Symplectic Methods

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Definition

This entry, concerned with the practical task of integrating numerically Hamiltonian systems, follows up the entry ▸ Hamiltonian Systems and keeps the notation and terminology used there.

Each one-step numerical integrator is specified by a smooth map $\Psi^H_{t_{n+1},t_n}$ that advances the numerical solution from a time level t_n to the next t_{n+1}

$$(p^{n+1}, q^{n+1}) = \Psi^H_{t_{n+1},t_n}(p^n, q^n); \qquad (1)$$

the superscript H refers to the Hamiltonian function $H(p, q; t)$ of the system being integrated. For instance for the explicit Euler rule

$$(p^{n+1}, q^{n+1}) = (p^n, q^n) + (t_{n+1} - t_n)\big(f(p^n, q^n; t_n), g(p^n, q^n; t_n)\big);$$

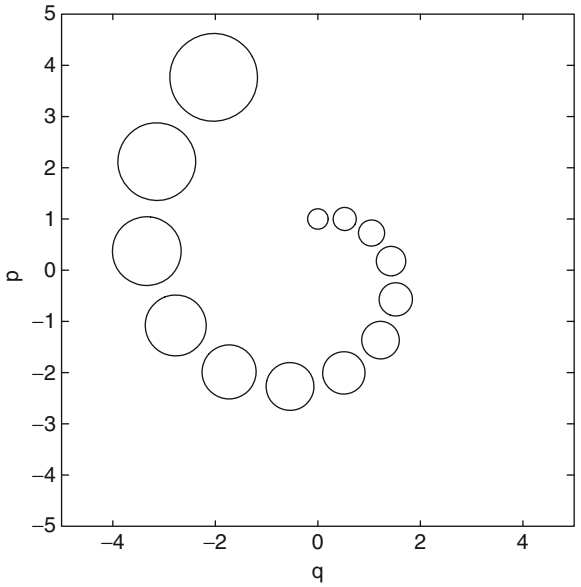
here and later f and g denote the d-dimensional real vectors with entries $-\partial H/\partial q_i$, $\partial H/\partial p_i$ (d is the number of degrees of freedom) so that (f, g) is the canonical vector field associated with H (in simpler words: the right-hand side of Hamilton's equations). For the integrator to make sense, $\Psi^H_{t_{n+1},t_n}$ has to approximate the solution operator $\Phi^H_{t_{n+1},t_n}$ that advances the true solution from its value at t_n to its value at t_{n+1}:

$$\big(p(t_{n+1}), q(t_{n+1})\big) = \Phi^H_{t_{n+1},t_n}\big(p(t_n), q(t_n)\big).$$

For a method of (consistency) order ν, $\Psi^H_{t_{n+1},t_n}$ differs from $\Phi^H_{t_{n+1},t_n}$ in terms of magnitude $\mathcal{O}\big((t_{n+1}-t_n)^{\nu+1}\big)$.

The solution map $\Phi^H_{t_{n+1},t_n}$ is a canonical (symplectic) transformation in phase space, an important fact that substantially constrains the dynamics of the true solution $\big(p(t), q(t)\big)$. If we wish the approximation Ψ^H to retain the "Hamiltonian" features of Φ^H, we should insist on Ψ^H also being a symplectic transformation. However, most standard numerical integrators – including explicit Runge–Kutta methods, regardless of their order ν – replace Φ^H by a nonsymplectic mapping Ψ^H. This is illustrated in Fig. 1 that corresponds to the Euler rule as applied to the harmonic oscillator $\dot{p} = -q$, $\dot{q} = p$. The (constant) step size is $t_{n+1} - t_n = 2\pi/12$. We have taken as a family of initial conditions the points of a circle centered at $p = 1, q = 0$ and seen the evolution after $1, 2, \ldots, 12$ steps. Clearly the circle, which should move clockwise without changing area, gains area as the integration proceeds: The numerical Ψ^H is not symplectic. As a result, the origin, a center in the true dynamics, is turned by the discretization procedure into an unstable spiral point, i.e., into something that cannot arise in Hamiltonian dynamics. For the implicit Euler rule, the corresponding integration loses area and gives rise to a family of smaller and smaller circles that spiral toward the origin. Again, such a stable focus is incompatible with Hamiltonian dynamics.

