $h\sum b_i\mathbf{f}(\mathbf{Y}_i)$. Furthermore, the terms $h\mathbf{f}$ being weighted have the form of the increment in the Euler (i.e. simplest conceivable) method. In a similar vein, Miesbach and Pesch suggest methods where the Poincaré generating function is a weighted sum of terms, each term being the simplest generating function hH (i.e. that corresponding to the implicit midpoint rule) evaluated at some suitable inner stage. The resulting method is Runge–Kutta-like in that no higher derivatives of H are required; however it is not a symplectic Runge–Kutta method like those considered in Section 6.

11. Back to symplectic Runge–Kutta methods: the canonical theory of the order

The symplectic Runge–Kutta methods (6.1), (6.4) define a symplectic transformation which as $h \to 0$ approaches the identity. Hence they must have an S^3 generating function. Lasagni (1990) has found the corresponding expression

$$S^3(\mathbf{p}_n, \mathbf{q}_{n+1}; h) = \mathbf{p}_n^T\mathbf{q}_{n+1} - h\sum_i b_i H(\mathbf{P}_i, \mathbf{Q}_i) - h^2\sum_{ij} b_i a_{ij} H_{\mathbf{p}}(\mathbf{P}_i, \mathbf{Q}_i) H_{\mathbf{q}}(\mathbf{P}_j, \mathbf{Q}_j)^T.$$

Here $H_{\mathbf{p}}$ and H are row vectors of partial derivatives and the stages should be interpreted as functions of $\mathbf{p}_n$, $\mathbf{q}_{n+1}$ and h implicitly defined in (6.2), (6.3). (Actually, in Section 9 we showed that a generating function would exist if the domain Ω were simply connected. Lasagni's recipe for S^3 works for all domains. Symplectic RK have generating functions regardless of the geometry of Ω and therefore, in symplectic geometry jargon, they give rise to *exact symplectic* transformations, i.e. transformations for which (9.1) holds. Actually, the flow of a Hamiltonian system is also an exact symplectic transformation.)

In a manner similar to that used for symplectic PRK, Abia and Sanz-Serna (1990) find the generating function

$$S^3(\mathbf{p}_n, \mathbf{q}_{n+1}; h) = \mathbf{p}_n^T\mathbf{q}_{n+1} - h\sum_i b_i V(\mathbf{Q}_i) - h\sum_i B_i T(\mathbf{P}_i) + h^2\sum_{ij} B_i a_{ij}\mathbf{g}(\mathbf{P}_i)^T\mathbf{f}(\mathbf{Q}_j),$$

and for symplectic RKN schemes the generating function is given by (Calvo and Sanz-Serna, 1991a)

$$S^3(\mathbf{p}_n, \mathbf{q}_{n+1}; h) = \mathbf{p}_n^T\mathbf{q}_{n+1} - h\sum_i b_i V(\mathbf{Q}_i) - \frac{h}{2}\mathbf{p}_n^T\mathbf{p}_n + \frac{h^3}{2}\sum_{ij} b_i(\beta_j - \alpha_{ij})\,\mathbf{f}(\mathbf{Q}_i)^T\mathbf{f}(\mathbf{Q}_j).$$

We emphasize that, unlike the situation with the methods considered in Section 10, these generating functions are not needed to derive or to implement the RK and related methods introduced in Section 6. However explicit knowledge of the generating function can be put to good use. In fact we can study the order of consistency by simply substituting the expression for S^3 with $h = t$ in $H + \partial S^3/\partial t$: an $\mathcal{O}(t^r)$ behaviour is, as we know, equivalent to order r. This is the methodology suggested by Sanz-Serna and Abia (1991). For the case of RK methods these authors give systematic rules, based on graph theory, to write the Taylor expansion of $H + \partial S^3/\partial t$ in powers of t. It turns out that the graphs to be used are *nonsuperfluous trees*: at the t^ρ level, $\rho > 1$, the Taylor expansion contains a term for each nonsuperfluous tree with ρ nodes. Hence the number of order conditions is the number of nonsuperfluous trees. Furthermore the coefficients that must be annihilated to impose $H + \partial S^3/\partial t = \mathcal{O}(t^r)$ are just the right-hand sides of the homogeneous order conditions we described at the end of Section 7, see e.g. (7.5)–(7.6). Thus the use of the Hamilton–Jacobi equation gives a very clear meaning to the results presented in Section 7.

