Chapter VI.
Symplectic Integration of Hamiltonian Systems

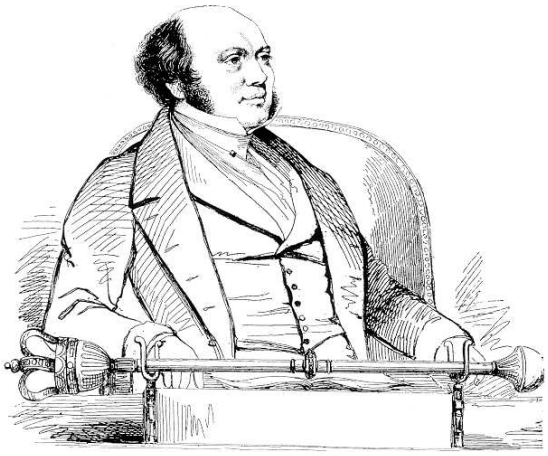
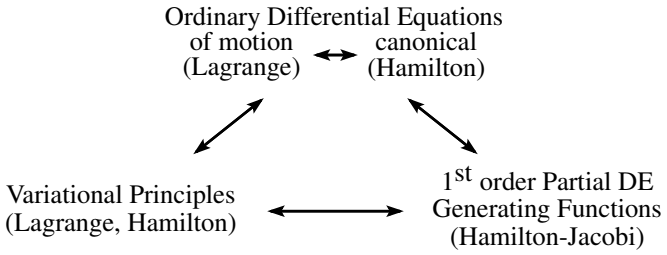


Fig. 0.1. Sir William Rowan Hamilton, born: 4 August 1805 in Dublin, died: 2 September 1865. Famous for research in optics, mechanics, and for the invention of quaternions.

Hamiltonian systems form the most important class of ordinary differential equations in the context of 'Geometric Numerical Integration'. An outstanding property of these systems is the symplecticity of the flow. As indicated in the following diagram,



Hamiltonian theory operates in three different domains (equations of motion, partial differential equations and variational principles) which are all interconnected. Each of these viewpoints, which we will study one after the other, leads to the construction of methods preserving the symplecticity.

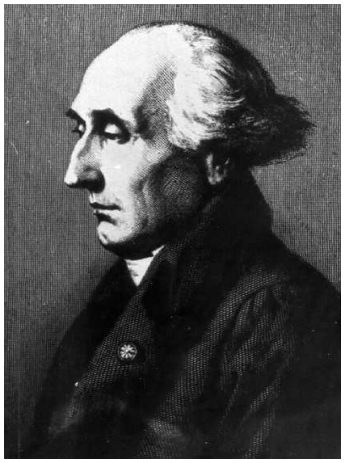
VI.1 Hamiltonian Systems

Hamilton's equations appeared first, among thousands of other formulas, and inspired by previous research in optics, in Hamilton (1834). Their importance was immediately recognized by Jacobi, who stressed and extended the fundamental ideas, so that, a couple of years later, all the long history of research of Galilei, Newton, Euler and Lagrange, was, in the words of Jacobi (1842), "to be considered as an introduction". The next mile-stones in the exposition of the theory were the monumental three volumes of Poincaré (1892,1893,1899) on celestial mechanics, Siegel's "Lectures on Celestial Mechanics" (1956), English enlarged edition by Siegel & Moser (1971), and the influential book of V.I. Arnold (1989; first Russian edition 1974). Beyond that, Hamiltonian systems became fundamental in many branches of physics. One such area, the dynamics of particle accelerators, actually motivated the construction of the first symplectic integrators (Ruth 1983).

VI.1.1 Lagrange's Equations

> Équations différentielles pour la solution de tous les problèmes de Dynamique. (J.-L. Lagrange 1788)

The problem of computing the dynamics of general mechanical systems began with Galilei (published 1638) and Newton's *Principia* (1687). The latter allowed one to reduce the movement of free mass points (the "mass points" being such planets as Mars or Jupiter) to the solution of differential equations (see Sect. I.2). But the movement of more complicated systems such as rigid bodies or bodies attached to each other by rods or springs, were the subject of long and difficult developments, until Lagrange (1760, 1788) found an elegant way of treating such problems in general.



Joseph-Louis Lagrange[1]

We suppose that the position of a mechanical system with d degrees of freedom is described by $q = (q_1, \ldots, q_d)^T$ as *generalized coordinates* (this can be for example Cartesian coordinates, angles, arc lengths along a curve, etc.). The theory is then built upon two pillars, namely an expression

$$T = T(q, \dot{q}) \tag{1.1}$$

which represents the *kinetic energy* (and which is often of the form $\frac{1}{2}\dot{q}^T M(q)\dot{q}$ where $M(q)$ is symmetric and positive definite), and by a function

[1] Joseph-Louis Lagrange, born: 25 January 1736 in Turin, Sardinia–Piedmont (now Italy), died: 10 April 1813 in Paris.

$$U = U(q) \tag{1.2}$$

representing the *potential energy*. Then, after denoting by

$$L = T - U \tag{1.3}$$

the corresponding *Lagrangian*, the coordinates $q_1(t), \dots, q_d(t)$ obey the differential equations

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot q}\right) = \frac{\partial L}{\partial q}\ , \tag{1.4}$$

which constitute the *Lagrange equations* of the system. A numerical (or analytical) integration of these equations allows one to predict the motion of any such system from given initial values ("Ce sont ces équations qui serviront à déterminer la courbe décrite par le corps M et sa vitesse à chaque instant"; Lagrange 1760, p. 369).

Example 1.1. For a mass point of mass m in $\mathbb{R}^3$ with Cartesian coordinates $x = (x_1, x_2, x_3)^T$ we have $T(\dot x) = m(\dot x_1^2 + \dot x_2^2 + \dot x_3^2)/2$. We suppose the point to move in a conservative force field $F(x) = -\nabla U(x)$. Then, the Lagrange equations (1.4) become $m\ddot x = F(x)$, which is Newton's second law. The equations (I.2.2) for the planetary motion are precisely of this form.

Example 1.2 (Pendulum). For the mathematical pendulum of Sect. I.1 we take the angle α as coordinate. The kinetic and potential energies are given by $T = m(\dot x^2 + \dot y^2)/2 = m\ell^2\dot\alpha^2/2$ and $U = mgy = -mg\ell\cos\alpha$, respectively, so that the Lagrange equations become $-mg\ell\sin\alpha - m\ell^2\ddot\alpha = 0$ or equivalently $\ddot\alpha + \frac{g}{\ell}\sin\alpha = 0$.

VI.1.2 Hamilton's Canonical Equations

> An diese *Hamiltonsche* Form der Differentialgleichungen werden die ferneren Untersuchungen, welche den Kern dieser Vorlesung bilden, anknüpfen; das Bisherige ist als Einleitung dazu anzusehen.
>
> (C.G.J. Jacobi 1842, p. 143)

Hamilton (1834) simplified the structure of Lagrange's equations and turned them into a form that has remarkable symmetry, by

- introducing Poisson's variables, the conjugate *momenta*

$$p_k = \frac{\partial L}{\partial \dot q_k}(q, \dot q) \qquad \text{for} \quad k = 1, \dots, d, \tag{1.5}$$

- considering the *Hamiltonian*

$$H := p^T\dot q - L(q, \dot q) \tag{1.6}$$

  as a function of p and q, i.e., taking $H = H(p, q)$ obtained by expressing $\dot q$ as a function of p and q via (1.5).

Here it is, of course, required that (1.5) defines, for every q, a continuously differentiable bijection $\dot q \leftrightarrow p$. This map is called the *Legendre transform*.

Theorem 1.3. *Lagrange's equations (1.4) are equivalent to Hamilton's equations*

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}(p,q), \qquad \dot{q}_k = \frac{\partial H}{\partial p_k}(p,q), \qquad k = 1,\dots,d. \tag{1.7}$$

Proof. The definitions (1.5) and (1.6) for the momenta p and for the Hamiltonian H imply that

$$\begin{aligned} \frac{\partial H}{\partial p} &= \dot{q}^T + p^T \frac{\partial \dot{q}}{\partial p} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial p} \;=\; \dot{q}^T, \\ \frac{\partial H}{\partial q} &= p^T \frac{\partial \dot{q}}{\partial q} - \frac{\partial L}{\partial q} - \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q} \;=\; -\frac{\partial L}{\partial q}. \end{aligned}$$

The Lagrange equations (1.4) are therefore equivalent to (1.7). □

Case of Quadratic T. In the case that $T = \frac{1}{2}\dot{q}^T M(q)\dot{q}$ is quadratic, where $M(q)$ is a symmetric and positive definite matrix, we have, for a fixed q, $p = M(q)\dot{q}$, so that the existence of the Legendre transform is established. Further, by replacing the variable $\dot{q}$ by $M(q)^{-1}p$ in the definition (1.6) of $H(p,q)$, we obtain

$$\begin{aligned} H(p,q) &= p^T M(q)^{-1} p - L\big(q, M(q)^{-1}p\big) \\ &= p^T M(q)^{-1} p - \frac{1}{2}\, p^T M(q)^{-1} p + U(q) \;=\; \frac{1}{2}\, p^T M(q)^{-1} p + U(q) \end{aligned}$$

and the Hamiltonian is $H = T + U$, which is the *total energy* of the mechanical system.

In Chap. I we have seen several examples of Hamiltonian systems, e.g., the pendulum (I.1.13), the Kepler problem (I.2.2), the outer solar system (I.2.12), etc. In the following we consider Hamiltonian systems (1.7) where the Hamiltonian $H(p,q)$ is arbitrary, and so not necessarily related to a mechanical problem.

VI.2 Symplectic Transformations

> The name "complex group" formerly advocated by me in allusion to line complexes, ... has become more and more embarrassing through collision with the word "complex" in the connotation of complex number. I therefore propose to replace it by the Greek adjective "symplectic."
>
> (H. Weyl (1939), p. 165)

A first property of Hamiltonian systems, already seen in Example 1.2 of Sect. IV.1, is that the Hamiltonian $H(p,q)$ is a *first integral* of the system (1.7). In this section we shall study another important property – the *symplecticity* of its flow. The basic objects to be studied are two-dimensional parallelograms lying in $\mathbb{R}^{2d}$. We suppose the parallelogram to be spanned by two vectors

$$\xi = \begin{pmatrix} \xi^p \\ \xi^q \end{pmatrix}, \qquad \eta = \begin{pmatrix} \eta^p \\ \eta^q \end{pmatrix}$$

in the (p,q) space (ξ^p, ξ^q, η^p, η^q are in $\mathbb{R}^d$) as

$$P = \big\{ t\xi + s\eta \mid 0 \le t \le 1,\ 0 \le s \le 1 \big\}.$$

In the case $d = 1$ we consider the *oriented area*

$$\text{or.area}\,(P) = \det \begin{pmatrix} \xi^p & \eta^p \\ \xi^q & \eta^q \end{pmatrix} = \xi^p \eta^q - \xi^q \eta^p \tag{2.1}$$

(see left picture of Fig. 2.1). In higher dimensions, we replace this by the *sum of the oriented areas of the projections of P onto the coordinate planes (p_i, q_i)*, i.e., by

$$\omega(\xi, \eta) := \sum_{i=1}^{d} \det \begin{pmatrix} \xi_i^p & \eta_i^p \\ \xi_i^q & \eta_i^q \end{pmatrix} = \sum_{i=1}^{d} (\xi_i^p \eta_i^q - \xi_i^q \eta_i^p). \tag{2.2}$$

This defines a bilinear map acting on vectors of $\mathbb{R}^{2d}$, which will play a central role for Hamiltonian systems. In matrix notation, this map has the form

$$\omega(\xi, \eta) = \xi^T J \eta \qquad \text{with} \qquad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{2.3}$$

where I is the identity matrix of dimension d.

Definition 2.1. A linear mapping $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called *symplectic* if

$$A^T J A = J$$

or, equivalently, if $\omega(A\xi, A\eta) = \omega(\xi, \eta)$ for all $\xi, \eta \in \mathbb{R}^{2d}$.

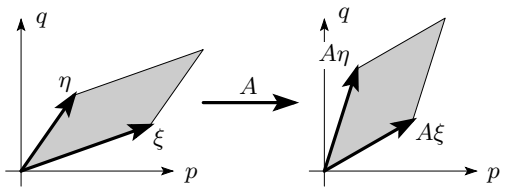


Fig. 2.1. Symplecticity (area preservation) of a linear mapping.

In the case $d = 1$, where the expression $\omega(\xi, \eta)$ represents the area of the parallelogram P, symplecticity of a linear mapping A is therefore the *area preservation* of A (see Fig. 2.1). In the general case ($d > 1$), symplecticity means that the sum of the oriented areas of the projections of P onto (p_i, q_i) is the same as that for the transformed parallelograms $A(P)$.

We now turn our attention to nonlinear mappings. Differentiable functions can be locally approximated by linear mappings. This justifies the following definition.

Definition 2.2. A differentiable map $g : U \to \mathbb{R}^{2d}$ (where $U \subset \mathbb{R}^{2d}$ is an open set) is called *symplectic* if the Jacobian matrix $g'(p, q)$ is everywhere symplectic, i.e., if

$$g'(p,q)^T J\, g'(p,q) = J \qquad \text{or} \qquad \omega(g'(p,q)\xi, g'(p,q)\eta) = \omega(\xi, \eta).$$

Let us give a geometric interpretation of symplecticity for nonlinear mappings. Consider a 2-dimensional sub-manifold M of the $2d$-dimensional set U, and suppose that it is given as the image $M = \psi(K)$ of a compact set $K \subset \mathbb{R}^2$, where

$\psi(s,t)$ is a continuously differentiable function. The manifold M can then be considered as the limit of a union of small parallelograms spanned by the vectors

$$\frac{\partial\psi}{\partial s}(s,t)\,ds \qquad \text{and} \qquad \frac{\partial\psi}{\partial t}(s,t)\,dt.$$

For one such parallelogram we consider (as above) the sum over the oriented areas of its projections onto the (p_i,q_i) plane. We then sum over all parallelograms of the manifold. In the limit this gives the expression

$$\Omega(M)=\iint_K \omega\left(\frac{\partial\psi}{\partial s}(s,t),\frac{\partial\psi}{\partial t}(s,t)\right)ds\,dt. \tag{2.4}$$

The transformation formula for double integrals implies that $\Omega(M)$ is independent of the parametrization ψ of M.

Lemma 2.3. *If the mapping $g:U\to\mathbb{R}^{2d}$ is symplectic on U, then it preserves the expression $\Omega(M)$, i.e.,*

$$\Omega\big(g(M)\big)=\Omega(M)$$

holds for all 2-dimensional manifolds M that can be represented as the image of a continuously differentiable function ψ.

Proof. The manifold $g(M)$ can be parametrized by $g\circ\psi$. We have

$$\Omega\big(g(M)\big)=\iint_K \omega\left(\frac{\partial(g\circ\psi)}{\partial s}(s,t),\frac{\partial(g\circ\psi)}{\partial t}(s,t)\right)ds\,dt=\Omega(M),$$

because $(g\circ\psi)'(s,t)=g'\big(\psi(s,t)\big)\psi'(s,t)$ and g is a symplectic transformation. □

For $d=1$, M is already a subset of $\mathbb{R}^2$ and we choose $K=M$ with ψ the identity map. In this case, $\Omega(M)=\iint_M ds\,dt$ represents the area of M. Hence, Lemma 2.3 states that all symplectic mappings (also nonlinear ones) are *area preserving*.

We are now able to prove the main result of this section. We use the notation $y=(p,q)$, and we write the Hamiltonian system (1.7) in the form

$$\dot y=J^{-1}\nabla H(y), \tag{2.5}$$

where J is the matrix of (2.3) and $\nabla H(y)=H'(y)^T$.

Recall that the flow $\varphi_t:U\to\mathbb{R}^{2d}$ of a Hamiltonian system is the mapping that advances the solution by time t, i.e., $\varphi_t(p_0,q_0)=(p(t,p_0,q_0),q(t,p_0,q_0))$, where $p(t,p_0,q_0)$, $q(t,p_0,q_0)$ is the solution of the system corresponding to initial values $p(0)=p_0$, $q(0)=q_0$.

Theorem 2.4 (Poincaré 1899). *Let $H(p,q)$ be a twice continuously differentiable function on $U\subset\mathbb{R}^{2d}$. Then, for each fixed t, the flow φ_t is a symplectic transformation wherever it is defined.*

Proof. The derivative $\partial\varphi_t/\partial y_0$ (with $y_0=(p_0,q_0)$) is a solution of the variational equation which, for the Hamiltonian system (2.5), is of the form $\dot\Psi=J^{-1}\nabla^2H\big(\varphi_t(y_0)\big)\Psi$, where $\nabla^2H(p,q)$ is the Hessian matrix of $H(p,q)$ ($\nabla^2H(p,q)$

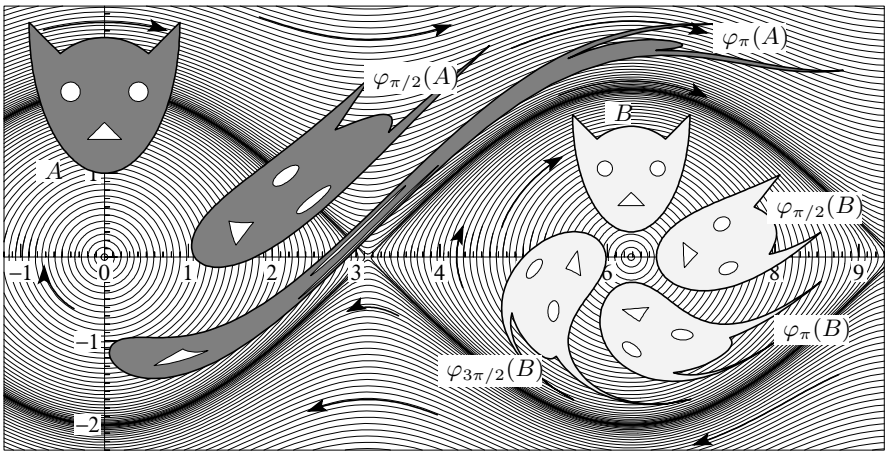


Fig. 2.2. Area preservation of the flow of Hamiltonian systems

is symmetric). We therefore obtain

$$\frac{d}{dt}\left(\left(\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{\partial\varphi_t}{\partial y_0}\right)\right) = \left(\frac{d}{dt}\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{\partial\varphi_t}{\partial y_0}\right) + \left(\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{d}{dt}\frac{\partial\varphi_t}{\partial y_0}\right)$$
$$= \left(\frac{\partial\varphi_t}{\partial y_0}\right)^T \nabla^2 H\big(\varphi_t(y_0)\big) J^{-T} J\left(\frac{\partial\varphi_t}{\partial y_0}\right) + \left(\frac{\partial\varphi_t}{\partial y_0}\right)^T \nabla^2 H\big(\varphi_t(y_0)\big)\left(\frac{\partial\varphi_t}{\partial y_0}\right) = 0,$$

because $J^T = -J$ and $J^{-T}J = -I$. Since the relation

$$\left(\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{\partial\varphi_t}{\partial y_0}\right) = J \tag{2.6}$$

is satisfied for $t = 0$ (φ_0 is the identity map), it is satisfied for all t and all (p_0, q_0), as long as the solution remains in the domain of definition of H. □

Example 2.5. We illustrate this theorem with the pendulum problem (Example 1.2) using the normalization $m = \ell = g = 1$. We have $q = \alpha$, $p = \dot\alpha$, and the Hamiltonian is given by

$$H(p, q) = p^2/2 - \cos q.$$

Fig. 2.2 shows level curves of this function, and it also illustrates the area preservation of the flow φ_t. Indeed, by Theorem 2.4 and Lemma 2.3, the areas of A and $\varphi_t(A)$ as well as those of B and $\varphi_t(B)$ are the same, although their appearance is completely different.

We next show that symplecticity of the flow is a characteristic property for Hamiltonian systems. We call a differential equation $\dot y = f(y)$ *locally Hamiltonian*, if for every $y_0 \in U$ there exists a neighbourhood where $f(y) = J^{-1}\nabla H(y)$ for some function H.

Theorem 2.6. *Let $f : U \to \mathbb{R}^{2d}$ be continuously differentiable. Then, $\dot y = f(y)$ is locally Hamiltonian if and only if its flow $\varphi_t(y)$ is symplectic for all $y \in U$ and for all sufficiently small t.*

Proof. The necessity follows from Theorem 2.4. We therefore assume that the flow φ_t is symplectic, and we have to prove the local existence of a function $H(y)$ such that $f(y) = J^{-1}\nabla H(y)$. Differentiating (2.6) and using the fact that $\partial\varphi_t/\partial y_0$ is a solution of the variational equation $\dot\Psi = f'\big(\varphi_t(y_0)\big)\Psi$, we obtain

$$\frac{d}{dt}\left(\Big(\frac{\partial\varphi_t}{\partial y_0}\Big)^T J\Big(\frac{\partial\varphi_t}{\partial y_0}\Big)\right) = \Big(\frac{\partial\varphi_t}{\partial y_0}\Big)\Big(f'\big(\varphi_t(y_0)\big)^T J + Jf'\big(\varphi_t(y_0)\big)\Big)\Big(\frac{\partial\varphi_t}{\partial y_0}\Big) = 0.$$

Putting $t = 0$, it follows from $J = -J^T$ that $Jf'(y_0)$ is a symmetric matrix for all y_0. The Integrability Lemma 2.7 below shows that $Jf(y)$ can be written as the gradient of a function $H(y)$. □

The following integrability condition for the existence of a potential was already known to Euler and Lagrange (see e.g., Euler's *Opera Omnia*, vol. 19. p. 2-3, or Lagrange (1760), p. 375).

Lemma 2.7 (Integrability Lemma). *Let $D \subset \mathbb{R}^n$ be open and $f : D \to \mathbb{R}^n$ be continuously differentiable, and assume that the Jacobian $f'(y)$ is symmetric for all $y \in D$. Then, for every $y_0 \in D$ there exists a neighbourhood and a function $H(y)$ such that*

$$f(y) = \nabla H(y) \tag{2.7}$$

on this neighbourhood. In other words, the differential form $f_1(y)\,dy_1 + \ldots + f_n(y)\,dy_n = dH$ is a total differential.

