Structure preserving discretisations

J. Frauendiener

Department of Mathematics and Statistics
University of Otago, Dunedin, New Zealand
and
Centre of Mathematics for Applications
University of Oslo, Norway

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Introduction

Consider the following system

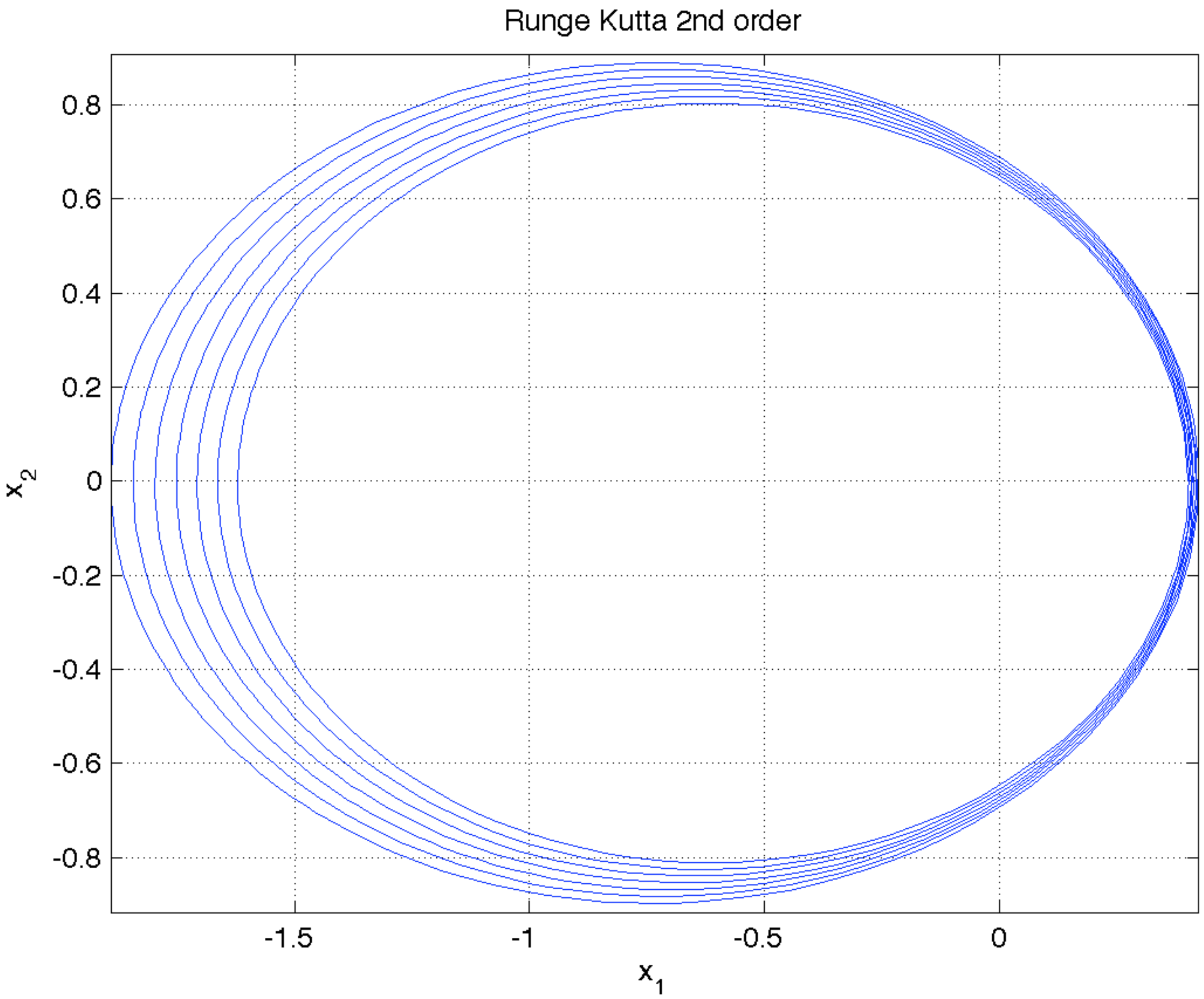
$$\dot{x}_1 = x_3, \qquad \dot{x}_3 = -\frac{x_1}{(x_1^2 + x_2^2)^{3/2}}$$
$$\dot{x}_2 = x_4, \qquad \dot{x}_4 = -\frac{x_2}{(x_1^2 + x_2^2)^{3/2}}$$

general form of autonomous system

$$\dot{x} = f(x)$$

Can be numerically integrated with e.g. a Runge-Kutta method

Introduction



Introduction

On the other hand, writing the same system as

$$\dot{q}_1 = p_1, \qquad \dot{p}_1 = -\frac{q_1}{(q_1^2 + q_2^2)^{3/2}}$$

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shows, that it is Hamiltonian