12. Properties of symplectic integrators: backward error interpretation

Now that we have introduced the families of symplectic integrators available in the literature, it is time to investigate the general properties of symplectic integrators. The *a priori* motivation for resorting to symplectic methods was presented in Section 5: by making the integrator symplectic we reproduce an important property of the true flow. However there is a big gap in numerical analysis between a reasonably motivated method and a method that works well. It is therefore essential that theoretical analysis and numerical experiments are presented that show the advantages, if any, of symplectic integrators.

In our opinion, to the numerical analyst, the most appealing feature of symplectic integration is the possibility of *backward error interpretation*. This idea is very similar to the *method of modified equations*, see Warming and Hyett (1974) and, for a more rigorous treatment, Griffiths and Sanz-Serna (1986). Let us begin with an example. Consider the Hamiltonian $H = \frac{1}{2}p^2 + V(q)$, leading to the system

$$\mathrm{d}p/\mathrm{d}t = f(q), \qquad \mathrm{d}q/\mathrm{d}t = p, \tag{12.1}$$

where $f = -V'$. We assume that $f(0) = 0$ and $f'(0) < 0$; the first hypothesis implies that the origin is an equilibrium of (12.1), the second implies that this equilibrium is a stable centre (the origin is a minimum of the potential energy V). The system (12.1) is integrated by the following first-order, symplectic PRK method

$$p^{n-1} = p^n + hf(q^{n+1}), \qquad q^{n+1} = q^n + hp^n. \tag{12.2}$$

In order to describe the behaviour of the points (p^n, q^n) computed by (12.2), we could just say that they approximately behave like the solutions $(p(t_n), q(t_n))$ of (12.1). This would not be a very precise description, even for h small, because $\phi_{h,H}$ and $\psi_{h,H}$ differ in $\mathcal{O}(h^2)$ terms (first order of consistency). Can we find *another* differential system $\mathcal{S}_2$ so that (12.2) is consistent with the *second* order with $\mathcal{S}_2$? The points (p^n, q^n) would then be closer to the solutions of $\mathcal{S}_2$ than to the solutions of the system we want to integrate. To find the *modified* system $\mathcal{S}_2$ use an ansatz

$$\mathrm{d}p/\mathrm{d}t = f(q) + hF_1(p,q), \qquad \mathrm{d}q/\mathrm{d}t = p + hG_1(p,q)$$

(note that h features here as a parameter so that $\mathcal{S}_2 = \mathcal{S}_2(h)$), substitute the solutions of the modified system in the difference equations and ask for an $\mathcal{O}(h^3)$ residual. This leads to

$$\frac{\mathrm{d}p}{\mathrm{d}t} = f(q) + \frac{h}{2}pf'(q), \qquad \frac{\mathrm{d}q}{\mathrm{d}t} = p - \frac{h}{2}f(q), \tag{12.3}$$

a Hamiltonian system, with Hamiltonian

$$H_2(h) = \tfrac{1}{2}p^2 + V(q) - (h/2)pf(q).$$

If we are not satisfied with $\mathcal{S}_2(h)$, we can find a differential system $\mathcal{S}_3(h)$ for which (12.2) is consistent with the third order. Again $\mathcal{S}_3(h)$ turns out to be a Hamiltonian problem; the expression for the Hamiltonian is

$$H_3(h) = (1/2)p^2 + V(q) - (h/2)pf(q) + (h^2/12)[f(q)^2 - p^2 f'(q)].$$

There is no limit: for any positive integer ρ a Hamiltonian system $\mathcal{S}_{H_\rho}(h)$ can be found such that the method $\psi_{h,H}$ differs from the flow $\phi_{h,H_\rho(h)}$ in $\mathcal{O}(h^{\rho+1})$ terms (see e.g. MacKay (1991)). By going from local to global errors, in any bounded time interval, the computed points are $\mathcal{O}(h^\rho)$ away from the solution of $\mathcal{S}_{H_\rho}(h)$.

