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

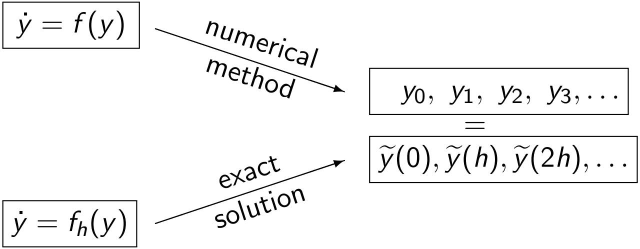
- **Part II. Differential equations with multiple time-scales**
  - Highly oscillatory problems, Fermi–Pasta–Ulam-type problems, trigonometric integrators, adiabatic invariants
  - Modulated Fourier expansion, near-preservation of energy and of adiabatic invariants, application to wave equations

Lecture 2. Backward error analysis

1. **Modified differential equation**
   - Construction of the modified differential equation
   - Hamiltonian systems – symplectic methods
2. **Long-time error analysis**
   - Near-energy preservation
   - Linear error growth for integrable systems
3. **Application to charged particle dynamics**
   - Basic properties
   - Main result - energy preservation
   - Numerical experiments
   - Proof – backward error analysis

Modified differential equation

Given a differential equation $\dot{y} = f(y)$ and a method $y_{n+1} = \Phi_h(y_n)$



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

$$\dot{y} = f(y) + h\, f_2(y) + h^2 f_3(y) + h^3 f_4(y) + \ldots$$

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

Construction of the modified differential equation

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

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

Ansatz for the **modified equation**

$$\dot y = f(y) + hf_2(y) + h^2 f_3(y) + \dots, \qquad y(0) = y_0$$

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

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

Comparison of like powers of h yields

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

Modified equations for the pendulum equation

explicit Euler:

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

implicit Euler: same equation with h replaced by $-h$.

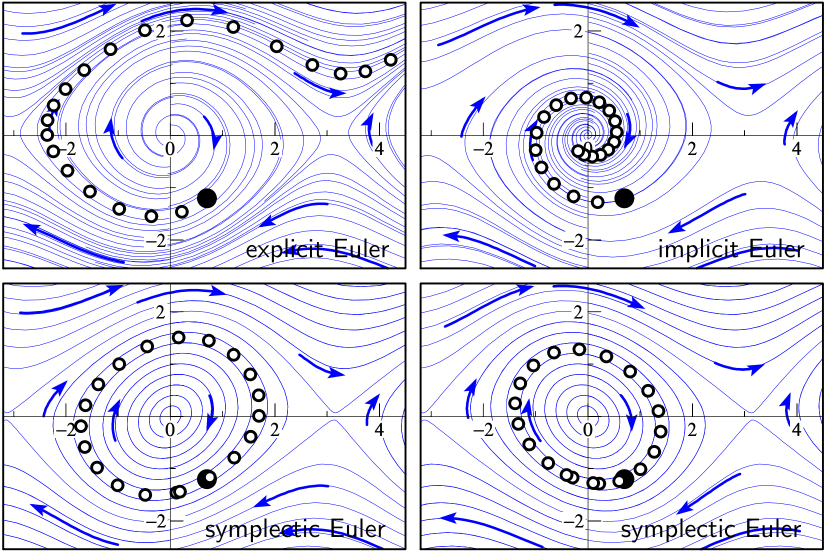
symplectic Euler (explicit in q, implicit in p):

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

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

same equation with h replaced by $-h$

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



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

Quadrature

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

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

The modified differential equation is of the form

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

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

$$(e^h - 1)(1 + hb_1 + h^2 b_2 + \ldots) \;=\; \frac{h}{2}(e^h + 1)$$

This is the generating function for the Bernoulli numbers; we have

$$b_k \approx c\,(2\pi)^{-k}$$

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

Hamiltonian systems

Consider a Hamiltonian system

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

and a one-step method

$$y_{n+1} = \Phi_h(y_n)$$

What can be said about its modified differential equation?

Example (pendulum)
explicit and implicit Euler: modified equation is **not** Hamiltonian
symplectic Euler: modified equation is Hamiltonian with

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

Is this true in general?

Modified equation for symplectic methods

Theorem

Consider

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

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

There are several proofs for this result.