Proof. Assume $y_0 = 0$, and consider a ball around y_0 which is contained in D. On this ball we define

$$H(y) = \int_0^1 y^T f(ty)\,dt + Const.$$

Differentiation with respect to y_k, and using the symmetry assumption $\partial f_i/\partial y_k = \partial f_k/\partial y_i$ yields

$$\frac{\partial H}{\partial y_k}(y) = \int_0^1 \Big(f_k(ty) + y^T\frac{\partial f}{\partial y_k}(ty)t\Big)\,dt = \int_0^1 \frac{d}{dt}\Big(tf_k(ty)\Big)\,dt = f_k(y),$$

which proves the statement. □

For $D = \mathbb{R}^{2d}$ or for star-shaped regions D, the above proof shows that the function H of Lemma 2.7 is globally defined. Hence the Hamiltonian of Theorem 2.6 is also globally defined in this case. This remains valid for simply connected sets D. A counter-example, which shows that the existence of a global Hamiltonian in Theorem 2.6 is not true for general D, is given in Exercise 6.

An important property of symplectic transformations, which goes back to Jacobi (1836, "Theorem X"), is that they preserve the Hamiltonian character of the differential equation. Such transformations have been termed *canonical* since the 19th century. The next theorem shows that canonical and symplectic transformations are the same.

Theorem 2.8. *Let $\psi : U \to V$ be a change of coordinates such that ψ and ψ^{-1} are continuously differentiable functions. If ψ is symplectic, the Hamiltonian system $\dot y = J^{-1}\nabla H(y)$ becomes in the new variables $z = \psi(y)$*

$$\dot z = J^{-1}\nabla K(z) \qquad \textit{with} \qquad K(z) = H(y). \tag{2.8}$$

Conversely, if ψ transforms every Hamiltonian system to another Hamiltonian system via (2.8), then ψ is symplectic.

Proof. Since $\dot z = \psi'(y)\dot y$ and $\psi'(y)^T\nabla K(z) = \nabla H(y)$, the Hamiltonian system $\dot y = J^{-1}\nabla H(y)$ becomes

$$\dot z = \psi'(y)J^{-1}\psi'(y)^T\nabla K(z) \tag{2.9}$$

in the new variables. It is equivalent to (2.8) if

$$\psi'(y)J^{-1}\psi'(y)^T = J^{-1}. \tag{2.10}$$

Multiplying this relation from the right by $\psi'(y)^{-T}$ and from the left by $\psi'(y)^{-1}$ and then taking its inverse yields $J = \psi'(y)^T J\psi'(y)$, which shows that (2.10) is equivalent to the symplecticity of ψ.

For the inverse relation we note that (2.9) is Hamiltonian for all $K(z)$ if and only if (2.10) holds. □

VI.3 First Examples of Symplectic Integrators

Since symplecticity is a characteristic property of Hamiltonian systems (Theorem 2.6), it is natural to search for numerical methods that share this property. Pioneering work on symplectic integration is due to de Vogelaere (1956), Ruth (1983), and Feng Kang (1985). Books on the now well-developed subject are Sanz-Serna & Calvo (1994) and Leimkuhler & Reich (2004).

Feng Kang[2]

Definition 3.1. A numerical one-step method is called *symplectic* if the one-step map

$$y_1 = \Phi_h(y_0)$$

is symplectic whenever the method is applied to a smooth Hamiltonian system.

[2] Feng Kang, born: 9 September 1920 in Nanjing (China), died: 17 August 1993 in Beijing; picture obtained from Yuming Shi with the help of Yifa Tang.

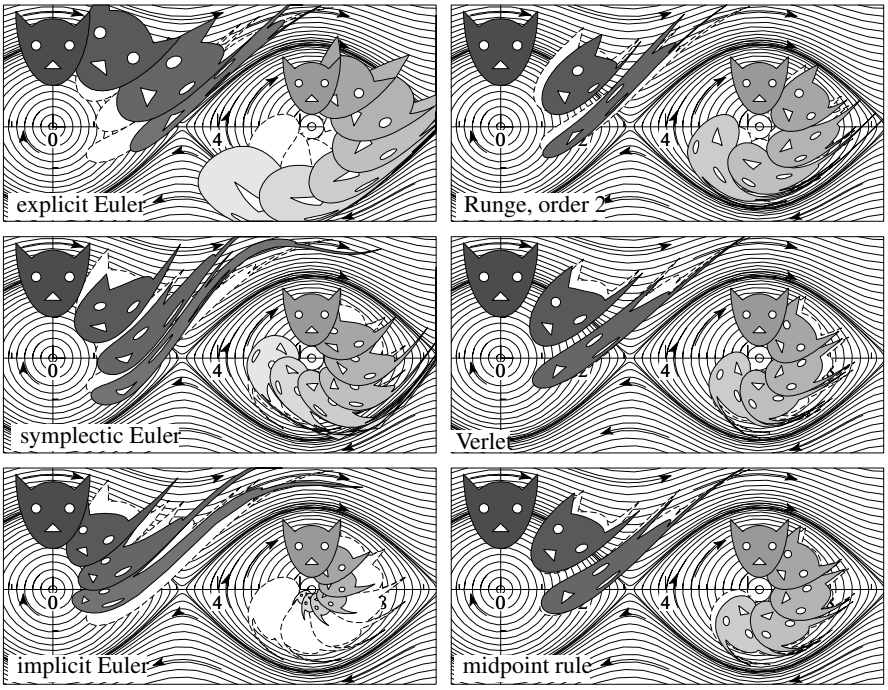


Fig. 3.1. Area preservation of numerical methods for the pendulum; same initial sets as in Fig. 2.2; first order methods (left column): $h = \pi/4$; second order methods (right column): $h = \pi/3$; dashed: exact flow.

Example 3.2. We consider the pendulum problem of Example 2.5 with the same initial sets as in Fig. 2.2. We apply six different numerical methods to this problem: the explicit Euler method (I.1.5), the symplectic Euler method (I.1.9), and the implicit Euler method (I.1.6), as well as the second order method of Runge (II.1.3) (the right one), the Störmer–Verlet scheme (I.1.17), and the implicit midpoint rule (I.1.7). For two sets of initial values (p_0, q_0) we compute several steps with step size $h = \pi/4$ for the first order methods, and $h = \pi/3$ for the second order methods. One clearly observes in Fig. 3.1 that the explicit Euler, the implicit Euler and the second order explicit method of Runge are not symplectic (not area preserving). We shall prove below that the other methods are symplectic. A different proof of their symplecticity (using generating functions) will be given in Sect. VI.5.

In the following we show the symplecticity of various numerical methods from Chapters I and II when they are applied to the Hamiltonian system in the variables $y = (p, q)$,

$$\begin{aligned} \dot p &= -H_q(p,q) \\ \dot q &= H_p(p,q) \end{aligned} \qquad \text{or equivalently} \qquad \dot y = J^{-1}\nabla H(y),$$

where H_p and H_q denote the column vectors of partial derivatives of the Hamiltonian $H(p, q)$ with respect to p and q, respectively.

Theorem 3.3 (de Vogelaere 1956). *The so-called symplectic Euler methods (I.1.9)*

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{aligned} \quad \textit{or} \quad \begin{aligned} p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \\ q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \end{aligned} \tag{3.1}$$

are symplectic methods of order 1.

Proof. We consider only the method to the left of (3.1). Differentiation with respect to (p_n, q_n) yields

$$\begin{pmatrix} I + hH_{qp}^T & 0 \\ -hH_{pp} & I \end{pmatrix} \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right) = \begin{pmatrix} I & -hH_{qq} \\ 0 & I + hH_{qp} \end{pmatrix},$$

where the matrices $H_{qp}, H_{pp}, \ldots$ of partial derivatives are all evaluated at (p_{n+1}, q_n). This relation allows us to compute $\frac{\partial(p_{n+1},q_{n+1})}{\partial(p_n,q_n)}$ and to check in a straightforward way the symplecticity condition $\big(\frac{\partial(p_{n+1},q_{n+1})}{\partial(p_n,q_n)}\big)^T J \big(\frac{\partial(p_{n+1},q_{n+1})}{\partial(p_n,q_n)}\big) = J$. □

The methods (3.1) are implicit for general Hamiltonian systems. For separable $H(p, q) = T(p) + U(q)$, however, both variants turn out to be explicit. It is interesting to mention that there are more general situations where the symplectic Euler methods are explicit. If, for a suitable ordering of the components,

$$\frac{\partial H}{\partial q_i}(p, q) \quad \text{does not depend on } p_j \text{ for } j \geq i, \tag{3.2}$$

then the left method of (3.1) is explicit, and the components of p_{n+1} can be computed one after the other. If, for a possibly different ordering of the components,

$$\frac{\partial H}{\partial p_i}(p, q) \quad \text{does not depend on } q_j \text{ for } j \geq i, \tag{3.3}$$

then the right method of (3.1) is explicit. As an example consider the Hamiltonian

$$H(p_r, p_\varphi, r, \varphi) = \frac{1}{2}\Big(p_r^2 + r^{-2}p_\varphi^2\Big) - r\cos\varphi + (r-1)^2,$$

which models a spring pendulum in polar coordinates. For the ordering $\varphi < r$, condition (3.2) is fulfilled, and for the inverse ordering $r < \varphi$ condition (3.3). Consequently, both symplectic Euler methods are explicit for this problem. The methods remain explicit if the conditions (3.2) and (3.3) hold for blocks of components instead of single components.

We consider next the extension of the Störmer–Verlet scheme (I.1.17), considered in Table II.2.1.

Theorem 3.4. *The Störmer–Verlet schemes (I.1.17)*

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2}H_q(p_{n+1/2}, q_n) \\ q_{n+1} &= q_n + \frac{h}{2}\Big(H_p(p_{n+1/2}, q_n) + H_p(p_{n+1/2}, q_{n+1})\Big) \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2}H_q(p_{n+1/2}, q_{n+1}) \end{aligned} \tag{3.4}$$

and

$$\begin{aligned} q_{n+1/2} &= q_n + \frac{h}{2} H_q(p_n, q_{n+1/2}) \\ p_{n+1} &= p_n - \frac{h}{2}\Big(H_p(p_n, q_{n+1/2}) + H_p(p_{n+1}, q_{n+1/2})\Big) \\ q_{n+1} &= q_{n+1/2} + \frac{h}{2} H_q(p_{n+1}, q_{n+1/2}) \end{aligned} \tag{3.5}$$

are symplectic methods of order 2.

Proof. This is an immediate consequence of the fact that the Störmer–Verlet scheme is the composition of the two symplectic Euler methods (3.1). Order 2 follows from its symmetry. □

We note that the Störmer–Verlet methods (3.4) and (3.5) are explicit for separable problems and for Hamiltonians that satisfy both conditions (3.2) and (3.3).

Theorem 3.5. *The implicit midpoint rule*

$$y_{n+1} = y_n + hJ^{-1}\nabla H\big((y_{n+1} + y_n)/2\big) \tag{3.6}$$

is a symplectic method of order 2.

Proof. Differentiation of (3.6) yields

$$\Big(I - \frac{h}{2}J^{-1}\nabla^2 H\Big)\Big(\frac{\partial y_{n+1}}{\partial y_n}\Big) = \Big(I + \frac{h}{2}J^{-1}\nabla^2 H\Big).$$

Again it is straightforward to verify that $\big(\frac{\partial y_{n+1}}{\partial y_n}\big)^T J\big(\frac{\partial y_{n+1}}{\partial y_n}\big) = J$. Due to its symmetry, the midpoint rule is known to be of order 2 (see Theorem II.3.2). □

The next two theorems are a consequence of the fact that the composition of symplectic transformations is again symplectic. They are also used to prove the existence of symplectic methods of arbitrarily high order, and to explain why the theory of composition methods of Chapters II and III is so important for geometric integration.

Theorem 3.6. *Let Φ_h denote the symplectic Euler method (3.1). Then, the composition method (II.4.6) is symplectic for every choice of the parameters α_i, β_i.*

If $\widehat{\Phi}_h$ is symplectic and symmetric (e.g., the implicit midpoint rule or the Störmer–Verlet scheme), then the composition method (V.3.8) is symplectic too. □

Theorem 3.7. *Assume that the Hamiltonian is given by $H(y) = H_1(y) + H_2(y)$, and consider the splitting*

$$\dot{y} = J^{-1}\nabla H(y) = J^{-1}\nabla H_1(y) + J^{-1}\nabla H_2(y).$$

The splitting method (II.5.6) is then symplectic. □

VI.4 Symplectic Runge–Kutta Methods

The systematic study of symplectic Runge–Kutta methods started around 1988, and a complete characterization has been found independently by Lasagni (1988) (using the approach of generating functions), and by Sanz-Serna (1988) and Suris (1988) (using the ideas of the classical papers of Burrage & Butcher (1979) and Crouzeix (1979) on algebraic stability).

VI.4.1 Criterion of Symplecticity

We follow the approach of Bochev & Scovel (1994), which is based on the following important lemma.

Lemma 4.1. *For Runge–Kutta methods and for partitioned Runge–Kutta methods the following diagram commutes:*

$$\begin{array}{ccc} \dot y = f(y),\ \ y(0) = y_0 & \longrightarrow & \begin{array}{c} \dot y = f(y),\ \ y(0) = y_0 \\ \dot\Psi = f'(y)\Psi,\ \ \Psi(0) = I \end{array} \\ \Big\downarrow \textit{method} & & \Big\downarrow \textit{method} \\ \{y_n\} & \longrightarrow & \{y_n, \Psi_n\} \end{array}$$

(horizontal arrows mean a differentiation with respect to y_0). Therefore, the numerical result y_n, Ψ_n, obtained from applying the method to the problem augmented by its variational equation, is equal to the numerical solution for $\dot y = f(y)$ augmented by its derivative $\Psi_n = \partial y_n / \partial y_0$.

Proof. The result is proved by implicit differentiation. Let us illustrate this for the explicit Euler method

$$y_{n+1} = y_n + hf(y_n).$$

We consider y_n and y_{n+1} as functions of y_0, and we differentiate with respect to y_0 the equation defining the numerical method. For the Euler method this gives

$$\frac{\partial y_{n+1}}{\partial y_0} = \frac{\partial y_n}{\partial y_0} + hf'(y_n)\,\frac{\partial y_n}{\partial y_0},$$

which is exactly the relation that we get from applying the method to the variational equation. Since $\partial y_0 / \partial y_0 = I$, we have $\partial y_n / \partial y_0 = \Psi_n$ for all n. □

The main observation now is that the symplecticity condition (2.6) is a quadratic first integral of the variational equation: we write the Hamiltonian system together with its variational equation as

$$\dot y = J^{-1}\nabla H(y), \qquad \dot\Psi = J^{-1}\nabla^2 H(y)\Psi. \tag{4.1}$$

It follows from

$$(J^{-1}\nabla^2 H(y)\Psi)^T J\Psi + \Psi^T J(J^{-1}\nabla^2 H(y)\Psi) = 0$$

(see also the proof of Theorem 2.4) that $\Psi^T J\Psi$ is a quadratic first integral of the augmented system (4.1).

Therefore, every Runge–Kutta method that preserves quadratic first integrals, is a symplectic method. From Theorem IV.2.1 and Theorem IV.2.2 we thus obtain the following results.

Theorem 4.2. *The Gauss collocation methods of Sect. II.1.3 are symplectic.* □

Theorem 4.3. *If the coefficients of a Runge–Kutta method satisfy*

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \qquad \textit{for all } \; i,j = 1,\dots,s, \tag{4.2}$$

then it is symplectic. □

Similar to the situation in Theorem V.2.4, diagonally implicit, symplectic Runge–Kutta methods are composition methods.

Theorem 4.4. *A diagonally implicit Runge–Kutta method satisfying the symplecticity condition (4.2) and $b_i \neq 0$ is equivalent to the composition*

$$\Phi^M_{b_s h} \circ \ldots \circ \Phi^M_{b_2 h} \circ \Phi^M_{b_1 h},$$

where Φ^M_h stands for the implicit midpoint rule.

Proof. For $i = j$ condition (4.2) gives $a_{ii} = b_i/2$ and, together with $a_{ji} = 0$ (for $i > j$), implies $a_{ij} = b_j$. This proves the statement. □

The assumption "$b_i \neq 0$" is not restrictive in the sense that for diagonally implicit Runge–Kutta methods satisfying (4.2) the internal stages corresponding to "$b_i = 0$" do not influence the numerical result and can be removed.

To understand the symplecticity of partitioned Runge–Kutta methods, we write the solution Ψ of the variational equation as

$$\Psi = \begin{pmatrix} \Psi^p \\ \Psi^q \end{pmatrix}.$$

Then, the Hamiltonian system together with its variational equation (4.1) is a partitioned system with variables (p, Ψ^p) and (q, Ψ^q). Every component of

$$\Psi^T J\Psi = (\Psi^p)^T \Psi^q - (\Psi^q)^T \Psi^p$$

is of the form (IV.2.5), so that Theorem IV.2.3 and Theorem IV.2.4 yield the following results.

Theorem 4.5. *The Lobatto IIIA - IIIB pair is a symplectic method.* □

Theorem 4.6. *If the coefficients of a partitioned Runge–Kutta method (II.2.2) satisfy*

$$b_i\widehat{a}_{ij} + \widehat{b}_j a_{ji} = b_i\widehat{b}_j \qquad \text{for } i,j = 1,\dots,s, \tag{4.3}$$

$$b_i = \widehat{b}_i \qquad \text{for } i = 1,\dots,s, \tag{4.4}$$

then it is symplectic.

If the Hamiltonian is of the form $H(p,q) = T(p) + U(q)$, i.e., it is separable, then the condition (4.3) alone implies the symplecticity of the numerical flow. □

We have seen in Sect. V.2.2 that within the class of partitioned Runge–Kutta methods it is possible to get explicit, symmetric methods for separable systems $\dot y = f(z)$, $\dot z = g(y)$. A similar result holds for symplectic methods. However, as in Theorem V.2.6, such methods are not more general than composition or splitting methods as considered in Sect. II.5. This has first been observed by Okunbor & Skeel (1992).

Theorem 4.7. *Consider a partitioned Runge–Kutta method based on two diagonally implicit methods (i.e., $a_{ji} = \widehat{a}_{ji} = 0$ for $i > j$), assume $a_{ii} \cdot \widehat{a}_{ii} = 0$ for all i, and apply it to a separable Hamiltonian system with $H(p,q) = T(p) + U(q)$. If (4.3) holds, then the numerical result is the same as that obtained from the splitting method (II.5.6).*

By (II.5.8), such a method is equivalent to a composition of symplectic Euler steps.

Proof. We first notice that the stage values $k_i = f(Z_i)$ (for i with $b_i = 0$) and $\ell_i = g(Y_i)$ (for i with $\widehat{b}_i = 0$) do not influence the numerical solution and can be removed. This yields a scheme with non-zero b_i and $\widehat{b}_i$, but with possibly non-square matrices (a_{ij}) and $(\widehat{a}_{ij})$.

Since the method is explicit for separable problems, one of the reduced matrices (a_{ij}) or $(\widehat{a}_{ij})$ has a row consisting only of zeros. Assume that it is the first row of (a_{ij}), so that $a_{1j} = 0$ for all j. The symplecticity condition thus implies $\widehat{a}_{i1} = \widehat{b}_1 \neq 0$ for all $i \geq 1$, and $a_{i1} = b_1 \neq 0$ for $i \geq 2$. This then yields $\widehat{a}_{22} \neq 0$, because otherwise the first two stages of $(\widehat{a}_{ij})$ would be identical and one could be removed. By our assumption we get $a_{22} = 0$, $\widehat{a}_{i2} = \widehat{b}_2 \neq 0$ for $i \geq 2$, and $a_{i2} = b_2$ for $i \geq 3$. Continuing this procedure we see that the method becomes

$$\dots \circ \varphi^{[2]}_{\widehat{b}_2 h} \circ \varphi^{[1]}_{b_2 h} \circ \varphi^{[2]}_{\widehat{b}_1 h} \circ \varphi^{[1]}_{b_1 h},$$

where $\varphi^{[1]}_t$ and $\varphi^{[2]}_t$ are the exact flows corresponding to the Hamiltonians $T(p)$ and $U(q)$, respectively. □

The necessity of the conditions of Theorem 4.3 and Theorem 4.6 for symplectic (partitioned) Runge–Kutta methods will be discussed at the end of this chapter in Sect. VI.7.4.

A second order differential equation $\ddot{y} = g(y)$, augmented by its variational equation, is again of this special form. Furthermore, the diagram of Lemma 4.1 commutes for Nyström methods, so that Theorem IV.2.5 yields the following result originally obtained by Suris (1988, 1989).

Theorem 4.8. *If the coefficients of a Nyström method (IV.2.11) satisfy*

$$\begin{aligned} \beta_i &= b_i(1-c_i) \qquad \textit{for } i = 1,\dots,s, \\ b_i(\beta_j - a_{ij}) &= b_j(\beta_i - a_{ji}) \qquad \textit{for } i,j = 1,\dots,s, \end{aligned} \tag{4.5}$$

then it is symplectic. □

VI.4.2 Connection Between Symplectic and Symmetric Methods

There exist symmetric methods that are not symplectic, and there exist symplectic methods that are not symmetric. For example, the *trapezoidal rule*

$$y_1 = y_0 + \frac{h}{2}\Big(f(y_0) + f(y_1)\Big) \tag{4.6}$$

is symmetric, but it does not satisfy the condition (4.2) for symplecticity. In fact, this is true of all Lobatto IIIA methods (see Example II.2.2). On the other hand, any composition $\Phi_{\gamma_1 h} \circ \Phi_{\gamma_2 h}$ ($\gamma_1 + \gamma_2 = 1$) of symplectic methods is symplectic but symmetric only if $\gamma_1 = \gamma_2$.

However, for (non-partitioned) Runge–Kutta methods and for quadratic Hamiltonians $H(y) = \frac{1}{2} y^T C y$ (C is a symmetric real matrix), where the corresponding system (2.5) is linear,

$$\dot{y} = J^{-1} C y, \tag{4.7}$$

we shall see that both concepts are equivalent.

