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Introduction to geometric numerical integration

Ernst Hairer, Geneva

Main reference

Geometric Numerical Integration
Structure-Preserving Algorithms for Ordinary Differential Equations
E. Hairer, C. Lubich, G. Wanner
Springer Series in Computational Mathematics, Vol. 31
Springer, Berlin, 2002

Developments in solving ODEs numerically

- **Classical period, nonstiff problems (since $\sim$ 1855)**
  multistep methods, Adams (1855, 1883)
  Runge-Kutta methods, Runge (1895), Kutta (1901)
- **Stiff differential equations (since $\sim$ 1960)**
  chemical reactions with different time scales,
  semi-discretized parabolic PDEs
  BDF methods (Curtiss & Hirschfelder 1952, Gear 1972)
  implicit RK-methods (Butcher 1964, Ehle 1968, . . .)
- **Geometric integration, structured probl. (since $\sim$ 1985)**
  Hamiltonian and reversible systems
  symplectic and symmetric integrators, splitting methods
  Feng Kang (1985), Sanz-Serna (1988), . . .

Geometric numerical integration – structures in ODEs

- Hamiltonian ODE – symplectic flow
- divergence-free ODE – volume-preserving flow
- reversible ODE – time-reversible flow
- ODE on manifold – flow preserves invariants
- . . .

Outline of the lecture

Part I
Hamiltonian systems
simple geometric integrators
higher order extensions

Part II
Idea of backward error analysis
rigorous estimates

I.1 Hamiltonian systems

Differential equation:

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

or (in a more compact notation)

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

where $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$
d . . . number of degrees of freedom of the system.

Flow: $\varphi_t : (p_0, q_0) \mapsto (p(t), q(t))$

Example (classical mechanics):

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

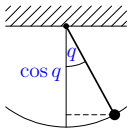
Property (P1): Conservation of the Hamiltonian

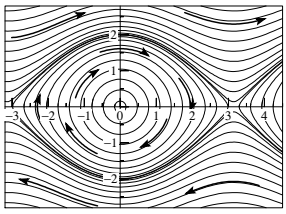
The Hamiltonian is constant along solutions:

$$H(p(t), q(t)) = const$$

Example (pendulum)

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





Conservation of further invariants in special systems:

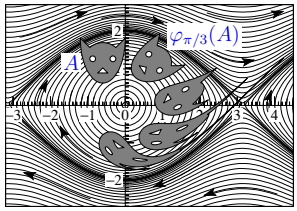
- linear and angular momentum in N-body problems
- completely integrable systems (d first integrals)

Property (P2): Symplecticity

The flow $\varphi_t(y)$ is symplectic (Poincaré 1899), i.e.

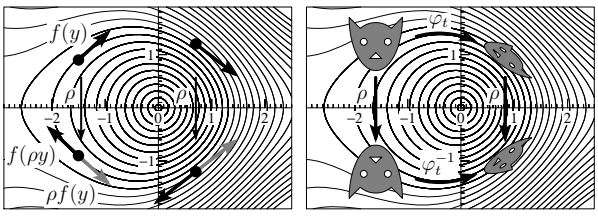
$$\varphi_t'(y)^T J \, \varphi_t'(y) = J$$

This implies $\det \varphi_t'(y) = 1$, hence
volume preservation $\mu(\varphi_t(A)) = \mu(A)$ for $A \subset \mathbb{R}^{2d}$,
and is equivalent to area preservation for $d = 1$.



Property (P3): Reversibility

Let ρ be a linear transformation, e.g., $\rho(p,q) = (-p,q)$.



The system $\dot y = f(y) = J^{-1}\nabla H(y)$ is *ρ-reversible*, if
$(\rho \circ f)(y) = -(f \circ \rho)(y)$ i.e. $H(-p,q) = H(p,q)$

This is equivalent to the *ρ-reversibility* of its flow $\varphi_t(y)$:

$$(\rho \circ \varphi_t)(y) = (\varphi_t^{-1} \circ \rho)(y)$$

I.2 Simple geometric integrators

For a Hamiltonian system

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

consider the numerical method $\Phi_h : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$

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

Properties of the method:

(P2) it is symplectic: $\Phi_h'(y)^T J \Phi_h'(y) = J$
(P1) it nearly conserves most first integrals
and exactly conserves quadratic first integrals $p^T C\, q$

Attention:

