Lecture 2: Symplectic integrators

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A numerical one-step method $y_{n+1} = \Phi_h(y_n)$ is called *symplectic* if, when applied to a Hamiltonian system, the discrete flow $y \mapsto \Phi_h(y)$ is a symplectic transformation for all sufficiently small step sizes. Pioneering work on symplectic integrators is due to de Vogelaere (1956)[1], Ruth (1983)[2], and Feng Kang (1985)[3].

1 Basic symplectic integration schemes

The most simple symplectic integrators are motivated by the theory of generating functions for symplectic transformations (see Lecture 1). We consider the Hamiltonian system in the variables $y = (p, q)$,

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

[1] R. de Vogelaere, *Methods of integration which preserve the contact transformation property of the Hamiltonian equations*, Report No. 4, Dept. Math., Univ. of Notre Dame, Notre Dame, Ind. (1956)

[2] R.D. Ruth, *A canonical integration technique*, IEEE Trans. Nuclear Science NS-30 (1983) 2669–2671.

[3] K. Feng, *On difference schemes and symplectic geometry*, Proceedings of the 5-th Intern. Symposium on differential geometry & differential equations, Aug. 1984, Beijing (1985) 42–58.

Theorem 1 (symplectic Euler) *The so-called symplectic Euler methods*

$$\begin{aligned} p_{n+1} &= p_n - h\nabla_q H(p_{n+1}, q_n) \\ q_{n+1} &= q_n + h\nabla_p H(p_{n+1}, q_n) \end{aligned} \qquad \textit{or} \qquad \begin{aligned} p_{n+1} &= p_n - h\nabla_q H(p_n, q_{n+1}) \\ q_{n+1} &= q_n + h\nabla_p H(p_n, q_{n+1}) \end{aligned} \tag{1}$$

are symplectic methods of order 1.

Proof. Symplecticity is an immediate consequence of the first two characterizations of Theorem 5 (Lecture 1). Consistency of the scheme is obvious. □

The methods (1) are implicit for general Hamiltonian systems. For separable $H(p,q) = T(p) + U(q)$, however, both variants turn out to be explicit. This is also the case for the methods of the next theorem.

Theorem 2 (Störmer–Verlet) *The Störmer–Verlet schemes*

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

and

$$\begin{aligned} q_{n+1/2} &= q_n + \frac{h}{2}\,\nabla_p H(p_n, q_{n+1/2}) \\ p_{n+1} &= p_n - \frac{h}{2}\Big(\nabla_q H(p_n, q_{n+1/2}) + \nabla_q H(p_{n+1}, q_{n+1/2})\Big) \\ q_{n+1} &= q_{n+1/2} + \frac{h}{2}\,\nabla_p H(p_{n+1}, q_{n+1/2}) \end{aligned} \tag{3}$$

are symplectic methods of order 2.

Proof. The statement follows from the fact that the Störmer–Verlet scheme is the composition of the two symplectic Euler methods (1) with step size $h/2$. Even order 2 follows from its symmetry. □

For a second order differential equation $\ddot{q} = -\nabla U(q)$, for which the Hamiltonian is $H(p,q) = \frac{1}{2}\,p^{\mathsf{T}}p + U(q)$, method (2) becomes

$$q_{n+1} - 2\,q_n + q_{n-1} = -h^2\,\nabla U(q_n), \qquad p_n = \frac{q_{n+1} - q_{n-1}}{2h}. \tag{4}$$

Theorem 3 (implicit midpoint) *The implicit midpoint rule*

$$y_{n+1} = y_n + hJ^{-1}\nabla H\Big(\frac{y_{n+1} + y_n}{2}\Big) \tag{5}$$

is a symplectic method of order 2.

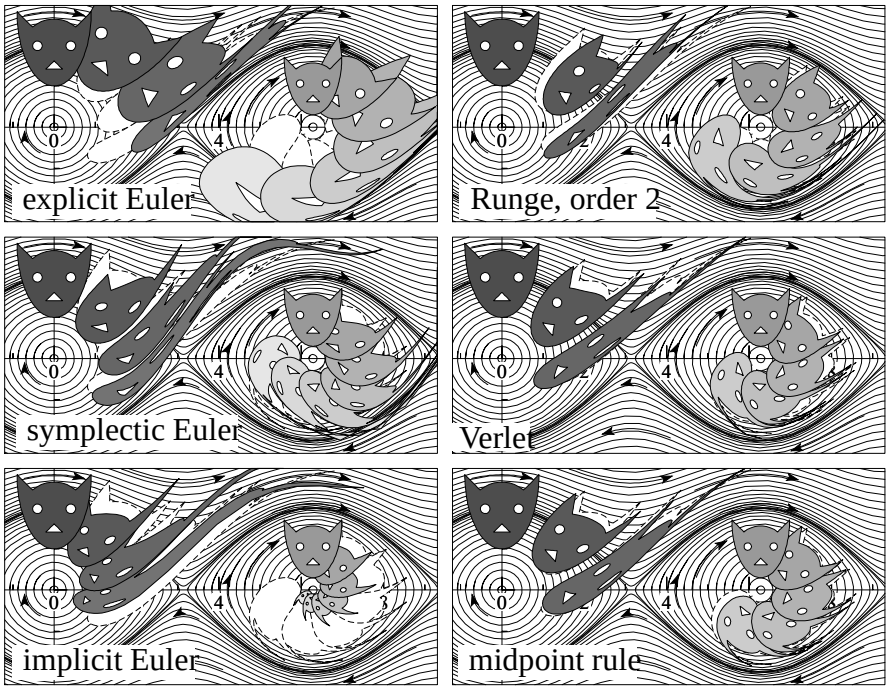


Figure 1: Area preservation of numerical methods for the pendulum; same initial sets as in Figure 3 of Lecture 1; first order methods (left column): $h = \pi/4$; second order methods (right column): $h = \pi/3$; dashed: exact flow.