A Runge–Kutta method, applied with step size h to a linear system $\dot{y} = Ly$, is equivalent to

$$y_1 = R(hL)y_0, \tag{4.8}$$

where the rational function $R(z)$ is given by

$$R(z) = 1 + z b^T (I - zA)^{-1} \mathbb{1}, \tag{4.9}$$

$A = (a_{ij})$, $b^T = (b_1,\dots,b_s)$, and $\mathbb{1}^T = (1,\dots,1)$. The function $R(z)$ is called the *stability function* of the method, and it is familiar to us from the study of stiff differential equations (see e.g., Hairer & Wanner (1996), Chap. IV.3).

For the explicit Euler method, the implicit Euler method and the implicit midpoint rule, the stability function $R(z)$ is given by

$$1 + z, \qquad \frac{1}{1-z}, \qquad \frac{1 + z/2}{1 - z/2}.$$

Theorem 4.9. *For Runge–Kutta methods the following statements are equivalent:*

- *the method is symmetric for linear problems $\dot y = Ly$;*
- *the method is symplectic for problems (4.7) with symmetric C;*
- *the stability function satisfies $R(-z)R(z) = 1$ for all complex z.*

Proof. The method $y_1 = R(hL)y_0$ is symmetric, if and only if $y_0 = R(-hL)y_1$ holds for all initial values y_0. But this is equivalent to $R(-hL)R(hL) = I$.

Since $\Phi_h'(y_0) = R(hL)$, symplecticity of the method for the problem (4.7) is defined by $R(hJ^{-1}C)^T J R(hJ^{-1}C) = J$. For $R(z) = P(z)/Q(z)$ this is equivalent to

$$P(hJ^{-1}C)^T J P(hJ^{-1}C) = Q(hJ^{-1}C)^T J Q(hJ^{-1}C). \tag{4.10}$$

By the symmetry of C, the matrix $L := J^{-1}C$ satisfies $L^T J = -JL$ and hence also $(L^k)^T J = J(-L)^k$ for $k = 0, 1, 2, \ldots$. Consequently, (4.10) is equivalent to

$$P(-hJ^{-1}C)P(hJ^{-1}C) = Q(-hJ^{-1}C)Q(hJ^{-1}C),$$

which is nothing other than $R(-hJ^{-1}C)R(hJ^{-1}C) = I$. □

VI.5 Generating Functions

> ... by which the study of the motions of all free systems of attracting or repelling points is reduced to the search and differentiation of one central relation, or characteristic function. (W.R. Hamilton 1834)

> Professor Hamilton hat ... das merkwürdige Resultat gefunden, dass ... sich die Integralgleichungen der Bewegung ... sämmtlich durch die partiellen Differentialquotienten einer einzigen Function darstellen lassen. (C.G.J. Jacobi 1837)

We enter here the second heaven of Hamiltonian theory, the realm of partial differential equations and generating functions. The starting point of this theory was the discovery of Hamilton that the motion of the system is completely described by a "characteristic" function S, and that S is the solution of a partial differential equation, now called the *Hamilton–Jacobi differential equation*.

It was noticed later, especially by Siegel (see Siegel & Moser 1971, §3), that such a function S is directly connected to any symplectic map. It received the name *generating function*.

VI.5.1 Existence of Generating Functions

We now consider a fixed Hamiltonian system and a fixed time interval and denote by the column vectors p and q the *initial values* $p_1, \ldots, p_d$ and $q_1, \ldots, q_d$ at t_0 of a trajectory. The *final values* at t_1 are written as P and Q. We thus have a mapping $(p, q) \mapsto (P, Q)$ which, as we know, is symplectic on an open set U.

The following results are conveniently formulated in the notation of differential forms. For a function F we denote by $dF = F'$ its (Fréchet) derivative. We denote by $dq = (dq_1, \ldots, dq_d)^T$ the derivative of the coordinate projection $(p, q) \mapsto q$.

Theorem 5.1. *A mapping $\varphi : (p, q) \mapsto (P, Q)$ is symplectic if and only if there exists locally a function $S(p, q)$ such that*

$$P^T\, dQ - p^T\, dq = dS. \tag{5.1}$$

This means that $P^T\, dQ - p^T\, dq$ is a total differential.

Proof. We split the Jacobian of φ into the natural 2×2 block matrix

$$\frac{\partial(P, Q)}{\partial(p, q)} = \begin{pmatrix} P_p & P_q \\ Q_p & Q_q \end{pmatrix}.$$

Inserting this into (2.6) and multiplying out shows that the three conditions

$$P_p^T Q_p = Q_p^T P_p, \qquad P_p^T Q_q - I = Q_p^T P_q, \qquad Q_q^T P_q = P_q^T Q_q \tag{5.2}$$

are equivalent to symplecticity. We now insert $dQ = Q_p\, dp + Q_q\, dq$ into the left-hand side of (5.1) and obtain

$$\left(P^T Q_p,\ P^T Q_q - p^T\right) \begin{pmatrix} dp \\ dq \end{pmatrix} = \begin{pmatrix} Q_p^T P \\ Q_q^T P - p \end{pmatrix}^T \begin{pmatrix} dp \\ dq \end{pmatrix}.$$

To apply the Integrability Lemma 2.7, we just have to verify the symmetry of the Jacobian of the coefficient vector,

$$\begin{pmatrix} Q_p^T P_p & Q_p^T P_q \\ Q_q^T P_p - I & Q_q^T P_q \end{pmatrix} + \sum_i P_i\, \frac{\partial^2 Q_i}{\partial(p, q)^2}. \tag{5.3}$$

Since the Hessians of Q_i are symmetric anyway, it is immediately clear that the symmetry of the matrix (5.3) is equivalent to the symplecticity conditions (5.2). □

Reconstruction of the Symplectic Map from S. Up to now we have considered all functions as depending on p and q. The essential idea now is to introduce new coordinates; namely (5.1) suggests using $z = (q, Q)$ instead of $y = (p, q)$. This is a well-defined local change of coordinates $y = \psi(z)$ if p can be expressed in terms of the coordinates (q, Q), which is possible by the implicit function theorem if $\frac{\partial Q}{\partial p}$ is invertible. Abusing our notation we again write $S(q, Q)$ for the transformed function $S(\psi(z))$. Then, by comparing the coefficients of $dS = \frac{\partial S(q,Q)}{\partial q}\, dq + \frac{\partial S(q,Q)}{\partial Q}\, dQ$ with (5.1), we arrive at[3]

$$P = \frac{\partial S}{\partial Q}(q, Q), \qquad p = -\frac{\partial S}{\partial q}(q, Q). \tag{5.4}$$

If the transformation $(p, q) \mapsto (P, Q)$ is symplectic, then it can be reconstructed from the scalar function $S(q, Q)$ by the relations (5.4). By Theorem 5.1 the converse

[3] On the right-hand side we should have put the gradient $\nabla_Q S = (\partial S/\partial Q)^T$. We shall not make this distinction between row and column vectors when there is no danger of confusion.

is also true: *any sufficiently smooth and nondegenerate function $S(q,Q)$ "generates" via (5.4) a symplectic mapping $(p,q) \mapsto (P,Q)$*. This gives us a powerful tool for creating symplectic methods.

Mixed-Variable Generating Functions. Another often useful choice of coordinates for generating symplectic maps are the mixed variables (P,q). For any continuously differentiable function $\widehat{S}(P,q)$ we clearly have $d\widehat{S} = \frac{\partial \widehat{S}}{\partial P}\,dP + \frac{\partial \widehat{S}}{\partial q}\,dq$. On the other hand, since $d(P^TQ) = P^T dQ + Q^T dP$, the symplecticity condition (5.1) can be rewritten as $Q^T dP + p^T dq = d(Q^TP - S)$ for some function S. It therefore follows from Theorem 5.1 that the equations

$$Q = \frac{\partial \widehat{S}}{\partial P}(P,q), \qquad p = \frac{\partial \widehat{S}}{\partial q}(P,q) \tag{5.5}$$

define (locally) a symplectic map $(p,q) \mapsto (P,Q)$ if $\partial^2 \widehat{S}/\partial P \partial q$ is invertible.

Example 5.2. Let $Q = \chi(q)$ be a change of position coordinates. With the generating function $\widehat{S}(P,q) = P^T\chi(q)$ we obtain via (5.5) an extension to a symplectic mapping $(p,q) \mapsto (P,Q)$. The conjugate variables are thus related by $p = \chi'(q)^T P$.

Mappings Close to the Identity. We are mainly interested in the situation where the mapping $(p,q) \mapsto (P,Q)$ is close to the identity. In this case, the choices (p,Q) or (P,q) or $\big((P+p)/2, (Q+q)/2\big)$ of independent variables are convenient and lead to the following characterizations.

Lemma 5.3. *Let $(p,q) \mapsto (P,Q)$ be a smooth transformation, close to the identity. It is symplectic if and only if one of the following conditions holds locally:*

- $Q^T dP + p^T dq = d(P^Tq + S^1)$ *for some function $S^1(P,q)$;*
- $P^T dQ + q^T dp = d(p^TQ - S^2)$ *for some function $S^2(p,Q)$;*
- $(Q-q)^T d(P+p) - (P-p)^T d(Q+q) = 2\,dS^3$ *for some function $S^3\big((P+p)/2, (Q+q)/2\big)$.*

Proof. The first characterization follows from the discussion before formula (5.5) if we put S^1 such that $P^Tq + S^1 = \widehat{S} = Q^TP - S$. For the second characterization we use $d(p^Tq) = p^T dq + q^T dp$ and the same arguments as before. The last one follows from the fact that (5.1) is equivalent to $(Q-q)^T d(P+p) - (P-p)^T d(Q+q) = d\big((P+p)^T(Q-q) - 2S\big)$. □

The generating functions S^1, S^2, and S^3 have been chosen such that we obtain the identity mapping when they are replaced with zero. Comparing the coefficient functions of dq and dP in the first characterization of Lemma 5.3, we obtain

$$p = P + \frac{\partial S^1}{\partial q}(P,q), \qquad Q = q + \frac{\partial S^1}{\partial P}(P,q). \tag{5.6}$$

Whatever the scalar function $S^1(P,q)$ is, the relation (5.6) defines a symplectic transformation $(p,q) \mapsto (P,Q)$. For $S^1(P,q) := hH(P,q)$ we recognize the symplectic Euler method (I.1.9). This is an elegant proof of the symplecticity of this method. The second characterization leads to the adjoint of the symplectic Euler method.

The third characterization of Lemma 5.3 can be written as

$$\begin{aligned} P &= p - \partial_2 S^3\big((P+p)/2, (Q+q)/2\big), \\ Q &= q + \partial_1 S^3\big((P+p)/2, (Q+q)/2\big), \end{aligned} \tag{5.7}$$

which, for $S^3 = hH$, is nothing other than the implicit midpoint rule (I.1.7) applied to a Hamiltonian system. We have used the notation ∂_1 and ∂_2 for the derivative with respect to the first and second argument, respectively. The system (5.7) can also be written in compact form as

$$Y = y + J^{-1}\nabla S^3\big((Y+y)/2\big), \tag{5.8}$$

where $Y = (P,Q)$, $y = (p,q)$, $S^3(w) = S^3(u,v)$ with $w = (u,v)$, and J is the matrix of (2.3).

VI.5.2 Generating Function for Symplectic Runge–Kutta Methods

We have just seen that all symplectic transformations can be written in terms of generating functions. What are these generating functions for symplectic Runge–Kutta methods? The following result, proved by Lasagni in an unpublished manuscript (with the same title as the note Lasagni (1988)), gives an alternative proof for Theorem 4.3.

Theorem 5.4. *Suppose that*

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad \textit{for all } \ i,j \tag{5.9}$$

(see Theorem 4.3). Then, the Runge–Kutta method

$$\begin{aligned} P &= p - h\sum_{i=1}^{s} b_i H_q(P_i,Q_i), \qquad & P_i &= p - h\sum_{j=1}^{s} a_{ij} H_q(P_j,Q_j), \\ Q &= q + h\sum_{i=1}^{s} b_i H_p(P_i,Q_i), \qquad & Q_i &= q + h\sum_{j=1}^{s} a_{ij} H_p(P_j,Q_j) \end{aligned} \tag{5.10}$$

can be written as (5.6) with

$$S^1(P,q,h) = h\sum_{i=1}^{s} b_i H(P_i,Q_i) - h^2 \sum_{i,j=1}^{s} b_i a_{ij} H_q(P_i,Q_i)^T H_p(P_j,Q_j). \tag{5.11}$$

Proof. We first differentiate $S^1(P,q,h)$ with respect to q. Using the abbreviations $H[i] = H(P_i,Q_i)$, $H_p[i] = H_p(P_i,Q_i)$, ..., we obtain

$$\begin{aligned}\frac{\partial}{\partial q}\Big(\sum_i b_i H[i]\Big) &= \sum_i b_i H_p[i]^T\Big(\frac{\partial p}{\partial q} - h\sum_j a_{ij}\frac{\partial}{\partial q}H_q[j]\Big)\\ &+ \sum_i b_i H_q[i]^T\Big(I + h\sum_j a_{ij}\frac{\partial}{\partial q}H_p[j]\Big).\end{aligned}$$

With

$$0 = \frac{\partial p}{\partial q} - h\sum_j b_j\frac{\partial}{\partial q}H_q[j]$$

(this is obtained by differentiating the first relation of (5.10)), Leibniz' rule

$$\frac{\partial}{\partial q}\big(H_q[i]^T H_p[j]\big) = H_q[i]^T\frac{\partial}{\partial q}H_p[j] + H_p[j]^T\frac{\partial}{\partial q}H_q[i]$$

and the condition (5.9) therefore yield the first relation of

$$\frac{\partial S^1(P,q,h)}{\partial q} = h\sum_i b_i H_q[i], \qquad \frac{\partial S^1(P,q,h)}{\partial P} = h\sum_i b_i H_p[i].$$

The second relation is proved in the same way. This shows that the Runge–Kutta formulas (5.10) are equivalent to (5.6). □

It is interesting to note that, whereas Lemma 5.3 guarantees the *local* existence of a generating function S^1, the explicit formula (5.11) shows that for Runge–Kutta methods this generating function is *globally* defined. This means that it is well-defined in the same region where the Hamiltonian $H(p,q)$ is defined.

Theorem 5.5. *A partitioned Runge–Kutta method (II.2.2), satisfying the symplecticity conditions (4.3) and (4.4), is equivalent to (5.6) with*

$$S^1(P,q,h) = h\sum_{i=1}^s b_i H(P_i,Q_i) - h^2\sum_{i,j=1}^s b_i\widehat{a}_{ij}H_q(P_i,Q_i)^T H_p(P_j,Q_j).$$

If the Hamiltonian is of the form $H(p,q) = T(p) + U(q)$, i.e., it is separable, then the condition (4.3) alone implies that the method is of the form (5.6) with

$$S^1(P,q,h) = h\sum_{i=1}^s\Big(b_i U(Q_i) + \widehat{b}_i T(P_i)\Big) - h^2\sum_{i,j=1}^s b_i\widehat{a}_{ij}U_q(Q_i)^T T_p(P_j,).$$

Proof. This is a straightforward extension of the proof of the previous theorem. □

VI.5.3 The Hamilton–Jacobi Partial Differential Equation

C.G.J. Jacobi[4]

We now return to the above construction of S for a symplectic transformation $(p,q) \mapsto (P,Q)$ (see Theorem 5.1). This time, however, we imagine the point $P(t), Q(t)$ to move in the flow of the Hamiltonian system (1.7). We wish to determine a smooth generating function $S(q,Q,t)$, now also depending on t, which generates via (5.4) the symplectic map $(p,q) \mapsto \big(P(t),Q(t)\big)$ of the *exact flow* of the Hamiltonian system.

In accordance with equation (5.4) we have to satisfy

$$\begin{aligned} P_i(t) &= \frac{\partial S}{\partial Q_i}\big(q, Q(t), t\big), \\ p_i &= -\frac{\partial S}{\partial q_i}\big(q, Q(t), t\big). \end{aligned} \tag{5.12}$$

Differentiating the second relation with respect to t yields

$$0 = \frac{\partial^2 S}{\partial q_i \partial t}\big(q,Q(t),t\big) + \sum_{j=1}^{d} \frac{\partial^2 S}{\partial q_i \partial Q_j}\big(q,Q(t),t\big) \cdot \dot{Q}_j(t) \tag{5.13}$$

$$= \frac{\partial^2 S}{\partial q_i \partial t}\big(q,Q(t),t\big) + \sum_{j=1}^{d} \frac{\partial^2 S}{\partial q_i \partial Q_j}\big(q,Q(t),t\big) \cdot \frac{\partial H}{\partial P_j}\big(P(t),Q(t)\big) \tag{5.14}$$

where we have inserted the second equation of (1.7) for $\dot{Q}_j$. Then, using the chain rule, this equation simplifies to

$$\frac{\partial}{\partial q_i}\left(\frac{\partial S}{\partial t} + H\Big(\frac{\partial S}{\partial Q_1}, \ldots, \frac{\partial S}{\partial Q_d}, Q_1, \ldots, Q_d\Big)\right) = 0. \tag{5.15}$$

This motivates the following surprisingly simple relation.

Theorem 5.6. *If $S(q,Q,t)$ is a smooth solution of the partial differential equation*

$$\frac{\partial S}{\partial t} + H\Big(\frac{\partial S}{\partial Q_1}, \ldots, \frac{\partial S}{\partial Q_d}, Q_1, \ldots, Q_d\Big) = 0 \tag{5.16}$$

with initial values satisfying $\frac{\partial S}{\partial q_i}(q,q,0) + \frac{\partial S}{\partial Q_i}(q,q,0) = 0$, and if the matrix $\big(\frac{\partial^2 S}{\partial q_i \partial Q_j}\big)$ is invertible, then the map $(p,q) \mapsto \big(P(t),Q(t)\big)$ defined by (5.12) is the flow $\varphi_t(p,q)$ of the Hamiltonian system (1.7).

Equation (5.16) is called the 'Hamilton–Jacobi partial differential equation'.

[4] Carl Gustav Jacob Jacobi, born: 10 December 1804 in Potsdam (near Berlin), died: 18 February 1851 in Berlin.

Proof. The invertibility of the matrix $\left(\frac{\partial^2 S}{\partial q_i \partial Q_j}\right)$ and the implicit function theorem imply that the mapping $(p,q) \mapsto \big(P(t),Q(t)\big)$ is well-defined by (5.12), and, by differentiation, that (5.13) is true as well.

Since, by hypothesis, $S(q,Q,t)$ is a solution of (5.16), the equations (5.15) and hence also (5.14) are satisfied. Subtracting (5.13) and (5.14), and once again using the invertibility of the matrix $\left(\frac{\partial^2 S}{\partial q_i \partial Q_j}\right)$, we see that necessarily $\dot{Q}(t) = H_p\big(P(t),Q(t)\big)$. This proves the validity of the second equation of the Hamiltonian system (1.7).

The first equation of (1.7) is obtained as follows: differentiate the first relation of (5.12) with respect to t and the Hamilton–Jacobi equation (5.16) with respect to Q_i, then eliminate the term $\frac{\partial^2 S}{\partial Q_i \partial t}$. Using $\dot{Q}(t) = H_p\big(P(t),Q(t)\big)$, this leads in a straightforward way to $\dot{P}(t) = -H_q\big(P(t),Q(t)\big)$. The condition on the initial values of S ensures that $(P(0),Q(0)) = (p,q)$. □

In the hands of Jacobi (1842), this equation turned into a powerful tool for the analytic integration of many difficult problems. One has, in fact, to find a solution of (5.16) which contains sufficiently many parameters. This is often possible with the method of separation of variables. An example is presented in Exercise 11.

Hamilton–Jacobi Equation for S^1, S^2, and S^3. We now express the Hamilton–Jacobi differential equation in the coordinates used in Lemma 5.3. In these coordinates it is also possible to prescribe initial values for S at $t = 0$.

From the proof of Lemma 5.3 we know that the generating functions in the variables (q,Q) and (P,q) are related by

$$S^1(P,q,t) = P^T(Q-q) - S(q,Q,t). \tag{5.17}$$

We consider P, q, t as independent variables, and we differentiate this relation with respect to t. Using the first relation of (5.12) this gives

$$\frac{\partial S^1}{\partial t}(P,q,t) = P^T \frac{\partial Q}{\partial t} - \frac{\partial S}{\partial Q}(q,Q,t)\frac{\partial Q}{\partial t} - \frac{\partial S}{\partial t}(q,Q,t) = -\frac{\partial S}{\partial t}(q,Q,t).$$

Differentiating (5.17) with respect to P yields

$$\frac{\partial S^1}{\partial P}(P,q,t) = Q - q + P^T \frac{\partial Q}{\partial P} - \frac{\partial S}{\partial Q}(q,Q,t)\frac{\partial Q}{\partial P} = Q - q.$$

Inserting $\frac{\partial S}{\partial Q} = P$ and $Q = q + \frac{\partial S^1}{\partial P}$ into the Hamilton–Jacobi equation (5.16) we are led to the equation of the following theorem.

Theorem 5.7. *If $S^1(P,q,t)$ is a solution of the partial differential equation*

$$\frac{\partial S^1}{\partial t}(P,q,t) \;=\; H\Big(P, q + \frac{\partial S^1}{\partial P}(P,q,t)\Big), \qquad S^1(P,q,0) = 0, \tag{5.18}$$

then the mapping $(p,q) \mapsto \big(P(t),Q(t)\big)$, defined by (5.6), is the exact flow of the Hamiltonian system (1.7).

Proof. Whenever the mapping $(p,q) \mapsto \big(P(t),Q(t)\big)$ can be written as (5.12) with a function $S(q,Q,t)$, and when the invertibility assumption of Theorem 5.6 holds, the proof is done by the above calculations. Since our mapping, for $t=0$, reduces to the identity and cannot be written as (5.12), we give a direct proof.