(P3) it is **not** symmetric, hence **not** ρ-reversible

Störmer–Verlet method

Composition of symplectic Euler with its adjoint:

$$p_{n+1/2} = p_n - \frac{h}{2}\nabla_q H(p_{n+1/2}, q_n)$$
$$q_{n+1} = q_n + \frac{h}{2}\left(\nabla_p H(p_{n+1/2}, q_n) + \nabla_p H(p_{n+1/2}, q_{n+1})\right)$$
$$p_{n+1} = p_{n+1/2} - \frac{h}{2}\nabla_q H(p_{n+1/2}, q_{n+1})$$

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

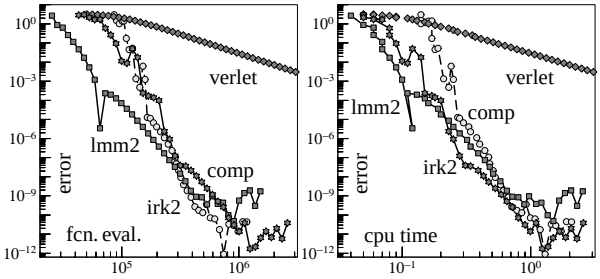
Properties of the method $\Phi_h : (p_n, q_n) \mapsto (p_{n+1}, q_{n+1})$

(P2) it is symplectic: $\Phi_h'(y)^T J \Phi_h'(y) = J$
(P3) it is symmetric: $\Phi_{-h} \circ \Phi_h = id$, hence also ρ-reversible
(P1) it nearly conserves most first integrals
and exactly conserves quadratic first integrals $p^T C\, q$

I.3 Higher order extensions

- (partitioned) Runge-Kutta methods,
- (partitioned) multistep methods,
- composition and splitting methods.

Comparison. Kepler problem, 200 periods, $e = 0.6$.



gnicodes (http://www.unige.ch/math/folks/hairer)

Symmetric composition methods

For an arbitrary method Φ_h, consider the composition

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

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

Motivation.
a) Φ_h symplectic $\Rightarrow$ Ψ_h symplectic,
b) Φ_h symmetric, $\gamma_{s+1-i} = \gamma_i$ $\Rightarrow$ Ψ_h symmetric.
c) Φ_h nearly conserves invariants $\Rightarrow$ Ψ_h also ....

Lemma. *Let Φ_h be of order p. If*

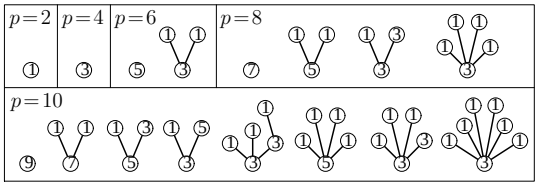
$$\gamma_1 + \ldots + \gamma_s = 1 \quad \textit{and} \quad \gamma_1^{p+1} + \ldots + \gamma_s^{p+1} = 0$$

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

Theorem *For composition methods*

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

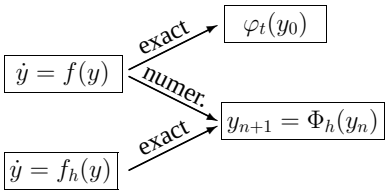
with symmetric Φ_h and $\gamma_{s+1-i} = \gamma_i$, the order conditions are in one-to-one correspondence to the following trees.



E.g., $\sum_{k=1}^s \gamma_k^5 = 0$, $\quad \sum_{k=1}^s \gamma_k^3 (\sum_{l=1}^{k'} \gamma_l)^2 = 0$

p	2	4	5	8	10
s	1	3	7	15	31

II.1 Backward error analysis (idea)



Idea. Find a *modified differential equation* $\dot y = f_h(y)$ of the form

$$\dot y = f(y) + h f_2(y) + h^2 f_3(y) + \ldots,$$

such that its solution $\widetilde y(t)$ satisfies formally $\quad y_n = \widetilde y(nh)$.