Proof. Symplecticity is a consequence of the third characterization of Theorem 5 (Lecture 1), and order 2 follows from the symmetry of the method. □

We consider the pendulum problem with Hamiltonian $H(p, q) = \frac{1}{2}p^2 - \cos q$. We apply six different numerical methods to this problem: the explicit Euler method, the symplectic Euler method (1), and the implicit Euler method, as well as a second order method of Runge, the Störmer–Verlet scheme (2), and the implicit midpoint rule (5). 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 Figure 1[4] that the explicit Euler, the implicit Euler and the second order explicit method of Runge are not symplectic (not area preserving).

[4]This figure and most of the text are taken from the monograph *Geometric Numerical Integration* by Hairer, Lubich & Wanner.

2 Symplectic Runge–Kutta methods

An s-stage Runge–Kutta method, applied to an initial value problem $\dot{y} = f(t, y)$, $y(t_0) = y_0$ is given by the formulas

$$\begin{aligned} k_i &= f\Big(t_0 + c_i h, y_0 + h \sum_{j=1}^{s} a_{ij} k_j\Big), \quad i = 1, \ldots, s \\ y_1 &= y_0 + h \sum_{i=1}^{s} b_i k_i, \end{aligned} \tag{6}$$

where $c_i = \sum_{j=1}^{s} a_{ij}$. We allow a full matrix (a_{ij}) of non-zero coefficients, so that the slopes k_i are defined implicitly. For the study of their symplecticity we follow the approach of Bochev & Scovel[5]. It relates symplecticity to the conservation of quadratic first integrals. Recall that a function $I(y)$ is a *first integral* of the differential equation $\dot{y} = f(y)$, if $I'(y)f(y) = 0$ for all y.

Theorem 4 *If a Runge–Kutta method (6) conserves quadratic first integrals (i.e., $I(y_1) = I(y_0)$ whenever $I(y) = y^{\mathsf{T}} C y$, with symmetric matrix C, is a first integral of $\dot{y} = f(y)$), then it is symplectic.*

Proof. Symplecticity of the discrete flow $y \mapsto \Phi_h(y)$ means that for a Hamiltonian problem the quadratic expression $\Psi^{\mathsf{T}} J \Psi$ (with $\Psi = \Phi_h'(y)$) is a first integral of the variational equation. The statement of the theorem is therefore a consequence of the fact that for Runge–Kutta methods the following diagram commutes:

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

(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 $\Psi_n = \partial y_n / \partial y_0$.

[5] P.B. Bochev & C. Scovel, *On quadratic invariants and symplectic structure*, BIT 34 (1994) 337–345.

The commutativity of the above diagram 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. □

An elegant proof of symplecticity is possible for Gauss collocation methods. They are defined as follows: let $c_1, \ldots, c_s$ be the zeros of the shifted Legendre polynomial $\frac{d^s}{dx^s}\big(x^s(1-x)^s\big)$, and let $u(t)$ be the polynomial of degree s satisfying

$$\begin{aligned} u(t_0) &= y_0 \\ \dot u(t_0 + c_i h) &= f\big(t_0 + c_i h, u(t_0 + c_i h)\big), \quad i = 1, \ldots, s, \end{aligned} \tag{7}$$

then the numerical solution of the *Gauss collocation method* is defined by $y_1 = u(t_0 + h)$.

Putting $k_i = \dot u(t_0 + c_i h)$, and expressing $\dot u(t_0 + \tau h)$ and by integration also $u(t_0 + \tau h)$ in terms of the k_i, one see that these methods are special case of implicit Runge–Kutta methods. The implicit midpoint rule (5) is the special case $s = 1$ of the Gauss methods.

Theorem 5 *The Gauss collocation methods conserve quadratic first integrals and are thus symplectic by Theorem 4.*

Proof. Let $u(t)$ be the collocation polynomial of the Gauss methods, and assume that $I(y) = y^{\mathsf T} C\, y$, with symmetric C, is a first integral of $\dot y = f(y)$. Since $\frac{d}{dt} I\big(u(t)\big) = 2u(t)^{\mathsf T} C \dot u(t)$, it follows from $u(t_0) = y_0$ and $u(t_0 + h) = y_1$ that

$$y_1^{\mathsf T} C\, y_1 - y_0^{\mathsf T} C\, y_0 = 2 \int_{t_0}^{t_0+h} u(t)^{\mathsf T} C\, \dot u(t)\, dt. \tag{8}$$

The integrand $u(t)^{\mathsf T} C \dot u(t)$ is a polynomial of degree $2s - 1$, which is integrated without error by the s-stage Gaussian quadrature formula. It therefore follows from the collocation condition

$$u(t_0 + c_i h)^{\mathsf T} C\, \dot u(t_0 + c_i h) = u(t_0 + c_i h)^{\mathsf T} C\, f\big(u(t_0 + c_i h)\big) = 0$$

that the integral in (8) vanishes. □

The following criterion on the conservation of quadratic first integrals is due to Cooper[6], that on the symplecticity has been found independently by Lasagni[7], Sanz-Serna[8], and Suris[9].

Theorem 6 *If the coefficients of a Runge–Kutta method satisfy*

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \qquad \textit{for all } \; i, j = 1, \ldots, s, \tag{9}$$

then it conserves quadratic first integrals and it is symplectic (by Theorem 4).