This failure of well-known methods in mimicking Hamiltonian dynamics motivated the consideration of integrators that generate a symplectic mapping Ψ^H when applied to a Hamiltonian problem. Such methods are called *symplectic* or *canonical.* Since symplectic transformations also preserve volume, symplectic integrators applied to Hamiltonian problems are automatically *volume preserving*. On the other hand, while many important symplectic integrators are time-



Symplectic Methods, Fig. 1 The harmonic oscillator integrated by the explicit Euler method

reversible (symmetric), reversibility is neither sufficient nor necessary for a method to be symplectic ([8], Remark 6.5).

Even though early examples of symplectic integration may be traced back to the 1950s, the systematic exploration of the subject started with the work of Feng Kang (1920–1993) in the 1980s. An early short monograph is [8] and later books are the comprehensive [5] and the more applied [6]. Symplectic integration was the first step in the larger endeavor of developing structure-preserving integrators, i.e., of what is now often called, following [7], *geometric integration*.

Limitations of space restrict this entry to one-step methods and *canonical* Hamiltonian problems. For noncanonical Hamiltonian systems and multistep integrators the reader is referred to [5], Chaps. VII and XV.

Integrators Based on Generating Functions

The earliest systematic approaches by Feng Kang and others to the construction of symplectic integrators (see [5], Sect. VI.5.4 and [8], Sect. 11.2) exploited the following well-known result of the canonical formalism: The canonical transformation $\Phi^H_{t_{n+1},t_n}$ possesses a generating function S_2 that solves an initial value problem for the associated Hamilton–Jacobi equation. It is then possible, by Taylor expanding that equation, to obtain an approximation $\widetilde{S}_2$ to S_2. The transformation $\Psi^H_{t_{n+1},t_n}$ generated by $\widetilde{S}_2$ will automatically be canonical and therefore will define a symplectic integrator. If $\widetilde{S}_2$ differs from S_2 by terms $\mathcal{O}\big((t_{n+1}-t_n)^{\nu+1}\big)$, the integrator will be of order ν. Generally speaking, the high-order methods obtained by following this procedure are more difficult to implement than those derived by the techniques discussed in the next two sections.

Runge–Kutta and Related Integrators

In 1988, Lasagni, Sanz-Serna, and Suris (see [8], Chap. 6) discovered independently that some well-known families of numerical methods contain symplectic integrators.

Runge–Kutta Methods

Symplecticness Conditions

When the Runge–Kutta (RK) method with s stages specified by the tableau

$$\begin{array}{c|ccc} a_{11} & \cdots & a_{1s} \\ \vdots & \ddots & \vdots \\ a_{s1} & \cdots & a_{ss} \\ \hline b_1 & \cdots & b_s \end{array} \tag{2}$$

is applied to the integration of the Hamiltonian system with Hamiltonian function H, the relation (1) takes the form

$$p^{n+1} = p^n + h_{n+1} \sum_{i=1}^{s} b_i \, f(P_i, Q_i; t_n + c_i h_{n+1}),$$

$$q^{n+1} = q^n + h_{n+1} \sum_{i=1}^{s} b_i \, g(P_i, Q_i; t_n + c_i h_{n+1}),$$

where $c_i = \sum_j a_{ij}$ are the abscissae, $h_{n+1} = t_{n+1} - t_n$ is the step size and P_i, Q_i, $i = 1, \ldots, s$ are the internal stage vectors defined through the system

$$P_i = p^n + h_{n+1} \sum_{j=1}^{s} a_{ij} \, f(P_j, Q_j; t_n + c_j h_{n+1}), \tag{3}$$

$$Q_i = q^n + h_{n+1} \sum_{j=1}^{s} a_{ij} \, g(P_j, Q_j; t_n + c_j h_{n+1}). \tag{4}$$

Lasagni, Sanz-Serna, and Suris proved that if the coefficients of the method in (2) satisfy

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i, j = 1, \ldots, s, \tag{5}$$

then the method is symplectic. Conversely ([8], Sect. 6.5), the relations (5) are essentially necessary for the method to be symplectic. Furthermore for symplectic RK methods the transformation (1) is in fact *exact symplectic* ([8], Remark 11.1).

