Geometric Numerical Integration of Differential Equations

Ernst Hairer

Université de Genève

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E. Hairer, Ch. Lubich and G. Wanner, Geometric Numerical Integration, Second edition, Springer-Verlag, 2006

Summerschool in Aveiro (Sept. 2018), Ernst Hairer

- **Part I. Geometric numerical integration**
  - Hamiltonian systems, symplectic mappings, geometric integrators, Störmer–Verlet, composition and splitting, variational integrator
  - Backward error analysis, modified Hamiltonian, long-time energy conservation, application to charged particle dynamics

- **Part II. Differential equations with multiple time-scales**
  - Highly oscillatory problems, Fermi–Pasta–Ulam-type problems, trigonometric integrators, adiabatic invariants
  - Modulated Fourier expansion, near-preservation of energy and of adiabatic invariants, application to wave equations

Lecture 1. Introduction to geometric integration

1. **Introduction and examples**
   - Explicit, implicit, and symplectic Euler
   - Kepler and N-body problems

2. **Hamiltonian systems**
   - Symplectic mappings
   - Theorem of Poincaré
   - Symplectic Euler methods
   - Störmer–Verlet integrator

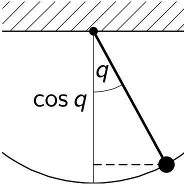
3. **Symplectic integration methods**
   - Runge–Kutta methods
   - Composition and splitting methods
   - Variational integrators

Mathematical pendulum

$$\ddot{q} + \sin q = 0$$

or

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\sin q \end{aligned}$$

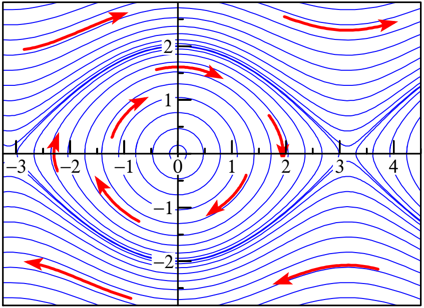


The energy

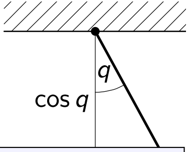
$$H(p,q) = \tfrac{1}{2}\, p^2 - \cos q$$

is constant along solutions:

$$H\big(p(t), q(t)\big) = \text{Const.}$$



Mathematical pendulum



$$\ddot{q} + \sin q = 0$$

or

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\sin q \end{aligned}$$

Proof. $\dfrac{\mathrm{d}}{\mathrm{d}t} H\big(p(t), q(t)\big) = p(t)\dot{p}(t) + \sin(q(t))\dot{q}(t) = 0$

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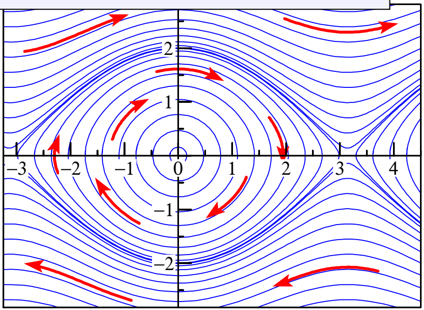
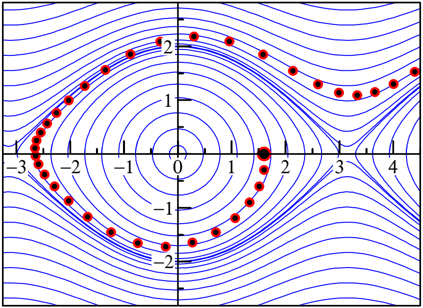


Explicit Euler

$$
\begin{aligned}
q_{n+1} &= q_n + h\,p_n \\
p_{n+1} &= p_n - h\,\sin q_n
\end{aligned}
$$



Implicit Euler

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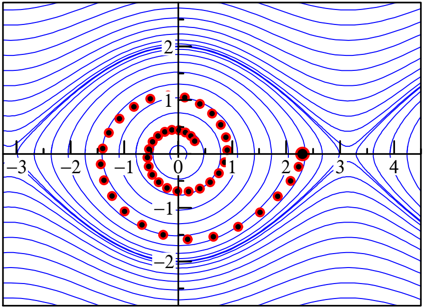

Constant step size $h = 0.3$ in both cases.
Initial values: large symbols.