Proof. The Runge–Kutta relation $y_1 = y_0 + h \sum_{i=1}^{s} b_i k_i$ yields

$$y_1^T C y_1 = y_0^T C y_0 + h \sum_{i=1}^{s} b_i \, k_i^T C y_0 + h \sum_{j=1}^{s} b_j \, y_0^T C k_j + h^2 \sum_{i,j=1}^{s} b_i b_j \, k_i^T C k_j. \tag{10}$$

We then write $k_i = f(Y_i)$ with $Y_i = y_0 + h \sum_{j=1}^{s} a_{ij} k_j$. The main idea is to compute y_0 from this relation and to insert it into the central expressions of (10). This yields (using the symmetry of C)

$$y_1^T C y_1 = y_0^T C y_0 + 2h \sum_{i=1}^{s} b_i \, Y_i^T C f(Y_i) + h^2 \sum_{i,j=1}^{s} (b_i b_j - b_i a_{ij} - b_j a_{ji}) \, k_i^T C k_j.$$

The condition (9) together with the assumption $y^T C f(y) = 0$, which states that $y^T C y$ is a first integral of $\dot y = f(y)$, imply $y_1^T C y_1 = y_0^T C y_0$. □

All results of this section can be extended to *partitioned Runge–Kutta methods*, where the components of p and q in a Hamiltonian system are treated by different Runge-Kutta methods. The most prominent examples are the symplectic Euler method (combination of explicit and implicit Euler) and the Störmer–Verlet method (combination of the trapezoidal rule and the implicit midpoint rule).

[6] G.J. Cooper, *Stability of Runge–Kutta methods for trajectory problems*, IMA J. Numer. Anal. 7 (1987) 1–13.

[7] F.M. Lasagni, *Canonical Runge–Kutta methods*, ZAMP 39 (1988) 952–953.

[8] J.M. Sanz-Serna, *Runge–Kutta schemes for Hamiltonian systems*, BIT 28 (1988) 877–883.

[9] Y.B. Suris, *On the conservation of the symplectic structure in the numerical solution of Hamiltonian systems* (in Russian), In: Numerical Solution of Ordinary Differential Equations, ed. S.S. Filippov, Keldysh Inst. of Appl. Math., USSR Academy of Sciences, Moscow, 1988, 148–160.

3 The Adjoint of a Method

The flow φ_t of an autonomous differential equation $\dot{y} = f(y)$ satisfies $\varphi_{-t}^{-1} = \varphi_t$. This property is in general not shared by the one-step map Φ_h of a numerical method. An illustration is presented in the upper picture of Figure 2 (a), where we see that the one-step map Φ_h for the explicit Euler method is different from the inverse of Φ_{-h}, which is the implicit Euler method.

Definition 1 The *adjoint method* Φ_h^* of a method Φ_h is the inverse map of the original method with reversed time step $-h$, i.e.,

$$\Phi_h^* := \Phi_{-h}^{-1} \tag{11}$$

(see Figure 2 (b)). In other words, $y_1 = \Phi_h^*(y_0)$ is implicitly defined by the relation $\Phi_{-h}(y_1) = y_0$. A method for which $\Phi_h^* = \Phi_h$ is called *symmetric*.

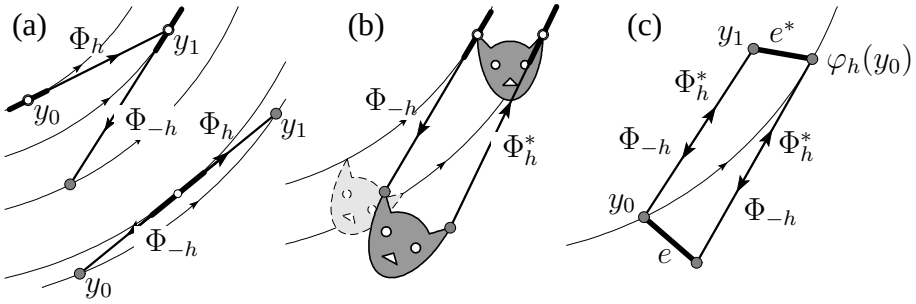


Figure 2: Definition and properties of the adjoint method

The adjoint method satisfies the usual properties such as $(\Phi_h^*)^* = \Phi_h$ and $(\Phi_h \circ \Psi_h)^* = \Psi_h^* \circ \Phi_h^*$ for any two one-step methods Φ_h and Ψ_h. The implicit Euler method is the adjoint of the explicit Euler method. The implicit midpoint rule is symmetric (see the lower picture of Figure 2 (a)), and the trapezoidal rule and the Störmer–Verlet method are also symmetric.

Theorem 7 *Let φ_t be the exact flow of $\dot{y} = f(y)$ and let Φ_h be a one-step method of order r satisfying*

$$\Phi_h(y_0) = \varphi_h(y_0) + C(y_0)h^{r+1} + \mathcal{O}(h^{r+2}). \tag{12}$$

The adjoint method Φ_h^* then has the same order r and we have

$$\Phi_h^*(y_0) = \varphi_h(y_0) + (-1)^r C(y_0)h^{r+1} + \mathcal{O}(h^{p+r}). \tag{13}$$

If the method is symmetric, its (maximal) order is even.

Proof. The idea of the proof is exhibited in drawing (c) of Figure 2. From a given initial value y_0 we compute $\varphi_h(y_0)$ and $y_1 = \Phi_h^*(y_0)$, whose difference e^* is the local error of Φ_h^*. This error is then projected back by Φ_{-h} to become e. We see that $-e$ is the local error of Φ_{-h}, i.e., by hypothesis (12),

$$e = (-1)^r C(\varphi_h(y_0))h^{r+1} + \mathcal{O}(h^{r+2}). \tag{14}$$

Since $\varphi_h(y_0) = y_0 + \mathcal{O}(h)$ and $e = (I + \mathcal{O}(h))e^*$, it follows that

$$e^* = (-1)^r C(y_0)h^{r+1} + \mathcal{O}(h^{r+2})$$

which proves (13). The statement for symmetric methods is an immediate consequence of this result, because $\Phi_h = \Phi_h^*$ implies $C(y_0) = (-1)^r C(y_0)$, and therefore $C(y_0)$ can be different from zero only for even r. □

4 Composition methods

Let Φ_h be a basic method and $\gamma_1, \ldots, \gamma_s$ real numbers. Then we call its composition with step sizes $\gamma_1 h, \gamma_2 h, \ldots, \gamma_s h$, i.e.,

$$\Psi_h = \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_1 h}, \tag{15}$$

the corresponding composition method (see Figure 3(a)). The aim is to increase the order while preserving desirable properties like symplecticity of the basic method.