What is the situation when using a nonsymplectic method? Take the standard forward Euler method as an illustration. Again a modified system $\mathcal{S}_2(h)$ can be found for which consistency is of the second order. This now reads

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \left[f(q) + \frac{h}{2}pf'(q)\right] - hpf'(q), \qquad \frac{\mathrm{d}q}{\mathrm{d}t} = \left[p - \frac{h}{2}f(q)\right];$$

the terms in brackets replicate the Hamiltonian system (12.3), but there is an extra term $-hf'(q)p$. Since $f'(0) < 0$ this extra term introduces negative dissipation near the origin: in any bounded time interval, the computed points are $\mathcal{O}(h)$ away from the solutions of the Hamiltonian system we want to solve, but $\mathcal{O}(h^2)$ away from the solutions of a system where the Hamiltonian character has been lost and the origin is an unstable focus.

Even though these considerations have been presented by means of an example, they hold for all symplectic methods: provided that the system

(2.1) is smooth enough, for arbitrarily high ρ, a modified Hamiltonian system $\mathcal{S}_{H_\rho(h)}$ can be found such that the method $\psi_{h,H}$ differs from the flow $\phi_{h,H_\rho(h)}$ in $\mathcal{O}(h^{\rho+1})$ terms. The difference between the true Hamiltonian H and the modified Hamiltonian $H_\rho(h)$ is $\mathcal{O}(h^r)$, with r the order of the method.

As shown in this example, the functions $H_\rho(h)$, $\rho = 2, 3, \ldots$, are truncations of a power series in h. If this power series converges, its sum $H_\infty(h)$ gives rise to a modified Hamiltonian problem *that is integrated exactly by the symplectic numerical method*: $\psi_{h,H} \equiv \phi_{h,H_\infty(h)}$. In the previous example with $V(q) = \frac{1}{2}q^2$ (i.e. the harmonic oscillator (2.5)) this modified Hamiltonian problem is given by Beyn (1991, p. 221)

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} p \\ q \end{bmatrix} = \left(h^{-1}\log\begin{bmatrix} 1-h^2 & -h \\ h & 1 \end{bmatrix}\right)\begin{bmatrix} p \\ q \end{bmatrix}; \tag{12.4}$$

when solving this system analytically the matrix in brackets is exponentiated and the equations (12.2) of the numerical method are recovered.

In general, for nonlinear problems, the series does not converge: the computed points are not quite an exact solution of a differential problem (Sanz-Serna, 1991a, p. 168). However if H is very smooth, it can be shown (Neishtadt, 1984; cf. Lasagni, 1990; MacKay, 1991) that a Hamiltonian $H_\infty(h)$ can be constructed for which the corresponding h-flow differs from $\psi_{h,H}$ in terms that tend to 0 exponentially fast as $h \to 0$.

In any case the conclusion is the same: for a symplectic integrator applied to (2.1) modified Hamiltonian problems exist so that the computed points lie either exactly or 'very approximately' on the exact trajectories of the modified problem. This makes a backward error interpretation of the numerical results possible (cf. Sanz-Serna (1990)): the computed solutions are solving exactly (or 'very approximately') a nearby Hamiltonian problem. In a modelling situation where the exact form of the Hamiltonian H may be in doubt, or some coefficients in H may be the result of experimental measurements, the fact that integrating the model numerically introduces perturbations to H comparable with the uncertainty in H inherent in the model is the most one can hope for.

On the other hand, when a nonsymplectic formula is used the modified system is not Hamiltonian: the process of numerical integration perturbs the model in such a way as to take it out of the Hamiltonian class. The acceptability of such nonHamiltonian perturbations is a question that should be decided in each individual modelling problem.

12.1. An alternative approach

If

$$(\mathbf{p}, \mathbf{q}) = \psi_{h,H}(\mathbf{p}^0, \mathbf{q}^0) \tag{12.5}$$

is a numerical method, it is a simple matter to find a differential equation satisfied by the functions $(\mathbf{p}(h), \mathbf{q}(h))$: we differentiate (12.5) with respect to h and eliminate $(\mathbf{p}^0, \mathbf{q}^0)$ in the result by using (12.5).

For the symplectic method (12.2) this procedure yields the system

$$\frac{\mathrm{d}p}{\mathrm{d}h} = f(q) + hpf'(q) - h^2 f(q)f'(q), \qquad \frac{\mathrm{d}q}{\mathrm{d}h} = p - hf(q),$$

which (this should not be surprising by now) is a Hamiltonian system, with Hamiltonian $\tilde{H}(p,q;h) = \frac{1}{2}(p - hf(q))^2 + V(q)$. Since h is our 'time', the system is nonautonomous. Moving from $t = 0$ to $t = h$ with the method (12.2) is moving from $t = 0$ to $t = h$ with a nonautonomous system with Hamiltonian $\tilde{H}$. The fact that H and $\tilde{H}$ differ in $\mathcal{O}(h)$ terms is a reflection of the first-order accuracy of the method.