Local existence of the Hamiltonian $H_k(y)$

simple proof by induction without additional assumption
idea goes back to Moser (1968),
Benettin & Giorgilli (1994), Tang (1994)

Global existence of the Hamiltonian $H_k(y)$

needs additional assumptions (satisfied by RK methods)
proof via generating functions: Murua (1994)
algebraic proof for B-series integrators: Hairer (1994)

Proof by induction (local existence)

We prove by induction on N that

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

is Hamiltonian. This is obviously true for $N = 1$.
Assume that (1) is Hamiltonian for N. Its flow $\varphi_{N,t}(y)$ satisfies

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

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

$$\begin{aligned} J &= \Phi_h'(y)^{\mathsf{T}} J \, \Phi_h'(y) = \ldots \\ &= J + h^{N+1}\big(f_{N+1}'(y)^{\mathsf{T}} J + J \, f_{N+1}'(y)\big) + \mathcal{O}(h^{N+2}), \end{aligned}$$

so that $J \, f_{N+1}'(y)$ is symmetric. The integrability lemma implies the local existence of $H_{N+1}(y)$ such that $J \, f_{N+1}(y) = \nabla H_{N+1}(y)$. □

Modified equation for symmetric methods

Theorem (adjoint method)

a) Let $f_j(y)$ *be the coefficient functions of the modified differential equation for a method* $\Phi_h(y)$*. The coefficient functions of the modified equation for the adjoint method* $\Phi_h^*(y) = \Phi_{-h}^{-1}(y)$ *are then given by*

$$f_j^*(y) = (-1)^{j+1} f_j(y).$$

b) The modified equation of a symmetric method has an expansion in even powers of h.

Proof.

The solution $\widetilde{y}(t)$ of the modified equation for Φ_h^* has to satisfy

$$\widetilde{y}(t) = \Phi_{-h}\big(\widetilde{y}(t+h)\big) \qquad \text{and hence} \qquad \widetilde{y}(t-h) = \Phi_{-h}\big(\widetilde{y}(t)\big)$$

Replacing h by $-h$, we get the solution of the modified equation for the method Φ_h. □

Structure preservation

There are many similar results that can all be proved by the same induction argument.

- divergence-free vector fields $\dot{y} = f(y)$, i.e., $\mathrm{div} f(y) = 0$, and volume-preserving flows,
- Poisson systems $\dot{y} = B(y)\nabla H(y)$ and Poisson mappings,
- vector fields on a manifold and flows on the manifold,
- special case, where the manifold is a Lie group,
- differential equations with first integrals.

Always when a numerical integrator shares a characteristic property of the exact flow, the modified differential equation retains the structure of the problem.

Lecture 3. Backward error analysis

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2. **Long-time error analysis**
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3. **Application to charged particle dynamics**
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Estimates of the local error

Since the modified equation is in general divergent, we have to truncate it. What is the induced error?

Theorem (local error estimation)

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

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

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

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

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.

Exponentially small error estimates

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

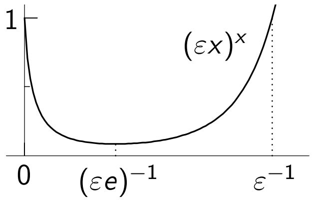
$$C_N(y_0) \leq \alpha(\omega N)^N$$

Optimal choice of N:
the estimate

$$C_N(y_0)h^{N+1} \leq h\alpha(\omega h N)^N$$

is minimal, when

$$N = (\omega h e)^{-1}.$$



This choice of N yields

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

Estimation of the global error

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

- **Typical situation:** if we know that

  $$\|\widetilde{\varphi}_t(y_0) - \widetilde{\varphi}_t(z_0)\| \le c\, e^{\omega t}\, \|y_0 - z_0\|,$$

  then we have for $t = nh$

  $$\|y_n - \widetilde{\varphi}_t(y_0)\| \le \alpha\, e^{-\gamma/h}\, t\, e^{\omega t}$$

  exponentially close on intervals of length $\mathcal{O}(1)$.

- **Integrable systems:** 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 $t = nh$

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

  exponentially close on exponentially long time intervals.