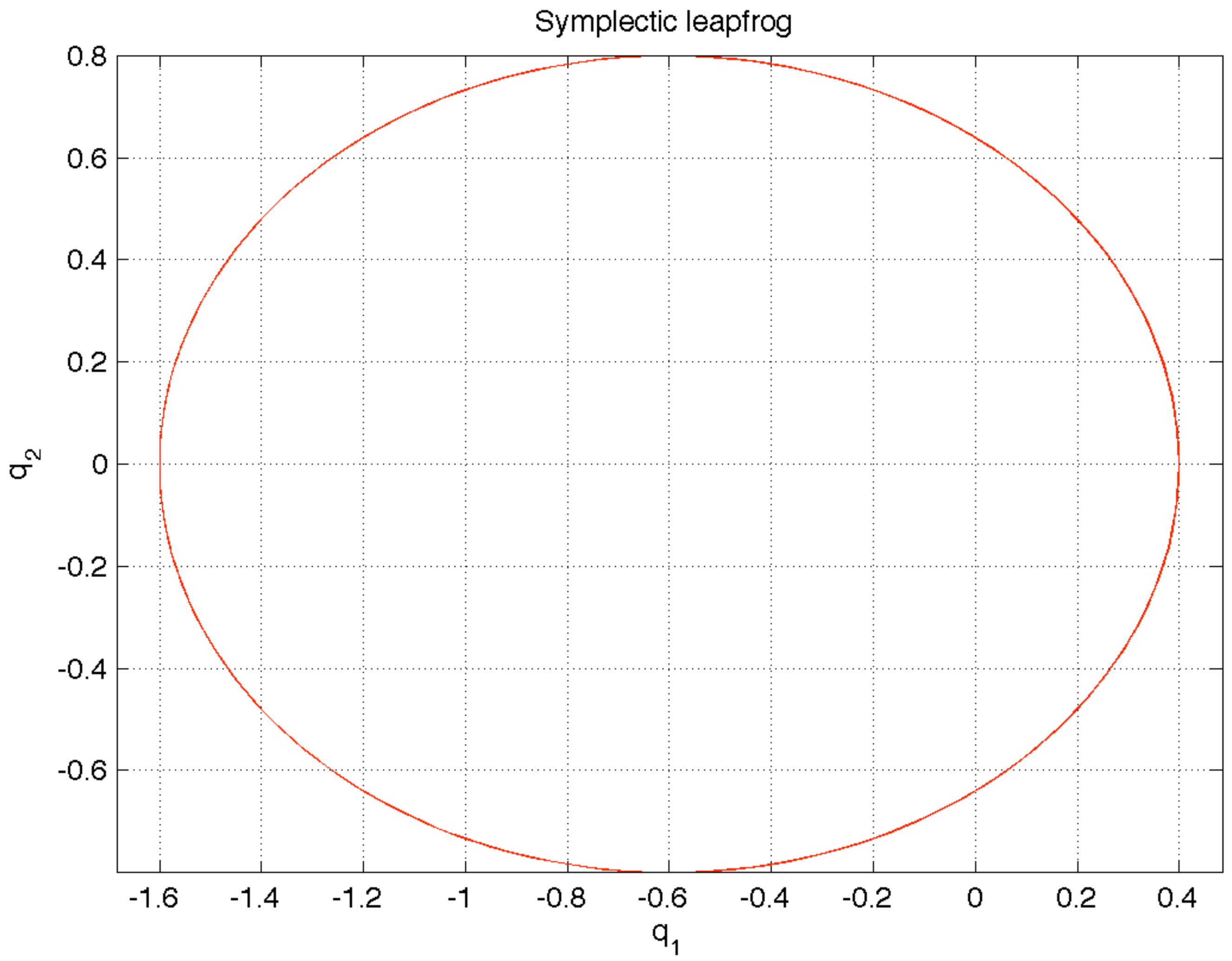
$$\dot{q}_1 = \frac{\partial H}{\partial p_1}, \qquad \dot{p}_1 = -\frac{\partial H}{\partial q_1}$$

$$\dot{q}_2 = \frac{\partial H}{\partial p_2}, \qquad \dot{p}_2 = -\frac{\partial H}{\partial q_2}$$

for the Hamiltonian function

$$H = \frac{1}{2}\left(p_1^2+p_2^2\right) - \frac{1}{\sqrt{q_1^2+q_2^2}}$$

Introduction



In fact, the Hamiltonian

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specifies a planar Kepler problem