What is unsatisfactory with this approach is that taking two steps $0 \rightarrow h \rightarrow 2h$ with the numerical method is *not* going from $t = 0$ to $t = 2h$ with $S_{\tilde{H}}$: given an initial condition, to move from 0 to $2h$ in a nonautonomous differential system is not quite the same as advancing the initial condition to $t = h$ and then using the result as new initial condition for another $0 \rightarrow h$ forward shift. There is a way around this problem: for $0 \le t < h$ we keep the Hamiltonian $\tilde{H}(p,q;t)$ found earlier and for $h \le t < 2h$, $2h \le t < 3h$, ..., we repeat it periodically. The good news is that now the nonautonomous system is such that the transformation that moves the initial condition from $t = 0$ to $t = nh$ is the nth power of the transformation that advances the initial condition from $t = 0$ to $t = h$. Hence, the numerically computed points exactly lie on solutions of this nonautonomous system. The bad news is that the new Hamiltonian is not only nonautonomous, but also discontinuous as a function of t. Such a lack of smoothness is not very welcome.

The canonical formalism of generating functions provides a very clever way of finding $\tilde{H}$ without having to differentiate $\psi_{h,H}$. The initial conditions $(\mathbf{p}^0, \mathbf{q}^0)$ do not vary with t: we could see them as solutions of the 0 Hamiltonian. By using Theorem 9.1, the functions $(\mathbf{p}(h), \mathbf{q}(h))$ then evolve with the Hamiltonian $\tilde{H} = -\partial S^3/\partial h$. In the example, the generating function is $S^3 = p^0 q - (h/2)(p^0)^2 - hV(q)$ (now p and q play the role played by p^* and q^* in Section 9, while p^0 and q^0 play now the role of 'old' variables). Differentiation with respect to h in S^3 leads to $\tilde{H} = \frac{1}{2}(p^0)^2 + V(q)$; in view of (12.2) this equals $\frac{1}{2}(p - hf(q))^2 + V(q)$, the same expression we found before.

McLachlan and Atela (1991) use the discrepancy between H and $\tilde{H}$ as a measure of the accuracy of the method $\psi_{h,H}$. Since such a discrepancy equals $H + \partial S^3/\partial h$ this is just using the Hamilton–Jacobi methodology introduced by Sanz-Serna and Abia (1991).

13. Properties of symplectic integrators: conservation of energy

For the system (2.1) the Hamiltonian H is a conserved quantity: $H(\mathbf{p}(t),\mathbf{q}(t))$ does not vary with t if $(\mathbf{p}(t), \mathbf{q}(t))$ is a solution of (2.1). In applications in mechanics conservation of H usually corresponds to conservation of total mechanical energy. Do symplectic integrators possess the analogous property that, except for rounding errors, $H(\mathbf{p}^n, \mathbf{q}^n)$ does not vary with n along a numerically computed solution? Sometimes they do: if (2.1) is a *linear* system and the integrator is a symplectic RK method (6.1)–(6.4), then H is conserved along numerical trajectories. In fact in this case H is a quadratic function and symplectic RK methods conserve all quadratic functions that are conserved by the Hamiltonian system being integrated, Sanz-Serna (1988). However if we still assume linearity in the system and we use a PRK or a RKN method, conservation of H no longer holds. This is easily seen in the case of the harmonic oscillator (2.5) integrated by the method (12.2). We have noticed earlier that the computed points exactly lie on trajectories of the modified system (12.4) and hence on the lines $H_\infty(p,q;h) =$ constant in the (p,q) plane. But, for h small, these lines can be seen to be ellipses, while for conservation of energy we wanted the points to be on circles $p^2 + q^2 =$ constant. As $h \rightarrow 0$ the eccentricity of the ellipses decreases and they look more like circles: smaller values of h lead to smaller energy errors, as in the consistent method. Furthermore the fact that the computed points stay exactly on an ellipse near the theoretical circle implies that the error in energy remains bounded even if t gets very large.