Symplectic Euler methods

$$\begin{aligned} q_{n+1} &= q_n + h\, p_n \\ p_{n+1} &= p_n - h \sin q_{n+1} \end{aligned}$$

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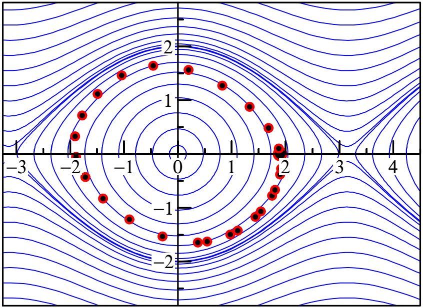
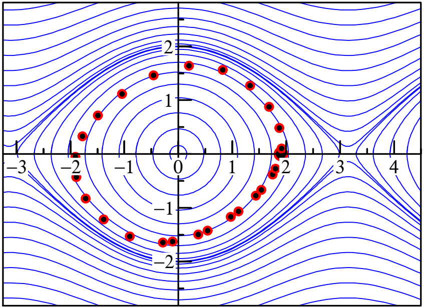


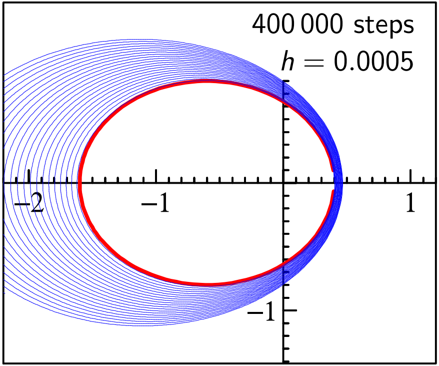


Constant step size $h = 0.4$ in both cases.
Same initial values: large symbols.

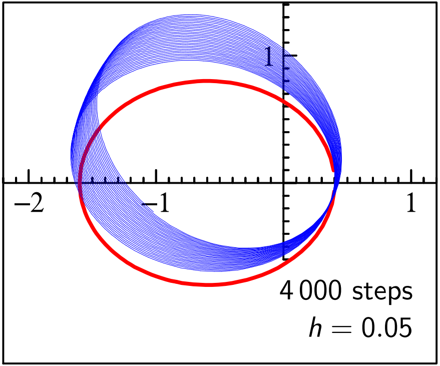
Kepler problem (two-body problem)

$$\dot{q}_i = p_i, \qquad \dot{p}_i = -\frac{q_i}{(q_1^2 + q_2^2)^{3/2}}, \qquad i = 1, 2$$

exact solution in (q_1, q_2)-space is an ellipse (drawn in red)



explicit Euler



symplectic Euler

N-body problems

The differential equation is given by

$$\dot q_i = \frac{\partial H}{\partial p_i}(p,q), \quad \dot p_i = -\frac{\partial H}{\partial q_i}(p,q), \quad i = 1,\ldots,N$$

where

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}\,p_i^{\mathsf T} p_i + \sum_{i=2}^{N}\sum_{j=1}^{i-1} V_{ij}\big(\|q_i - q_j\|\big)$$

Astronomy (solar system): $V_{ij}(r) = -G\,\dfrac{m_i m_j}{r}$

Molecular dynamics (Lennard–Jones): $V_{ij}(r) = \varepsilon_{ij}\left(\left(\dfrac{\sigma_{ij}}{r}\right)^{12} - \left(\dfrac{\sigma_{ij}}{r}\right)^{6}\right)$

Further examples of Hamiltonian systems

- Integrable Hamiltonian systems
  - Toda lattice
  - discretized Schrödinger equation
- chaotic systems
  - double (multiple) pendulum
  - Hénon–Heiles system
- rigid body dynamics
  - free rigid body
  - top, levitron

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Hamiltonian systems

Differential equation:

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}(p,q), \quad \dot{q}_i = \frac{\partial H}{\partial p_i}(p,q), \quad i = 1,\ldots,d,$$

where $H : U \to \mathbb{R}$ and $U \subset \mathbb{R}^d \times \mathbb{R}^d$.

d ... degree of freedom of the system.

Different notation:

$$\dot{p} = -\nabla_q H(p,q), \qquad \dot{q} = \nabla_p H(p,q),$$

or

$$\dot{y} = J^{-1}\nabla H(y) \qquad y = \begin{pmatrix} p \\ q \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

Example: classical mechanical systems

minimal coordinates ... $q \in \mathbb{R}^d$

kinetic energy ... $T(q,\dot q) = \frac{1}{2}\,\dot q^{\mathsf T} M(q)\dot q$

potential energy ... $U(q)$

---

variational principle: $\int \big(T(q,\dot q) - U(q)\big)\,dt \to \min$

Euler-Lagrange equ. $\frac{d}{dt}\big(M(q)\dot q\big) = \frac{\partial}{\partial q}\big(T(q,\dot q) - U(q)\big)$

---

momenta (or Poisson variables) ... $p := M(q)\dot q$

Euler-Lagrange is equivalent to the Hamilton system with

$$\boxed{H(p,q) = \frac{1}{2}\,p^{\mathsf T} M(q)^{-1} p + U(q)}$$

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$$H(p,q) = \frac{1}{2}\,p^{\mathsf T} M(q)^{-1} p + U(q)$$