Order Conditions

Due to symmetry considerations, the relations (5) impose $s(s+1)/2$ independent equations on the $s^2 + s$

elements of the RK tableau (2), so that there is no shortage of symplectic RK methods. The available free parameters may be used to increase the accuracy of the method. It is well known that the requirement that an RK formula has a target order leads to a set of nonlinear relations (order conditions) between the elements of the corresponding tableau (2). For order $\geq \nu$ there is an order condition associated with each rooted tree with $\leq \nu$ vertices and, if the a_{ij} and b_i are free parameters, the order conditions are mutually independent. For symplectic methods however the tableau coefficients are constrained by (5), and Sanz-Serna and Abia proved in 1991 that then there are redundancies between the order conditions ([8], Sect. 7.2). In fact to ensure order $\geq \nu$ when (5) holds it is necessary and sufficient to impose an order condition for each so-called nonsuperfluous (nonrooted) tree with $\leq \nu$ vertices.

Examples of Symplectic Runge–Kutta Methods

Setting $j = i$ in (5) shows that explicit RK methods (with $a_{ij} = 0$ for $i \leq j$) cannot be symplectic.

Sanz-Serna noted in 1988 ([8], Sect. 8.1) that the *Gauss method* with s stages, $s = 1, 2, \ldots$, (i.e., the unique method with s stages that attains the maximal order $2s$) *is* symplectic. When $s = 1$ the method is the familiar *implicit midpoint rule*. Since for all Gauss methods the matrix (a_{ij}) is full, the computation of the stage vectors P_i and Q_i require, at each step, the solution of the system (3) and (4) that comprises $s \times 2d$ scalar equations. In non-stiff situations this system is readily solved by functional iteration, see [8] Sects. 5.4 and 5.5 and [5] Sect. VIII.6, and then the Gauss methods combine the advantages of symplecticness, easy implementation, and high order with that of being applicable to all canonical Hamiltonian systems.

If the system being solved is stiff (e.g., it arises through discretization of the spatial variables of a Hamiltonian partial differential equation), Newton iteration has to be used to solve the stage equations (3) and (4), and for high-order Gauss methods the cost of the linear algebra may be prohibitive. It is then of interest to consider the possibility of *diagonally implicit* symplectic RK methods, i.e., methods where $a_{ij} = 0$ for $i < j$ and therefore (3) and (4) demand the successive solution of s systems of dimension $2d$, rather than that of a single $(s \times 2d)$–dimensional system. It turns out ([8], Sect. 8.2) that such methods are necessarily composition methods (see below) obtained by concatenating implicit midpoint sub-steps of lengths $b_1 h_{n+1}, \ldots, b_s h_{n+1}$. The determination of the free parameters b_i is a task best accomplished by means of the techniques used to analyze composition methods.

The B-series Approach

In 1994, Calvo and Sanz-Serna ([5], Sect. VI.7.2) provided an indirect technique for the derivation of the symplecticness conditions (5). The first step is to identify conditions for the symplecticness of the associated B-series (i.e., the series that expands the transformation (1)) in powers of the step size. Then the conditions (on the B-series) obtained in this way are shown to be equivalent to (5). This kind of approach has proved to be very powerful in the theory of geometric integration, where extensive use is made of formal power series.

Partitioned Runge–Kutta Methods

Partitioned Runge–Kutta (PRK) methods differ from standard RK integrators in that they use *two* tableaux of coefficients of the form (2): one to advance p and the other to advance q. Most developments of the theory of symplectic RK methods are easily adapted to cover the partitioned situation, see e.g., [8], Sects. 6.3, 7.3, and 8.4.

The main reason ([8], Sect. 8.4) to consider the class of PRK methods is that it contains integrators that are both *explicit* and symplectic when applied to *separable* Hamiltonian systems with $H(p, q; t) = T(p) + V(q; t)$, a format that often appears in the applications. It turns out ([8], Remark 8.1, [5], Sect. VI.4.1, Theorem 4.7) that such explicit, symplectic PRK methods may always be viewed as splitting methods (see below). Moreover it is advantageous to perform their analysis by interpreting them as splitting algorithms.

Runge–Kutta–Nyström Methods

In the special but important case where the (separable) Hamiltonian is of the form $H = (1/2)p^T M^{-1} p + V(q; t)$ (M a positive-definite symmetric matrix) the canonical equations

$$\frac{d}{dt} p = -\nabla V(q; t), \qquad \frac{d}{dt} q = M^{-1} p \tag{6}$$

lead to

$$\frac{d^2}{dt^2} q = -M^{-1} \nabla V(q; t),$$

a second-order system whose right-hand side is independent of $(d/dt)q$. Runge–Kutta–Nyström (RKN) methods may then be applied to the second-order form and are likely to improve on RK integrations of the original first-order system (6).