The same ideas apply more generally. When problem (2.1) is very smooth but nonlinear, the computed points do not remain exactly on trajectories of the modified problem $S_{H_\infty(h)}$. Nevertheless, the drift of the points away from the modified trajectories is very slow: the numerical scheme has exponentially small local truncation errors when seen as an approximation to the modified system. Therefore $H_\infty(h)$ is conserved by the numerical solutions, except for exponentially small errors, for long $(\mathcal{O}(h^{-1}))$ periods of time. This in turn implies that the errors in $H = H_\infty(h) + \mathcal{O}(h^r)$ possess an $\mathcal{O}(h^r)$ bound on time intervals of length $\mathcal{O}(h^{-1})$ (Lasagni, 1988).

For 'general' Hamiltonians, Ge and Marsden (1988) prove that a symplectic method $\psi_{h,H}$ cannot exactly conserve energy (except for the trivial cases where the function $\psi_{h,H}$ actually coincides with or is a time reparameterization of the true flow $\phi_{h,H}$). Hence conservation of the symplectic structure and conservation of energy are conflicting requirements that, in general, cannot be satisfied simultaneously by a numerical scheme. Since both the Hamiltonian and the symplectic structure are conserved by Hamiltonian systems, the question naturally arises of whether when constructing an integrator we should choose to conserve symplecticness and violate con-

servation of energy or *vice versa*. This is a question that should probably be answered differently for each specific application. However it should be pointed out that, as mentioned in Section 4, symplecticness is a property that fully characterizes Hamiltonian problems, while conservation of an energy-like function is a feature also present in many nonHamiltonian systems. Furthermore conservation of energy restricts the dynamics of the numerical solution by forcing the computed points to be on the correct $(2d-1)$-dimensional manifold H = constant, but otherwise poses no restriction to the dynamics: within the manifold the points are free to move anywhere and only motions orthogonal to the manifold are forbiden. When d is large this is clearly a rather weak restriction. On the other hand, symplecticness restricts the dynamics in a more global way: all directions in phase space are taken into account.

The literature has devoted a great deal of attention to the construction of numerical schemes that exactly conserve H (or more generally, to the construction of integrators for a system $\mathrm{d}\mathbf{y}/\mathrm{d}t = \mathbf{f}(\mathbf{y})$ that exactly conserve one or more invariants of motion). Several ideas have been suggested:

1 stepping from t_n to t_{n+1} with a standard method and then projecting the numerical result onto the correct energy surface;
2 adding the conservation constraints to the differential system to obtain a system of differential-algebraic equations; and
3 constructing *ad hoc* schemes. However conservation of energy is not the theme of this paper and we shall not attempt to review the relevant literature.

14. Properties of symplectic integrators: KAM theory

The Kolmogorov–Arnold–Moser (KAM) theory for Hamiltonian problems explains the behaviour of Hamiltonian systems that are perturbations of so-called integrable Hamiltonian systems (i.e. of Hamiltonian systems that can be explicitly solved in terms of quadratures). This material is covered in the books by Moser (1973), Arnold (1988, 1989) and MacKay and Meiss (1987). The theory also caters for the case of symplectic mappings that are perturbations of integrable symplectic mappings. Therefore KAM results can often be applied to the mappings $\psi_{h,H}$ associated with symplectic integrators.

To get the flavour of this sort of application, let us consider once more the method (12.2) applied to (12.1). Recall that the origin is a (stable) centre for the system (12.1). For the discrete equations (12.2), linearization around the origin leads to

$$p^{n+1} = p^n + hf(0)q^{n+1}, \qquad q^{n+1} = q^n + hp^n, \tag{14.1}$$

a system that has, for h small, unit modulus eigenvalues. Thus the origin

is also a centre for (14.1). However to go from (14.1) to the discretization (12.2) we must include the effects of the nonlinear terms that were discarded in the process of linearization. Since (14.1) is only neutrally stable, it may be feared that the nonlinear effects, small as they may be, will render the origin unstable for (12.2). The KAM theory can be used to show that the symplecticness of the method implies that such a destabilization does not occur. Full details of this example have been given in Sanz-Serna (1991a). Incidentally, we would like to point out that it is this mechanism that renders the standard explicit midpoint rule stable in many nonlinear problems, even though this rule is only neutrally stable in a linear analysis. The interested reader is referred to Sanz-Serna and Vadillo (1986, 1987).