Proof.
$$\dot q = M(q)^{-1} p = \nabla_p H(p,q)$$
$$\dot p = \frac{1}{2}\dot q^{\top} \nabla_q M(q)\dot q - \nabla_q U(q) = -\nabla_q H(p,q)$$

Symplectic mappings – differential form

Let P be the parallelogram spanned by

$$\xi = (\xi_1^p, \ldots, \xi_d^p, \xi_1^q, \ldots, \xi_d^q)^\mathsf{T} \quad \text{and}$$

$$\eta = (\eta_1^p, \ldots, \eta_d^p, \eta_1^q, \ldots, \eta_d^q)^\mathsf{T}$$

and

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

the *sum of the oriented areas of the projections of P onto the coordinate planes (p_i, q_i).*

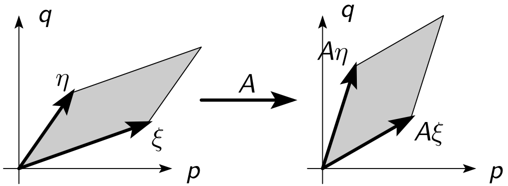
This bilinear form $\omega(\xi, \eta)$ can also be written as

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

Symplectic mappings – definition

Definition

A linear map $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is *symplectic* if $\omega(A\xi, A\eta) = \omega(\xi, \eta)$ for all $\xi, \eta \in \mathbb{R}^{2d}$ or, equivalently, if $A^{\mathsf{T}} J A = J$.



Definition

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

$$g'(p, q)^{\mathsf{T}} J \, g'(p, q) = J.$$

Theorem of Poincaré

We write the Hamiltonian system as

$$\dot{y} = J^{-1}\nabla H(y) \qquad \text{with} \qquad H : U \to \mathbb{R}. \tag{1}$$

Theorem (Poincaré 1899)

For every fixed t, the flow φ_t of (1) is a symplectic transformation wherever it is defined.

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For every fixed t, the flow φ_t of (1) is a symplectic transformation wherever it is defined.

Proof.

The derivative $\partial\varphi_t/\partial y_0$ is a solution of the variational equation $\dot{\Psi} = J^{-1}\nabla^2 H\big(\varphi_t(y_0)\big)\Psi$. Hence,

$$\frac{d}{dt}\bigg(\Big(\frac{\partial\varphi_t}{\partial y_0}\Big)^{\mathsf{T}} J \Big(\frac{\partial\varphi_t}{\partial y_0}\Big)\bigg) = \ldots = 0.$$

Since $\Big(\frac{\partial\varphi_t}{\partial y_0}\Big)^{\mathsf{T}} J \Big(\frac{\partial\varphi_t}{\partial y_0}\Big) = J$ is satisfied for $t = 0$ (φ_0 is the identity map), it is satisfied for all t and all y_0. $\square$

Symplecticity is characteristic for Hamiltonian systems

Theorem

The flow φ_t *of* $\dot{y} = f(y)$ *is a symplectic transformation for all* t *if and only if locally* $f(y) = J^{-1}\nabla H(y)$ *for some* $H(y)$.

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Proof.

Since $\partial\varphi_t/\partial y_0$ is a solution of the variational equation $\dot\Psi = f'\big(\varphi_t(y_0)\big)\Psi$, we obtain

$$\begin{aligned} 0 &= \frac{d}{dt}\Big(\Big(\frac{\partial\varphi_t}{\partial y_0}\Big)^{\mathsf T} J\,\Big(\frac{\partial\varphi_t}{\partial y_0}\Big)\Big) \\ &= \Big(\frac{\partial\varphi_t}{\partial y_0}\Big)\Big(f'\big(\varphi_t(y_0)\big)^{\mathsf T} J + J\,f'\big(\varphi_t(y_0)\big)\Big)\Big(\frac{\partial\varphi_t}{\partial y_0}\Big). \end{aligned}$$

Putting $t = 0$, it follows from $J = -J^{\mathsf T}$ that $J\,f'(y_0)$ is a symmetric matrix for all y_0. The Integrability Lemma thus shows that $J\,f(y)$ is locally of the form $\nabla H(y)$. □

Lemma (Integrability Lemma)

Let $g : U \to \mathbb{R}^n$ have a symmetric Jacobian $g'(y)$. Then, there exists locally a function $H(y)$ such that

$$g(y) = \nabla H(y).$$

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Proof.