Let $S^1(P,q,t)$ be given by the Hamilton–Jacobi equation (5.18), and assume that $(p,q) \mapsto (P,Q) = \big(P(t),Q(t)\big)$ is the transformation given by (5.6). Differentiation of the first relation of (5.6) with respect to time t and using (5.18) yields[5]

$$\Big(I + \frac{\partial^2 S^1}{\partial P \partial q}(P,q,t)\Big)\dot{P} \;=\; -\frac{\partial^2 S^1}{\partial t \partial q}(P,q,t) \;=\; -\Big(I + \frac{\partial^2 S^1}{\partial P \partial q}(P,q,t)\Big)\frac{\partial H}{\partial Q}(P,Q).$$

Differentiation of the second relation of (5.6) gives

$$\begin{aligned}\dot{Q} \;&=\; \frac{\partial^2 S^1}{\partial t \partial P}(P,q,t) + \frac{\partial^2 S^1}{\partial P^2}(P,q,t)\dot{P} \\ &=\; \frac{\partial H}{\partial P}(P,Q) + \frac{\partial^2 S^1}{\partial P^2}(P,q,t)\Big(\frac{\partial H}{\partial Q}(P,Q) + \dot{P}\Big).\end{aligned}$$

Consequently, $\dot{P} = -\frac{\partial H}{\partial Q}(P,Q)$ and $\dot{Q} = \frac{\partial H}{\partial P}(P,Q)$, so that $\big(P(t),Q(t)\big) = \varphi_t(p,q)$ is the exact flow of the Hamiltonian system. □

Writing the Hamilton–Jacobi differential equation in the variables $(P+p)/2$, $(Q+q)/2$ gives the following formula.

Theorem 5.8. *Assume that $S^3(u,v,t)$ is a solution of*

$$\frac{\partial S^3}{\partial t}(u,v,t) \;=\; H\Big(u - \frac{1}{2}\frac{\partial S^3}{\partial v}(u,v,t), v + \frac{1}{2}\frac{\partial S^3}{\partial u}(u,v,t)\Big) \tag{5.19}$$

with initial condition $S^3(u,v,0) = 0$. Then, the exact flow $\varphi_t(p,q)$ of the Hamiltonian system (1.7) satisfies the system (5.7).

Proof. As in the proof of Theorem 5.7, one considers the transformation $(p,q) \mapsto \big(P(t),Q(t)\big)$ defined by (5.7), and then checks by differentiation that $\big(P(t),Q(t)\big)$ is a solution of the Hamiltonian system (1.7). □

Writing $w = (u,v)$ and using the matrix J of (2.3), the Hamilton–Jacobi equation (5.19) can also be written as

$$\frac{\partial S^3}{\partial t}(w,t) \;=\; H\Big(w + \frac{1}{2}J^{-1}\nabla S^3(w,t)\Big), \qquad S^3(w,0) = 0. \tag{5.20}$$

The solution of (5.20) is anti-symmetric in t, i.e.,

$$S^3(w,-t) = -S^3(w,t). \tag{5.21}$$

[5] Due to an inconsistent notation of the partial derivatives $\frac{\partial H}{\partial Q}$, $\frac{\partial S^1}{\partial q}$ as column or row vectors, this formula may be difficult to read. Use indices instead of matrices in order to check its correctness.

This can be seen as follows: let $\varphi_t(w)$ be the exact flow of the Hamiltonian system $\dot y = J^{-1}\nabla H(y)$. Because of (5.8), $S^3(w,t)$ is defined by

$$\varphi_t(w) - w = J^{-1}\nabla S^3\big((\varphi_t(w)+w)/2, t\big).$$

Replacing t with $-t$ and then w with $\varphi_t(w)$ we get from $\varphi_{-t}\big(\varphi_t(t)\big) = w$ that

$$w - \varphi_t(w) = J^{-1}\nabla S^3\big((w+\varphi_t(w))/2, -t\big).$$

Hence $S^3(w,t)$ and $-S^3(w,-t)$ are generating functions of the same symplectic transformation. Since generating functions are unique up to an additive constant (because $dS = 0$ implies $S = \mathit{Const}$), the anti-symmetry (5.21) follows from the initial condition $S^3(w,0) = 0$.

VI.5.4 Methods Based on Generating Functions

To construct symplectic numerical methods of high order, Feng Kang (1986), Feng Kang, Wu, Qin & Wang (1989) and Channell & Scovel (1990) proposed computing an approximate solution of the Hamilton–Jacobi equation. For this one inserts the ansatz

$$S^1(P,q,t) = tG_1(P,q) + t^2G_2(P,q) + t^3G_3(P,q) + \dots$$

into (5.18), and compares like powers of t. This yields

$$\begin{aligned}
G_1(P,q) &= H(P,q),\\
G_2(P,q) &= \frac{1}{2}\Big(\frac{\partial H}{\partial P}\frac{\partial H}{\partial q}\Big)(P,q),\\
G_3(P,q) &= \frac{1}{6}\bigg(\frac{\partial^2 H}{\partial P^2}\Big(\frac{\partial H}{\partial q}\Big)^2 + \frac{\partial^2 H}{\partial P \partial q}\frac{\partial H}{\partial P}\frac{\partial H}{\partial q} + \frac{\partial^2 H}{\partial q^2}\Big(\frac{\partial H}{\partial P}\Big)^2\bigg)(P,q).
\end{aligned}$$

If we use the truncated series

$$S^1(P,q) = hG_1(P,q) + h^2G_2(P,q) + \dots + h^rG_r(P,q) \tag{5.22}$$

and insert it into (5.6), the transformation $(p,q) \mapsto (P,Q)$ defines a symplectic one-step method of order r. Symplecticity follows at once from Lemma 5.3 and order r is a consequence of the fact that the truncation of $S^1(P,q)$ introduces a perturbation of size $\mathcal{O}(h^{r+1})$ in (5.18). We remark that for $r \geq 2$ the methods obtained require the computation of higher derivatives of $H(p,q)$, and for separable Hamiltonians $H(p,q) = T(p) + U(q)$ they are no longer explicit (compared to the symplectic Euler method (3.1)).

The same approach applied to the third characterization of Lemma 5.3 yields

$$S^3(w,h) = hG_1(w) + h^3G_3(w) + \dots + h^{2r-1}G_{2r-1}(w),$$

where $G_1(w) = H(w)$,

$$G_3(w) \;=\; \frac{1}{24}\,\nabla^2 H(w)\Big(J^{-1}\nabla H(w), J^{-1}\nabla H(w)\Big),$$

and further $G_j(w)$ can be obtained by comparing like powers of h in (5.20). In this way we get symplectic methods of order $2r$. Since $S^3(w,h)$ has an expansion in odd powers of h, the resulting method is symmetric.

The Approach of Miesbach & Pesch. With the aim of avoiding higher derivatives of the Hamiltonian in the numerical method, Miesbach & Pesch (1992) propose considering generating functions of the form

$$S^3(w,h) = h\sum_{i=1}^{s} b_i H\Big(w + hc_i J^{-1}\nabla H(w)\Big), \tag{5.23}$$

and to determine the free parameters b_i, c_i in such a way that the function of (5.23) agrees with the solution of the Hamilton–Jacobi equation (5.20) up to a certain order. For $b_{s+1-i} = b_i$ and $c_{s+1-i} = -c_i$ this function satisfies $S^3(w,-h) = -S^3(w,h)$, so that the resulting method is symmetric. A straightforward computation shows that it yields a method of order 4 if

$$\sum_{i=1}^{s} b_i = 1, \qquad \sum_{i=1}^{s} b_i c_i^2 = \frac{1}{12}.$$

For $s = 3$, these equations are fulfilled for $b_1 = b_3 = 5/18$, $b_2 = 4/9$, $c_1 = -c_3 = \sqrt{15}/10$, and $c_2 = 0$. Since the function S^3 of (5.23) has to be inserted into (5.20), these methods still need second derivatives of the Hamiltonian.

VI.6 Variational Integrators

A third approach to symplectic integrators comes from using discretized versions of Hamilton's principle, which determines the equations of motion from a variational problem. This route has been taken by Suris (1990), MacKay (1992) and in a series of papers by Marsden and coauthors, see the review by Marsden & West (2001) and references therein. Basic theoretical properties were formulated by Maeda (1980,1982) and Veselov (1988,1991) in a non-numerical context.

VI.6.1 Hamilton's Principle

> Ours, according to Leibniz, is the best of all possible worlds, and the laws of nature can therefore be described in terms of extremal principles.
>
> (C.L. Siegel & J.K. Moser 1971, p. 1)

> Man scheint dies Princip früher ... unbemerkt gelassen zu haben. *Hamilton* ist der erste, der von diesem Princip ausgegangen ist.
>
> (C.G.J. Jacobi 1842, p. 58)

> Hamilton gave an improved mathematical formulation of a principle which was well established by the fundamental investigations of Euler and Lagrange; the integration process employed by him was likewise known to Lagrange. The name "Hamilton's principle", coined by Jacobi, was not adopted by the scientists of the last century. It came into use, however, through the textbooks of more recent date.
>
> (C. Lanczos 1949, p. 114)

Lagrange's equations of motion (1.4) can be viewed as the Euler–Lagrange equations for the variational problem of extremizing the *action integral*

$$\mathcal{S}(q) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t))\, dt \tag{6.1}$$

among all curves $q(t)$ that connect two given points q_0 and q_1:

$$q(t_0) = q_0\ , \quad q(t_1) = q_1\ . \tag{6.2}$$

In fact, assuming $q(t)$ to be extremal and considering a variation $q(t) + \varepsilon\, \delta q(t)$ with the same end-points, i.e., with $\delta q(t_0) = \delta q(t_1) = 0$, gives, using a partial integration,

$$0 = \frac{d}{d\varepsilon}\Big|_{\varepsilon=0} \mathcal{S}(q + \varepsilon\, \delta q) = \int_{t_0}^{t_1} \Big(\frac{\partial L}{\partial q}\, \delta q + \frac{\partial L}{\partial \dot{q}}\, \delta \dot{q} \Big) dt = \int_{t_0}^{t_1} \Big(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \Big) \delta q\, dt\,,$$

which leads to (1.4). The principle that the motion extremizes the action integral is known as *Hamilton's principle*.

We now consider the action integral as a function of (q_0, q_1), for the solution $q(t)$ of the Euler–Lagrange equations (1.4) with these boundary values (this exists uniquely locally at least if q_0, q_1 are sufficiently close),

$$S(q_0, q_1) = \int_{t_0}^{t_1} L(q(t), \dot{q}(t))\, dt\ . \tag{6.3}$$

The partial derivative of S with respect to q_0 is, again using partial integration,

$$\begin{aligned} \frac{\partial S}{\partial q_0} &= \int_{t_0}^{t_1} \Big(\frac{\partial L}{\partial q} \frac{\partial q}{\partial q_0} + \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q_0} \Big)\, dt \\ &= \frac{\partial L}{\partial \dot{q}} \frac{\partial q}{\partial q_0}\Big|_{t_0}^{t_1} + \int_{t_0}^{t_1} \Big(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \Big) \frac{\partial q}{\partial q_0}\, dt = -\frac{\partial L}{\partial \dot{q}}(q_0, \dot{q}_0) \end{aligned}$$

with $\dot{q}_0 = \dot{q}(t_0)$, where the last equality follows from (1.4) and (6.2). In view of the definition (1.5) of the conjugate momenta, $p = \partial L / \partial \dot{q}$, the last term is simply $-p_0$. Computing $\partial S / \partial q_1 = p_1$ in the same way, we thus obtain for the differential of S

$$dS = \frac{\partial S}{\partial q_1}\, dq_1 + \frac{\partial S}{\partial q_0}\, dq_0 = p_1\, dq_1 - p_0\, dq_0 \tag{6.4}$$

which is the basic formula for symplecticity generating functions (see (5.1) above), obtained here by working with the Lagrangian formalism.

VI.6.2 Discretization of Hamilton's Principle

Discrete-time versions of Hamilton's principle are of mathematical interest in their own right, see Maeda (1980,1982), Veselov (1991) and references therein. Here they are considered with the aim of deriving or understanding numerical approximation schemes. The discretized Hamilton principle consists of extremizing, for given q_0 and q_N, the sum

$$\mathcal{S}_h(\{q_n\}_0^N) = \sum_{n=0}^{N-1} L_h(q_n, q_{n+1}) \,. \tag{6.5}$$

We think of the *discrete Lagrangian* L_h as an approximation

$$L_h(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L(q(t), \dot{q}(t))\, dt \,, \tag{6.6}$$

where $q(t)$ is the solution of the Euler–Lagrange equations (1.4) with boundary values $q(t_n) = q_n$, $q(t_{n+1}) = q_{n+1}$. If equality holds in (6.6), then it is clear from the continuous Hamilton principle that the exact solution values $\{q(t_n)\}$ of the Euler–Lagrange equations (1.4) extremize the action sum $\mathcal{S}_h$. Before we turn to concrete examples of approximations L_h, we continue with the general theory which is analogous to the continuous case.

The requirement $\partial \mathcal{S}_h / \partial q_n = 0$ for an extremum yields the *discrete Euler–Lagrange equations*

$$\frac{\partial L_h}{\partial y}(q_{n-1}, q_n) + \frac{\partial L_h}{\partial x}(q_n, q_{n+1}) = 0 \tag{6.7}$$

for $n = 1, \ldots, N-1$, where the partial derivatives refer to $L_h = L_h(x, y)$. This gives a three-term difference scheme for determining $q_1, \ldots, q_{N-1}$.

We now set

$$S_h(q_0, q_N) = \sum_{n=0}^{N-1} L_h(q_n, q_{n+1})$$

where $\{q_n\}$ is a solution of the discrete Euler–Lagrange equations (6.7) with the boundary values q_0 and q_N. With (6.7) the partial derivatives reduce to

$$\frac{\partial S_h}{\partial q_0} = \frac{\partial L_h}{\partial x}(q_0, q_1), \qquad \frac{\partial S_h}{\partial q_N} = \frac{\partial L_h}{\partial y}(q_{N-1}, q_N) \,.$$

We introduce the *discrete momenta* via a discrete Legendre transformation,

$$p_n = -\frac{\partial L_h}{\partial x}(q_n, q_{n+1}) \,. \tag{6.8}$$

The above formula and (6.7) for $n = N$ then yield

$$dS_h = p_N\, dq_N - p_0\, dq_0. \tag{6.9}$$

If (6.8) defines a bijection between p_n and q_{n+1} for given q_n, then we obtain a one-step method $\Phi_h : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ by composing the inverse discrete Legendre transform, a step with the discrete Euler–Lagrange equations, and the discrete Legendre transformation as shown in the diagram:

$$\begin{array}{ccc} & \overset{(6.7)}{} & \\ (q_n, q_{n+1}) & \longrightarrow & (q_{n+1}, q_{n+2}) \\ (6.8)\uparrow & & \downarrow(6.8) \\ (p_n, q_n) & & (p_{n+1}, q_{n+1}) \end{array}$$

The method is symplectic by (6.9) and Theorem 5.1. A short-cut in the computation is obtained by noting that (6.7) and (6.8) (for $n+1$ instead of n) imply

$$p_{n+1} = \frac{\partial L_h}{\partial y}(q_n, q_{n+1}) \,, \tag{6.10}$$

which yields the scheme

$$(p_n, q_n) \overset{(6.8)}{\longrightarrow} (q_n, q_{n+1}) \overset{(6.10)}{\longrightarrow} (p_{n+1}, q_{n+1}) \,.$$

Let us summarize these considerations, which can be found in Maeda (1980), Suris (1990), Veselov (1991) and MacKay (1992).

Theorem 6.1. *The discrete Hamilton principle for (6.5) gives the discrete Euler–Lagrange equations (6.7) and the symplectic method*

$$p_n = -\frac{\partial L_h}{\partial x}(q_n, q_{n+1}) \,, \quad p_{n+1} = \frac{\partial L_h}{\partial y}(q_n, q_{n+1}) \,. \tag{6.11}$$

These formulas also show that L_h is a generating function (5.4) for the symplectic map $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$. Conversely, since every symplectic method has a generating function (5.4), it can be interpreted as resulting from Hamilton's principle with the generating function (5.4) as the discrete Lagrangian. The classes of symplectic integrators and variational integrators are therefore identical.

We now turn to simple examples of variational integrators obtained by choosing a discrete Lagrangian L_h with (6.6).

Example 6.2 (MacKay 1992). Choose $L_h(q_n, q_{n+1})$ by approximating $q(t)$ of (6.6) as the linear interpolant of q_n and q_{n+1} and approximating the integral by the trapezoidal rule. This gives

$$L_h(q_n, q_{n+1}) \,=\, \frac{h}{2}\, L\Big(q_n, \frac{q_{n+1}-q_n}{h}\Big) + \frac{h}{2}\, L\Big(q_{n+1}, \frac{q_{n+1}-q_n}{h}\Big) \tag{6.12}$$

and hence the symplectic scheme, with $v_{n+1/2} = (q_{n+1} - q_n)/h$ for brevity,

$$\begin{aligned} p_n &= \frac{1}{2}\frac{\partial L}{\partial \dot q}(q_n, v_{n+1/2}) + \frac{1}{2}\frac{\partial L}{\partial \dot q}(q_{n+1}, v_{n+1/2}) - \frac{h}{2}\frac{\partial L}{\partial q}(q_n, v_{n+1/2}) \\ p_{n+1} &= \frac{1}{2}\frac{\partial L}{\partial \dot q}(q_n, v_{n+1/2}) + \frac{1}{2}\frac{\partial L}{\partial \dot q}(q_{n+1}, v_{n+1/2}) + \frac{h}{2}\frac{\partial L}{\partial q}(q_{n+1}, v_{n+1/2}) \,. \end{aligned}$$

For a mechanical Lagrangian $L(q,\dot q) = \frac{1}{2}\dot q^T M\dot q - U(q)$ this reduces to the Störmer–Verlet method

$$\begin{aligned} Mv_{n+1/2} &= p_n + \frac{1}{2}hF_n \\ q_{n+1} &= q_n + hv_{n+1/2} \\ p_{n+1} &= Mv_{n+1/2} + \frac{1}{2}hF_{n+1} \end{aligned}$$

where $F_n = -\nabla U(q_n)$. In this case, the discrete Euler–Lagrange equations (6.7) become the familiar second-difference formula $M(q_{n+1} - 2q_n + q_{n-1}) = h^2 F_n$.

Example 6.3 (Wendlandt & Marsden 1997). Approximating the integral in (6.6) instead by the midpoint rule gives

$$L_h(q_n, q_{n+1}) = hL\Big(\frac{q_{n+1}+q_n}{2}, \frac{q_{n+1}-q_n}{h}\Big). \tag{6.13}$$

This yields the symplectic scheme, with the abbreviations $q_{n+1/2} = (q_{n+1}+q_n)/2$ and $v_{n+1/2} = (q_{n+1}-q_n)/h$,

$$\begin{aligned} p_n &= \frac{\partial L}{\partial \dot q}(q_{n+1/2}, v_{n+1/2}) - \frac{h}{2}\frac{\partial L}{\partial q}(q_{n+1/2}, v_{n+1/2}) \\ p_{n+1} &= \frac{\partial L}{\partial \dot q}(q_{n+1/2}, v_{n+1/2}) + \frac{h}{2}\frac{\partial L}{\partial q}(q_{n+1/2}, v_{n+1/2}) \,. \end{aligned}$$

For $L(q,\dot q) = \frac{1}{2}\dot q^T M\dot q - U(q)$ this becomes the implicit midpoint rule

$$\begin{aligned} Mv_{n+1/2} &= p_n + \frac{1}{2}hF_{n+1/2} \\ q_{n+1} &= q_n + hv_{n+1/2} \\ p_{n+1} &= Mv_{n+1/2} + \frac{1}{2}hF_{n+1/2} \end{aligned}$$

with $F_{n+1/2} = -\nabla U(\frac{1}{2}(q_{n+1}+q_n))$.

VI.6.3 Symplectic Partitioned Runge–Kutta Methods Revisited

To obtain higher-order variational integrators, Marsden & West (2001) consider the discrete Lagrangian

$$L_h(q_0, q_1) = h\sum_{i=1}^{s} b_i L\big(u(c_i h), \dot u(c_i h)\big) \tag{6.14}$$

where $u(t)$ is the polynomial of degree s with $u(0) = q_0$, $u(h) = q_1$ which extremizes the right-hand side. They then show that the corresponding variational integrator can be realized as a partitioned Runge–Kutta method. We here consider the slightly more general case

$$L_h(q_0, q_1) = h \sum_{i=1}^{s} b_i L(Q_i, \dot{Q}_i) \tag{6.15}$$

where

$$Q_i = q_0 + h \sum_{j=1}^{s} a_{ij} \dot{Q}_j$$

and the $\dot{Q}_i$ are chosen to extremize the above sum under the constraint

$$q_1 = q_0 + h \sum_{i=1}^{s} b_i \dot{Q}_i \; .$$

We assume that all the b_i are non-zero and that their sum equals 1. Note that (6.14) is the special case of (6.15) where the a_{ij} and b_i are integrals (II.1.10) of Lagrange polynomials as for collocation methods.