Theorem 8 *Let Φ_h be a one-step method of order r. If*

$$\begin{aligned} \gamma_1 + \ldots + \gamma_s &= 1 \\ \gamma_1^{r+1} + \ldots + \gamma_s^{r+1} &= 0, \end{aligned} \tag{16}$$

then the composition method (15) *is at least of order $r + 1$.*

Proof. The proof is presented in Figure 3(b) for $s = 3$. It is very similar to the proof of Theorem 7. Starting with y_0, we let $y_i = \Phi_{\gamma_i h}(y_{i-1})$, so that $\Psi_h(y_0) = y_s$. By hypothesis we have $e_{i+1} = \varphi_{\gamma_i h}(y_i) - \Phi_{\gamma_i h}(y_i) = C(y_i)\,\gamma_i^{r+1} h^{r+1} + \mathcal{O}(h^{r+2})$, and the transported local error satisfies $E_i = (I + \mathcal{O}(h))e_i$ for all i. Because of $y_i = y_0 + \mathcal{O}(h)$ it follows from $\sum_{i=1}^s \gamma_i = 1$ (consistency requirement) that

$$\varphi_h(y_0) - \Psi_h(y_0) = E_1 + \ldots + E_s = C(y_0)(\gamma_1^{r+1} + \ldots + \gamma_s^{r+1})h^{r+1} + \mathcal{O}(h^{r+2})$$

which shows that under conditions (16) the $\mathcal{O}(h^{r+1})$-term vanishes. □

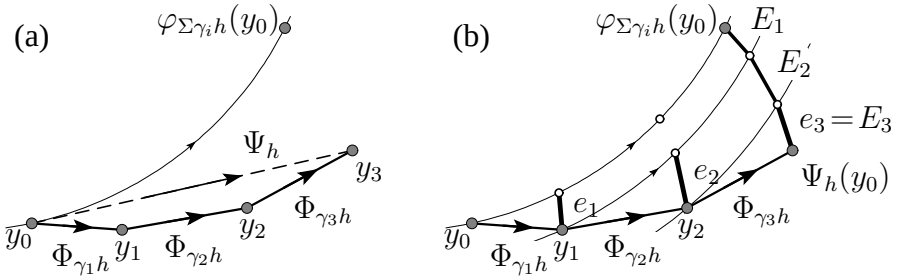


Figure 3: Composition of method Φ_h with three step sizes

Example 1 (The Triple Jump) Equations (16) have no real solution for odd r. Therefore, the order increase is only possible for even r. In this case, the smallest s which allows a solution is $s = 3$. We then have some freedom for solving the two equations. If we impose symmetry $\gamma_1 = \gamma_3$, then we obtain (Creutz & Gocksch[10], Forest[11], Suzuki[12], Yoshida[13])

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{1/(r+1)}}, \qquad \gamma_2 = -\frac{2^{1/(r+1)}}{2 - 2^{1/(r+1)}} \; . \tag{17}$$

This procedure can be repeated: we start with a symmetric method of order 2, apply (17) with $r = 2$ to obtain order 3; due to the symmetry of the γ's this new method is in fact of order 4 (see Theorem 7). With this new method we repeat (17) with $r = 4$ and obtain a symmetric 9-stage composition method of order 6, then with $r = 6$ a 27-stage symmetric composition method of order 8, and so on. One obtains in this way *any* order, however, at the price of a terrible zig-zag of the step points (see Figure 4).

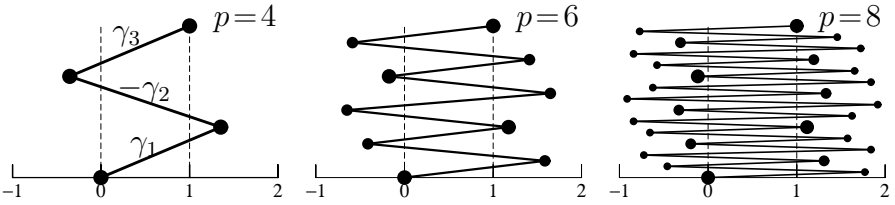


Figure 4: The Triple Jump of order 4 and its iterates of orders 6 and 8

[10]M. Creutz & A. Gocksch, *Higher-order hybrid Monte Carlo algorithms*, Phys. Rev. Lett. 63 (1989) 9–12.

[11]E. Forest, *Canonical integrators as tracking codes*, AIP Conference Proceedings 184 (1989) 1106–1136.

[12]M. Suzuki, *Fractal decomposition of exponential operators with applications to many-body theories and Monte Carlo simulations*, Phys. Lett. A 146 (1990) 319–323.

[13]H. Yoshida, *Construction of higher order symplectic integrators*, Phys. Lett. A 150 (1990) 262–268.

Example 2 (Suzuki's Fractals) If one desires methods with smaller values of γ_i, one has to increase s even more. For example, for $s = 5$ the best solution of (16) has the sign structure $++-++$ with $\gamma_1 = \gamma_2$ (Suzuki 1990). This leads to

$$\gamma_1 = \gamma_2 = \gamma_4 = \gamma_5 = \frac{1}{4 - 4^{1/(r+1)}}, \qquad \gamma_3 = -\frac{4^{1/(r+1)}}{4 - 4^{1/(r+1)}} \; . \tag{18}$$

The repetition of this algorithm for $r = 2, 4, 6, \ldots$ leads to a fractal structure of the step points (see Figure 5).