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

$$H(y) = \int_0^1 y^{\mathsf{T}} g(ty)\, dt + \text{const} .$$

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

$$\frac{\partial H}{\partial y_k}(y) = \int_0^1 \Big(g_k(ty) + y^{\mathsf{T}} \frac{\partial g}{\partial y_k}(ty)\, t \Big) dt = \int_0^1 \frac{d}{dt} \Big(t g_k(ty) \Big) dt \; = \; g_k(y).$$

$\square$

Symplectic Euler method

For a Hamiltonian system

$$\dot{p} = -\nabla_q H(p,q), \quad \dot{q} = \nabla_p H(p,q),$$

we consider the numerical method

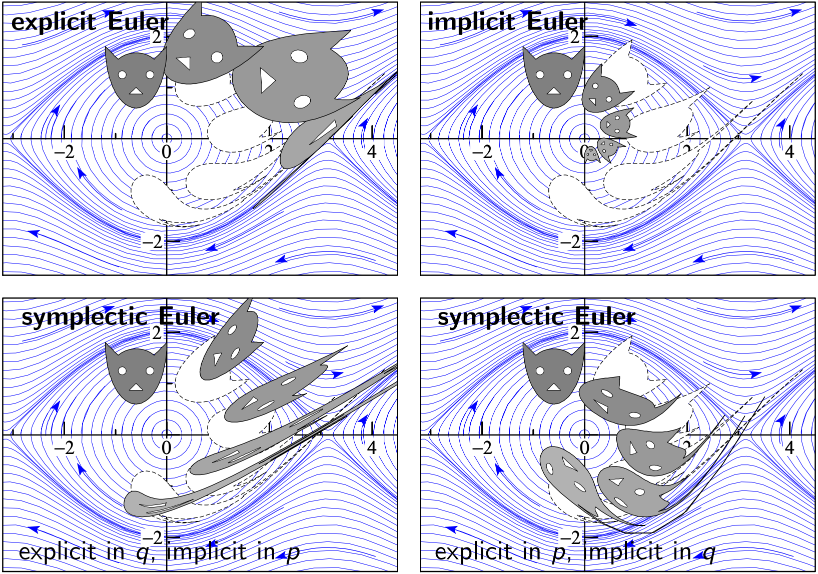
$$\begin{aligned} p_{n+1} &= p_n - h\nabla_q H(p_{n+1}, q_n) \\ q_{n+1} &= q_n + h\nabla_p H(p_{n+1}, q_n) \end{aligned}$$

Theorem (R. de Vogelaere, 1956)

This numerical scheme defines a symplectic transformation

$$\Phi_h : \begin{pmatrix} p_n \\ q_n \end{pmatrix} \mapsto \begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix}.$$

Area preservation (order 1, step size $h = \pi/4$)



Proof of symplecticity: separable Hamiltonian

For $H(p,q) = T(p) + U(q)$ the method reads

$$p_{n+1} = p_n - h\nabla_q U(q_n), \quad q_{n+1} = q_n + h\nabla_p T(p_{n+1}).$$

It is the composition

$$\begin{pmatrix} p_n \\ q_n \end{pmatrix} \xrightarrow{\varphi_h^U} \begin{pmatrix} p_{n+1} \\ q_n \end{pmatrix} \xrightarrow{\varphi_h^T} \begin{pmatrix} p_{n+1} \\ q_{n+1} \end{pmatrix},$$

where φ_t^U and φ_t^T are the exact flows of the Hamiltonian systems

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

corresponding to the Hamiltonians $U(q)$ and $T(p)$. $\square$

Proof of symplecticity: general Hamiltonian

Differentiating the formulas

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

with respect to (p_n, q_n) yields

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

where the matrices $H_{qp}, H_{pp}, \ldots$ of partial derivatives are all evaluated at (p_{n+1}, q_n). One verifies straightforwardly

$$\left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right)^{\mathsf{T}} J \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right) = J. \qquad \square$$

Symmetric methods

A numerical integrator $y_{n+1} = \Phi_h(y_n)$ is called *symmetric*, if

$$\Phi_h = \Phi_h^* \quad \text{with} \quad \Phi_h^* := \Phi_{-h}^{-1} \quad (\Phi_h^* \text{ is the adjoint method})$$

Example: "implicit Euler" is the adjoint method of "explicit Euler";

Theorem

Let Ψ_h be an arbitrary method of order one, then

$$\Psi_{h/2} \circ \Psi_{h/2}^* \qquad \text{and} \qquad \Psi_{h/2}^* \circ \Psi_{h/2}$$

are symmetric and of order two.