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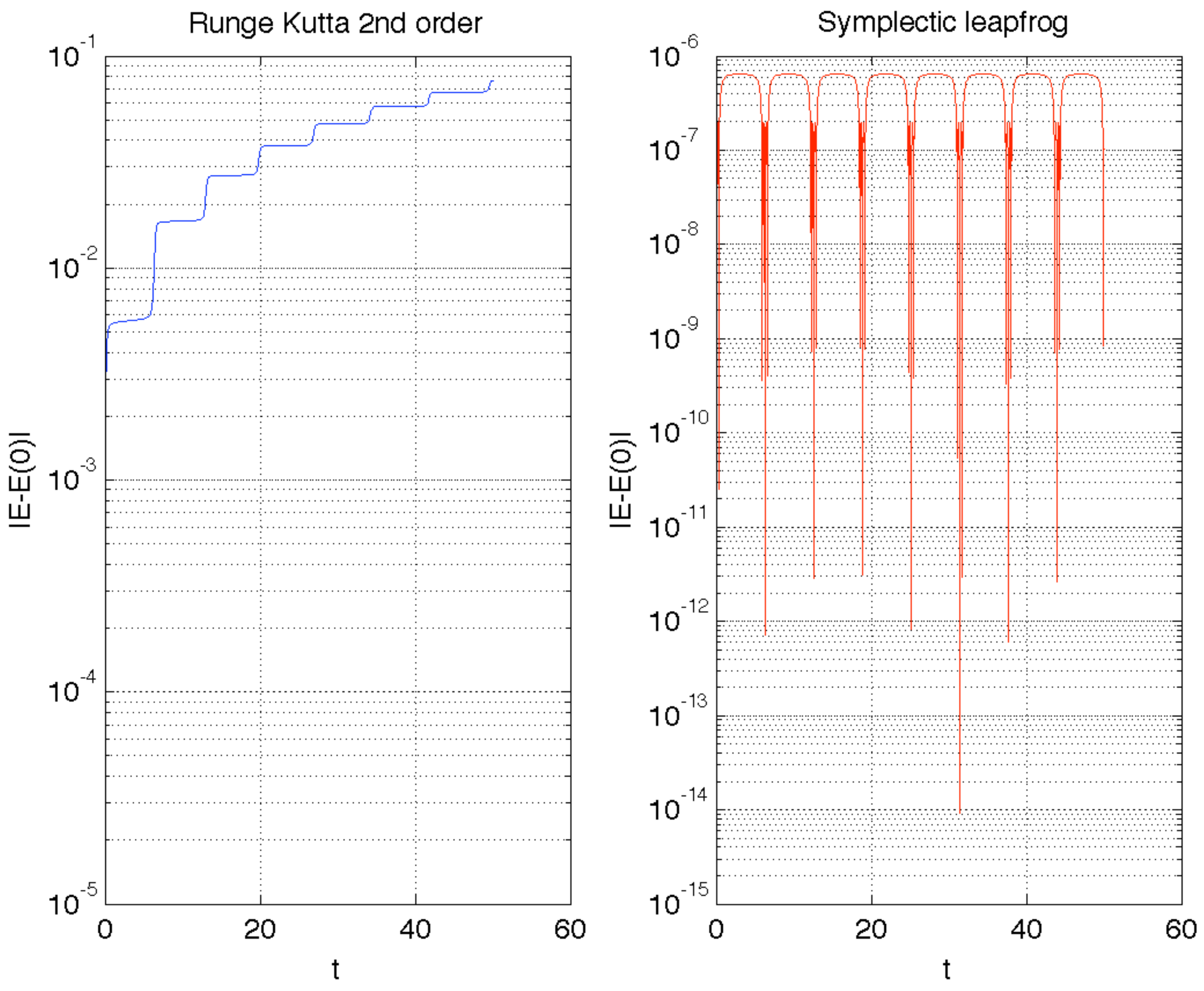
One expects

- Closed orbits
- Conservation of energy i.e.