Near-energy preservation

Theorem

Consider a symplectic method of order r with global modified Hamiltonian

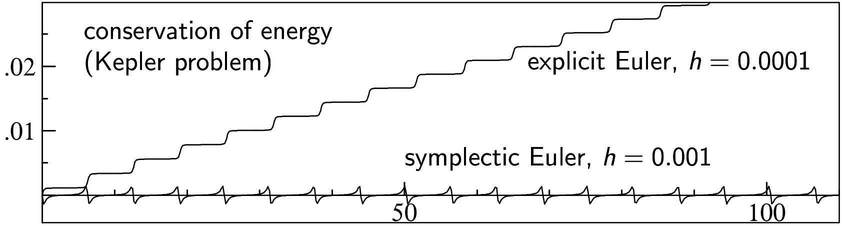
$$\widetilde{H}(p,q) = H(p,q) + h^r H_{r+1}(p,q) + \ldots + h^{N-1} H_N(p,q).$$

Then, the numerical solution satisfies

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

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

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



Completely integrable systems

Consider a Hamiltonian system

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

Definition

A Hamiltonian system with d degrees of freedom ($H : M \to \mathbb{R}$ with an open set $M \subset \mathbb{R}^d \times \mathbb{R}^d$) is called *completely integrable* if there exist smooth functions $F_1 = H, F_2, \ldots, F_d$ such that

- $F_1, \ldots, F_d$ are in convolution, i.e., $\{F_i, F_j\} = \nabla F_i^{\mathsf{T}} J^{-1} \nabla F_j = 0$,
- The gradients of $F_1, \ldots, F_d$ are everywhere linearly independent,
- The solution trajectories of the Hamiltonian systems with F_i ($i = 1, \ldots, d$) exist for all times and remain in M.

Note that the first condition implies that all function F_j are first integrals (conserve quantities) of the Hamiltonian system.

Completely integrable systems – examples

- Hamiltonian systems with **one** degree of freedom, e.g., harmonic oscillator, mathematical pendulum
- Kepler problem
  first integrals are: energy H and angular momentum $L = q_1 p_2 - q_2 p_1$
- Toda lattice with $H(p,q) = \sum_{k=1}^{n} \Big(\frac{1}{2}\, p_k^2 + \exp(q_k - q_{k+1}) \Big)$
  related to a Lax pair $\dot{L} = [B(L), L]$ with skew-symmetric $B(L)$
- Ablowitz–Ladik discrete nonlinear Schrödinger equation
- Volterra lattices

Arnold–Liouville Theorem

For a *completely integrable* Hamiltonian system there exists a symplectic transformation

$$(p,q) = \psi(a,\theta) \quad (2\pi\text{-periodic in } \theta)$$

to *action-angle variables* such that the Hamiltonian becomes

$$H(p,q) = H(\psi(a,\theta)) = K(a).$$

In the action-angle variables, the system becomes

$$\dot a_i = 0, \quad \dot\theta_i = \omega_i(a), \qquad i = 1,\dots,d$$

with $\omega_i(a) = \partial K/\partial a_i(a)$, and can be solved directly

$$a_i(t) = a_{i0}, \quad \theta_i(t) = \theta_{i0} + \omega_i(a_0)t$$

so that

$$(p(t),q(t)) = \psi(a_0, \theta_0 + \omega(a_0)t)$$

(periodic or quasi-periodic flow).

Linear error growth for integrable systems

Assumptions

- completely integrable Hamiltonian system with real-analytic Hamiltonian, action variables $a = I(p, q)$
- symplectic integrator of order r
- some technical assumptions.

Then, there exist constants C, h_0 such that for $h \le h_0$ and for $t = nh \le h^{-r}$ the numerical solution satisfies

$$\|(p_n, q_n) - (p(t), q(t))\| \le C\, t\, h^r \qquad \text{(linear error growth)}$$

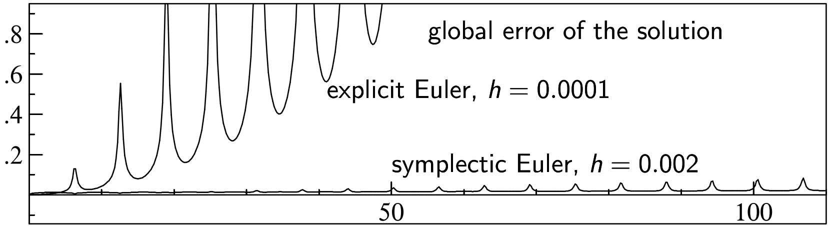
$$\|I(p_n, q_n) - I(p_0, q_0)\| \le C\, h^r \qquad \text{(near-conserv. of actions)}$$

Remark. The same statement is true if we replace
"Hamiltonian" by "reversible" and
"symplectic" by "symmetric".