Proof: it holds $(\Phi_h^*)^* = \Phi_h$ and $(\Phi_h \circ \Psi_h)^* = \Psi_h^* \circ \Phi_h^*$. □

Example. Let Ψ_h be the explicit Euler method. Then,

$$\Psi_{h/2} \circ \Psi_{h/2}^* : \quad y_{n+1} = y_n + hf\Big(\frac{y_n + y_{n+1}}{2}\Big) \quad \text{(implicit midpoint rule)}$$

$$\Psi_{h/2}^* \circ \Psi_{h/2} : \quad y_{n+1} = y_n + \frac{h}{2}\big(f(y_n) + f(y_{n+1})\big) \quad \text{(trapezoidal rule).}$$

Störmer–Verlet integrator

Let Ψ_h be the symplectic Euler method. Then, the method $\Phi_h = \Psi^*_{h/2} \circ \Psi_{h/2}$ is given by

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

For $H(p,q) = \frac{1}{2} p^{\mathsf{T}} p + U(q)$, where $\ddot{q} = -\nabla U(q)$, this method becomes

$$
q_{n+1} - 2q_n + q_{n-1} = -h^2 \nabla U(q_n)
$$

(Newton, Delambre, Encke, Störmer, Verlet).

Properties of the Störmer–Verlet integrator

- method of order two,
- symplectic method,
- symmetric method,
- explicit for separable Hamiltonians $T(p) + U(q)$,
- exact conservation of quadratic first integrals $p^\mathsf{T} Cq$, e.g., angular momentum, ...

This is an excellent, widely used method (in particular in molecular dynamics).

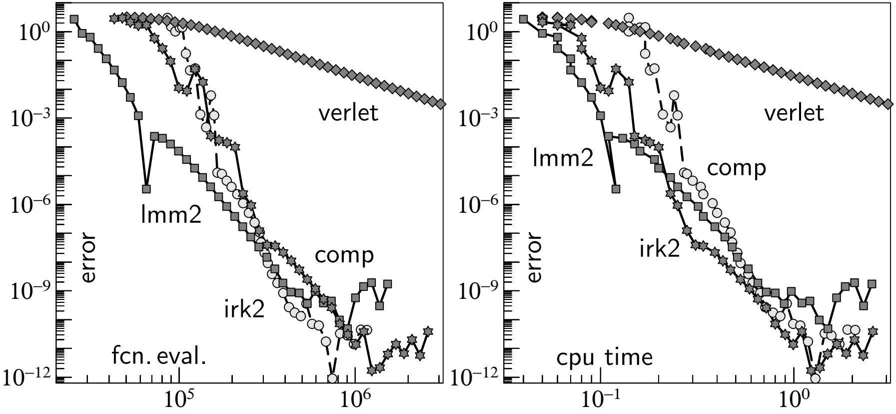
The only disadvantage is its low order.

Why do we need higher order methods?

Comparison with higher order methods

implicit Runge–Kutta, composition, symmetric multistep

Problem: Kepler problem, 200 periods, $e = 0.6$.



gnicodes (http://www.unige.ch/∼hairer/software.html)

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Symplectic Runge–Kutta methods

For a Hamiltonian system $\dot{y} = J^{-1}\nabla H(y)$ we consider (denoting the vector field by $f(y) = J^{-1}\nabla H(y)$)

$$\begin{aligned} Y_i &= y_n + h\sum_{j=1}^{s} a_{ij}\, f(Y_j) \\ y_{n+1} &= y_n + h\sum_{i=1}^{s} b_i\, f(Y_i) \end{aligned}$$

Theorem (Lasagni 1988, Sanz-Serna 1988, Suris 1988)

A Runge–Kutta method, when applied to a Hamiltonian system, defines a symplectic mapping $y_n \mapsto y_{n+1}$ if

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \qquad \textit{for all} \;\; i, j.$$

Examples of symplectic Runge–Kutta methods

Implicit midpoint rule

$$y_{n+1} = y_n + h\, f\Big(\frac{y_n + y_{n+1}}{2}\Big)$$

Gauss collocation (order $2s$, coefficients for $s = 2$)

$$\begin{array}{c|cc}
\frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\
\frac{1}{2} + \frac{\sqrt{3}}{6} & \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \\
\hline
 & \frac{1}{2} & \frac{1}{2}
\end{array}$$

DIRK methods ($c_i = \sum_{j=1}^{i} a_{ij}$)

$$\begin{array}{c|cccc}
c_1 & b_1/2 & & & \\
c_2 & b_1 & b_2/2 & & \\
c_3 & b_1 & b_2 & b_3/2 & \\
c_4 & b_1 & b_2 & b_3 & b_4/2 \\
\hline
 & b_1 & b_2 & b_3 & b_4
\end{array}$$

First proof (Lasagni 1988)

We write the Hamiltonian system as $\dot{p} = -\nabla_q H(p,q)$, $\dot{q} = \nabla_p H(p,q)$ and the numerical solution of a Runge–Kutta method as $y_n = (p_n, q_n)$.