Construction of the modified equation

Numerical Method for $\dot y = f(y)$

$$y_1 = \Phi_h(y_0) = y_0 + hf(y_0) + h^2 d_2(y_0) + h^3 d_3(y_0) + \ldots$$

Ansatz for the **modified equation**

$$\dot y = f(y) + h f_2(y) + h^2 f_3(y) + \ldots, \qquad y(0) = y_0,$$

Taylor series expansion of its solution $\widetilde y(t)$ at $t = h$

$$\begin{aligned}\widetilde y(h) &= y_0 + h\widetilde y'(0) + \tfrac{h^2}{2!}\widetilde y''(0) + \tfrac{h^3}{3!}\widetilde y'''(0) + \ldots \\ &= y_0 + h(f + hf_2 + h^2 f_3 + \ldots)_0 \\ &+ \tfrac{h^2}{2!}(f' + hf_2' + \ldots)(f + hf_2 + \ldots)_0 + \ldots .\end{aligned}$$

Comparison of like powers of h yields

$$\begin{aligned} d_2(y) &= f_2(y) + \tfrac{1}{2!} f'f(y) \\ d_3(y) &= f_3(y) + \tfrac{1}{2!}(f'f_2 + f_2' f)(y) + \tfrac{1}{3!}(f''(f,f) + f'f'f)(y) \\ &\ldots \end{aligned}$$

Modified equations for the pendulum equation

explicit Euler:

$$\begin{pmatrix}\dot q \\ \dot p\end{pmatrix} = \begin{pmatrix} p \\ -\sin q\end{pmatrix} + \frac{h}{2}\begin{pmatrix}\sin q \\ p\cos q\end{pmatrix} + \frac{h^2}{12}\begin{pmatrix}-4\,p\cos q \\ (p^2 + 4\cos q)\sin q\end{pmatrix} + \ldots$$

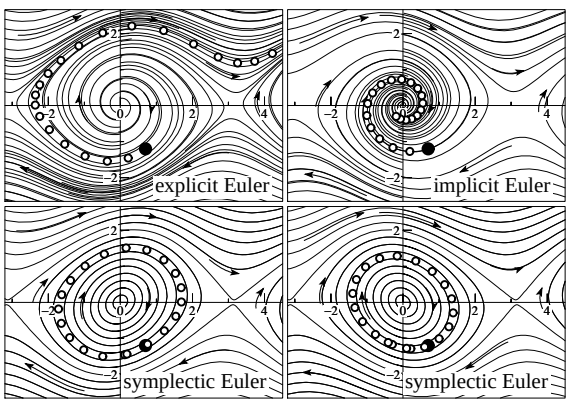
symplectic Euler (explicit in q, implicit in p):

$$\begin{pmatrix}\dot q \\ \dot p\end{pmatrix} = \begin{pmatrix} p \\ -\sin q\end{pmatrix} + \frac{h}{2}\begin{pmatrix}-\sin q \\ p\cos q\end{pmatrix} + \frac{h^2}{12}\begin{pmatrix}2\,p\cos q \\ (p^2 - 2\cos q)\sin q\end{pmatrix} + \ldots$$

this modified equation is Hamiltonian with

$$\widetilde H(p,q) = \frac{1}{2}p^2 - \cos q - \frac{h}{2}\,p\,\sin q + \frac{h^2}{12}(p^2 - \cos q)\cos q + \ldots$$

Numerical illustration: pendulum $\dot q = p,\ \dot p = -\sin q$



expl.in p, impl. in q expl.in q, impl. in p

Divergence of modified equation

Problem: $\dot y = f(t),\ \ y(0) = 0$

Method: $y_{n+1} = y_n + \frac{h}{2}(f(t_{n+1}) + f(t_n))$

The modified differential equation is of the form

$$\dot{\tilde y} = f(t) + hb_1 f'(t) + h^2 b_2 f''(t) + h^3 b_3 f'''(t) + \dots$$

The coefficients can be obtained by putting $f(t) = e^t$:

$$(e^h - 1)(1 + hb_1 + h^2 b_2 + \dots) \ = \ \tfrac{h}{2}(e^h + 1)$$

This is the generating function for the Bernoulli numbers; we have $b_k \approx const(2\pi)^{-k}$.

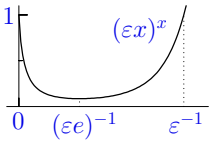
As soon as $f^{(k)}(t) \approx k!\, M\, R^{-k}$, the series of the modified equation diverges for all $h \neq 0$.

Exponentially small estimates

Typically (e.g., when $f(y)$ is real-analytic) one cannot expect a better estimate than

$$C_N(y_0) \le \alpha(\beta N)^N$$

Optimal choice of N:
the estimate
$C_N(y_0)h^{N+1} \le h\alpha(\beta hN)^N$
is minimal, when
$N = (\beta he)^{-1}$.