There are *explicit, symplectic* RKN integrators ([8], Sect. 8.5). However their application (see [8], Remark 8.5) is always equivalent to the application of an explicit, symplectic PRK method to the first-order equations (6) and therefore – in view of a consideration made above – to the application of a splitting algorithm.

Integrators Based on Splitting and Composition

The related ideas of splitting and composition are extremely fruitful in deriving practical symplectic integrators in many fields of application. The corresponding methods are typically *ad hoc* for the problem at hand and do not enjoy the universal off-the-shelf applicability of, say, Gaussian RK methods; however, when applicable, they may be highly efficient. In order to simplify the exposition, we assume hereafter that the Hamiltonian H is *time-independent* $H = H(p,q)$; we write $\phi^H_{h_{n+1}}$ and $\psi^H_{h_{n+1}}$ rather than $\Phi^H_{t_{n+1},t_n}$ and $\Psi^H_{t_{n+1},t_n}$. Furthermore, we shall denote the time step by h omitting the possible dependence on the step number n.

Splitting

Simplest Splitting

The easiest possibility of splitting occurs when the Hamiltonian H may be written as $H_1 + H_2$ and the Hamiltonian systems associated with H_1 and H_2 may be explicitly integrated. If the corresponding flows are denoted by $\phi_t^{H_1}$ and $\phi_t^{H_2}$, the recipe (Lie–Trotter splitting, [8], Sect. 12.4.2, [5], Sect. II.5)

$$\psi_h^H = \phi_h^{H_2} \circ \phi_h^{H_1} \tag{7}$$

defines the map (1) of a first-order integrator that is symplectic (the mappings being composed in the right-hand side are Hamiltonian flows and therefore symplectic). Splittings of H in more than two pieces are feasible but will not be examined here.

A particular case of (7) of great practical significance is provided by the *separable* Hamiltonian $H(p,q) = T(p) + V(q)$ with $H_1 = T$, $H_2 = V$; the flows associated with H_1 and H_2 are respectively given by

$$(p,q) \mapsto (p, q + t\nabla T(p)), \quad (p,q) \mapsto (p - t\nabla V(q), q).$$

Thus, in this particular case the scheme (7) reads

$$p^{n+1} = p^n - h\nabla V(q^{n+1}), \quad q^{n+1} = q^n + h\nabla T(p^n), \tag{8}$$

and it is sometimes called the *symplectic Euler* rule (it is obviously possible to interchange the roles of p and q). Alternatively, (8) may be considered as a one-stage, explicit, symplectic PRK integrator as in [8], Sect. 8.4.3.

As a second example of splitting, one may consider (nonseparable) formats $H = H_1(p,q) + V^*(q)$, where the Hamiltonian system associated with H_1 can be integrated in closed form. For instance, H_1 may correspond to a set of uncoupled harmonic oscillators and $V^*(q)$ represent the potential energy of the interactions between oscillators. Or H_1 may correspond to the Keplerian motion of a point mass attracted to a fixed gravitational center and V^* be a potential describing some sort of perturbation.

Strang Splitting

With the notation in (7), the symmetric Strang formula ([8], Sect. 12.4.3, [5], Sect. II.5)

$$\bar{\psi}_h^H = \phi_{h/2}^{H_2} \circ \phi_h^{H_1} \circ \phi_{h/2}^{H_2} \tag{9}$$

defines a time-reversible, *second-order* symplectic integrator $\bar{\psi}_h^H$ that improves on the first order (7).

In the separable Hamiltonian case $H = T(p) + V(q)$, (9) leads to

$$\begin{aligned} p^{n+1/2} &= p^n - \frac{h}{2}\nabla V(q^n), \\ q^{n+1} &= q^n + h\nabla T(p^{n+1/2}), \\ p^{n+1} &= p^{n+1/2} - \frac{h}{2}\nabla V(q^{n+1}). \end{aligned}$$

This is the Störmer–Leapfrog–Verlet method that plays a key role in molecular dynamics [6]. It is also possible

to regard this integrator as an explicit, symplectic PRK with two stages ([8], Sect. 8.4.3).