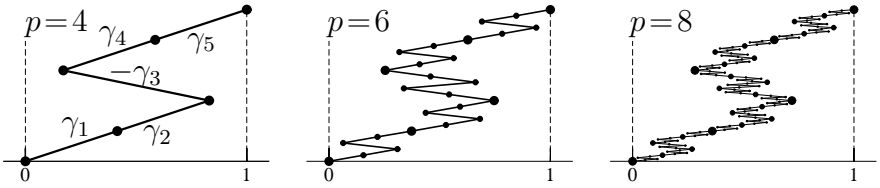


Figure 5: Suzuki's 'fractal' composition methods

Composition with the Adjoint Method. If we replace the composition (15) by the more general formula

$$\Psi_h = \Phi_{\alpha_s h} \circ \Phi^*_{\beta_s h} \circ \ldots \circ \Phi^*_{\beta_2 h} \circ \Phi_{\alpha_1 h} \circ \Phi^*_{\beta_1 h}, \tag{19}$$

the condition for order $r+1$ becomes, by using the result (13) and a similar proof as above,

$$\begin{aligned} \beta_1 + \alpha_1 + \beta_2 + \ldots + \beta_s + \alpha_s &= 1 \\ (-1)^r \beta_1^{r+1} + \alpha_1^{r+1} + (-1)^r \beta_2^{r+1} + \ldots + (-1)^r \beta_s^{r+1} + \alpha_s^{r+1} &= 0. \end{aligned} \tag{20}$$

This allows an order increase for odd r as well. In particular, we see at once the solution $\alpha_1 = \beta_1 = 1/2$ for $r = s = 1$, which turns every consistent one-step method of order 1 into a second-order symmetric method

$$\Psi_h = \Phi_{h/2} \circ \Phi^*_{h/2}. \tag{21}$$

For example, if Φ_h is the explicit (resp. implicit) Euler method, then Ψ_h in (21) becomes the implicit midpoint (resp. trapezoidal) rule. If Φ_h is the symplectic Euler method, then the composed method Ψ_h in (21) is the Störmer–Verlet method.

A Numerical Example. To demonstrate the numerical performance of the above methods, we choose the Kepler problem on the interval $[0, 7.5]$ with initial values corresponding to an eccentricity $e = 0.6$ (see Lecture 1). As the basic method we use the Störmer–Verlet scheme and compare in Figure 6 the Triple Jump (17) and Suzuki (18) compositions for a large number of different equidistant basic step sizes and for orders $r = 4, 6, 8, 10, 12$. The maximal final error is compared with

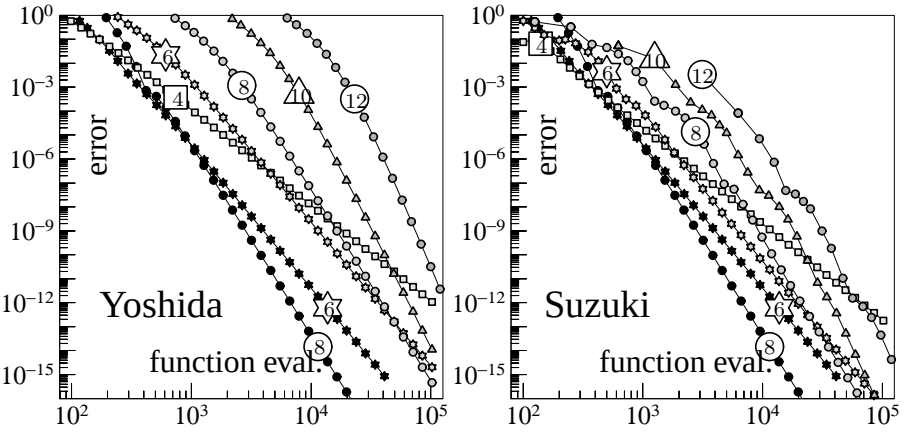
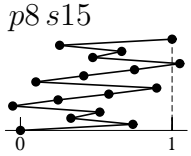


Figure 6: Numerical results of the Triple Jump and Suzuki step sequences (grey symbols) compared to optimal methods (black symbols)

the total number of function evaluations in double logarithmic scales. We observe that the wild zig-zag of the Triple Jump (17) is a more serious handicap than the large number of small steps of the Suzuki sequence (18).

Optimized composition methods. The construction of optimal methods (large order with minimal s) needs an elaborate order theory and cumbersome numerical search algorithms. We just present the coefficients of an 8th order method [14] [15] [16]

$$
\begin{aligned}
\gamma_1 = \gamma_{15} &= 0.74167036435061295344822780 \\
\gamma_2 = \gamma_{14} &= -0.40910082580003159399730010 \\
\gamma_3 = \gamma_{13} &= 0.19075471029623837995387626 \\
\gamma_4 = \gamma_{12} &= -0.57386247111608226665638773 \\
\gamma_5 = \gamma_{11} &= 0.29906418130365592384446354 \\
\gamma_6 = \gamma_{10} &= 0.33462491824529818378495798 \\
\gamma_7 = \gamma_9 \phantom{{}_{10}} &= 0.31529309239676659663205666 \\
\gamma_8 \phantom{{}_{10}} &= -0.79688793935291635401978884
\end{aligned}
\qquad
\begin{array}{c} p8\,s15 \\ \\ \\ \\ \\ \\ \\ \\ \end{array}
$$



(22)

The results of this 8th order method and of an optimized method of order 6 are included in Figure 6 with black symbols. They outperform those of the previous approaches.

[14] M. Suzuki & K. Umeno, *Higher-order decomposition theory of exponential operators and its applications to QMC and nonlinear dynamics*, Springer Proceedings in Physics 76 (1993) 74–86.

[15] M. Suzuki, *Quantum Monte Carlo methods and general decomposition theory of exponential operators and symplectic integrators*, Physica A 205 (1994) 65–79.