Lasagni (1988) noticed that (symplectic Euler)

$$\begin{aligned} p_{n+1} &= p_n - h\nabla_q S(p_{n+1}, q_n, h) \\ q_{n+1} &= q_n + h\nabla_p S(p_{n+1}, q_n, h) \end{aligned}$$

where

$$\begin{aligned} S(p_{n+1}, q_n, h) &= \textstyle\sum_{i=1}^s b_i\, H(P_i, Q_i) \\ &\quad - h \textstyle\sum_{i,j=1}^s b_i\, a_{ij} \nabla_q H(P_i, Q_i)^\mathsf{T} \nabla_p H(P_j, Q_j) \end{aligned}$$

This follows from a tedious but direct computation (differentiation of S).

The function $S(p,q,h)$ is called *generating function* of the symplectic transformation.

Symplecticity versus preservation of quadratic invariants (Bochev & Scovel 1994)

For RK-methods (and many more methods) the following diagram commutes (horizontal arrow indicates differentiation with respect to y_0)

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

- y_n and $\Psi_n = \partial y_n / \partial y_0$ are a R-K solution of the augmented system,
- the symplecticity condition means that $\Psi^{\mathsf T} J \Psi$ is a quadratic first integral of the augmented system,
- consequence:
  preservation of quadratic first integrals implies symplecticity.

Proof for Gauss methods (inspired by Wanner 1976)

Problem. $\dot y = f(y)$ with $Q(y) = y^{\mathsf T} C\, y$ satisfying $y^{\mathsf T} C\, f(y) = 0$, where C is a symmetric matrix.

Gauss collocation method. $y_{n+1} = u(t_n + h)$ where the polynomial $u(t)$ of degree s is defined by

$$u(t_n) = y_n \quad \text{and}$$
$$\dot u(t_n + c_i h) = f\big(u(t_n + c_i h)\big) \quad \text{for} \quad i = 1, \ldots, s.$$

Proof. Since $\frac{d}{dt} Q\big(u(t)\big) = 2\, u(t)^{\mathsf T} C\, \dot u(t)$ and the Gaussian quadrature integrates polynomials of degree $2s-1$ without error,

$$\begin{aligned} y_{n+1}^{\mathsf T} C\, y_{n+1} \; - \; y_n^{\mathsf T} C\, y_n \; &= \; 2 \int_{t_n}^{t_n+h} u(t)^{\mathsf T} C\, \dot u(t)\, dt \\ &= \; 2h \sum_{i=1}^{s} b_i\, u(t_n + c_i h)^{\mathsf T} C\, f\big(u(t_n + c_i h)\big) \; = \; 0 \end{aligned}$$

This implies conservation of $y^{\mathsf T} C\, y$ and hence also symplecticity.

Second proof (Cooper 1987, Sanz-Serna 1988, Suris 1988), inspired by (Burrage & Butcher 1979, Crouzeix 1979)

Problem. $\dot{y} = f(y)$ with $Q(y) = y^{\mathsf{T}} C\, y$ satisfying $y^{\mathsf{T}} C\, f(y) = 0$.

Using the relations

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i\, f(Y_i), \qquad Y_i = y_n + h \sum_{j=1}^{s} a_{ij}\, f(Y_j)$$

and the abbreviation $k_i = f(Y_i)$, one obtains

$$\begin{aligned} y_{n+1}^{\mathsf{T}} C\, y_{n+1} - y_n^{\mathsf{T}} C\, y_n &= 2h \sum_{i=1}^{s} b_i\, Y_i^{\mathsf{T}} C\, k_i \\ &+ h^2 \sum_{i,j=1}^{s} \Big(b_i b_j - b_i a_{ij} - b_j a_{ji} \Big)\, k_i^{\mathsf{T}} C\, k_j \end{aligned}$$

Consequently, the condition $b_i a_{ij} + b_j a_{ji} = b_i b_j$ implies preservation of $y^{\mathsf{T}} C\, y$, and hence also symplecticity.

Basic idea of composition methods

For an arbitrary method Φ_h, consider the composition

$$\boxed{\Psi_h = \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_2 h} \circ \Phi_{\gamma_1 h}}$$

and determine $\gamma_1, \ldots, \gamma_s$ such that Ψ_h has a higher order (is more accurate).

Motivation.

- Φ_h symplectic $\Rightarrow$ Ψ_h symplectic,
- Φ_h symmetric, $\gamma_{s+1-i} = \gamma_i$ $\Rightarrow$ Ψ_h symmetric.

Lemma

Let Φ_h be of order p. If

$$\gamma_1 + \ldots + \gamma_s = 1 \qquad \text{and} \qquad \gamma_1^{p+1} + \ldots + \gamma_s^{p+1} = 0$$

then the composition method Ψ_h is at least of order $p+1$.