More Sophisticated Formulae

A further generalization of (7) is

$$\phi^{H_2}_{\beta_s h} \circ \phi^{H_1}_{\alpha_s h} \circ \phi^{H_2}_{\beta_{s-1} h} \circ \cdots \circ \phi^{H_2}_{\beta_1 h} \circ \phi^{H_1}_{\alpha_1 h} \tag{10}$$

where the coefficients α_i and β_i, $\sum_i \alpha_i = 1, \sum_i \beta_i = 1$, are chosen so as to boost the order ν of the method. A systematic treatment based on trees of the required order conditions was given by Murua and Sanz-Serna in 1999 ([5], Sect. III.3). There has been much recent activity in the development of accurate splitting coefficients α_i, β_i and the reader is referred to the entry ▸ Splitting Methods in this encyclopedia.

In the particular case where the splitting is given by $H = T(p) + V(q)$, the family (10) provides the most general explicit, symplectic PRK integrator.

Splitting Combined with Approximations

In (7), (9), or (10) use is made of the exact solution flows $\phi^{H_1}_t$ and $\phi^{H_2}_t$. Even if one or both of these flows are not available, it is still possible to employ the idea of splitting to construct symplectic integrators. A simple example will be presented next, but many others will come easily to mind.

Assume that we wish to use a Strang-like method but $\phi^{H_1}_t$ is not available. We may then advance the numerical solution via

$$\phi^{H_2}_{h/2} \circ \widehat{\psi}^{H_1}_h \circ \phi^{H_2}_{h/2}, \tag{11}$$

where $\widehat{\psi}^{H_1}_h$ denotes a consistent method for the integration of the Hamiltonian problem associated with H_1. If $\widehat{\psi}^{H_1}_h$ is time-reversible, the composition (11) is also time-reversible and hence of order $\nu = 2$ (at least). And if $\widehat{\psi}^{H_1}_h$ is symplectic, (11) will define a symplectic method.

Composition

A step of a composition method ([5], Sect. II.4) consists of a concatenation of a number of sub-steps performed with one or several simpler methods. Often the aim is to create a high-order method out of low-order integrators; the composite method automatically inherits the conservation properties shared by the methods being composed. The idea is of particular appeal within the field of geometric integration, where it is frequently not difficult to write down first- or second-order integrators with good conservation properties.

A useful example, due to Suzuki, Yoshida, and others (see [8], Sect. 13.1), is as follows. Let ψ^H_h be a time-reversible integrator that we shall call the *basic* method and define the composition method $\widehat{\psi}^H_h$ by

$$\widehat{\psi}^H_h = \psi^H_{\alpha h} \circ \psi^H_{(1-2\alpha)h} \circ \psi^H_{\alpha h};$$

if the basic method is symplectic, then $\widehat{\psi}^H_h$ will obviously be a symplectic method. It may be proved that, if $\alpha = (1/3)(2 + 2^{1/3} + 2^{-1/3})$, then $\widehat{\psi}^H_h$ will have order $\nu = 4$. By using this idea one may perform symplectic, fourth-order accurate integrations while really implementing a simpler second-order integrator. The approach is particularly attractive when the direct application of a fourth-order method (such as the two-stage Gauss method) has been ruled out on implementation grounds, but a suitable basic method (for instance the implicit midpoint rule or a scheme derived by using Strang splitting) is available.

If the (time-reversible) basic method is of order 2μ and $\alpha = \left(2 - 2^{1/(2\mu+1)}\right)^{-1}$ then $\widehat{\psi}^H_h$ will have order $\nu = 2\mu + 2$; the recursive application of this idea shows that it is possible to reach arbitrarily high orders starting from a method of order 2.

For further possibilities, see the entry ▸ Composition Methods and [8], Sect. 13.1, [5], Sects. II.4 and III.3.

The Modified Hamiltonian

The properties of symplectic integrators outlined in the next section depend on the crucial fact that, when a symplectic integrator is used, a numerical solution of the Hamiltonian system with Hamiltonian H may be viewed as an (almost) exact solution of a Hamiltonian system whose Hamiltonian function $\widetilde{H}$ (the so-called modified Hamiltonian) is a perturbation of H.