With a Lagrange multiplier $\lambda = (\lambda_1, \ldots, \lambda_d)$ for the constraint, the extremality conditions obtained by differentiating (6.15) with respect to $\dot{Q}_j$ for $j = 1, \ldots, s$, read

$$\sum_{i=1}^{s} b_i \frac{\partial L}{\partial q}(Q_i, \dot{Q}_i) h a_{ij} + b_j \frac{\partial L}{\partial \dot{q}}(Q_j, \dot{Q}_j) = b_j \lambda \; .$$

With the notation

$$\dot{P}_i = \frac{\partial L}{\partial q}(Q_i, \dot{Q}_i) \; , \qquad P_i = \frac{\partial L}{\partial \dot{q}}(Q_i, \dot{Q}_i) \tag{6.16}$$

this simplifies to

$$b_j P_j = b_j \lambda - h \sum_{i=1}^{s} b_i a_{ij} \dot{P}_i \; . \tag{6.17}$$

The symplectic method of Theorem 6.1 now becomes

$$\begin{aligned} p_0 &= -\frac{\partial L_h}{\partial x}(q_0, q_1) \\ &= -h \sum_{i=1}^{s} b_i \dot{P}_i \Big(I + h \sum_{j=1}^{s} a_{ij} \frac{\partial \dot{Q}_j}{\partial q_0} \Big) - h \sum_{j=1}^{s} b_j P_j \frac{\partial \dot{Q}_j}{\partial q_0} \\ &= -h \sum_{i=1}^{s} b_i \dot{P}_i + \lambda \; . \end{aligned}$$

In the last equality we use (6.17) and $h \sum_j b_j \partial \dot{Q}_j / \partial q_0 = -I$, which follows from differentiating the constraint. In the same way we obtain

$$p_1 = \frac{\partial L_h}{\partial y}(q_0, q_1) = \lambda \, .$$

Putting these formulas together, we see that (p_1, q_1) result from applying a partitioned Runge–Kutta method to the Lagrange equations (1.4) written as a differential-algebraic system

$$\dot p = \frac{\partial L}{\partial q}(q, \dot q) \, , \quad p = \frac{\partial L}{\partial \dot q}(q, \dot q) \, . \tag{6.18}$$

That is

$$\begin{aligned} p_1 &= p_0 + h \sum_{i=1}^{s} b_i \dot P_i \, , & q_1 &= q_0 + h \textstyle\sum_{i=1}^{s} b_i \dot Q_i \, , \\ P_i &= p_0 + h \sum_{j=1}^{s} \widehat a_{ij} \dot P_j \, , & Q_i &= q_0 + h \textstyle\sum_{j=1}^{s} a_{ij} \dot Q_j \, , \end{aligned} \tag{6.19}$$

with $\widehat a_{ij} = b_j - b_j a_{ji}/b_i$ so that the symplecticity condition (4.3) is fulfilled, and with $P_i, Q_i, \dot P_i, \dot Q_i$ related by (6.16). Since equations (6.16) are of the same form as (6.18), the proof of Theorem 1.3 shows that they are equivalent to

$$\dot P_i = -\frac{\partial H}{\partial q}(P_i, Q_i) \, , \quad \dot Q_i = \frac{\partial H}{\partial p}(P_i, Q_i) \tag{6.20}$$

with the Hamiltonian $H = p^T \dot q - L(q, \dot q)$ of (1.6). We have thus proved the following, which is similar in spirit to a result of Suris (1990).

Theorem 6.4. *The variational integrator with the discrete Lagrangian (6.15) is equivalent to the symplectic partitioned Runge–Kutta method (6.19), (6.20) applied to the Hamiltonian system with the Hamiltonian (1.6).* □

In particular, as noted by Marsden & West (2001), choosing Gaussian quadrature in (6.14) gives the Gauss collocation method applied to the Hamiltonian system, while Lobatto quadrature gives the Lobatto IIIA - IIIB pair.

VI.6.4 Noether's Theorem

> . . . enthält Satz I alle in Mechanik u.s.w. bekannten Sätze über erste Integrale. (E. Noether 1918)

We now return to the subject of Chap. IV, i.e., the existence of first integrals, but here in the context of Hamiltonian systems. E. Noether found the surprising result that continuous *symmetries* in the Lagrangian lead to such first integrals. We give in the following a version of her "Satz I", specialized to our needs, with a particularly short proof.

Theorem 6.5 (Noether 1918). *Consider a system with Hamiltonian $H(p, q)$ and Lagrangian $L(q, \dot q)$. Suppose $\{g_s : s \in \mathbb{R}\}$ is a one-parameter group of transformations ($g_s \circ g_r = g_{s+r}$) which leaves the Lagrangian invariant:*

$$L(g_s(q), g_s'(q)\dot{q}) = L(q, \dot{q}) \quad \textit{for all } s \textit{ and all } (q, \dot{q}). \tag{6.21}$$

Let $a(q) = (d/ds)|_{s=0}\, g_s(q)$ *be defined as the vector field with flow* $g_s(q)$*. Then*

$$I(p, q) = p^T a(q) \tag{6.22}$$

is a first integral of the Hamiltonian system.

Example 6.6. Let G be a matrix Lie group with Lie algebra $\mathfrak{g}$ (see Sect. IV.6). Suppose $L(Qq, Q\dot{q}) = L(q, \dot{q})$ for all $Q \in G$. Then $p^T Aq$ is a first integral for every $A \in \mathfrak{g}$. (Take $g_s(q) = \exp(sA)q$.) For example, $G = SO(n)$ yields conservation of angular momentum.

We prove Theorem 6.5 by using the discrete analogue, which reads as follows.

Theorem 6.7. *Suppose the one-parameter group of transformations* $\{g_s : s \in \mathbb{R}\}$ *leaves the discrete Lagrangian* $L_h(q_0, q_1)$ *invariant:*

$$L_h(g_s(q_0), g_s(q_1)) = L_h(q_0, q_1) \quad \textit{for all } s \textit{ and all } (q_0, q_1). \tag{6.23}$$

Then (6.22) is a first integral of the method (6.11), i.e., $p_{n+1}^T a(q_{n+1}) = p_n^T a(q_n)$.

Proof. Differentiating (6.23) with respect to s gives

$$0 = \frac{d}{ds}\Big|_{s=0} L_h(g_s(q_0), g_s(q_1)) = \frac{\partial L_h}{\partial x}(q_0, q_1)a(q_0) + \frac{\partial L_h}{\partial y}(q_0, q_1)a(q_1).$$

By (6.11) this becomes $0 = -p_0^T a(q_0) + p_1^T a(q_1)$. □

Theorem 6.5 now follows by choosing $L_h = S$ of (6.3) and noting (6.4) and

$$\begin{aligned} S(q(t_0), q(t_1)) &= \int_{t_0}^{t_1} L\big(q(t), \dot{q}(t)\big)\, dt \\ &= \int_{t_0}^{t_1} L\Big(g_s(q(t)), \frac{d}{dt} g_s(q(t))\Big)\, dt = S\Big(g_s(q(t_0)), g_s(q(t_1))\Big). \end{aligned}$$

Theorem 6.7 has the appearance of giving a rich source of first integrals for symplectic methods. However, it must be noted that, unlike the case of the exact flow map in the above formula, the invariance (6.21) of the Lagrangian L does not in general imply the invariance (6.23) of the discrete Lagrangian L_h of the numerical method. A noteworthy exception arises for linear transformations g_s as in Example 6.6, for which Theorem 6.7 yields the conservation of quadratic first integrals $p^T Aq$, such as angular momentum, by symplectic partitioned Runge–Kutta methods — a property we already know from Theorem IV.2.4. For Hamiltonian systems with an associated Lagrangian $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M\dot{q} - U(q)$, all first integrals originating from Noether's Theorem are quadratic (see Exercise 13).

VI.7 Characterization of Symplectic Methods

Up to now in this chapter, we have presented sufficient conditions for the symplecticity of numerical integrators (usually in terms of certain coefficients). Here, we will prove *necessary* conditions for symplecticity, i.e., answer the question as to which methods are *not* symplectic. It will turn out that the sufficient conditions of Sect. VI.4, under an irreducibility condition on the method, are also necessary. The main tool is the Taylor series expansion of the numerical flow $y_0 \mapsto \Phi_h(y_0)$, which we assume to be a B-series (or a P-series).

VI.7.1 B-Series Methods Conserving Quadratic First Integrals

The numerical solution of a Runge–Kutta method (II.1.4) can be written as a B-series

$$y_1 \;=\; B(a, y_0) \;=\; y_0 + \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)}\, a(\tau)\, F(\tau)(y_0) \tag{7.1}$$

with coefficients $a(\tau)$ given by

$$a(\tau) = \sum_{i=1}^{s} b_i \mathbf{g}_i(\tau) \qquad \text{for} \quad \tau \in T \tag{7.2}$$

(see (III.1.16) and Sect. III.1.2). Our aim is to express the sufficient condition for the exact conservation of quadratic first integrals (which is the same as for symplecticity) in terms of the coefficients $a(\tau)$. For this we multiply (4.2) by $\mathbf{g}_i(u) \cdot \mathbf{g}_j(v)$ (where $u = [u_1, \ldots, u_m]$ and $v = [v_1, \ldots, v_l]$ are trees in T) and we sum over all i and j. Using (III.1.13) and the recursion (III.1.15) this yields

$$\sum_{i=1}^{s} b_i \mathbf{g}_i(u \circ v) + \sum_{j=1}^{s} b_j \mathbf{g}_j(v \circ u) \;=\; \Big(\sum_{i=1}^{s} b_i \mathbf{g}_i(u)\Big)\Big(\sum_{j=1}^{s} b_j \mathbf{g}_j(v)\Big),$$

where we have used the Butcher product (see, e.g., Butcher (1987), Sect. 143)

$$u \circ v = [u_1, \ldots, u_m, v], \qquad v \circ u = [v_1, \ldots, v_l, u] \tag{7.3}$$

(compare also Definition III.3.7 and Fig. 7.1 below). Because of (7.2), this implies

$$a(u \circ v) + a(v \circ u) = a(u) \cdot a(v) \qquad \text{for} \quad u, v \in T. \tag{7.4}$$

We now forget that the B-series (7.1) has been obtained from a Runge–Kutta method, and we ask the following question: is the condition (7.4) sufficient for a B-series method defined by (7.1) to conserve exactly quadratic first integrals (and to be symplectic)? The next theorem shows that this is indeed true, and we shall see later that condition (7.4) is also necessary (cf. Chartier, Faou & Murua 2005).

Theorem 7.1. *Consider a B-series method $\Phi_h(y) = B(a,y)$ and problems $\dot y = f(y)$ having $Q(y) = y^T C y$ (with symmetric matrix C) as first integral.*

If the coefficients $a(\tau)$ satisfy (7.4), then the method exactly conserves $Q(y)$ and it is symplectic.

Proof. a) Under the assumptions of the theorem we shall prove in part (c) that

$$B(a,y)^T C B(a,y) = y^T C y + \sum_{u,v\in T} \frac{h^{|u|+|v|}}{\sigma(u)\sigma(v)} m(u,v)\, F(u)(y)^T C F(v)(y) \quad (7.5)$$

with $m(u,v) = a(u)\cdot a(v) - a(u\circ v) - a(v\circ u)$. Condition (7.4) is equivalent to $m(u,v) = 0$ and thus implies the exact conservation of $Q(y) = y^T C y$.

To prove symplecticity of the method it is sufficient to show that the diagram of Lemma 4.1 commutes for general B-series methods. This is seen by differentiating the elementary differentials and by comparing them with those for the augmented system (Exercise 8). Symplecticity of the method thus follows as in Sect. VI.4.1 form the fact that the symplecticity relation is a quadratic first integral of the augmented system.

b) Since $Q(y) = y^T C y$ is a first integral of $\dot y = f(y)$, we have $y^T C f(y) = 0$ for all y. Differentiating m times this relation with respect to y yields

$$\sum_{j=1}^{m} k_j^T C f^{(m-1)}(y)\big(k_1,\dots,k_{j-1},k_{j+1}\dots,k_m\big) + y^T C f^{(m)}(y)\big(k_1,\dots,k_m\big) = 0.$$

Putting $k_j = F(\tau_j)(y)$ we obtain the formula

$$y^T C F([\tau_1,\dots,\tau_m])(y) = -\sum_{j=1}^{m} F(\tau_j)(y)^T C F([\tau_1,\dots,\tau_{j-1},\tau_{j+1},\dots,\tau_m])(y),$$

which can also be written in the form

$$y^T C\, \frac{F(\tau)(y)}{\sigma(\tau)} \;=\; -\sum_{u,v\in T,\, v\circ u=\tau} \frac{F(u)(y)^T}{\sigma(u)}\, C\, \frac{F(v)(y)}{\sigma(v)}. \quad (7.6)$$

c) With (7.1) the expression $y_1^T C y_1$ becomes

$$\begin{aligned} B(a,y)^T C B(a,y) \;&=\; y^T C y + 2 y^T C \sum_{\tau\in T} \frac{h^{|\tau|}}{\sigma(\tau)}\, a(\tau)\, F(\tau)(y) \\ &+\; \sum_{u,v\in T} \frac{h^{|u|+|v|}}{\sigma(u)\sigma(v)}\, a(u)\, a(v)\, F(u)(y)^T C F(v)(y). \end{aligned}$$

Since C is symmetric, formula (7.6) remains true if we sum over trees u, v such that $u\circ v = \tau$. Inserting both formulas into the sum over τ leads directly to (7.5). □

Extension to P-Series. All the previous results can be extended to partitioned methods. To find the correct conditions on the coefficients of the P-series, we use the fact that the numerical solution of a partitioned Runge–Kutta method (II.2.2) is a P-series

$$\begin{pmatrix} p_1 \\ q_1 \end{pmatrix} = \begin{pmatrix} P_p(a,(p_0,q_0)) \\ P_q(a,(p_0,q_0)) \end{pmatrix} = \begin{pmatrix} p_0 \\ q_0 \end{pmatrix} + \begin{pmatrix} \sum_{u\in TP_p} \frac{h^{|u|}}{\sigma(u)}\, a(u)\, F(u)(p_0,q_0) \\ \sum_{v\in TP_q} \frac{h^{|v|}}{\sigma(v)}\, a(v)\, F(v)(p_0,q_0) \end{pmatrix} \tag{7.7}$$

with coefficients $a(\tau)$ given by

$$a(\tau) = \begin{cases} \sum_{i=1}^s b_i \phi_i(\tau) & \text{for} \quad \tau \in TP_p \\ \sum_{i=1}^s \widehat{b}_i \phi_i(\tau) & \text{for} \quad \tau \in TP_q \end{cases} \tag{7.8}$$

(see Theorem III.2.4). We assume here that the elementary differentials $F(\tau)(p,q)$ originate from a partitioned sytem

$$\dot p = f_1(p,q), \quad \dot q = f_2(p,q), \tag{7.9}$$

such as the Hamiltonian system (1.7). This time we multiply (4.3) by $\phi_i(u)\cdot\phi_j(v)$ (where $u=[u_1,\dots,u_m]_p \in TP_p$ and $v=[v_1,\dots,v_l]_q \in TP_q$) and we sum over all i and j. Using the recursion (III.2.7) this yields

$$\sum_{i=1}^s b_i\phi_i(u\circ v) + \sum_{j=1}^s \widehat{b}_j\phi_j(v\circ u) = \Big(\sum_{i=1}^s b_i\phi_i(u)\Big)\Big(\sum_{j=1}^s \widehat{b}_j\phi_j(v)\Big), \tag{7.10}$$

where $u\circ v=[u_1,\dots,u_m,v]_p$ and $v\circ u=[v_1,\dots,v_l,u]_q$. Because of (7.8), this implies the relation

$$a(u\circ v)+a(v\circ u) = a(u)\cdot a(v) \qquad \text{for} \quad u\in TP_p,\ v\in TP_q. \tag{7.11}$$

Since $\phi_i(\tau)$ is independent of the colour of the root of τ, condition (4.4) implies

$$a(\tau) \text{ is independent of the colour of the root of } \tau. \tag{7.12}$$

Theorem 7.2. *Consider a P-series method $(p_1,q_1)=\Phi_h(p_0,q_0)$ given by (7.7), and a problem (7.9) having $Q(p,q)=p^TEq$ as first integral.*

i) If the coefficients $a(\tau)$ satisfy (7.11) and (7.12), the method exactly conserves $Q(p,q)$ and it is symplectic for general Hamiltonian systems (1.7).

ii) If the coefficients $a(\tau)$ satisfy only (7.11), the method exactly conserves $Q(p,q)$ for problems of the form $\dot p = f_1(q)$, $\dot q = f_2(p)$, and it is symplectic for separable Hamiltonian systems where $H(p,q)=T(p)+U(q)$.

Proof. This is very similar to that of Theorem 7.1. If $Q(p,q)=p^TEq$ is a first integral of (7.9), we have $f_1(p,q)^TEq + p^TEf_2(p,q)=0$ for all p and q. Differentiating m times with respect to p and n times with respect to q yields

$$
\begin{aligned}
0 \;=\;& D_p^m D_q^n f_1(p,q)\big(k_1,\dots,k_m,\ell_1,\dots,\ell_n\big)^T E\, q \\
+\;& p^T E\, D_p^m D_q^n f_2(p,q)\big(k_1,\dots,k_m,\ell_1,\dots,\ell_n\big) \\
+\;& \sum_{j=1}^{n} D_p^m D_q^{n-1} f_1(p,q)\big(k_1,\dots,k_m,\ell_1,\dots,\ell_{j-1},\ell_{j+1},\dots,\ell_n\big)^T E\,\ell_j \\
+\;& \sum_{i=1}^{m} k_i^T E\, D_p^{m-1} D_q^n f_2(p,q)\big(k_1,\dots,k_{i-1},k_{i+1},\dots,k_m,\ell_1,\dots,\ell_n\big).
\end{aligned}
\tag{7.13}
$$

Putting $k_i = F(u_i)(p,q)$ with $u_i \in TP_p$, $\ell_j = F(v_j)(p,q)$ with $v_j \in TP_q$, $\tau_p = [u_1,\dots,u_m,v_1,\dots,v_n]_p$ and $\tau_q = [u_1,\dots,u_m,v_1,\dots,v_n]_q$, we obtain as in part (b) of the proof of Theorem 7.1 that

$$
\begin{aligned}
&\frac{F(\tau_p)(p,q)^T}{\sigma(\tau_p)} E\, q + p^T E\, \frac{F(\tau_q)(p,q)}{\sigma(\tau_q)} \\
&= \sum_{u\circ v=\tau_p} \frac{F(u)(p,q)^T}{\sigma(u)} E\, \frac{F(v)(p,q)}{\sigma(v)} + \sum_{v\circ u=\tau_q} \frac{F(u)(p,q)^T}{\sigma(u)} E\, \frac{F(v)(p,q)}{\sigma(v)},
\end{aligned}
\tag{7.14}
$$

where the sums are over $u \in TP_p$ and $v \in TP_q$.

With (7.7) the expression $p_1^T E\, q_1$ becomes

$$
\begin{aligned}
&P_p(a,(p,q))^T E\, P_q(a,(p,q)) \;=\; p^T E\, q \\
&+ \sum_{u\in TP_p} \frac{h^{|u|}}{\sigma(u)}\, a(u)\, F(u)(p,q)^T E\, q \;+\; p^T E \sum_{v\in TP_q} \frac{h^{|v|}}{\sigma(v)}\, a(v)\, F(v)(p,q) \\
&+ \sum_{u\in TP_p, v\in TP_q} \frac{h^{|u|+|v|}}{\sigma(u)\sigma(v)}\, a(u)a(v)\, F(u)(p,q)^T E\, F(v)(p,q).
\end{aligned}
\tag{7.15}
$$

Condition (7.12) implies that $a(\tau_p) = a(\tau_q)$ for the trees in (7.14). Since also $|\tau_p| = |\tau_q|$ and $\sigma(\tau_p) = \sigma(\tau_q)$, two corresponding terms in the sums of the second line in (7.15) can be jointly replaced by the use of (7.14). As in part (c) of the proof of Theorem 7.1 this together with (7.11) then yields

$$
P_p(a,(p,q))^T E\, P_q(a,(p,q)) = p^T E\, q,
$$

which proves the conservation of quadratic first integrals $p^T E\, q$. Symplecticity follows as before, because the diagram of Lemma 4.1 also commutes for general P-series methods.

For the proof of statement (ii) we notice that $f_1(q)^T E\, q + p^T E\, f_2(p) = 0$ implies that $f_1(q)^T E\, q = 0$ and $p^T E\, f_2(p) = 0$ vanish separately. Instead of (7.14) we thus have two identities: the term $F(\tau_p)(p,q)^T E\, q/\sigma(\tau_p)$ becomes equal to the first sum in (7.14), and $p^T E\, F(\tau_q)(p,q)/\sigma(\tau_q)$ to the second sum. Consequently, the previous argumentation can be applied without the condition $a(\tau_p) = a(\tau_q)$. □

Second Order Differential Equations. We next consider partitioned systems of the particular form

$$\dot p = f_1(q), \qquad \dot q = Cp + c, \tag{7.16}$$

where C is a matrix and c a vector. Since problems of this type are second order differential equations $\ddot q = Cf_1(q)$, partitioned Runge–Kutta methods become equivalent to Nyström methods (see Sects. II.2.3 and IV.2.3).

An important special case are Hamiltonian systems

$$\dot p = -\nabla U(q), \qquad \dot q = Cp + c \tag{7.17}$$

(or, equivalently, $\ddot q = -C\nabla U(q)$). They correspond to Hamiltonian functions

$$H(p,q) = \frac{1}{2}\, p^T C p + c^T p + U(q), \tag{7.18}$$

where the kinetic energy is at most quadratic in p (here, C is usually symmetric).

In a P-series representation of the numerical solution, many elementary differentials vanish identically. Only those trees have to be considered, whose neighbouring vertices have different colour (the problem is separable) and whose white vertices have at most one son[6] (second component is linear). We denote this set of trees by

$$TN_p = \left\{ \tau \in TP_p \;\middle|\; \begin{array}{c} \text{neighbouring vertices of } \tau \text{ have different colour} \\ \text{white vertices of } \tau \text{ have at most one son} \end{array} \right\}, \tag{7.19}$$

and we let TN_q be the corresponding subset of TP_q.

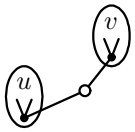
The same procedure as for partitioned methods permits us to write the symplecticity condition of Theorem 4.8 in terms of the coefficients $a(\tau)$ of the P-series. Assuming $a(\bullet) = a(\circ) = 1$, the two conditions of (4.5) lead to

$$a(\circ\circ u) + a(u\circ\circ) = a(u)\,a(\circ) \qquad \text{for } u \in TN_p \tag{7.20}$$

$$a(u)a(\circ\circ v) - a(u\circ\!\circ v) = a(\circ\circ u)a(v) - a(v\circ\!\circ u) \quad \text{for } u, v \in TN_p \tag{7.21}$$

where we use the abbreviating notation

$$u\circ\!\circ v = u\circ(\circ\circ v) = [u_1,\dots,u_m,[v]_q]_p \tag{7.22}$$



if $u = [u_1,\dots,u_m]_p$. Notice that for $u, v \in TN_p$, the trees $u\circ\circ$, $u\circ\!\circ v$ and $v\circ\!\circ u$ are in TN_p, and $\circ\circ u$ is in TN_q.