Proof of the Lemma

The local error satisfies

$$\Phi_{\gamma_i h}(y_0) - y(\gamma_i h) = C(y_0)(\gamma_i h)^{p+1} + \mathcal{O}(h^{p+2}).$$

For a fixed number of steps, the dominant term of the composition error is the sum of the local errors, i.e.

$$\begin{aligned} \Psi_h(y_0) \; - \; & y\big((\gamma_1 + \ldots + \gamma_s)h\big) \\ = \; & C(y_0)(\gamma_1^{p+1} + \ldots + \gamma_s^{p+1})h^{p+1} + \mathcal{O}(h^{p+2}). \end{aligned}$$

Remark.

The order can be increased (with real γ_i) only if p is even.

Yoshida's methods (triple jump) 1990

Take a symmetric method of order $p = 2k$, put $s = 3$, and solve

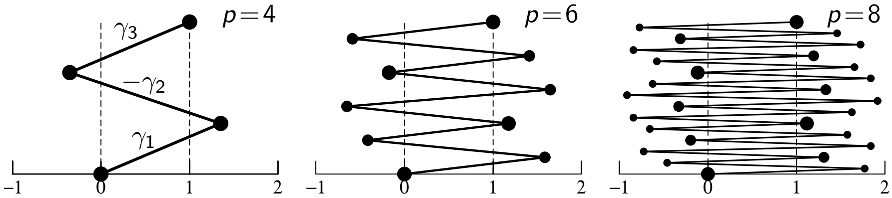
$$\gamma_1 + \gamma_2 + \gamma_3 = 1, \quad \gamma_1^{p+1} + \gamma_2^{p+1} + \gamma_3^{p+1} = 0 \quad \text{with} \quad \gamma_1 = \gamma_3.$$

This yields

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{1/(p+1)}}, \quad \gamma_2 = -\frac{2^{1/(p+1)}}{2 - 2^{1/(p+1)}}$$

The composition $\Phi_{\gamma_3 h} \circ \Phi_{\gamma_2 h} \circ \Phi_{\gamma_1 h}$ is symmetric, hence of order $p+2$.

Important fact. Starting with a method of order 2, the procedure can be repeated and yields methods of arbitrarily high order.



Suzuki's methods (1990)

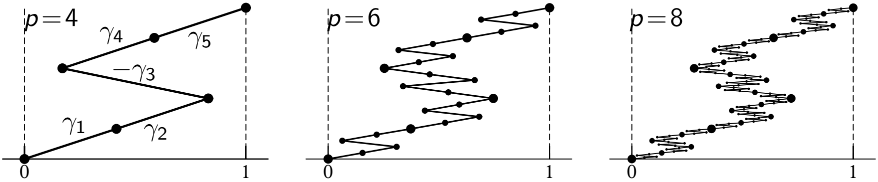
Take a symmetric method of order $p = 2k$, put $s = 5$, and solve

$$\gamma_1 + \ldots + \gamma_5 = 1, \quad \gamma_1^{p+1} + \ldots + \gamma_5^{p+1} = 0 \qquad \text{with} \quad \gamma_1 = \gamma_2 = \gamma_4 = \gamma_5.$$

This yields

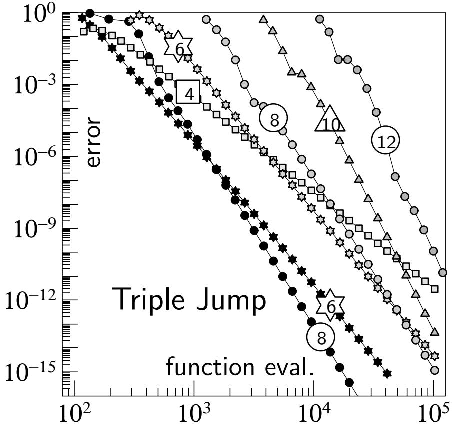
$$\gamma_1 = \gamma_2 = \gamma_4 = \gamma_5 = \frac{1}{4 - 4^{1/(p+1)}}, \quad \gamma_3 = -\frac{4^{1/(p+1)}}{4 - 4^{1/(p+1)}}$$

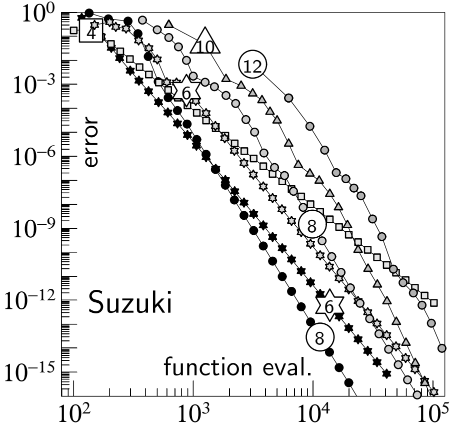
The composition $\Phi_{\gamma_5 h} \circ \Phi_{\gamma_4 h} \circ \Phi_{\gamma_3 h} \circ \Phi_{\gamma_2 h} \circ \Phi_{\gamma_1 h}$ is symmetric and of order $p + 2$.