15. Practical performance of symplectic integrators

Numerical tests provide the final verdict on the usefulness of any numerical method. For Hamiltonian problems, are symplectic methods more advantageous in practice than their nonsymplectic counterparts? Before we answer this question, let us observe that many symplectic methods are implicit. Even though explicit symplectic algorithms exist in the PRK and RKN families, they are only applicable to restricted classes of Hamiltonians. Furthermore, when deriving such explicit methods, free parameters are used to ensure symplecticness which could otherwise be directed at increasing accuracy. The result is that, to achieve a given order, a symplectic explicit PRK or RKN method usually needs more stages than a standard PRK or RKN method. All these considerations show that there is a price to pay for symplecticness. Symplecticness is expected to pay back when performing very long time integrations: then a symplectic scheme has some inbuilt features that may guarantee the right long-term qualitative behaviour and even result in a favourable error propagation mechanism. On the other hand for short-time integrations, where accuracy is of paramount importance, a good standard code is expected to outperform any symplectic method.

Menyuk (1984), Feng and Qin (1987), Sanz-Serna (1989), Channell and Scovel (1990), Miesbach and Pesch (1990), Candy and Rozmus (1991), McLachlan and Atela (1991), Okunbor and Skeel (1991) and Pullin and Saffman (1991) provide numerical experiments involving symplectic integrators. The sort of experiment performed often consists of the application of a symplectic method to the long-time integration of a Hamiltonian problem; some sort of graphic output is then examined. The conclusions appear to be that symplectic integrators are very successful in identifying most relevant qualitative features of Hamiltonian flows. In most of the papers cited here, the symplectic method is tested against a standard method of the same order of accuracy. The standard method is usually proved to require much smaller step-sizes to correctly identify the true dynamics.

This sort of experimentation, encouraging as it may be to the developer of symplectic methods, is open to criticism. To begin with, the reference standard method being used tends to be either the classical fourth-order RK method or a low accuracy RK formula like the modified Euler scheme. These reference methods are far away from state of the art numerical integrators. Furthermore, in the experiments we are discussing, both the symplectic integrator and the reference standard method are implemented with constant step-sizes, which again is far away from current numerical ODE practice. It is legitimate to ask what would happen if in the comparisons the nonsymplectic method would have been chosen to be a modern variable step-size code. On the other hand, this criticism may not be entirely fair: standard methods have been under development for several decades, while we are at the stone age of symplectic integration; it may then make sense to compare our symplectic integrators with stone-age standard methods.

A somewhat more severe test has been conducted by Calvo and Sanz-Serna (1991b,c). A fourth-order, explicit, symplectic RKN method is constructed which is optimal in the sense that the error constants have been minimized following a methodology due to Dormand *et al.* (1987). First, this symplectic integrator, implemented with ***constant step-sizes***, is compared with a *variable step*-code based on an optimal fourth-order nonsymplectic formula of Dormand *et al.* (1987). The result of the comparison is that, in long time integrations, the symplectic method definitely needs less work to achieve a given accuracy. This holds even in cases where the solution possesses several time scales along the integration interval and the code is much benefiting from the step-changing facility. In the integration of Kepler's problem, it can be shown rigorously (Calvo and Sanz-Serna, 1991c) that for symplectic integrators the errors grow linearly with t, while for nonsymplectic methods grow like t^2. Hence the symplectic methods are guaranteed to win if t is large enough.

15.1. Variable step-sizes

Calvo and Sanz-Serna (1991b) then go on to compare the nonsymplectic code with a variable step-size implementation of the symplectic formula. For this implementation, due care was exercised in constructing the error estimator, etc. Before the experiments were conducted it was expected that the combination of the advantages of symplecticness with those of variable step-sizes would lead to a very efficient algorithm. The numerical results were very disappointing: in the variable step-size implementation, the symplectic formula does not show any advantage in the long-time error propagation mechanism. For instance, for Kepler's problem the error growth is quadratic, just as if a nonsymplectic formula were used. Since the cost per step of the simplectic algorithm is higher than that of the standard code (see earlier), the conclusion is that the variable step-size simplectic algorithm is not competitive with the standard code.

It thus appears that there is a future for the practical application of symplectic integration, especially if high order symplectic formulae are developed and if advances are made in efficiently implementing the implicit symplectic methods. However such a future seems to be limited to constant step-size implementations!