Theorem 7.3. *Consider a P-series method (7.7) for differential equations (7.16) having $Q(p,q) = p^T Eq$ as first integral.*

If the coefficients $a(\tau)$ satisfy (7.20) and (7.21), the method exactly conserves $Q(p,q)$ and it is symplectic for Hamiltonian systems with $H(p,q)$ of the form (7.18).

[6] Attention: with respect to (III.2.10) the vertices have opposite colour, because the linear dependence is in the second component in (7.17) whereas it is in the first component in (III.2.9).

Proof. Since the elementary differentials $F(\tau)(p,q)$ vanish identically for $\tau \notin TN_p \cup TN_q$, we can arbitrarily define $a(\tau)$ for trees outside $TN_p \cup TN_q$ without changing the method (throughout this proof we implicitly assume that for the considered trees neighbouring vertices have different colour). We shall do this in such a way that (7.11) holds.

Consider first the tree $u \circ\!\circ v$. There is exactly one vertex between the roots of u and v. Making this vertex to the root gives the tree $[u,v]_q$ which is not in TN_q. We define for $u, v \in TN_p$

$$a([u,v]_q) := a(u)a(\circ\circ v) - a(u \circ\!\circ v).$$

Condition (7.21) shows that $a([u,v]_q)$ is independent of permuting u and v and is thus well-defined. For trees that are neither in $TN_p \cup TN_q$ nor of the form $[u,v]_q$ with $u, v \in TN_p$ we let $a(\tau) = 0$. This extension of $a(\tau)$ implies that condition (7.11) holds for all trees, and part (ii) of Theorem 7.2 yields the statement. Notice that for problems $\dot p = f_1(q)$, $\dot q = f_2(p)$ only trees, for which neighbouring vertices have different colour, are relevant. □

VI.7.2 Characterization of Symplectic P-Series (and B-Series)

A characterization of symplectic B-series was first obtained by Calvo & Sanz-Serna (1994). We also consider P-series with various important special situations.

Theorem 7.4. *Consider a P-series method (7.7) applied to a general partitioned differential equation (7.9). Equivalent are:*

1) the coefficients $a(\tau)$ satisfy (7.11) and (7.12),

2) quadratic first integrals of the form $Q(p,q) = p^T E\, q$ are exactly conserved,

3) the method is symplectic for general Hamiltonian systems (1.7).

Proof. The implication (1)⇒(2) follows from part (i) of Theorem 7.2, (2)⇒(3) is a consequence of the fact that the symplecticity condition is a quadratic first integral of the variational equation (see the proof of Theorem 7.2). The remaining implication (3)⇒(1) will be proved in the following two steps.

a) We fix two trees $u \in TP_p$ and $v \in TP_q$, and we construct a (polynomial) Hamiltonian such that the transformation (7.7) satisfies

$$\Big(\frac{\partial(p_1,q_1)}{\partial p_0^1}\Big)^T J \Big(\frac{\partial(p_1,q_1)}{\partial q_0^2}\Big) \;=\; C\Big(a(u\circ v) + a(v\circ u) - a(u)\cdot a(v)\Big) \quad (7.23)$$

with $C \neq 0$ (here, p_0^1 denotes the first component of p_0, and q_0^2 the second component of q_0). The symplecticity of (7.7) implies that the expression in (7.23) vanishes, so that condition (7.11) has to be satisfied.

For given $u \in TP_p$ and $v \in TP_q$ we define the Hamiltonian as follows: to the branches of $u \circ v$ we attach the numbers $3, \dots, |u| + |v| + 1$ such that the branch between the roots of u and v is labelled by 3. Then, the Hamiltonian is a sum of as many terms as vertices in the tree. The summand corresponding to a vertex is a

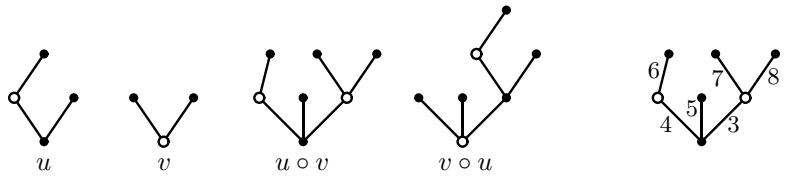


Fig. 7.1. Illustration of the Hamiltonian (7.24)

product containing the factor p^j (resp. q^j) if an upward leaving branch "j" is directly connected with a black (resp. white) vertex, and the factor q^i (resp. p^i) if the vertex itself is black (resp. white) and the downward leaving branch has label "i". Finally, the factors q^2 and p^1 are included in the terms corresponding to the roots of u and v, respectively. For the example of Fig. 7.1 we have

$$H(p,q) = q^2q^3q^4p^5 + p^1p^3p^7p^8 + p^4p^6 + q^5 + q^6 + q^7 + q^8. \tag{7.24}$$

The components $F^i(\tau)(p,q)$ of the elementary differentials corresponding to the Hamiltonian system (with the Hamiltonian constructed above) satisfy

$$\begin{aligned} F^2(u\circ v)(p,q) &= (-1)^{\delta(u\circ v)}\sigma(u\circ v)\cdot p^1, \\ F^1(v\circ u)(p,q) &= (-1)^{\delta(v\circ u)}\sigma(v\circ u)\cdot q^2, \\ F^3(u)(p,q) &= (-1)^{\delta(u)}\sigma(u)\cdot q^2 \\ F^3(v)(p,q) &= (-1)^{\delta(v)}\sigma(v)\cdot p^1, \end{aligned} \tag{7.25}$$

and for all other trees $\tau \in TP$ and components i we have

$$\frac{\partial F^i(\tau)}{\partial p^1}(0,0) \;=\; \frac{\partial F^i(\tau)}{\partial q^2}(0,0) \;=\; 0.$$

In (7.25), $\delta(\tau)$ counts the number of black vertices of τ, and the *symmetry coefficient* $\sigma(\tau)$ is that of (III.2.3). For example, $\sigma(u) = 1$ and $\sigma(v) = 2$ for the trees of Fig. 7.1. The verification of (7.25) is straightforward. The coefficient $(-1)^{\delta(\tau)}$ is due to the minus sign in the first part of the Hamiltonian system (1.7), and the symmetry coefficient $\sigma(\tau)$ appears in exactly the same way as in the multidimensional Taylor formula. Due to the zero initial values, no elementary differential other than those of (7.25) give rise to non-vanishing expressions in (7.23). Consider for example the second component of $F(\tau)(p,q)$ for a tree $\tau \in TP_p$. Since we are concerned with the Hamiltonian system (1.7), this expression starts with a derivative of H_{q^2}. Therefore, it contributes to (7.23) at $p_0 = q_0 = 0$ only if it contains the factor $H_{q^2q^3q^4p^5}$ (for the example of Fig. 7.1). This in turn implies the presence of factors $H_{p^3\ldots}$, $H_{p^4\ldots}$ and $H_{q^5\ldots}$. Continuing this line of reasoning, we find that $F^2(\tau)(p,q)$ contributes to (7.23) at $p_0 = q_0 = 0$ only if $\tau = u \circ v$. With similar arguments we see that only the elementary differentials of (7.25) have to be considered. We now insert (7.25) into (7.7), and we compute its derivatives with respect to p^1 and q^2. This then yields (7.23) with $C = (-1)^{\delta(u)+\delta(v)}h^{|u|+|v|}$, and completes the proof concerning condition (7.11).

b) The necessity of condition (7.12) is seen similarly. We fix a tree $\tau \in TP_p$ and we let $\overline{\tau} \in TP_q$ be the tree obtained from τ by changing the colour of the root. We then attach the numbers $3, \dots, |\tau| + 1$ to the branches of τ, and we define a Hamiltonian as above but, different from adding the factors q^2 and p^1, we include the factor $p^1 q^2$ to the term corresponding to the root. For the tree $\tau = u$ of Fig. 7.1 this yields

$$H(p,q) \;=\; p^1 q^2 q^3 p^4 + p^3 p^5 + q^4 + q^5.$$

With this Hamiltonian we get

$$\begin{aligned} F^2(\tau)(p,q) &= (-1)^{\delta(\tau)} \sigma(\tau) \cdot p^1, \\ F^1(\overline{\tau})(p,q) &= (-1)^{\delta(\tau)} \sigma(\tau) \cdot q^2, \end{aligned}$$

and these are the only elementary differentials contributing to the left-hand expression of (7.23). We thus get

$$\Big(\frac{\partial(p_1,q_1)}{\partial p_0^1}\Big)^T J \Big(\frac{\partial(p_1,q_1)}{\partial q_0^2}\Big) \;=\; (-1)^{\delta(\tau)} h^{|\tau|} \Big(a(\tau) - a(\overline{\tau})\Big),$$

which completes the proof of Theorem 7.4. □

Theorem 7.5. *Consider a P-series method (7.7) applied to a separable partitioned differential equation $\dot p = f_1(q)$, $\dot q = f_2(p)$. Equivalent are:*

1) the coefficients $a(\tau)$ satisfy (7.11),

2) quadratic first integrals of the form $Q(p,q) = p^T E\, q$ are exactly conserved,

3) the method is symplectic for separable Hamiltonians $H(p,q) = T(p) + U(q)$.

Proof. The implications (1)⇒(2)⇒(3) follow as before from part (ii) of Theorem 7.2. The remaining implication (3)⇒(1) is a consequence of the fact that the Hamiltonian constructed in part (a) of the proof of Theorem 7.4 is separable, when u and v have no neighbouring vertices of the same colour. □

Theorem 7.6. *Consider a B-series method (7.1) for $\dot y = f(y)$. Equivalent are:*

1) the coefficients $a(\tau)$ satisfy (7.4),

2) quadratic first integrals of the form $Q(y) = y^T C y$ are exactly conserved,

3) the method is symplectic for general Hamiltonian systems $\dot y = J^{-1} \nabla H(y)$.

Proof. The implications (1)⇒(2)⇒(3) follow from Theorem 7.1. The remaining implication (3)⇒(1) follows from Theorem 7.4, because a B-series with coefficients $a(\tau), \tau \in T$, applied to a partitioned differential equation, can always be interpreted as a P-series (Definition III.2.1), where $a(\tau) := a(\varphi(\tau))$ for $\tau \in TP$ and $\varphi : TP \to T$ is the mapping that forgets the colouring of the vertices. This follows from the fact that

$$\alpha(\tau) F(\tau)(y) \;=\; \begin{pmatrix} \sum_{u \in TP_p, \varphi(u) = \tau} \alpha(u)\, F(u)(p,q) \\ \sum_{v \in TP_q, \varphi(v) = \tau} \alpha(v)\, F(v)(p,q) \end{pmatrix}$$

for $\tau \in T$, because $\alpha(u) \cdot \sigma(u) = \alpha(v) \cdot \sigma(v) = \mathbf{e}(\tau) \cdot |\tau|!$. Here, $y = (p,q)$, the elementary differentials $F(\tau)(y)$ are those of Definition III.1.2, whereas $F(u)(p,q)$ and $F(v)(p,q)$ are those of Table III.2.1. □

Theorem 7.7. *Consider a P-series method (7.7) applied to the special partitioned system (7.16). Equivalent are:*

1) the coefficients $a(\tau)$ satisfy (7.20) and (7.21),

2) quadratic first integrals of the form $Q(p,q) = p^T E\, q$ are exactly conserved,

3) the method is symplectic for Hamiltonian systems of the form (7.17).

Proof. The implications (1)⇒(2)⇒(3) follow from Theorem 7.3. The remaining implication (3)⇒(1) can be seen as follows.

Condition (7.20) is a consequence of the the proof of Theorem 7.4, because for $u \in TN_p$ and $v = \circ$ the Hamiltonian constructed there is of the form (7.18).

To prove condition (7.21) we have to modify slightly the definition of $H(p,q)$. We take $u, v \in TN_p$ and define the polynomial Hamiltonian as follows: to the branches of $u \circ\circ v$ we attach the numbers $3, \dots, |u| + |v| + 2$. The Hamiltonian is then a sum of as many terms as vertices in the tree. The summands are defined as in the proof of Theorem 7.4 with the only exception that to the terms corresponding to the roots of u and v we include the factors q^2 and q^1, respectively, instead of q^2 and p^1. This gives a Hamiltonian of the form (7.18), for which the expression

$$\Big(\frac{\partial(p_1,q_1)}{\partial q_0^1}\Big)^T J \Big(\frac{\partial(p_1,q_1)}{\partial q_0^2}\Big) \tag{7.26}$$

becomes equal to

$$a(u)a(\circ\circ v) - a(u\circ\circ v) - a(\circ\circ u)a(v) + a(v\circ\circ u) \tag{7.27}$$

up to a nonzero constant. By symplecticity, (7.26) is zero so that also (7.27) has to vanish. This proves the validity of condition (7.21). □

VI.7.3 Irreducible Runge–Kutta Methods

We are now able to study to what extent the conditions of Theorem 4.3 and Theorem 4.6 are also necessary for symplecticity. Consider first the 2-stage method

$$\begin{array}{c|cc} 1/2 & \alpha & 1/2-\alpha \\ 1/2 & \beta & 1/2-\beta \\ \hline & 1/2 & 1/2 \end{array}.$$

The solution of the corresponding Runge–Kutta system (II.1.4) is given by $k_1 = k_2 = k$, where $k = f(y_0 + k/2)$, and hence $y_1 = y_0 + hk$. Whatever the values of α and β are, the numerical solution of the Runge–Kutta method is identical to that of the implicit midpoint rule, so that it defines a symplectic transformation. However, the condition (4.2) is only satisfied for $\alpha = \beta = 1/4$.

Definition 7.8. Two stages i and j of a Runge–Kutta method (II.1.4) are said to be *equivalent for a class ($\mathcal{P}$)* of initial value problems, if for every problem in ($\mathcal{P}$) and for every sufficiently small step size we have $k_i = k_j$ ($k_i = k_j$ and $\ell_i = \ell_j$ for partitioned Runge–Kutta methods (II.2.2)).

The method is called *irreducible for ($\mathcal{P}$)* if it does not have equivalent stages. It is called *irreducible* if it is irreducible for all sufficiently smooth initial value problems.

For a more amenable characterization of irreducible Runge–Kutta methods, we introduce an ordering on T (and on TP), and we consider the following $s \times \infty$ matrices

$\Phi_{\text{RK}} = \big(\phi(\tau); \tau \in T\big)$ with entries $\phi_i(\tau) = \mathbf{g}_i(\tau)$ given by (III.1.13),[7]
$\Phi_{\text{PRK}} = \big(\phi(\tau); \tau \in TP_p\big) = \big(\phi(\tau); \tau \in TP_q\big)$ with entries $\phi_i(\tau)$ given by (III.2.7); observe that $\phi_i(\tau)$ does not depend on the colour of the root,
$\Phi^*_{\text{PRK}} = \big(\phi(\tau); \tau \in TP^*_p\big) = \big(\phi(\tau); \tau \in TP^*_q\big)$ where TP^*_p (resp. TP^*_q) is the set of trees in TP_p (resp. TP_q) whose neighbouring vertices have different colours.

Lemma 7.9 (Hairer 1994). *A Runge–Kutta method is irreducible if and only if the matrix Φ_{RK} has full rank s.*

A partitioned Runge–Kutta method is irreducible if and only if the matrix Φ_{PRK} has full rank s.

A partitioned Runge–Kutta method is irreducible for separable problems $\dot p = f_1(q)$, $\dot q = f_2(p)$ if and only if the matrix Φ^*_{PRK} has full rank s.

Proof. If the stages i and j are equivalent, it follows from the expansion

$$k_i = \sum_{\tau \in T} \frac{h^{|\tau|}}{\sigma(\tau)}\, \phi_i(\tau)\, F(\tau)(y_0)$$

(see the proof of Theorem III.1.4) and from the independency of the elementary differentials (Exercise III.3) that $\phi_i(\tau) = \phi_j(\tau)$ for all $\tau \in T$. Hence, the rows i and j of the matrix Φ_{RK} are identical. The analogous statement for partitioned Runge–Kutta methods follows from Theorem III.2.4 and Exercise III.6. This proves the sufficiency of the 'full rank' condition.

We prove its necessity only for partitioned Runge–Kutta methods applied to separable problems (the other situations can be treated similarly). For separable problems, only trees in $TP^*_p \cup TP^*_q$ give rise to non-vanishing elementary differentials. Irreducibility therefore implies that for every pair (i, j) with $i \neq j$ there exists a tree $\tau \in TP^*_p$ such that $\phi_i(\tau) \neq \phi_j(\tau)$. Consequently, a certain finite linear combination of the columns of Φ^*_{PRK} has distinct elements, i.e., there exist vectors $\xi \in \mathbb{R}^\infty$ (only finitely many non zero elements) and $\eta \in \mathbb{R}^s$ with $\Phi^*_{\text{PRK}}\xi = \eta$ and $\eta_i \neq \eta_j$ for $i \neq j$. Due to the fact that $\phi_i([\tau_1, \dots, \tau_m]) = \phi_i([\tau_1]) \cdot \ldots \cdot \phi_i([\tau_m])$, the componentwise product of two columns of Φ^*_{PRK} is again a column of Φ^*_{PRK}. Continuing this argumentation and observing that $(1, \dots, 1)^T$ is a column of Φ^*_{PRK}, we obtain a matrix X such that $\Phi^*_{\text{PRK}} X = (\eta_i^{j-1})_{i,j=1}^s$ is a Vandermonde matrix. Since the η_i are distinct, the matrix Φ^*_{PRK} has to be of full rank s. □

[7] In this section we let $\phi(\tau) \in \mathbb{R}^s$ denote the vector whose elements are $\phi_i(\tau)$, $i = 1, \dots, s$. This should not be mixed up with the value $\phi(\tau)$ of (III.1.16).

VI.7.4 Characterization of Irreducible Symplectic Methods

The necessity of the condition (4.2) for symplectic Runge–Kutta methods was first stated by Lasagni (1988). Abia & Sanz-Serna (1993) extended his proof to partitioned methods. We follow here the ideas of Hairer (1994).

Theorem 7.10. *An irreducible Runge–Kutta method (II.1.4) is symplectic if and only if the condition (4.2) holds.*

An irreducible partitioned Runge–Kutta method (II.2.2) is symplectic if and only if the conditions (4.3) and (4.4) hold.

A partitioned Runge–Kutta method, irreducible for separable problems, is symplectic for separable Hamiltonians $H(p,q) = T(p) + U(q)$ if and only if the condition (4.3) holds.

Proof. The "if" part of all three statements has been proved in Theorem 4.3 and Theorem 4.6. We prove the "only if" part for partitioned Runge–Kutta methods applied to general Hamiltonian systems (the other two statements can be obtained in the same way).

We consider the $s \times s$ matrix M with entries $m_{ij} = b_i\widehat{a}_{ij} + \widehat{b}_j a_{ji} - b_i\widehat{b}_j$. The computation leading to formula (7.11) shows that for $u \in TP_p$ and $v \in TP_q$

$$\phi(u)^T M\, \phi(v) \;=\; a(u \circ v) + a(v \circ u) - a(u) \cdot a(v)$$

holds. Due to the symplecticity of the method, this expression vanishes and we obtain

$$\Phi_{\text{PRK}}^T M\, \Phi_{\text{PRK}} \;=\; 0,$$

where Φ_{PRK} is the matrix of Lemma 7.9. An application of this lemma then yields $M = 0$, which proves the necessity of (4.3).

For the vector d with components $d_i = b_i - \widehat{b}_i$ we get $d^T\Phi_{\text{PRK}} = 0$, and we deduce from Lemma 7.9 that $d = 0$, so that (4.4) is also seen to be necessary. □

VI.8 Conjugate Symplecticity

The symplecticity requirement may be too strong if we are interested in a correct long-time behaviour of a numerical integrator. Stoffer (1988) suggests considering methods that are not necessarily symplectic but conjugate to a symplectic method.

Definition 8.1. Two numerical methods Φ_h and Ψ_h are mutually *conjugate*, if there exists a global change of coordinates χ_h, such that

$$\Phi_h = \chi_h^{-1} \circ \Psi_h \circ \chi_h. \tag{8.1}$$

We assume that $\chi_h(y) = y + \mathcal{O}(h)$ uniformly for y varying in a compact set.

For a numerical solution $y_{n+1} = \Phi_h(y_n)$, lying in a compact subset of the phase space, the transformed values $z_n = \chi_h(y_n)$ constitute a numerical solution $z_{n+1} = \Psi_h(z_n)$ of the second method. Since $y_n - z_n = \mathcal{O}(h)$, both numerical solutions have the same long-time behaviour, independently of whether one method shares certain properties (e.g., symplecticity) with the other.

VI.8.1 Examples and Order Conditions

The most prominent pair of conjugate methods are the trapezoidal and midpoint rules. Their conjugacy has been originally exploited by Dahlquist (1975) in an investigation on nonlinear stability.

If we denote by Φ_h^E and Φ_h^I the explicit and implicit Euler methods, respectively, then the trapezoidal rule Φ_h^T and the implicit midpoint rule Φ_h^M can be written as

$$\Phi_h^T = \Phi_{h/2}^I \circ \Phi_{h/2}^E, \qquad \Phi_h^M = \Phi_{h/2}^E \circ \Phi_{h/2}^I$$

(see Fig. 8.1). This shows $\Phi_h^T = \chi_h^{-1} \Phi_h^M \chi_h$ with $\chi_h = \Phi_{h/2}^E$, implying that the trapezoidal and midpoint rules are mutually conjugate. The change of coordinates, which transforms the numerical solution of one method to that of the other, is $\mathcal{O}(h)$-close to the identity.

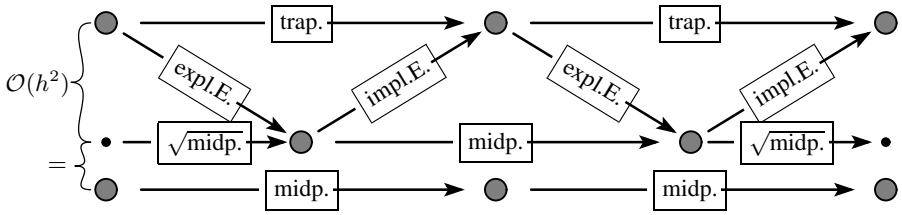


Fig. 8.1. Conjugacy of the trapezoidal rule and the implicit midpoint rule.