$$E = H(p(t), q(t)) = H(p(0), q(0))$$

  should be constant
- Conservation of angular momentum $L = p_1 q_2 - p_2 q_1$



Runge Kutta 2nd order
10^-1
10^-2
10^-3
10^-4
10^-5
IE-E(0)I
0
20
40
60
t
Symplectic leapfrog
10^-6
10^-7
10^-8
10^-9
10^-10
10^-11
10^-12
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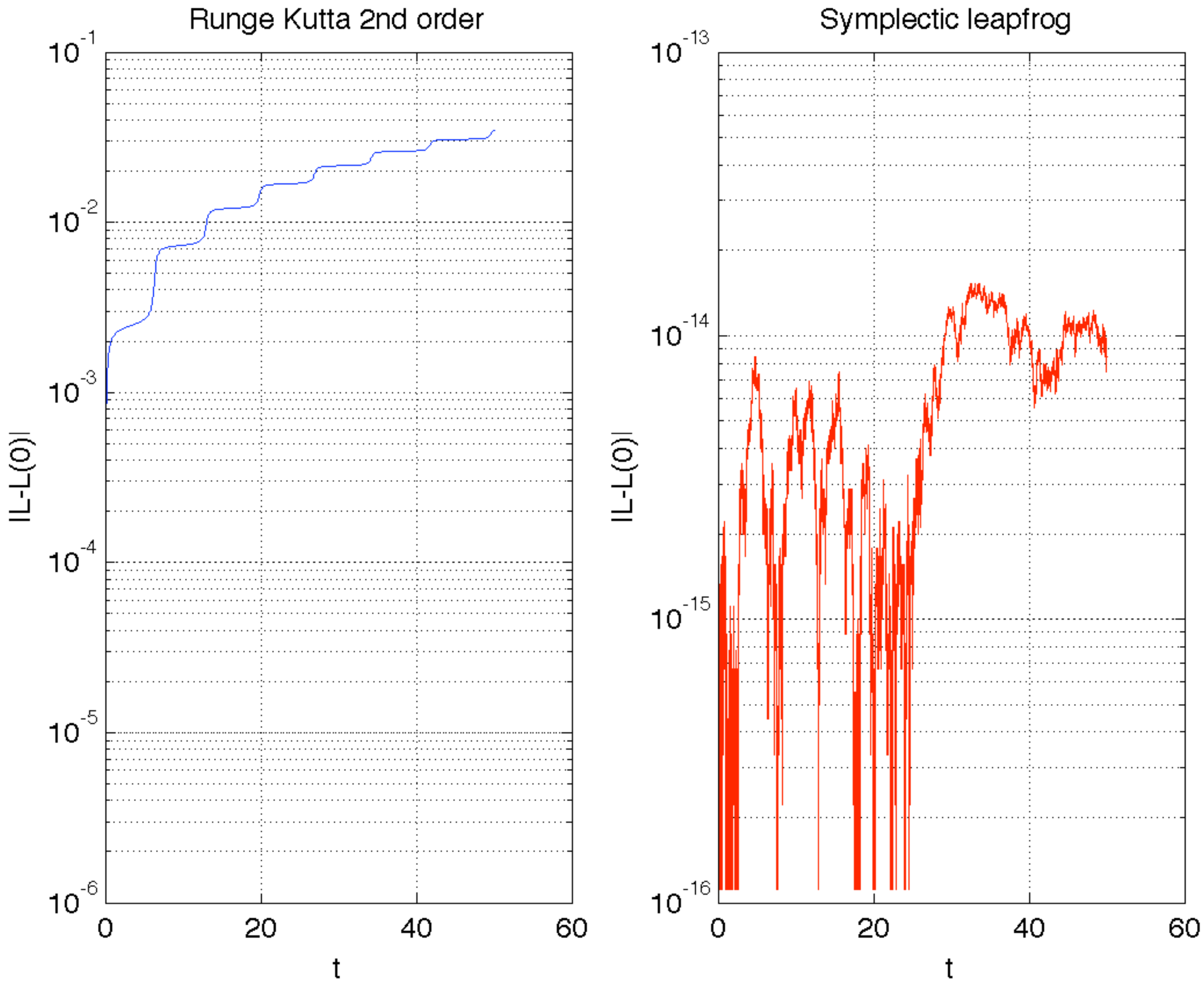
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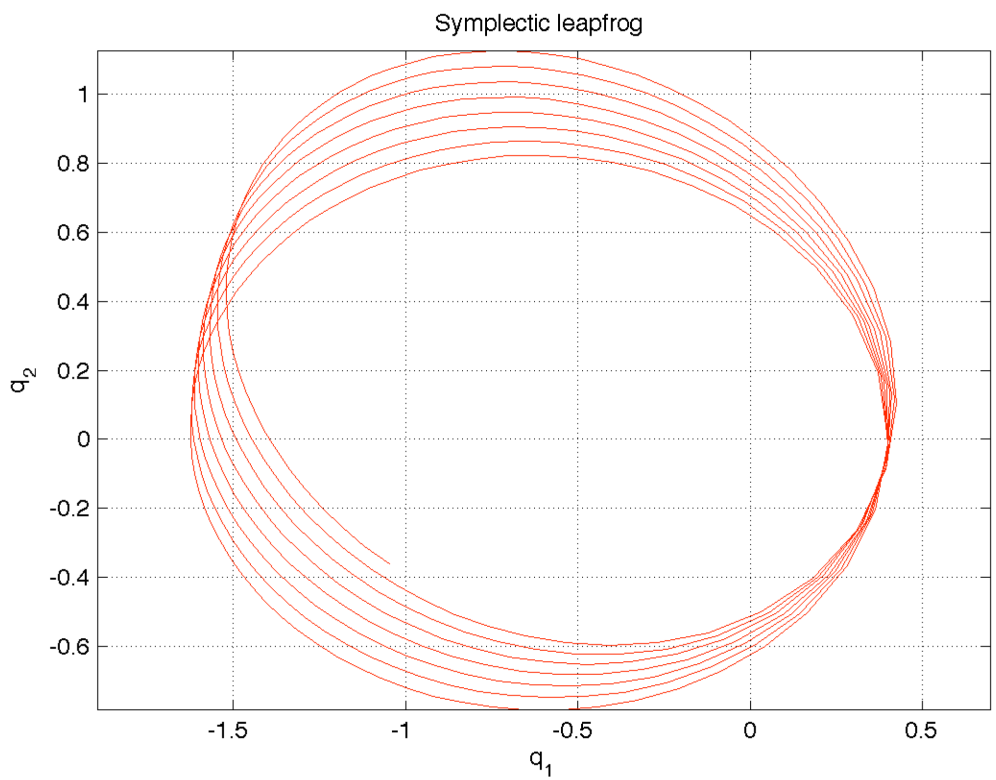
Comparison of the two methods (for general Hamiltonian systems)