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

Lecture 2. Backward error analysis

Charged particle dynamics

Newton's Second Law together with Lorentz's force equation yields (assuming suitable units)

$$\ddot{x} = \dot{x} \times B(x) + E(x)$$

where $E(x)$ is the electric field and $B(x)$ the magnetic field.

Boris algorithm

The most simple discretization is

$$x_{n+1} - 2x_n + x_{n-1} = \frac{h}{2}(x_{n+1} - x_{n-1}) \times B(x_n) + h^2 E(x_n)$$

J.P. Boris, *Relativistic plasma simulation-optimization of a hybrid code.* Proc. of 4th Conf. on Numer. Simul. of Plasmas (Nov. 1970)

Properties of the differential equation

We write

$$\ddot{x} = \dot{x} \times B(x) + E(x)$$

as

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= v \times B(x) + E(x) \end{aligned}$$

- the flow $\varphi_t(x, v)$ is volume preserving:

$$\mu\big(\varphi_t(K)\big) = \mu(K) \qquad \text{for all } t;$$

- if $E(x) = -\nabla U(x)$, the energy

$$H(x, v) = \tfrac{1}{2} v^{\top} v + U(x) \qquad \text{is preserved;}$$

- if $E(x) = -\nabla U(x)$ and $B(x) = \nabla_x \times A(x)$, the differential equations are the Euler–Lagrange equations with

$$L(x, v) = \tfrac{1}{2} v^{\top} v - U(x) + A(x)^{\top} v$$

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- if

Proof. Divergence of the vector field $= 0$, because $v \times B(x) = \widehat{B}(x)\, v$ with a skew-symmetric matrix $\widehat{B}(x)$.

- if $E(x) = -\nabla U(x)$ and $B(x) = \nabla_x \times A(x)$, the differential equations are the Euler–Lagrange equations with

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- if … ations
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Proof.

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t} H\big(x(t), v(t)\big) &= v^\top \dot{v} + \dot{x}^\top \nabla U(x) \\ &= v^\top \big(v \times B(x) - \nabla U(x)\big) + v^\top \nabla U(x) = 0 \end{aligned}$$

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- the flow $\varphi_t(x,v)$ is volume preserving;

- if

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(\nabla_v L\big) = \nabla_x L$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\big(v + A(x)\big) = -\nabla_x U + \nabla_x\big(A(x)^\top v\big)$$

and the statement follows from

$$\nabla_x\big(A(x)^\top v\big) - \frac{\mathrm{d}}{\mathrm{d}t}A(x) = \big(A'(x)^\top - A'(x)\big)v = v \times B(x)$$

- if $E(x) = -\nabla U(x)$ and $B(x) = \nabla_x \times A(x)$, the differential equations are the Euler–Lagrange equations with

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Boris algorithm as one-step method

$$
\begin{aligned}
x_{n+1} - 2x_n + x_{n-1} &= \frac{h}{2}\,(x_{n+1} - x_{n-1}) \times B(x_n) + h^2 E(x_n) \\
v_n &= \frac{1}{2h}\,(x_{n+1} - x_{n-1})
\end{aligned}
$$

With $v_{n+1/2} = \frac{1}{h}(x_{n+1} - x_n) = v_n + \frac{h}{2}\, v_n \times B(x_n) + \frac{h}{2} E(x_n)$ we have

$$
v_{n+1/2} - v_{n-1/2} = \frac{h}{2}\,(v_{n+1/2} + v_{n-1/2}) \times B(x_n) + h\, E(x_n)
$$

and the map $(x_n, v_{n-1/2}) \mapsto (x_{n+1}, v_{n+1/2})$ is implemented as

$$
\begin{aligned}
v^+_{n-1/2} &= v_{n-1/2} + \frac{h}{2}\, E(x_n) \\
v^-_{n+1/2} - v^+_{n-1/2} &= \frac{h}{2}\,(v^-_{n+1/2} + v^+_{n-1/2}) \times B(x_n) \\
v_{n+1/2} &= v^-_{n+1/2} + \frac{h}{2}\, E(x_n) \\
x_{n+1} &= x_n + h\, v_{n+1/2}
\end{aligned}
$$