In fact, we can do even better. If we let $\Phi_{h/2}$ be the square root of Φ_h^M (i.e., $\Phi_{h/2} \circ \Phi_{h/2} = \Phi_h^M$, see Lemma V.3.2), then we have (Fig. 8.1)

$$\Phi_h^T = (\Phi_{h/2}^E)^{-1} \circ \Phi_h^M \circ \Phi_{h/2}^E = (\Phi_{h/2}^E)^{-1} \circ \Phi_{h/2} \circ \Phi_{h/2} \circ \Phi_{h/2} \circ \Phi_{h/2}^{-1} \circ \Phi_{h/2}^E$$

so that the trapezoidal and the midpoint rules are conjugate via $\chi_h = \Phi_{h/2}^{-1} \circ \Phi_{h/2}^E$. Since $\Phi_{h/2}$ and $\Phi_{h/2}^E$ are both consistent with the same differential equation, the transformation χ_h is $\mathcal{O}(h^2)$-close to the identity. This shows that for every numerical solution of the trapezoidal rule there exists a numerical solution of the midpoint rule which remains $\mathcal{O}(h^2)$-close as long as it stays in a compact set. A single trajectory of the non-symplectic trapezoidal rule therefore behaves very much the same as a trajectory of the symplectic implicit midpoint rule.

A Study via B-Series. An investigation of Runge–Kutta methods, conjugate to a symplectic method, leads us to the following weaker requirement: we say that a numerical method Φ_h is *conjugate to a symplectic method Ψ_h up to order r*, if there exists a transformation $\chi_h(y) = y + \mathcal{O}(h)$ such that

$$\Phi_h(h) = \big(\chi_h^{-1} \circ \Psi_h \circ \chi_h\big)(y) + \mathcal{O}(h^{r+1}). \tag{8.2}$$

This implies that the error of such a method behaves as the superposition of the error of a symplectic method of order p with that of a non-symplectic method of order r.

In the following we assume that all methods considered as well as the conjugacy mapping χ_h can be represented as B-series

$$\Phi_h(y) = B(a, y), \qquad \Psi_h(y) = B(b, y), \qquad \chi_h(y) = B(c, y). \tag{8.3}$$

Using the composition formula (III.1.38) of B-series, condition (8.2) becomes

$$(ac)(\tau) = (cb)(\tau) \qquad \text{for} \quad |\tau| \le r. \tag{8.4}$$

The following results are taken from the thesis of P. Leone (2000).

Theorem 8.2. *Let $\Phi_h(y) = B(a, y)$ represent a numerical method of order 2.*
a) It is always conjugate to a symplectic method up to order 3.
b) It is conjugate to a symplectic method up to order 4, if and only if

$$a(\bullet, \vee) - 2a(\bullet, \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) = 0, \qquad a(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}, \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) - 2a(\bullet, \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) = 0. \tag{8.5}$$

Here, we use the abbreviation $a(u, v) = a(u) \cdot a(v) - a(u \circ v) - a(v \circ u)$.

Proof. The condition (8.4) allows us to express $b(\tau)$ as a function of $a(u)$ for $|u| \le |\tau|$ and of $c(v)$ for $|v| \le |\tau| - 1$ (use the formulas of Example III.1.11). All we have to do is to check the symplecticity conditions $b(u, v) = 0$ for $|u| + |v| \le r$ (see Theorem 7.6).

Since the method Φ_h is of order 2, we obtain $b(\bullet) = 1$ and $b(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) = 1/2$. We arbitrarily fix $c(\bullet) = 0$, so that the symplecticity condition $b(\bullet, \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) = 0$ becomes $2c(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) = a(\bullet, \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix})$. Defining $c(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix})$ by this relation proves statement (a).

For order 4, the three symplecticity conditions $b(\bullet, \vee) = b(\bullet, [[\bullet]]) = b(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}, \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) = 0$ have to be fulfilled. One of them can be satisfied by defining suitably $c(\vee) + c([[\bullet]])$; the other two conditions are then equivalent to (8.5). □

Theorem 8.3. *Let $\Phi_h(y) = B(a, y)$ represent a numerical method of order 4. It is conjugate to a symplectic method up to order 5, if and only if*

$$a(\bullet, \begin{smallmatrix} \bullet \\ \vee \\ \bullet \end{smallmatrix}) - 2a(\bullet, \begin{smallmatrix} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{smallmatrix}) = 0, \qquad a(\bullet, \begin{smallmatrix} \vee \\ \bullet \end{smallmatrix}) - 3a(\bullet, \begin{smallmatrix} \bullet \\ \vee \\ \bullet \end{smallmatrix}) + 3a(\bullet, \begin{smallmatrix} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{smallmatrix}) = 0,$$

$$a(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}, \vee) - a(\bullet, \begin{smallmatrix} \bullet \\ \vee \\ \bullet \end{smallmatrix}) - 2a(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}, \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}) + 3a(\bullet, \begin{smallmatrix} \bullet \\ | \\ \bullet \\ | \\ \bullet \end{smallmatrix}) = 0.$$

Proof. The idea of the proof is the same as in the preceding theorem. The verification is left as an exercise for the reader. □

Example 8.4. A direct computation shows that for the Lobatto IIIB method with $s = 3$ we have $a(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}, \vee) = 1/144$, and $a(u, v) = 0$ for all other pairs with $|u| + |v| = 5$. Theorem 8.3 therefore proves that this method is not conjugate to a symplectic method up to order 5.

For the Lobatto IIIA method with $s = 3$ we obtain $a(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}, \vee) = -1/144$, $a(\begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}, [[\bullet]]) = -1/288$, and $a(u, v) = 0$ for the remaining pairs with $|u| + |v| = 5$. This time the conditions of Theorem 8.3 are fulfilled, so that the Lobatto IIIA method with $s = 3$ is conjugate to a symplectic method up to order 5 at least.

VI.8.2 Near Conservation of Quadratic First Integrals

We have already met in Sect. VI.4.1 a close relationship between symplecticity and the conservation of quadratic first integrals. The aim of this section is to show a similar connection between conjugate symplecticity and the near conservation of quadratic first integrals. This has first been observed and proved by Chartier, Faou & Murua (2005) using the algebra of rooted trees.

Let $Q(y) = y^T C y$ (with symmetric matrix C) be a quadratic first integral of $\dot y = f(y)$, and assume that $\Phi_h(y)$ is conjugate to a method $\Psi_h(y)$ that exactly conserves quadratic first integrals (e.g., symplectic Runge–Kutta methods). This means that $y_{n+1} = \Phi_h(y_n)$ satisfies

$$\chi_h(y_{n+1})^T C \chi_h(y_{n+1}) = \chi_h(y_n)^T C \chi_h(y_n),$$

and the expression $\widetilde Q(y) = \chi_h(y)^T C \chi_h(y)$ is exactly conserved by the numerical solution of $\Phi_h(y)$. If $\chi_h(y) = B(c, y)$ is a B-series, this is of the form

$$\widetilde Q(y) = \sum_{\tau,\vartheta \in T \cup \{\emptyset\}} h^{|\tau|+|\vartheta|} \beta(\tau,\vartheta) F(\tau)(y)^T C\, F(\vartheta)(y), \tag{8.6}$$

where $F(\emptyset)(y) = y$ and $|\emptyset| = 0$ for the empty tree, and $\beta(\emptyset,\emptyset) = 1$. We have the following criterion for conjugate symplecticity, where all formulas have to be interpreted in the sense of formal series.

Theorem 8.5. *Assume that a one-step method $\Phi_h(y) = B(a, y)$ leaves (8.6) invariant for all problems $\dot y = f(y)$ having $Q(y) = y^T C y$ as first integral.*

Then, it is conjugate to a symplectic integrator $\Psi_h(z)$, i.e., there exists a transformation $z = \chi_h(y) = B(c, y)$ such that $\Psi_h(z) = \chi_h \circ \Phi_h \circ \chi_h^{-1}(z)$, or equivalently, $\Psi_h(z) = B(c^{-1}ac, z)$ is symplectic.

Proof. The idea is to search for a B-series $B(c, y)$ such that the expression (8.6) becomes

$$\widetilde Q(y) = B(c, y)^T C\, B(c, y).$$

The mapping $z = \chi_h(y) = B(c, y)$ then provides a change of variables such that the original first integral $Q(z) = z^T C z$ is invariant in the new variables. By Theorem 7.6 this then implies that Ψ_h is symplectic.

By Lemma 8.6 below, the expression (8.6) can be written as

$$\widetilde Q(y) = y^T C \Big(y + \sum_{\theta \in T} h^{|\theta|} \eta(\theta) F(\theta)(y) \Big), \tag{8.7}$$

where $\eta(\theta) = 0$ for $|\theta| < r$, if the perturbation in (8.6) is of size $\mathcal{O}(h^r)$. Using the same lemma once more, we obtain

$$\begin{aligned} B(c, y)^T C\, B(c, y) \;&=\; y^T C \Big(y + 2 \sum_{\theta \in T} \frac{h^{|\theta|}}{\sigma(\theta)}\, c(\theta) F(\theta)(y) \Big) \\ &+\; y^T C \Big(\sum_{\theta \in T} \Big(\frac{h^{|\theta|}}{\sigma(\theta)} \sum_{\tau,\vartheta \in T} \frac{\sigma(\theta)\kappa_{\tau,\vartheta}(\theta)}{\sigma(\tau)\sigma(\vartheta)}\, c(\tau) c(\vartheta) F(\theta)(y) \Big). \end{aligned} \tag{8.8}$$

A comparison of the coefficients in (8.7) and (8.8) uniquely defines $c(\theta)$ in a recursive manner. We have $c(\theta) = 0$ for $|\theta| < r$, so that the transformation $z = B(c, y)$ is $\mathcal{O}(h^r)$ close to the identity. □

The previous proof is based on the following result.

Lemma 8.6. *Let $Q(y) = y^T C y$ (with symmetric matrix C) be a first integral of $\dot y = f(y)$. Then, for every pair of trees $\tau, \vartheta \in T$, we have*

$$F(\tau)(y)^T C\, F(\vartheta)(y) = y^T C \Big(\sum_{\theta \in T} \kappa_{\tau,\vartheta}(\theta) F(\theta)(y) \Big).$$

This sum is finite and only over trees satisfying $|\theta| = |\tau| + |\vartheta|$.

Proof. By definition of a first integral we have $y^T C\, f(y) = 0$ for all y. Differentiation with respect to y gives

$$f(y)^T C\, k + y^T C\, f'(y) k = 0 \qquad \text{for all } \ k. \tag{8.9}$$

Putting $k = F(\vartheta)(y)$, this proves the statement for $\tau = \bullet$.

Differentiating once more yields

$$(f'(y)\ell)^T C\, k + \ell^T C\, f'(y) k + y^T C\, f''(y)(k, \ell) = 0.$$

Putting $\ell = f(y)$ and using (8.9), we get the statement for $\tau = \begin{smallmatrix} \bullet \\ | \\ \bullet \end{smallmatrix}$. With $\ell = F(\tau_1)(y)$ we obtain the statement for $\tau = [\tau_1]$ provided that it is already proved for τ_1. We need a further differentiation to get a similar statement for $\tau = [\tau_1, \tau_2]$, etc. The proof concludes by induction on the order of τ. □

Partitioned Methods. This criterion for conjugate symplecticity can be extended to partitioned P-series methods. For partitioned problems

$$\dot p = f_1(p, q), \qquad \dot q = f_2(p, q) \tag{8.10}$$

we consider first integrals of the form $L(p, q) = p^T E\, q$, where E is an arbitrary constant matrix. If $\Phi_h(p, q)$ is conjugate to a method that exactly conserves $L(p, q)$, then it will conserve a modified first integral of the form

$$\widetilde L(p, q) = \sum_{\tau \in TP_p \cup \{\emptyset_p\}, \vartheta \in TP_q \cup \{\emptyset_q\}} h^{|\tau|+|\vartheta|} \beta(\tau, \vartheta) F(\tau)(p, q)^T E\, F(\vartheta)(p, q), \tag{8.11}$$

where $\beta(\emptyset_p, \emptyset_q) = 1$, $F(\emptyset_p)(p, q) = p$, $F(\emptyset_q)(p, q) = q$. We first extend Lemma 8.6 to the new situation.

Lemma 8.7. *Let $L(p, q) = p^T E\, q$ be a first integral of (8.10). Then, for every pair of trees $\tau \in TP_p, \vartheta \in TP_q$, we have*

$$\begin{aligned} F(\tau)(p, q)^T E\, F(\vartheta)(p, q) \ &= \ p^T E \Big(\sum_{\theta \in TP_q} \kappa_{\tau,\vartheta}(\theta) F(\theta)(p, q) \Big) \\ &+ \ \Big(\sum_{\theta \in TP_p} \kappa_{\tau,\vartheta}(\theta) F(\theta)(p, q) \Big)^T E\, q. \end{aligned} \tag{8.12}$$

These sums are finite and only over trees satisfying $|\theta| = |\tau| + |\vartheta|$.

Proof. Since $L(p,q) = p^T E\, q$ is a first integral of the differential equation, we have $f_1(p,q)^T E\, q + p^T E\, f_2(p,q) = 0$ for all p and q. As in the proof of Lemma 8.6 the statement follows from differentiation of this relation. □

Theorem 8.8. *Assume that a partitioned one-step method $\Phi_h(p,q) = P(a,(p,q))$ leaves (8.11) invariant for all problems (8.10) having $L(p,q) = p^T E\, q$ as first integral.*

Then it is conjugate to a symplectic integrator $\Psi_h(u,v)$, i.e., there is a transformation $(u,v) = \chi_h(p,q) = P(c,(p,q))$ such that $\Psi_h(u,v) = \chi_h \circ \Phi_h \circ \chi_h^{-1}(u,v)$, or equivalently, $\Psi_h(u,v) = P(c^{-1}ac,(u,v))$ is symplectic.

Proof. We search for a P-series $P(c,(p,q)) = \big(P_p(c,(p,q)), P_q(c,(p,q))\big)^T$ such that the expression (8.11) can be written as

$$\widetilde{L}(p,q) = P_p(c,(p,q))^T E\, P_q(c,(p,q)).$$

As in the proof of Theorem 8.5 the mapping $(u,v) = \chi_h(p,q) = P(c,(p,q))$ then provides the searched change of variables.

Using Lemma 8.7 the expression (8.11) becomes

$$\widetilde{L}(p,q) = p^T E\Big(q + \sum_{\theta \in TP_q} h^{|\theta|}\eta(\theta)F(\theta)(p,q)\Big) + \Big(\sum_{\theta \in TP_p} h^{|\theta|}\eta(\theta)F(\theta)(p,q)\Big)^T E\, q.$$

Also $P_p(c,(p,q))^T E\, P_q(c,(p,q))$ can be written in such a form, and a comparison of the coefficients yields the coefficients $c(\tau)$ of the P-series $P(c,(p,q))$ in a recursive manner. We again have that $P(c,(p,q))$ is $\mathcal{O}(h^r)$ close to the identity, if the perturbation in (8.11) is of size $\mathcal{O}(h^r)$. □

The statement of Theorem 8.8 remains true in the class of second order differential equations $\ddot{q} = f_1(q)$, i.e., $\dot{p} = f_1(p)$, $\dot{q} = p$.

VI.9 Volume Preservation

The flow φ_t of a Hamiltonian system preserves volume in phase space: for every bounded open set $\Omega \subset \mathbb{R}^{2d}$ and for every t for which $\varphi_t(y)$ exists for all $y \in \Omega$,

$$\text{vol}(\varphi_t(\Omega)) = \text{vol}(\Omega)\ ,$$

where $\text{vol}(\Omega) = \int_\Omega dy$. This identity is often referred to as *Liouville's theorem*. It is a consequence of the transformation formula for integrals and the fact that

$$\det \frac{\partial \varphi_t(y)}{\partial y} = 1 \qquad \text{for all } t \text{ and } y, \tag{9.1}$$

which follows directly from the symplecticity and $\varphi_0 = \text{id}$. The same argument shows that every symplectic transformation, and in particular every symplectic integrator applied to a Hamiltonian system, preserves volume in phase space.

More generally than for Hamiltonian systems, volume is preserved by the flow of differential equations with a divergence-free vector field:

Lemma 9.1. *The flow of a differential equation $\dot{y} = f(y)$ in $\mathbb{R}^n$ is volume-preserving if and only if* $\operatorname{div} f(y) = 0$ *for all y.*

Proof. The derivative $Y(t) = \frac{\partial \varphi_t}{\partial y}(y_0)$ is the solution of the variational equation

$$\dot{Y} = A(t)Y\,, \quad Y(0) = I\,,$$

with the Jacobian matrix $A(t) = f'(y(t))$ at $y(t) = \varphi_t(y_0)$. From the proof of Lemma IV.3.1 we obtain the *Abel–Liouville–Jacobi–Ostrogradskii identity*

$$\frac{d}{dt} \det Y = \operatorname{trace} A(t) \cdot \det Y. \tag{9.2}$$

Note that here $\operatorname{trace} A(t) = \operatorname{div} f(y(t))$. Hence, $\det Y(t) = 1$ for all t if and only if $\operatorname{div} f(y(t)) = 0$ for all t. Since this is valid for all choices of initial values y_0, the result follows. □

Example 9.2 (ABC Flow). This flow, named after the three independent authors Arnold, Beltrami and Childress, is given by the equations

$$\begin{aligned} \dot{x} &= A \sin z + C \cos y \\ \dot{y} &= B \sin x + A \cos z \\ \dot{z} &= C \sin y + B \cos x \end{aligned} \tag{9.3}$$

and has all diagonal elements of f' identically zero. It is therefore volume preserving. In Arnold (1966, p. 347) it appeared in a footnote as an example of a flow with $\operatorname{rot} f$ parallel to f, thus violating Arnold's condition for the existence of invariant tori (Arnold 1966, p. 346). It was therefore expected to possess interesting chaotic properties and has since then been the object of many investigations showing their non-integrability (see e.g., Ziglin (1996)). We illustrate in Fig. 9.1 the action of this flow by transforming, in a volume preserving manner, a ball in $\mathbb{R}^3$. We see that, very soon, the set is strongly squeezed in one direction and dilated in two others. The solutions thus depend in a very sensitive way on the initial values.

Volume-Preserving Numerical Integrators. The question arises as to whether volume-preserving integrators can be constructed for every differential equation with volume-preserving flow. Already for linear problems, Lemma IV.3.2 shows that no standard method can be volume-preserving for dimension $n \geq 3$. Nevertheless, positive answers were found by Qin & Zhu (1993), Shang (1994a,1994b), Feng & Shang (1995) and Quispel (1995). In the following we present the approach of Feng & Shang (1995). The key is the following result which generalizes and reinterprets a construction of H. Weyl (1940) for $n = 3$.

Theorem 9.3 (Feng & Shang 1995). *Every divergence-free vector field $f : \mathbb{R}^n \to \mathbb{R}^n$ can be written as the sum of $n - 1$ vector fields*

$$f = f_{1,2} + f_{2,3} + \ldots + f_{n-1,n}$$

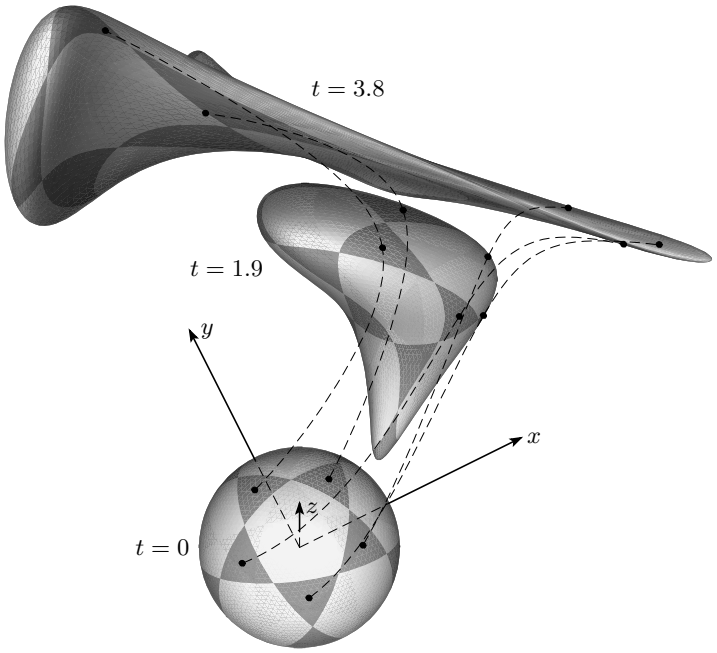


Fig. 9.1. Volume preserving deformation of the ball of radius 1, centred at the origin, by the ABC flow; $A = 1/2$, $B = C = 1$.

where each $f_{k,k+1}$ is Hamiltonian in the variables (y_k, y_{k+1}): there exist functions $H_{k,k+1} : \mathbb{R}^n \to \mathbb{R}$ such that

$$f_{k,k+1} = (0, \dots, 0, -\frac{\partial H_{k,k+1}}{\partial y_{k+1}}, \frac{\partial H_{k,k+1}}{\partial y_k}, 0, \dots, 0)^T \ .$$

Proof. In terms of the components of $f = (f_1, \dots, f_n)^T$, the functions $H_{k,k+1}$ must satisfy the equations

$$f_1 = -\frac{\partial H_{1,2}}{\partial y_2}, \quad f_2 = \frac{\partial H_{1,2}}{\partial y_1} - \frac{\partial H_{2,3}}{\partial y_3} \ , \dots ,$$

$$f_{n-1} = \frac{\partial H_{n-2,n-1}}{\partial y_{n-2}} - \frac{\partial H_{n-1,n}}{\partial y_n}, \quad f_n = \frac{\partial H_{n-1,n}}{\partial y_{n-1}} \ .$$

We thus set

$$H_{1,2} = -\int_0^{y_2} f_1 \, dy_2$$

and for $k = 2, \dots, n-2$

$$H_{k,k+1} = \int_0^{y_{k+1}} \Big(\frac{\partial H_{k-1,k}}{\partial y_{k-1}} - f_k \Big) \, dy_{k+1} \ .$$

It remains to construct $H_{n-1,n}$ from the last two equations. We see by induction that for $k \le n-2$,

$$\frac{\partial^2 H_{k,k+1}}{\partial y_k \partial y_{k+1}} = -\Big(\frac{\partial f_1}{\partial y_1} + \ldots + \frac{\partial f_k}{\partial y_k}\Big) ,$$

and hence the integrability condition for $H_{n-1,n}$,

$$\frac{\partial}{\partial y_{n-1}}\Big(\frac{\partial H_{n-2,n-1}}{\partial y_{n-2}} - f_{n-1}\Big) = \frac{\partial f_n}{\partial y_n} ,$$

reduces to the condition $\mathrm{div} f = 0$, which is satisfied by assumption. $H_{n-1,n}$ can thus be constructed as

$$H_{n-1,n} = \int_0^{y_n} \Big(\frac{\partial H_{n-2,n-1}}{\partial y_{n-2}} - f_{n-1}\Big)\, dy_n + \int_0^{y_{n-1}} f_n|_{y_n=0}\, dy_{n-1} ,$$

which completes the proof. □

The above construction also shows that

$$f_{k,k+1} = (0, \ldots, 0, f_k + g_k, -g_{k+1}, 0, \ldots, 0)$$

with

$$g_{k+1} = \int_0^{y_{k+1}} \Big(\frac{\partial f_1}{\partial y_1} + \ldots + \frac{\partial f_k}{\partial y_k}\Big)\, dy_{k+1}$$

for $1 \le k \le n-2$, and $g_1 = 0$ and $g_n = -f_n$.