Numerical comparison

Kepler problem. Initial values are such that the solution is an ellipse with eccentricity $e = 0.6$,
constant step size computation over the interval $[0, 7.5]$.



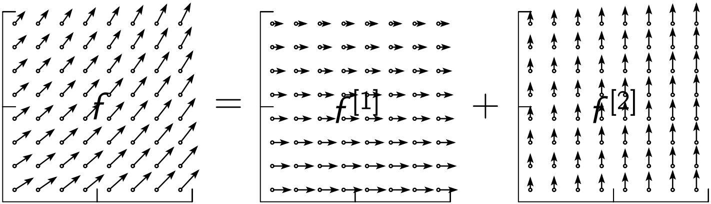


Basic idea of splitting methods

Situation. Consider a differential equation of the form

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

assume that the exact flows, $\varphi_t^{[1]}$ of $\dot{y} = f^{[1]}(y)$ and $\varphi_t^{[2]}$ of $\dot{y} = f^{[2]}(y)$, can be calculated explicitly.



Example. separable Hamiltonian $H(p,q) = T(p) + U(q)$

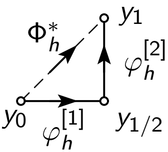
$$\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \begin{pmatrix} 0 \\ \nabla_p T(p) \end{pmatrix} + \begin{pmatrix} -\nabla_q U(q) \\ 0 \end{pmatrix}$$

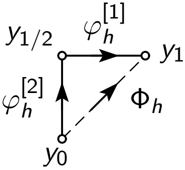
Splitting methods

Lie–Trotter splitting (order 1)

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

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



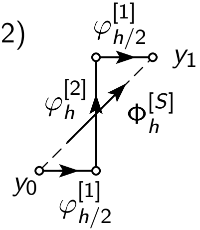


One checks that $(\varphi_h^{[1]} \circ \varphi_h^{[2]})(y_0) = \varphi_h(y_0) + \mathcal{O}(h^2)$.

Strang (Marchuk) splitting (symmetric, order 2)

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

we have $\Phi_h^{[S]} = \Phi_{h/2} \circ \Phi_{h/2}^*$.



General splitting procedure (higher order)

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

can be written as $\quad \Psi_h = \Phi_{\alpha_s h} \circ \Phi_{\beta_s h}^* \circ \ldots \circ \Phi_{\beta_2 h}^* \circ \Phi_{\alpha_1 h} \circ \Phi_{\beta_1 h}^*.$

Hamilton's variational principle

minimal coordinates ... $q \in \mathbb{R}^d$

kinetic energy ... $T(q, \dot q) = \frac{1}{2}\, \dot q^{\mathsf T} M(q) \dot q$

potential energy ... $U(q)$

Lagrangian ... $L(q, \dot q) = T(q, \dot q) - U(q)$

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variational principle: $\int L\big(q, \dot q\big)\, dt \to \min$

Euler–Lagrange equ. $\frac{d}{dt}\big(\frac{\partial}{\partial \dot q} L(q, \dot q)\big) = \frac{\partial}{\partial q} L(q, \dot q)$

---

discrete variational principle: $\sum_{n=0}^{N-1} L_h(q_n, q_{n+1}) \to \min$

discrete Euler–Lagrange equ. $D_2 L_h(q_{n-1}, q_n) + D_1 L_h(q_n, q_{n+1}) = 0$

D_1 derivative with respect to first argument

D_2 derivative with respect to second argument

Variational integrators

With $p_n = -D_1 L_h(q_n, q_{n+1})$, the discrete Euler–Lagrange equ. become

$$p_{n+1} = D_2 L_h(q_n, q_{n+1}), \qquad p_n = -D_1 L_h(q_n, q_{n+1})$$

Theorem

Any mapping $(p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$ *that satisfies the discrete Euler–Lagrange equations, is a symplectic transformation.*

Proof.

With the function (assuming that q_{n+1} can be expressed in terms of p_{n+1}, q_n)

$$S(p_{n+1}, q_n) := p_{n+1}^{\mathsf{T}}(q_{n+1} - q_n) - L_h(q_n, q_{n+1})$$

the Euler–Lagrange equations become

$$\begin{aligned} p_{n+1} &= p_n - \nabla_q S(p_{n+1}, q_n) \\ q_{n+1} &= q_n + \nabla_p S(p_{n+1}, q_n) \end{aligned}$$

which is the symplectic Euler method. □

Examples of variational integrators

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

Example (MacKay 1992)

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

reduces to the Störmer–Verlet method.

Example (Wendlandt & Marsden 1997)

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

reduces to the implicit midpoint rule.

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