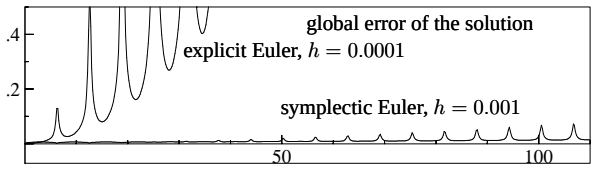


This choice of N yields

$$\|\Phi_h(y_0) - \varphi_{N,h}(y_0)\| \le h\alpha\, e^{-\gamma/h} \quad \text{with} \quad \gamma = (\beta e)^{-1} > 0.$$

Numerical experiment

Kepler problem (excentricity $e = 0.6$)
initial values, such that the orbit is elliptic with period 2π



Explicit Euler: quadratic error growth

Symplectic Euler: linear error growth

Theorem (energy conservation). *Consider a symplectic method of order r with globally defined modified Hamilt.*

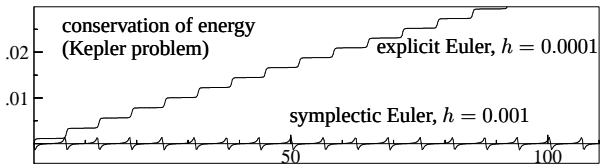
$$\widetilde H(p,q) = H(p,q) + h^r H_{r+1}(p,q) + \dots + h^{N-1} H_N(p,q).$$

Then, the numerical solution satisfies

$$H(p_n, q_n) \ = \ H(p_0, q_0) + \mathcal{O}(h^r) \quad \textit{for} \quad nh \le e^{\gamma/2h}$$

as long as the numerical solution stays in a compact set.

Proof. We have $|\widetilde H(p_n,q_n) - \widetilde H(p_0,q_0)| \le C\, nh\, e^{-\gamma/h}$. □



II.2 Rigorous estimates

Benettin & Giorgilli (1994), H. & Lubich (1997), Reich (1999)

Theorem. *Denote by $\varphi_{N,t}(y)$ the flow of the truncated modified differential equation*

$$\dot{\tilde y} = f(\tilde y) + hf_2(\tilde y) + h^2 f_3(\tilde y) + \dots + h^{N-1} f_N(\tilde y),$$

then there exists a constant $C_N(y_0)$ such that for $h \le h_0$

$$\|\Phi_h(y_0) - \varphi_{N,h}(y_0)\| \le C_N(y_0)\, h^{N+1}.$$

The proof is trivial. One even knows that

$$\Phi_h(y_0) - \varphi_{N,h}(y_0) = h^{N+1} f_{N+1}(y_0) + \mathcal{O}(h^{N+2}).$$

It is less trivial to study the dependence of $C_N(y_0)$ on N.

II.3 Linear error growth (integr. systems)

The previous estimates are purely **local**.

To get estimates of the global error, one has to know something about the error propagation of the modified differential equation.

For example, if we know that

$$\|\widetilde\varphi_t(y_0) - \widetilde\varphi_t(z_0)\| \le (a + b\,t)\, \|y_0 - z_0\|,$$

then we have for $t = nh$ (explain on blackboard)

$$\|y_n - \widetilde\varphi_t(y_0)\| \le \alpha\, e^{-\gamma/h}(at + bt^2/2)$$

i.e., the difference between the numerical solution and the exact solution of the modified equation is exponentially small on exponentially long time intervals.

II.4 Conservation of the Hamiltonian

Theorem. *Consider*

- *a Hamiltonian system with $H : U \to \mathbb{R}$*
- *a symplectic method $\Phi_h(y)$*

Then, the vector fields $f_k(y)$ of the modified equation are **locally** *Hamiltonian, i.e., locally $f_k(y) = J^{-1}\nabla H_k(y)$.*

Proof (by induction). Assume that

$$\dot y \ = \ f(y) + hf_2(y) + \dots + h^{N-1} f_N(y)$$

is Hamiltonian. Its flow $\varphi_{N,t}(y)$ satisfies

$$\Phi_h(y) \ = \ \varphi_{N,t}(y) + h^{N+1} f_{N+1}(y) + \mathcal{O}(h^{N+2}).$$

Since $\Phi_h(y)$ and $\varphi_{N,t}(y)$ are symplectic, it holds

$$J = \dots = J + h^{N+1}(f'_{N+1}(y_0)^T J + J f'_{N+1}(y_0)) + \mathcal{O}(h^{N+2}),$$

so that Jf'_{N+1} is symm. and locally $Jf_{N+1} = \nabla H_{N+1}$. □