Boris algorithm as one-step method

$$\begin{aligned} x_{n+1} - 2x_n + x_{n-1} &= \frac{h}{2}\,(x_{n+1} - x_{n-1}) \times B(x_n) + h^2 E(x_n) \\ v_n &= \frac{1}{2h}\,(x_{n+1} - x_{n-1}) \end{aligned}$$

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Boris algorithm as one-step method

$$\begin{aligned} x_{n+1} - 2x_n + x_{n-1} &= \tfrac{h}{2}\,(x_{n+1} - x_{n-1}) \times B(x_n) + h^2 E(x_n) \\ v_n &= \tfrac{1}{2h}\,(x_{n+1} - x_{n-1}) \end{aligned}$$

With $v_{n+1/2} = \frac{1}{h}(x_{n+1} - x_n) = v_n + \frac{h}{2}\, v_n \times B(x_n) + \frac{h}{2} E(x_n)$ we have

$$v_{n+1/2} - v_{n-1/2} = \tfrac{h}{2}\,(v_{n+1/2} + v_{n-1/2}) \times B(x_n) + h\, E(x_n)$$

and the map $(x_n, v_{n-1/2}) \mapsto (x_{n+1}, v_{n+1/2})$ is implemented as

$$\begin{aligned} v^+_{n-1/2} &= v_{n-1/2} + \tfrac{h}{2}\, E(x_n) \\ v^-_{n+1/2} - v^+_{n-1/2} &= \tfrac{h}{2}\,(v^-_{n+1/2} + v^+_{n-1/2}) \times B(x_n) \\ v_{n+1/2} &= v^-_{n+1/2} + \tfrac{h}{2}\, E(x_n) \\ x_{n+1} &= x_n + h\, v_{n+1/2} \end{aligned}$$

Boris algorithm as one-step method

With the splitting

$$\begin{pmatrix} \dot{x} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 \\ E(x) \end{pmatrix} + \begin{pmatrix} 0 \\ v \times B(x) \end{pmatrix} + \begin{pmatrix} v \\ 0 \end{pmatrix}$$

we have

$$\begin{pmatrix} x_{n+1} \\ v_{n+1/2} \end{pmatrix} = \varphi_h^V \circ \varphi_{h/2}^E \circ \Phi_h^B \circ \varphi_{h/2}^E \begin{pmatrix} x_n \\ v_{n-1/2} \end{pmatrix}$$

where φ_t^E and φ_t^V are the exact flows, and Φ_h^B is the discrete flow (mid-point rule) for the vector field in the middle.

Wi

and

$$\begin{aligned} v_{n-1/2}^{+} &= v_{n-1/2} + \frac{h}{2} E(x_n) \\ v_{n+1/2}^{-} - v_{n-1/2}^{+} &= \frac{h}{2} \left(v_{n+1/2}^{-} + v_{n-1/2}^{+} \right) \times B(x_n) \\ v_{n+1/2} &= v_{n+1/2}^{-} + \frac{h}{2} E(x_n) \\ x_{n+1} &= x_n + h\, v_{n+1/2} \end{aligned}$$

Properties of the Boris algorithm

$$
\begin{aligned}
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\end{aligned}
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- the mapping $(x_n, v_{n-1/2} \mapsto (x_{n+1}, v_{n+1/2})$ is volume preserving. Hence, the Boris method $(x_n, v_n) \mapsto (x_{n+1}, v_{n+1})$ is conjugate to a volume preserving mapping.
- the Boris method is a variational integrator only if $B(x) = Const.$ *(see Ellison & al., and part II of the talk)*
- What can be said about near energy preservation in the general case, where $B(x)$ is not a constant vector field? *This is the topic of the present talk.*

C. L. Ellison, J. W. Burby, and H. Qin, *Comment on "Symplectic integration of magnetic systems": A proof that the Boris algorithm is not variational. J. Comput. Phys. 301* (2015), 489–493

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Energy preservation - main result