[16] R.I. McLachlan, *On the numerical integration of ordinary differential equations by symmetric composition methods*, SIAM J. Sci. Comput. 16 (1995) 151–168.

5 Splitting methods

We consider an arbitrary system $\dot{y} = f(y)$ in $\mathbb{R}^n$, and suppose that the vector field is "split" as (Figure 7)

$$\dot{y} = f^{[1]}(y) + f^{[2]}(y). \tag{23}$$

If the exact flows $\varphi_t^{[1]}$ and $\varphi_t^{[2]}$ of the systems $\dot{y} = f^{[1]}(y)$ and $\dot{y} = f^{[2]}(y)$ can be calculated explicitly, we can compose them to get numerical approximations.

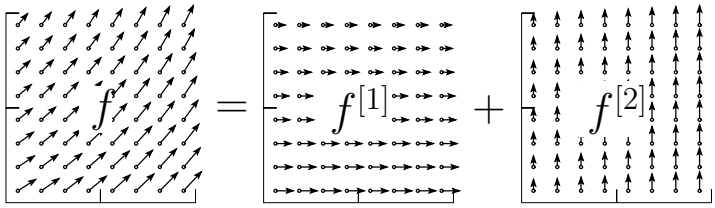
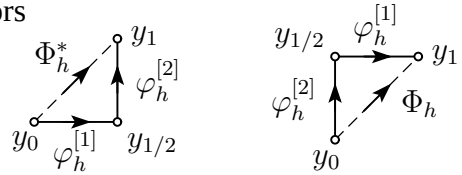


Figure 7: A splitting of a vector field.

Lie–Trotter[17] **splitting.** If, from a given initial value y_0, we first solve the first system to obtain a value $y_{1/2}$, and from this value integrate the second system to obtain y_1, we get numerical integrators

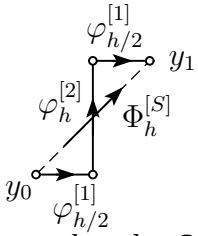
$$\Phi_h^* = \varphi_h^{[2]} \circ \varphi_h^{[1]} \qquad \Phi_h = \varphi_h^{[1]} \circ \varphi_h^{[2]} \tag{24}$$



where one is the adjoint of the other. By Taylor expansion we find that $(\varphi_h^{[1]} \circ \varphi_h^{[2]})(y_0) = \varphi_h(y_0) + \mathcal{O}(h^2)$, so that both methods give approximations of order 1 to the solution of (23).

Strang[18] **splitting or Marchuk**[19] **splitting.** Another idea is to use a symmetric version and put

$$\Phi_h^{[S]} = \varphi_{h/2}^{[1]} \circ \varphi_h^{[2]} \circ \varphi_{h/2}^{[1]}\,, \tag{25}$$



By breaking up in (25) $\varphi_h^{[2]} = \varphi_{h/2}^{[2]} \circ \varphi_{h/2}^{[2]}$, we see that the Strang splitting

[17] H.F. Trotter, *On the product of semi-groups of operators*, Proc. Am. Math. Soc.10 (1959) 545–551.

[18] G. Strang, *On the construction and comparison of difference schemes*, SIAM J. Numer. Anal. 5 (1968) 506–517.

[19] G. Marchuk, *Some applications of splitting-up methods to the solution of mathematical physics problems*, Aplikace Matematiky 13 (1968) 103–132.

$\Phi_h^{[S]} = \Phi_{h/2} \circ \Phi_{h/2}^*$ is the composition of the Lie-Trotter method and its adjoint with halved step sizes. The Strang splitting formula is therefore symmetric and of order 2 (see formula (21)).

Example 3 (The Symplectic Euler and the Störmer–Verlet Schemes) Suppose we have a Hamiltonian system with separable Hamiltonian $H(p,q) = T(p) + U(q)$. We consider this as the sum of two Hamiltonians, the first one depending only on p, the second one only on q. The corresponding Hamiltonian systems

$$\begin{aligned} \dot{p} &= 0 \\ \dot{q} &= \nabla_p T(p) \end{aligned} \qquad \text{and} \qquad \begin{aligned} \dot{p} &= -\nabla_q U(q) \\ \dot{q} &= 0 \end{aligned} \tag{26}$$

can be solved without problem to yield

$$\begin{aligned} p(t) &= p_0 \\ q(t) &= q_0 + t\,\nabla_p T(p_0) \end{aligned} \qquad \text{and} \qquad \begin{aligned} p(t) &= p_0 - t\,\nabla_q U(q_0) \\ q(t) &= q_0. \end{aligned} \tag{27}$$

Denoting the flows of these two systems by φ_t^T and φ_t^U, we see that the symplectic Euler method (1) is just the composition $\varphi_h^T \circ \varphi_h^U$, and its adjoint is $\varphi_h^U \circ \varphi_h^T$. The Störmer–Verlet scheme (2) is $\varphi_{h/2}^U \circ \varphi_h^T \circ \varphi_{h/2}^U$, the Strang splitting (25).

General Splitting Procedure. In a similar way to the general idea of composition methods (19), we can form with arbitrary coefficients $a_1, b_1, a_2, \ldots, a_m, b_m$ (where, eventually, a_1 or b_m, or both, are zero)

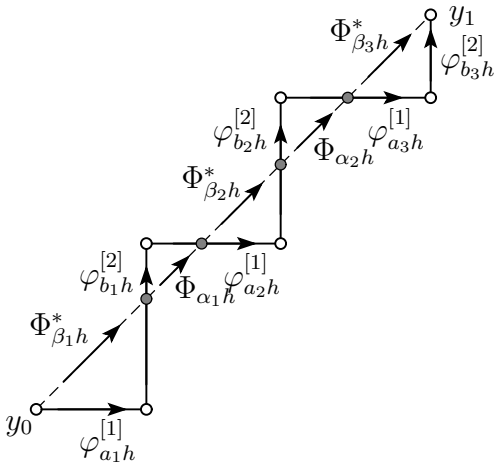
$$\Psi_h = \varphi_{b_m h}^{[2]} \circ \varphi_{a_m h}^{[1]} \circ \varphi_{b_{m-1} h}^{[2]} \circ \ldots \circ \varphi_{a_2 h}^{[1]} \circ \varphi_{b_1 h}^{[2]} \circ \varphi_{a_1 h}^{[1]} \tag{28}$$

and try to increase the order of the scheme by suitably determining the free coefficients.