With the decomposition of Lemma 9.3 at hand, a volume-preserving algorithm is obtained by applying a splitting method with symplectic substeps. For example, as proposed by Feng & Shang (1995), a second-order volume-preserving method is obtained by Strang splitting with symplectic Euler substeps:

$$\varphi_h \approx \Phi_h = \Phi_{h/2}^{[1,2]*} \circ \ldots \circ \Phi_{h/2}^{[n-1,n]*} \circ \Phi_{h/2}^{[n-1,n]} \circ \ldots \circ \Phi_{h/2}^{[1,2]}$$

where $\Phi_{h/2}^{[k,k+1]}$ is a symplectic Euler step of length $h/2$ applied to the system with right-hand side $f_{k,k+1}$, and $*$ denotes the adjoint method. In this method, one step $\widehat{y} = \Phi_h(y)$ is computed component-wise, in a Gauss-Seidel-like manner, as

$$\begin{aligned}
\overline{y}_1 &= y_1 + \frac{h}{2} f_1(\overline{y}_1, y_2, \ldots, y_n) \\
\overline{y}_k &= y_k + \frac{h}{2} f_k(\overline{y}_1, \ldots, \overline{y}_k, y_{k+1}, \ldots, y_n) + \frac{h}{2} g_k|_{y_k}^{\overline{y}_k} \quad \text{for } k = 2, \ldots, n-1 \\
\overline{y}_n &= y_n + \frac{h}{2} f_n(\overline{y}_1, \ldots, \overline{y}_{n-1}, y_n)
\end{aligned} \tag{9.4}$$

with $g_k|_{y_k}^{\overline{y}_k} = g_k(\overline{y}_1, \ldots, \overline{y}_k, y_{k+1}, \ldots, y_n) - g_k(\overline{y}_1, \ldots, \overline{y}_{k-1}, y_k, \ldots, y_n)$, and

$$\begin{aligned}
\widehat{y}_n &= \overline{y}_n + \frac{h}{2} f_n(\overline{y}_1, \dots, \widehat{y}_n) \\
\widehat{y}_k &= \overline{y}_k + \frac{h}{2} f_k(\overline{y}_1, \dots, \overline{y}_k, \widehat{y}_{k+1} \dots, \widehat{y}_n) - \frac{h}{2} \overline{g}_k|_{\overline{y}_k}^{\widehat{y}_k} \quad \text{for } k = n-1, \dots, 2 \\
\widehat{y}_1 &= \overline{y}_1 + \frac{h}{2} f_1(\overline{y}_1, \widehat{y}_2, \dots, \widehat{y}_n)
\end{aligned} \tag{9.5}$$

with $\overline{g}_k|_{\overline{y}_k}^{\widehat{y}_k} = g_k(\overline{y}_1, \dots, \overline{y}_{k-1}, \widehat{y}_k, \dots, \widehat{y}_n) - g_k(\overline{y}_1, \dots, \overline{y}_k, \widehat{y}_{k+1}, \dots, \widehat{y}_n)$. The method is one-dimensionally implicit in general, but becomes explicit in the particular case where $\partial f_k / \partial y_k = 0$ for all k.

Separable Partitioned Systems. For problems of the form

$$\dot{y} = f(z), \qquad \dot{z} = g(y) \tag{9.6}$$

with $y \in \mathbb{R}^m$, $z \in \mathbb{R}^n$, the scheme (9.4) becomes the symplectic Euler method, (9.5) its adjoint, and its composition the Lobatto IIIA - IIIB extension of the Störmer–Verlet method. Since symplectic explicit partitioned Runge–Kutta methods are compositions of symplectic Euler steps (Theorem VI.4.7), this observation proves that such methods are volume-preserving for systems (9.6). This fact was obtained by Suris (1996) by a direct calculation, without interpreting the methods as composition methods. The question arises as to whether more symplectic partitioned Runge–Kutta methods are volume-preserving for systems (9.6).

Theorem 9.4. *Every symplectic Runge–Kutta method with at most two stages is volume-preserving for systems (9.6) of arbitrary dimension.*

Proof. (a) The idea is to consider the Hamiltonian system with

$$H(u, v, y, z) = u^T f(z) + v^T g(y),$$

where (u, v) are the conjugate variables to (y, z). This system is of the form

$$\begin{aligned}
\dot{y} &= f(z) \qquad & \dot{u} &= -g'(y)^T v \\
\dot{z} &= g(y) \qquad & \dot{v} &= -f'(z)^T u.
\end{aligned} \tag{9.7}$$

Applying the Runge–Kutta method to this augmented system does not change the numerical solution for (y, z). For symplectic methods the matrix

$$\Big(\frac{\partial(y_1, z_1, u_1, v_1)}{\partial(y_0, z_0, u_0, v_0)}\Big) = M = \begin{pmatrix} R & 0 \\ S & T \end{pmatrix} \tag{9.8}$$

satisfies $M^T J M = J$ which implies $R T^T = I$. Below we shall show that $\det T = \det R$. This yields $\det R = 1$ which implies that the method is volume preserving.

(b) *One-stage methods*. The only symplectic one-stage method is the implicit midpoint rule for which R and T are computed as

$$\Big(I - \frac{h}{2}\,E_1\Big)R \;=\; I + \frac{h}{2}\,E_1 \tag{9.9}$$

$$\Big(I + \frac{h}{2}\,E_1^T\Big)T \;=\; I - \frac{h}{2}\,E_1^T, \tag{9.10}$$

where E_1 is the Jacobian of the system (9.6) evaluated at the internal stage value. Since

$$E_1 = \begin{pmatrix} 0 & f'(z_{1/2}) \\ g'(y_{1/2}) & 0 \end{pmatrix},$$

a similarity transformation with the matrix $D = \mathrm{diag}(I, -I)$ takes E_1 to $-E_1$. Hence, the transformed matrix satisfies

$$\Big(I - \frac{h}{2}\,E_1^T\Big)(D^{-1}TD) \;=\; I + \frac{h}{2}\,E_1^T.$$

A comparison with (9.9) and the use of $\det X^T = \det X$ proves $\det R = \det T$ for the midpoint rule.

(c) *Two-stage methods*. Applying a two-stage implicit Runge–Kutta method to (9.7) yields

$$\begin{pmatrix} I - ha_{11}E_1 & -ha_{12}E_2 \\ -ha_{21}E_1 & I - ha_{22}E_2 \end{pmatrix} \begin{pmatrix} R_1 \\ R_2 \end{pmatrix} \;=\; \begin{pmatrix} I \\ I \end{pmatrix},$$

where R_i is the derivative of the (y, z) components of the ith stage with respect to (y_0, z_0), and E_i is the Jacobian of the system (9.6) evaluated at the ith internal stage value. From the solution of this system the derivative R of (9.8) is obtained as

$$R \;=\; I + (b_1E_1, b_2E_2) \begin{pmatrix} I - ha_{11}E_1 & -ha_{12}E_2 \\ -ha_{21}E_1 & I - ha_{22}E_2 \end{pmatrix}^{-1} \begin{pmatrix} I \\ I \end{pmatrix}.$$

With the determinant identity

$$det(U)\,\det(X - WU^{-1}V) \;=\; \det \begin{pmatrix} U & V \\ W & X \end{pmatrix} \;=\; det(X)\,\det(U - VX^{-1}W),$$

which is seen by Gaussian elimination, this yields

$$\det R \;=\; \frac{\det\big(I \otimes I - h((A - \mathbb{1}b^T) \otimes I)\,E\big)}{\det\big(I \otimes I - h(A \otimes I)\,E\big)},$$

where A and b collect the Runge–Kutta coefficients, and $E = \mathrm{blockdiag}\,(E_1, E_2)$. For $D^{-1}TD$ we get the same formula with E replaced by E^T. If A is an arbitrary 2×2 matrix, it follows from block Gaussian elimination that

$$\det\big(I \otimes I - h(A \otimes I)\,E\big) \;=\; \det\big(I \otimes I - h(A \otimes I)\,E^T\big), \tag{9.11}$$

which then proves $\det R = \det T$. Notice that the identity (9.11) is no longer true in general if A is of dimension larger than two. □

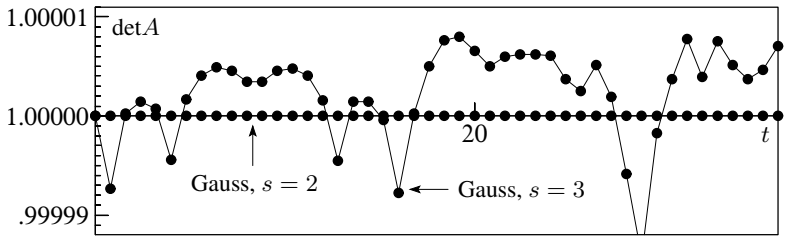


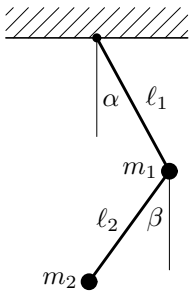
Fig. 9.2. Volume preservation of Gauss methods applied to (9.12) with $h = 0.8$.

We are curious to see whether Theorem 9.4 remains valid for symplectic Runge–Kutta methods with more than two stages. For this we apply the Gauss methods with $s = 2$ and $s = 3$ to the problem

$$\dot{x} = \sin z, \qquad \dot{y} = \cos z, \qquad \dot{z} = \sin y + \cos x \tag{9.12}$$

with initial value $(0, 0, 0)$. We show in Fig. 9.2 the determinant of the derivative of the numerical flow as a function of time. Only the two-stage method is volume-preserving for this problem which is in agreement with Theorem 9.4.

VI.10 Exercises



1. Let α and β be the generalized coordinates of the double pendulum, whose kinetic and potential energies are

$$\begin{aligned} T &= \frac{m_1}{2}(\dot{x}_1^2 + \dot{y}_1^2) + \frac{m_2}{2}(\dot{x}_2^2 + \dot{y}_2^2) \\ U &= m_1 g y_1 + m_2 g y_2. \end{aligned}$$

   Determine the generalized momenta of the corresponding Hamiltonian system.

2. A non-autonomous Hamiltonian system is given by a time-dependent Hamiltonian function $H(p, q, t)$ and the differential equations

$$\dot{p} = -H_q(p, q, t), \qquad \dot{q} = H_p(p, q, t).$$

   Verify that these equations together with $\dot{e} = -H_t(p, q, t)$ and $\dot{t} = 1$ are the canonical equations for the extended Hamiltonian $\widetilde{H}(\widetilde{p}, \widetilde{q}) = H(p, q, t) + e$ with $\widetilde{p} = (p, e)$ and $\widetilde{q} = (q, t)$.
3. Prove that a linear transformation $A : \mathbb{R}^2 \to \mathbb{R}^2$ is symplectic, if and only if $\det A = 1$.
4. Consider the transformation $(r, \varphi) \mapsto (p, q)$, defined by

$$p = \psi(r) \cos \varphi, \qquad q = \psi(r) \sin \varphi.$$

   For which function $\psi(r)$ is it a symplectic transformation?

5. Prove that the definition (2.4) of $\Omega(M)$ does not depend on the parametrization φ, i.e., the parametrization $\psi = \varphi \circ \alpha$, where α is a diffeomorphism between suitable domains of $\mathbb{R}^2$, leads to the same result.
6. On the set $U = \{(p,q)\,;\, p^2+q^2 > 0\}$ consider the differential equation

$$\begin{pmatrix} \dot p \\ \dot q \end{pmatrix} = \frac{1}{p^2+q^2} \begin{pmatrix} p \\ q \end{pmatrix}. \tag{10.1}$$

Prove that
a) its flow is symplectic everywhere on U;
b) on every simply-connected subset of U the vector field (10.1) is Hamiltonian (with $H(p,q) = \text{Im } \log(p+iq) + \mathit{Const}$);
c) it is not possible to find a differentiable function $H : U \to \mathbb{R}$ such that (10.1) is equal to $J^{-1}\nabla H(p,q)$ for all $(p,q) \in U$.
Remark. The vector field (10.1) is locally (but not globally) Hamiltonian.
7. (Burnton & Scherer 1998). Prove that all members of the one-parameter family of Nyström methods of order $2s$, constructed in Exercise III.9, are symplectic and symmetric.
8. Prove that the statement of Lemma 4.1 remains true for methods that are formally defined by a B-series, $\Phi_h(y) = B(a,y)$.
9. Compute the generating function $S^1(P,q,h)$ of a symplectic Nyström method applied to $\ddot q = U(q)$.
10. Find the Hamilton–Jacobi equation (cf. Theorem 5.7) for the generating function $S^2(p,Q)$ of Lemma 5.3.
11. (*Jacobi's method for exact integration*). Suppose we have a solution $S(q,Q,t,\alpha)$ of the Hamilton–Jacobi equation (5.16), depending on d parameters $\alpha_1,\dots,\alpha_d$ such that the matrix $\left(\frac{\partial^2 S}{\partial \alpha_i \partial Q_j}\right)$ is invertible. Since this matrix is the Jacobian of the system

$$\frac{\partial S}{\partial \alpha_i} = 0 \qquad i = 1,\dots,d, \tag{10.2}$$

this system determines a solution path $Q_1,\dots,Q_q$ which is locally unique. In possession of an additional parameter (and, including the partial derivatives with respect to t, an additional row and column in the Hessian matrix condition), we can also determine $Q_j(t)$ as function of t. Apply this method to the Kepler problem (I.2.2) in polar coordinates, where, with the generalized momenta $p_r = \dot r$, $p_\varphi = r^2\dot\varphi$, the Hamiltonian becomes

$$H = \frac{1}{2}\left(p_r^2 + \frac{p_\varphi^2}{r^2}\right) - \frac{M}{r}$$

and the Hamilton–Jacobi differential equation (5.16) is

$$S_t + \frac{1}{2}\big(S_r\big)^2 + \frac{1}{2r^2}\big(S_\varphi\big)^2 - \frac{M}{r} = 0.$$

Solve this equation by the ansatz $S(t,r,\varphi) = \theta_1(t)+\theta_2(r)+\theta_3(\varphi)$ (separation of variables).

Result. One obtains

$$S = \int \sqrt{2\alpha_1 r^2 + 2Mr - \alpha_2^2}\, \frac{dr}{r} + \alpha_2 \varphi - \alpha_1 t.$$

Putting, e.g., $\partial S/\partial \alpha_2 = 0$, we obtain $\varphi = \arcsin \frac{Mr-\alpha_2^2}{\sqrt{M^2+2\alpha_1\alpha_2^2}\, r}$ by evaluating an elementary integral. This, when resolved for r, leads to the elliptic movement of Kepler (Sect. I.2.2). This method turned out to be most effective for the exact integration of difficult problems. With the same ideas, just more complicated in the computations, Jacobi solves in "lectures" 24 through 30 of (Jacobi 1842) the Kepler motion in $\mathbb{R}^3$, the geodesics of ellipsoids (his greatest triumph), the motion with two centres of gravity, and proves a theorem of Abel.

12. (*Chan's Lobatto IIIS methods.*) Show that there exists a one-parameter family of symplectic, symmetric (and A-stable) Runge–Kutta methods of order $2s-2$ based on Lobatto quadrature (Chan 1990). A special case of these methods can be obtained by taking the arithmetic mean of the Lobatto IIIA and Lobatto IIIB method coefficients (Sun 2000).
Hint. Use the W-transformation (see Hairer & Wanner (1996), p. 77) by putting $X_{s,s-1} = -X_{s-1,s}$ an arbitrary constant.
13. For a Hamiltonian system with associated Lagrangian $L(q,\dot q) = \frac{1}{2}\dot q^T M \dot q - U(q)$, show that every first integral $I(p,q) = p^T a(q)$ resulting from Noether's Theorem has a linear $a(q) = Aq + c$ with skew-symmetric MA.
Hint. (a) It is sufficient to consider the case $M = I$.
(b) Show that $a'(q)$ is skew-symmetric.
(c) Let $a_{ij}(q) = \frac{\partial a_i}{\partial q_j}(q)$. Using the symmetry of the Hessian of each component $a_i(q)$, show that $a_{ij}(q)$ does not depend on q_i, q_j, and is at most linear in the remaining components q_k. With the skew-symmetry of $a'(q)$, conclude that $a'(q) = Const$.
14. Consider the unconstrained *optimal control problem*

$$\begin{aligned} & C\big(q(T)\big) \;\to\; \min \\ & \dot q(t) = f\big(q(t), u(t)\big), \quad q(0) = q_0 \end{aligned} \tag{10.3}$$

on the interval $[0,T]$, where the control function is assumed to be continuous. Prove that first-order necessary optimality conditions can be written as

$$\begin{aligned} \dot q(t) &= \nabla_p H\big(p(t),q(t),u(t)\big), & q(0) &= q_0 \\ \dot p(t) &= -\nabla_q H\big(p(t),q(t),u(t)\big), & p(T) &= \nabla_q C\big(q(T)\big) \\ 0 &= \nabla_u H\big(p(t),q(t),u(t)\big), \end{aligned} \tag{10.4}$$

where the Hamiltonian is given by

$$H(p,q,u) = p^T f(q,u)$$

(we assume that the Hessian $\nabla_u^2 H(p,q,u)$ is invertible, so that the third relation of (10.4) defines u as a function of (p,q)).

Hint. Consider a slightly perturbed control function $u(t) + \varepsilon\delta u(t)$, and let $q(t)+\varepsilon\delta q(t)+\mathcal{O}(\varepsilon^2)$ be the corresponding solution of the differential equation in (10.3). With the function $p(t)$ of (10.4) we then have

$$C'\big(q(T)\big)\,\delta q(T) \;=\; \int_0^T \frac{d}{dt}\Big(p(t)^T\delta q(t)\Big)dt = \int_0^T p(t)^T f_u\big(\ldots\big)\delta u(t)dt.$$

The algebraic relation of (10.4) then follows from the fundamental lemma of variational calculus.

15. A Runge–Kutta discretization of the problem (10.3) is

$$\begin{aligned} C(q_N) \;&\to\; \min \\ q_{n+1} \;&=\; q_n + h\textstyle\sum_{i=1}^s b_i f(Q_{ni}, U_{ni}) \\ Q_{ni} \;&=\; q_n + h\textstyle\sum_{j=1}^s a_{ij} f(Q_{nj}, U_{nj}) \end{aligned} \tag{10.5}$$

with $n = 0, \ldots, N-1$ and $h = T/N$. We assume $b_i \neq 0$ for all i. Introducing suitable Lagrange multipliers for the constrained minimization problem (10.5), prove that there exist p_n, P_{ni} such that the optimal solution of (10.5) satisfies (Hager 2000)

$$\begin{aligned} q_{n+1} \;&=\; q_n + h\textstyle\sum_{i=1}^s b_i \nabla_p H(P_{ni}, Q_{ni}, U_{ni}) \\ Q_{ni} \;&=\; q_n + h\textstyle\sum_{j=1}^s a_{ij} \nabla_p H(P_{nj}, Q_{nj}, U_{nj}) \\ p_{n+1} \;&=\; p_n - h\textstyle\sum_{i=1}^s \widehat{b}_i \nabla_q H(P_{ni}, Q_{ni}, U_{ni}) \\ P_{ni} \;&=\; p_n - h\textstyle\sum_{j=1}^s \widehat{a}_{ij} \nabla_q H(P_{nj}, Q_{nj}, U_{nj}) \\ 0 \;&=\; \nabla_u H(P_{ni}, Q_{ni}, U_{ni}) \end{aligned} \tag{10.6}$$

with $p_N = \nabla_q C(q_N)$ and given initial value q_0, where the coefficients $\widehat{b}_i$ and $\widehat{a}_{ij}$ are determined by

$$\widehat{b}_i = b_i, \qquad b_i\widehat{a}_{ij} + \widehat{b}_j a_{ji} = b_i\widehat{b}_j. \tag{10.7}$$

Consequently, (10.6) can be considered as a symplectic discretization of (10.4); see Bonnans & Laurent-Varin (2006).

16. (Hager 2000). For an explicit s-stage Runge–Kutta method of order $p = s$ and $b_i \neq 0$, consider the partitioned Runge–Kutta method with additional coefficients $\widehat{b}_i$ and $\widehat{a}_{ij}$ defined by (10.7). Prove the following:
a) For $p = s = 3$, the partitioned method is of order 3 if and only if $c_3 = 1$.
b) For $p = s = 4$, the partitioned method is of order 4 without any restriction.