Theorem

Assume that at least one of the following conditions is satisfied

- *the magnetic field* $B(x) = B$ *is constant,*
- *the scalar potential* $U(x) = \frac{1}{2} x^\top Q x + q^\top x$ *is quadratic,*

and that the numerical solution (x_n, v_n) *of the Boris method stays in a compact set. For every truncation index* N*, the energy* $H(x,v) = \frac{1}{2} v^\top v + U(x)$ *is bounded as*

$$|H(x_n, v_n) - H(x_0, v_0)| \le C_{2N} h^2 \quad \text{for} \quad nh \le h^{-2N}$$

with C *independent of* n *and* h *as long as* $nh \le h^{-2N}$.

What happens if none of the above two conditions is satisfied?

E. Hairer and Ch. Lubich, *Energy behaviour of the Boris method for charged-particle dynamics. BIT* (2018)

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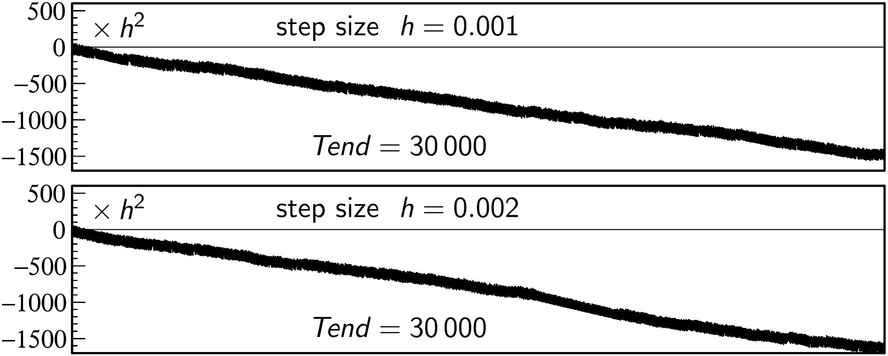
Example 1: linear growth

We consider the error in the energy for

$$U(x) = x_1^3 - x_2^3 + \frac{1}{5}x_1^4 + x_2^4 + x_3^4, \qquad B(x) = \begin{pmatrix} 0 \\ 0 \\ \sqrt{x_1^2 + x_2^2} \end{pmatrix}$$

$x(0) = (0.0, 1.0, 0.1)^\top$, $v(0) = (0.09, 0.55.0.30)^\top$.



Example 2: random walk

We consider the error in the energy for

$$U(x) = x_1^3 - x_2^3 + \frac{1}{5}x_1^4 + x_2^4 + x_3^4, \qquad B(x) = \frac{1}{2}\begin{pmatrix} x_2 - x_3 \\ x_1 + x_3 \\ x_2 - x_1 \end{pmatrix}$$

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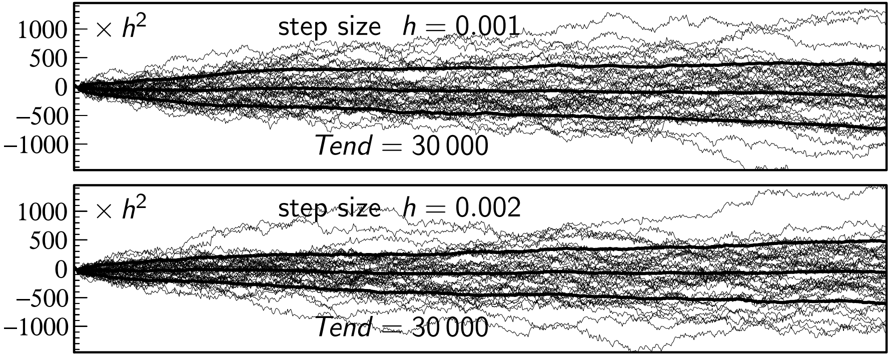

Backward error analysis (Boris algorithm)

For $x_n = y(nh)$ and $t = nh$ the Boris algorithm reads

$$y(t+h)-2y(t)+y(t-h) = \frac{h}{2}\Big(y(t+h)-y(t-h)\Big)\times B\big(y(t)\big)-h^2\nabla U\big(y(t)\big)$$