A close connection between the theories of splitting methods (28) and of composition methods (19) was discovered by McLachlan (1995). Indeed, if we put $\beta_1 = a_1$ and break up $\varphi_{b_1 h}^{[2]} = \varphi_{\alpha_1 h}^{[2]} \circ \varphi_{\beta_1 h}^{[2]}$ (group property of the exact flow) where α_1 is given in (30), further $\varphi_{a_2 h}^{[1]} = \varphi_{\beta_2 h}^{[1]} \circ \varphi_{\alpha_1 h}^{[1]}$ and so on (cf. Figure 8), we see, using (24), that Ψ_h of (28) is identical with Ψ_h of (19), where

$$\Phi_h = \varphi_h^{[1]} \circ \varphi_h^{[2]} \qquad \text{so that} \qquad \Phi_h^* = \varphi_h^{[2]} \circ \varphi_h^{[1]}. \tag{29}$$

A necessary and sufficient condition for the existence of α_i and β_i satisfying (30) is that $\sum a_i = \sum b_i$, which is the consistency condition anyway for method (28).



$$\begin{aligned} a_1 &= \beta_1 \\ b_1 &= \beta_1 + \alpha_1 \\ a_2 &= \alpha_1 + \beta_2 \\ b_2 &= \beta_2 + \alpha_2 \\ a_3 &= \alpha_2 + \beta_3 \\ b_3 &= \beta_3 \end{aligned} \tag{30}$$

Figure 8: Equivalence of splitting and composition methods.

Combining Exact and Numerical Flows. If the splitting (23) is such that only the flow of, say, $\dot{y} = f^{[1]}(y)$ can be computed exactly, we can consider

$$\Phi_h = \varphi_h^{[1]} \circ \Phi_h^{[2]}, \qquad \Phi_h^* = \Phi_h^{[2]*} \circ \varphi_h^{[1]} \tag{31}$$

as the basis of the composition method (19). Here $\varphi_t^{[1]}$ is the exact flow of $\dot{y} = f^{[1]}(y)$, and $\Phi_h^{[2]}$ is some first-order integrator applied to $\dot{y} = f^{[2]}(y)$. Since Φ_h of (31) is consistent with (23), the above interpretation of splitting methods as composition methods implies that the resulting method

$$\Psi_h = \varphi^{[1]}_{\alpha_s h} \circ \Phi^{[2]}_{\alpha_s h} \circ \Phi^{[2]*}_{\beta_s h} \circ \varphi^{[1]}_{(\beta_s+\alpha_{s-1})h} \circ \Phi^{[2]}_{\alpha_{s-1} h} \circ \ldots \circ \Phi^{[2]*}_{\beta_1 h} \circ \varphi^{[1]}_{\beta_1 h} \tag{32}$$

has the desired high order. Notice that replacing $\varphi_t^{[2]}$ with a low-order approximation $\Phi_t^{[2]}$ in (28) would not retain the high order of the composition, because $\Phi_t^{[2]}$ does not satisfy the group property.

Splitting into More than Two Vector Fields. Consider a differential equation

$$\dot{y} \;=\; f^{[1]}(y) + f^{[2]}(y) + \ldots + f^{[N]}(y), \tag{33}$$

where we assume that the flows $\varphi_t^{[j]}$ of the individual problems $\dot{y} = f^{[j]}(y)$ can be computed exactly. There are many possibilities for extending (28) and for writing the method as a composition of $\varphi^{[1]}_{a_j h}, \varphi^{[2]}_{b_j h}, \varphi^{[3]}_{c_j h}, \ldots$. A simple and efficient way is to consider the first-order method

$$\Phi_h = \varphi_h^{[1]} \circ \varphi_h^{[2]} \circ \ldots \circ \varphi_h^{[N]}$$

together with its adjoint as the basis of the composition (19). Without any additional effort this yields splitting methods for (33) of arbitrary high order.

6 Integrators based on generating functions

To construct symplectic numerical methods of high order, Feng Kang[20] and Channell & Scovel[21] proposed computing an approximate solution of the Hamilton–Jacobi equation.

Recall that a mapping $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ defined by

$$p_{n+1} = p_n - \nabla_q S^1(p_{n+1}, q_n), \qquad q_{n+1} = q_n + \nabla_p S^1(p_{n+1}, q_n) \tag{34}$$

is always symplectic (Section 5 of Lecture 1) and that it reproduces the exact solution (after time h) of the Hamiltonian system (Section 6 of Lecture 1) if

$$S^1(p, q, t) = h\, G_1(p, q) + h^2\, G_2(p, q) + h^3\, G_3(p, q) + \ldots$$

where

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

If we use the truncated series

$$S^1(p, q) = h\, G_1(p, q) + h^2\, G_2(p, q) + \ldots + h^r\, G_r(p, q) \tag{35}$$

and insert it into (34), we obtain a symplectic one-step method of order r. 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 (1)).

7 Variational integrators

All previous approaches start from extremizing the *action integral*

$$S(q) = \int_{t_0}^{t_N} L\big(q(t), \dot{q}(t)\big)\, dt,$$

then deriving the Euler–Lagrange equations and the equivalent Hamiltonian equations, and finally discretize the resulting differential equations.