An example. Consider the application of the symplectic Euler rule (8) to a one-degree-of-freedom system with separable Hamiltonian $H = T(p) + V(q)$. In order to describe the behavior of the points (p^n, q^n) computed by the algorithm, we could just say that they approximately behave like the solutions $(p(t_n), q(t_n))$ of the Hamiltonian system $\mathcal{S}$ being integrated. This would not be a very precise description because the

true flow ϕ_h^H and its numerical approximation ψ_h^H differ in $\mathcal{O}(h^2)$ terms. Can we find *another* differential system $\mathcal{S}_2$ (called a modified system) so that (8) is consistent of the *second* order with $\mathcal{S}_2$? The points (p^n, q^n) would then be closer to the solutions of $\mathcal{S}_2$ than to the solutions of the system $\mathcal{S}$ we want to integrate. Straightforward Taylor expansions ([8], Sect. 10.1) lead to the following expression for $\mathcal{S}_2$ (recall that $f = -\partial H/\partial q$, $g = \partial H/\partial p$)

$$\frac{d}{dt}p = f(q) + \frac{h}{2}g(p)f'(q), \qquad \frac{d}{dt}q = g(p) - \frac{h}{2}g'(p)f(q), \tag{12}$$

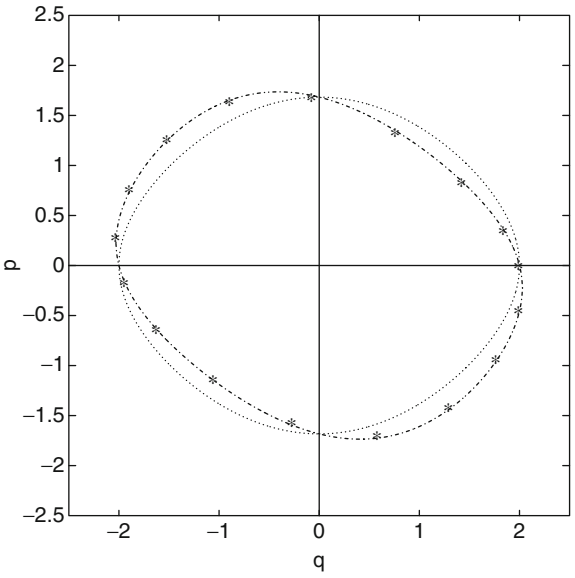
where we recognize the Hamiltonian system with (h-dependent!) Hamiltonian

$$\widetilde{H}_2^h = T(p) + V(q) + \frac{h}{2}T'(p)V'(q) = H + \mathcal{O}(h). \tag{13}$$

Figure 2 corresponds to the pendulum equations $g(p) = p$, $f(q) = -\sin q$ with initial condition $p(0) = 0$, $q(0) = 2$. The stars plot the numerical solution with $h = 0.5$. The dotted line $H =$ constant provides the true pendulum solution. The dash–dot line $\widetilde{H}_2^h =$ constant gives the solution of the modified system (12). The agreement of the computed points with the modified trajectory is very good.

The origin is a center of the modified system (recall that a small Hamiltonian perturbation of a Hamiltonian center is still a center); this matches the fact that, in the plot, the computed solution does not spiral in or out. On the other hand, the analogous modified system for the (nonsymplectic) integration in 1 is found not be a Hamiltonian system, but rather a system with negative dissipation: This agrees with the spiral behavior observed there.

By adding extra $\mathcal{O}(h^2)$ terms to the right-hand sides of (12), it is possible to construct a (more accurate) modified system $\mathcal{S}_3$ so that (8) is consistent of the *third* order with $\mathcal{S}_3$; thus, $\mathcal{S}_3$ would provide an even better description of the numerical solution. The procedure may be iterated to get modified systems $\mathcal{S}_4, \mathcal{S}_5, \ldots$ and all of them turn out to be Hamiltonian.



Symplectic Methods, Fig. 2 Computed points, true trajectory (*dotted line*) and modified trajectory (*dash–dot line*)

General case. Given an arbitrary Hamiltonian system with a smooth Hamiltonian H, a consistent symplectic integrator ψ_h^H and an arbitrary integer $\rho > 0$, it is possible ([8], Sect. 10.1) to construct a modified Hamiltonian system $\mathcal{S}_\rho$ with Hamiltonian function $\widetilde{H}_\rho^h$, such that ψ_h^H differs from the flow $\phi_h^{\widetilde{H}_\rho^h}$ in $\mathcal{O}(h^{\rho+1})$ terms. In fact, $\widetilde{H}_\rho^h$ may be chosen as a polynomial of degree $< \rho$ in h; the term independent of h coincides with H (cf. (13)) and for a method of order ν the terms in $h, \ldots, h^{\nu-1}$ vanish.