Expanding into powers of h and dividing by h^2 yields

$$\ddot{y} + \frac{h^2}{12}\ddddot{y} + \ldots = \Big(\dot{y} + \frac{h^2}{6}\dddot{y} + \ldots\Big)\times B(y) - \nabla U(y)$$

Eliminating third and higher derivatives by differentiation

$$\begin{aligned} \dddot{y} &= \ddot{y}\times B(y) + \dot{y}\times B'(y)\dot{y} - \nabla^2 U(y)\dot{y} + \mathcal{O}(h^2) \\ &= -\nabla U(y)\times B(y) + \dot{y}\times B'(y)\dot{y} - \nabla^2 U(y)\dot{y} + \mathcal{O}(h^2) \end{aligned}$$

gives the modified differential equation.

Similarly, we have $v_n = w(nh)$ for $t = nh$, where

$$w(t) = \frac{1}{2h}\Big(y(t+h)-y(t-h)\Big) = \dot{y} + \frac{h^2}{3!}\dddot{y} + \frac{h^4}{5!}y^{(5)} + \ldots$$

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Energy conservation - constant magnetic field

Consider the modified equation

$$\ddot{y} + \frac{h^2}{12}\ddddot{y} + \ldots = \Big(\dot{y} + \frac{h^2}{6}\dddot{y} + \ldots\Big) \times B(y) - \nabla U(y)$$

and take the scalar product with $\dot{y}$. This gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{2}\dot{y}^\top\dot{y} + U(y) + \frac{h^2}{12}\big(\dot{y}^\top\dddot{y} - \frac{1}{2}\ddot{y}^\top\ddot{y}\big) + \ldots\Big) = \frac{h^2}{6}\dot{y}^\top\big(\dddot{y} \times B(y)\big) + \ldots$$

Theorem

If the magnetic field $B(x) = B$ is constant, there exist $E_{2j}(x, v)$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{2}\dot{y}^\top\dot{y} + U(y) + h^2 E_2(y,\dot{y}) + \ldots + h^{2N} E_{2N}(y,\dot{y})\Big) = \mathcal{O}(h^{2N+2})$$

along solutions $(y, \dot{y})$ of the modified differential equation.

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Energy conservation - constant magnetic field

Consider the modified equation

$$\ddot y + \frac{h^2}{12}\, y^{(4)} + \ldots = \Big(\dot y + \frac{h^2}{6}\,\dddot y + \ldots\Big) \times B(y) - \nabla U(y)$$

and ta

because $\quad \dot y^\top(\dddot y \times B(y)) = \dot y^\top(\dddot y \times B) = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\dot y^\top(\ddot y \times B)\Big)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\frac{1}{2}\dot y^\top \dot y + U(y) + \frac{h^2}{12}\big(\dot y^\top \dddot y - \frac{1}{2}\ddot y^\top \ddot y\big) + \ldots\Big) = \frac{h^2}{6}\dot y^\top(\dddot y \times B(y)) + \ldots$$

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Energy conservation - quadratic electric potential

Consider the modified equation with $U(x) = \frac{1}{2}\, x^\top Q x + q^\top x$

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because $\quad \dddot y^\top \nabla U(y) = \dddot y^\top (Qy + q) = \frac{\mathrm{d}}{\mathrm{d}t}\Big(\ddot y^\top Q y - \frac{1}{2} \dot y^\top Q \dot y + \ddot y^\top q \Big)$

ar

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along solutions (y, w) *of the modified differential equation.*

Explanation of the numerical experiments

The numerical solution satisfies (formally) $x_n = y(nh)$, $v_n = w(nh)$, where

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(H(y,w)+h^2F(y,w)+\ldots\Big) = h^2G(y,w)+\mathcal{O}(h^4)$$

- integration shows that there is typically a linear drift of size th^2M, where M is an upper bound of $G(y,w)$,
- if the solution $(y(t),w(t))$ is ergodic on an invariant set A with invariant measure μ, then

$$\lim_{t\to\infty}\frac{1}{t}\int_0^t G\big(y(s),w(s)\big)\,\mathrm{d}s = \int_A G(x,v)\mu\big(d(x,v)\big)$$

  - if the integral to the right is non-zero, we will have a linear drift;
  - if it is zero, we will have a random walk: the error behaves like $\mathcal{O}(h^2)+\mathcal{O}(\sqrt{t}\,h^2)$.