Before closing this section it is appropriate to say some words on the failure of variable step-size symplectic methods. In Section 12 we pointed out that a symplectic integrator $\psi_{h,H}$ 'almost' provides the exact flow of a Hamiltonian problem $\phi_{h,H_\infty(h)}$. If h is held constant during the integration, the initial condition is numerically advanced to $t = t_n$ by

$$\overbrace{\psi_{h,H}\psi_{h,H}\cdots\psi_{h,H}}^{n}$$

which for t_n in a compact time interval differs from

$$\overbrace{\phi_{h,H_\infty(h)}\phi_{h,H_\infty(h)}\cdots\phi_{h,H_\infty(h)}}^{n} = \phi_{t_n,H_\infty(h)}$$

in exponentially small terms: the computed points stay very close of a modified Hamiltonian trajectory. The situation is quite different for variable step-sizes. Now the initial condition is advanced by

$$\psi_{h_n,H}\psi_{h_{n-1},H}\cdots\psi_{h_1,H}, \tag{15.1}$$

an approximation to

$$\phi_{h_n,H_\infty(h_n)}\phi_{h_{n-1},H_\infty(h_{n-1})}\cdots\phi_{h_1,H_\infty(h_1)}.$$

The last expression cannot be interpreted as the t_n-flow of a Hamiltonian problem: the Hamiltonians being used at different time steps are different. This shows that the backward error interpretation of symplectic integration does not hold for variable step-sizes.

There is a difficulty here: in a variable step-size code the step points t_n are actually functions of the initial point $(\mathbf{p}^0, \mathbf{q}^0)$ (and also of the initial guess for the first step-size). Therefore the algorithm does not really effect a transformation mapping the phase space Ω at $t = 0$ into the phase space Ω at time t, rather $(\Omega \times (t = 0))$ is mapped into some curved $2d$-dimensional surface in the $(2d+1)$-dimensional spacetime. It is then possible to question the relevance of (15.1) to the analysis of the variable step implementation. However in the experiments reported by Calvo and Sanz-Serna (1991b) only one fixed initial condition was used so that, in a 'mental experiment', one could pretend that the sequence of step-sizes $h_1, h_2, \ldots$, actually used in the integration was recorded and would have been used to integrate neighbouring initial conditions. In this context, compatible with the numerical

experiments, the initial condition is really advanced by the symplectic transformation (15.1).

The advantages of symplectic integration may well originate from the fact that one advances from $t = 0$ to time t_n by iterating n times a single symplectic mapping. Advancing by composing n *different* symplectic mappings does not appear to be as effective.

16. Concluding remarks

In the paper we have restricted ourselves to standard Hamiltonian problems (2.1) on a domain Ω in an even-dimensional oriented Euclidean space. One may also consider a so-called symplectic manifold, an even dimensional manifold endowed with a closed, nondegenerate differential 2-form that plays the role that was played here by $\mathbf{dp} \wedge \mathbf{dq}$ (Arnold, 1989; MacKay, 1991). In such a manifold to each scalar function H there corresponds a Hamiltonian-like system of differential equations. More generally one could consider a Poisson manifold. A reference where a symplectic integrator is derived for a Poisson system is de Frutos *et al.* (1990). Another area of active research in the physics literature is that of Lie–Poisson integrators, see e.g. Ge and Marsden (1988).

Many partial differential equations also possess a Hamiltonian structure. In connection with symplectic integration they pose two problems: how to discretize them in space to obtain a Hamiltonian semi-discretization and how to advance in time the semi-discrete solution to have an overall symplectic algorithm. Some references are Qin (1988), Li and Qin (1988), Qin and Zhang (1990), de Frutos *et al.* (1990).

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Error analysis of boundary integral methods

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Many of the boundary value problems traditionally cast as partial differential equations can be reformulated as integral equations over the boundary. After an introduction to boundary integral equations, this review describes some of the methods which have been proposed for their approximate solution. It discusses, as simply as possible, some of the techniques used in their error analysis, and points to areas in which the theory is still unsatisfactory.

CONTENTS

1. Introduction

In the past decade there has been a dramatic growth of engineering interest in boundary integral or boundary element methods, witnessed by the large number of recent conference proceedings with these words in the title. At the same time, the former rivalry between advocates of BIE (boundary integral equation) and PDE (partial differential equation) approaches seems to have softened, as the relative strengths and weaknesses of each have become better understood.

Boundary integral methods may be used for interior and exterior problems, but have a special advantage for the latter. As a first introduction,