The polynomials in h $\widetilde{H}_\rho^h$, $\rho = 2, 3, \ldots$ are the partial sums of a series in powers of h. Unfortunately this series does not in general converge for fixed h, so that, in particular, the modified flows $\phi_h^{\widetilde{H}_\rho^h}$ cannot converge to ψ_h^H as $\rho \uparrow \infty$. Therefore, in general, it is impossible to find a Hamiltonian $\widetilde{H}^h$ such that $\phi_h^{\widetilde{H}^h}$ coincides *exactly* with the integrator ψ_h^H. Neishtadt ([8], Sect. 10.1) proved that by retaining for each $h > 0$ a suitable number $N = N(h)$ of terms of the series it is possible to obtain a Hamiltonian $\widetilde{H}^h$ such that $\phi_h^{\widetilde{H}^h}$ differs from ψ_h^H in an exponentially small quantity.

Here is the conclusion for the practitioner: For a symplectic integrator applied to an autonomous

Hamiltonian system, modified autonomous Hamiltonian problems exist so that the computed points lie "very approximately" on the exact trajectories of the modified problems. This makes possible a backward error interpretation of the numerical results: The computed solutions are solving "very approximately" a nearby Hamiltonian problem. In a modeling situation where the exact form of the Hamiltonian H may be in doubt, or some coefficients in H may be the result of experimental measurements, the fact that integrating the model numerically introduces perturbations to H comparable to the uncertainty in H inherent in the model is the most one can hope for.

On the other hand, when a nonsymplectic formula is used the modified systems are not Hamiltonian: The process of numerical integration perturbs the model in such a way as to take it out of the Hamiltonian class.

Variable steps. An important point to be noted is as follows: *The backward error interpretation only holds if the numerical solution after n steps is computed by iterating n times one and the same symplectic map.* If, alternatively, one composes n symplectic maps (one from t_0 to t_1, a different one from t_1 to t_2, etc.) the backward error interpretation is lost, because the modified system changes at each step ([8], Sect. 10.1.3).

As a consequence, *most favorable properties of symplectic integrators (and of other geometric integrators) are lost when they are naively implemented with variable step sizes.* For a complete discussion of this difficulty and of ways to circumvent it, see [5], Sects. VIII 1–4.

Finding explicitly the modified Hamiltonians. The *existence* of a modified Hamiltonian system is a general result that derives directly from the symplecticness of the transformation ψ_h^H ([8], Sect. 10.1) and does not require any hypothesis on the particular nature of such a transformation. However, much valuable information may be derived from the *explicit construction* of the modified Hamiltonians. For RK and related methods, a way to compute systematically the $\widetilde{H}_\rho^h$'s was first described by Hairer in 1994 and then by Calvo, Murua, and Sanz-Serna ([5], Sect. IX.9). For splitting and composition integrators, the $\widetilde{H}_\rho^h$'s may be obtained by use of the Baker–Campbell–Hausdorff formula ([8], Sect. 12.3, [5], Sect. III.4) that provides a means to express as a single flow the composition of two flows. This kind of research relies very much on concepts and techniques from the theory of Lie algebras.

Properties of Symplectic Integrators

We conclude by presenting an incomplete list of favorable properties of symplectic integrators. Note that the advantage of symplecticness become more prominent as the integration interval becomes longer.

Conservation of energy. For autonomous Hamiltonians, the value of H is of course a conserved quantity and the invariance of H usually expresses conservation of physical energy. Ge and Marsden proved in 1988 ([8], Sect. 10.3.2) that the requirements of symplecticness and *exact* conservation of H cannot be met simultaneously by a *bona fide* numerical integrator. Nevertheless, symplectic integrators have very good energy behavior ([5], Sect. IX.8): Under very general hypotheses, for a symplectic integrator of order ν: $H(p^n, q^n) = H(p^0, q^0) + \mathcal{O}(h^\nu)$, where the constant implied in the $\mathcal{O}$ notation is independent of n over exponentially long time intervals $nh \leq \exp\left(h_0/(2h)\right)$.

Linear error growth in integrable systems. For a Hamiltonian problem that is integrable in the sense of the Liouville–Arnold theorem, it may be proved ([5], Sect. X.3) that, in (long) time intervals of length proportional to $h^{-\nu}$, the errors in the action variables are of magnitude $\mathcal{O}(h^\nu)$ and remain bounded, while the errors in angle variables are $\mathcal{O}(h^\nu)$ and exhibit a growth that is only linear in t. By implication the error growth in the components of p and q will be $\mathcal{O}(h^\nu)$ and grow, at most, linearly. Conventional integrators, including explicit Runge–Kutta methods, typically show *quadratic* error growth in this kind of situation and therefore cannot be competitive in a sufficiently long integration.