[20] K. Feng, *Difference schemes for Hamiltonian formalism and symplectic geometry*, J. Comp. Math. 4 (1986) 279–289.

[21] P.J. Channell & J.C. Scovel, *Symplectic integration of Hamiltonian systems*, Nonlinearity 3 (1990) 231–259.

Variational integrators start from discretizing the action integral followed by extremizing it in a finite dimensional space to obtain discrete Euler–Lagrange equations and (symplectic) numerical integrators.

For given q_0 and q_N, we consider the approximation

$$\mathcal{S}_h(\{q_n\}_0^N) = \sum_{n=0}^{N-1} L_h(q_n, q_{n+1}), \qquad L_h(q_n, q_{n+1}) \approx \int_{t_n}^{t_{n+1}} L(q(t), \dot{q}(t))\, dt$$

of the action integral, where L_h plays the role of a *discrete Lagrangian*. The requirement $\partial \mathcal{S}_h / \partial q_n = 0$ for an extremum yields the *discrete Euler–Lagrange equations*

$$\frac{\partial L_h}{\partial y}(q_{n-1}, q_n) + \frac{\partial L_h}{\partial x}(q_n, q_{n+1}) = 0 \tag{36}$$

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

$$p_n = -\frac{\partial L_h}{\partial x}(q_n, q_{n+1}), \tag{37}$$

so that the discrete Euler–Lagrange equations become equivalent to (substitute n for $n+1$ in (36))

$$p_{n+1} = \frac{\partial L_h}{\partial y}(q_n, q_{n+1}). \tag{38}$$

Under suitable assumptions on L_h, the two equations (37) and (38) define a mapping $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$.

Theorem 9 *The numerical method $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$, defined by (37) and (38), is a symplectic integrator.*

Proof. The differential of $L_h = L_h(q_n, q_{n+1})$ satisfies

$$dL_h = p_{n+1}\, dq_{n+1} - p_n\, dq_n,$$

which proves symplecticity by Theorem 4 of Lecture 1. □

Example 4 (MacKay[22]) Choose $L_h(q_n, q_{n+1})$ by approximating $q(t)$ as the linear interpolant of q_n and q_{n+1} and the integral by the trapezoidal rule. This gives

$$L_h(q_n, q_{n+1}) \;=\; \frac{h}{2}\, L\Big(q_n, \frac{q_{n+1} - q_n}{h}\Big) + \frac{h}{2}\, L\Big(q_{n+1}, \frac{q_{n+1} - q_n}{h}\Big) \tag{39}$$

[22] R. MacKay, *Some aspects of the dynamics of Hamiltonian systems*, in: D.S. Broomhead & A. Iserles, eds., *The Dynamics of Numerics and the Numerics of Dynamics*, Clarendon Press, Oxford, 1992, 137–193.

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 $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - U(q)$ and with the notation $p_{n+1/2} = M v_{n+1/2}$, this reduces to the Störmer–Verlet method

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2}\nabla U(q_n) \\ q_{n+1} &= q_n + h\, M^{-1} p_{n+1/2} \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2}\nabla U(q_{n+1}). \end{aligned}$$

In this case, the discrete Euler–Lagrange equations (36) become the familiar second order difference formula $M(q_{n+1} - 2q_n + q_{n-1}) = -h^2 \nabla U(q_n)$.

Example 5 (Wendlandt & Marsden[23]) Approximating the action integral instead by the midpoint rule gives

$$L_h(q_n, q_{n+1}) = hL\Big(\frac{q_{n+1} + q_n}{2}, \frac{q_{n+1} - q_n}{h}\Big). \tag{40}$$

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 $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - U(q)$ and $p_{n+1/2} = M v_{n+1/2}$, this becomes the implicit midpoint rule

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2}\nabla U(q_{n+1/2}) \\ q_{n+1} &= q_n + h\, M^{-1} p_{n+1/2} \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2}\nabla U(q_{n+1/2}), \end{aligned}$$

because we have $p_{n+1/2} = (p_{n+1} + p_n)/2$.

[23] J.M. Wendlandt & J.E. Marsden, *Mechanical integrators derived from a discrete variational principle*, Physica D 106 (1997) 223–246.

8 Exercises

1. Prove that under the condition (9) a Runge–Kutta method preserves all first integrals of the form $I(y) = y^T C y + d^T y + c$.

2. Prove that the Gauss methods of maximal oder $2s$ are the only collocation methods satisfying (9).

   Hint. Use the ideas of the proof of Lemma 13.9 in Hairer & Wanner[24].

3. Show that each of the symplectic Euler methods in (1) is the adjoint of the other.

4. Consider the composition method (15) with $s = 5$, $\gamma_5 = \gamma_1$, and $\gamma_4 = \gamma_2$. Among the solutions of

   $$2\gamma_1 + 2\gamma_2 + \gamma_3 = 1, \qquad 2\gamma_1^3 + 2\gamma_2^3 + \gamma_3^3 = 0$$

   find the one that minimizes $|2\gamma_1^5 + 2\gamma_2^5 + \gamma_3^5|$.

   Remark. This property motivates the choice of the γ_i in (18).

5. Design a symmetric splitting method for the Euler equations of a rigid body with given principal momenta of inertia I_1, I_2, I_3

   $$\dot{y} = B(y)\nabla H(y), \qquad B(y) = \begin{pmatrix} 0 & -y_3 & y_2 \\ y_3 & 0 & -y_1 \\ -y_2 & y_1 & 0 \end{pmatrix}$$

   by splitting the Hamiltonian

   $$H(y_1, y_2, y_3) = \frac{1}{2}\Big(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3} \Big)$$

   into three parts.

[24] E. Hairer & G. Wanner, *Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems, 2nd edition*, Springer Series in Computational Mathematics **14**, Springer-Verlag Berlin, 1996.