KAM theory. When the system is closed to integrable, the KAM theory ([5], Chap. X) ensures, among other things, the existence of a number of invariant tori that contribute to the stability of the dynamics (see [8], Sect. 10.4 for an example). On each invariant torus the motion is quasiperiodic. Symplectic integrators ([5], Chap. X, Theorem 6.2) possess invariant tori $\mathcal{O}(h^\nu)$ close to those of the system being integrated and

furthermore the dynamics on each invariant torus is conjugate to its exact counterpart.

Linear error growth in other settings. Integrable systems are not the only instance where symplectic integrators lead to linear error growth. Other cases include, under suitable hypotheses, periodic orbits, solitons, relative equilibria, etc., see, among others, [1–4].

Cross-References

- ▸ B-Series
- ▸ Composition Methods
- ▸ Euler Methods, Explicit, Implicit, Symplectic
- ▸ Gauss Methods
- ▸ Hamiltonian Systems
- ▸ Molecular Dynamics
- ▸ Nyström Methods
- ▸ One-Step Methods, Order, Convergence
- ▸ Runge–Kutta Methods, Explicit, Implicit
- ▸ Symmetric Methods

References

1. Cano, B., Sanz-Serna, J.M.: Error growth in the numerical integration of periodic orbits, with application to Hamiltonian and reversible systems. SIAM J. Numer. Anal. **34**, 1391–1417 (1997)
2. de Frutos, J., Sanz-Serna, J.M.: Accuracy and conservation properties in numerical integration: the case of the Korteweg-deVries equation. Numer. Math. **75**, 421–445 (1997)
3. Duran, A., Sanz-Serna, J.M.: The numerical integration of relative equilibrium solution. Geometric theory. Nonlinearity **11**, 1547–1567 (1998)
4. Duran, A., Sanz-Serna, J.M.: The numerical integration of relative equilibrium solutions. The nonlinear Schroedinger equation. IMA. J. Numer. Anal. **20**, 235–261 (1998)
5. Hairer, E., Lubich, Ch., Wanner, G.: Geometric Numerical Integration, 2nd edn. Springer, Berlin (2006)
6. Leimkuhler, B., Reich, S.: Simulating Hamiltonian Dynamics. Cambridge University Press, Cambridge (2004)
7. Sanz-Serna, J.M.: Geometric integration. In: Duff, I.S., Watson, G.A. (eds.) The State of the Art in Numerical Analysis. Clarendon Press, Oxford (1997)
8. Sanz-Serna, J.M., Calvo, M.P.: Numerical Hamiltonian Problems. Chapman & Hall, London (1994)

Systems Biology, Minimalist vs Exhaustive Strategies

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Introduction

Systems biology may be defined as the study of how physiology emerges from molecular interactions [11]. Physiology tells us about function, whether at the organismal, tissue, organ or cellular level; molecular interactions tell us about mechanism. How do we relate mechanism to function? This has always been one of the central problems of biology and medicine but it attains a particular significance in systems biology because the molecular realm is the base of the biological hierarchy. Once the molecules have been identified, there is nowhere left to go but up.

This is an enormous undertaking, encompassing, among other things, the development of multicellular organisms from their unicellular precursors, the hierarchical scales from molecules to cells, tissues, and organs, and the nature of malfunction, disease, and repair. Underlying all of this is evolution, without which biology can hardly be interpreted. Organisms are not designed to perform their functions, they have evolved to do so—variation, transfer, drift, and selection have tinkered with them over 3.5×10^9 years—and this has had profound implications for how their functions have been implemented at the molecular level [12].

The mechanistic viewpoint in biology has nearly always required a strongly quantitative perspective and therefore also a reliance on quantitative models. If this trend seems unfamiliar to those who have been reared on molecular biology, it is only because our historical horizons have shrunk. The quantitative approach would have seemed obvious to physiologists, geneticists, and biochemists of an earlier generation. Moreover, quantitative methods wax and wane within an individual discipline as new experimental techniques emerge and the focus shifts between the descriptive and the functional. The great Santiago Ramón y Cajal, to whom we owe the conception of the central nervous system as a network of neurons, classified "theorists" with "contemplatives, bibliophiles and polyglots,