method	**cost**	**error in E**	**error in L**	**global error**	**orbits**
RK2	2	$\mathcal{O}(t^2 h^2)$	$\mathcal{O}(t^2 h^2)$	$\mathcal{O}(t^2 h^2)$	open
SLF	1	$\mathcal{O}(h^2)$	0	$\mathcal{O}(t h^2)$	closed*

Introduction

symplectic leapfrog with large timestep



precession : same effect as a perturbation of the Hamiltonian
(→ backward error analysis)

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- here: focus on Hamiltonian (symplectic) systems

Hamiltonian system with n degrees of freedom

- state specified by $2n$ variables $x = (q, p) = (q^1, \dots, q^n, p_1, \dots, p_n)$

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Hamilton's principle

$$\delta \int p_i \dot{q}^i - H(q, p) \, \mathrm{d}t = 0$$

variational equations:

Hamilton's equations

$$\dot{q}^k = \frac{\partial H}{\partial p_k} \qquad \dot{p}_i = -\frac{\partial H}{\partial q^i} \iff \dot{x}^a = \Omega^{ab}\frac{\partial H}{\partial x^b} \quad \text{with} \quad \Omega^{ab} = \left(\begin{array}{c|c} 0 & \mathbf{1}_n \\ \hline -\mathbf{1}_n & 0 \end{array}\right) = -\Omega^{ba}$$

Poisson brackets

$$\{\cdot,\cdot\} : \mathscr{C}^\infty(M) \times \mathscr{C}^\infty(M) \to \mathscr{C}^\infty(M),$$
$$(f,g) \mapsto \{f,g\} := \partial_a f \Omega^{ab} \partial_b g$$

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In terms of (q,p)

$$\{f,g\} = \frac{\partial f}{\partial q^i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q^i}$$

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More general Poisson structure:

$\Omega^{ab}(x)$ with compatibility condition $\Omega^{e[c}\partial_e\Omega^{ab]} = 0$

could even be degenerate

Properties

1. anti-symmetry
$$\{f, g\} = -\{g, f\}$$
2. additivity
$$\{f + g, h\} = \{f, h\} + \{g, h\}$$
3. derivation property
$$\{fg, h\} = \{f, h\}g + f\{g, h\}$$
4. Jacobi identity
$$\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$$

For any function F one has

$$\{f+g,F\}=\{f,F\}, \qquad \{fg,F\}=\{f,F\}g+f\{g,H\}$$

hence $\{\cdot,F\}$ is a derivation on the ring $\mathscr{C}^\infty(M)$, a vectorfield X_F.

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The integral curves of the vectorfield are given by solutions of

$$\frac{\mathrm{d}x}{\mathrm{d}s} = X_F = \{x,F\} \iff \frac{\mathrm{d}x^a}{\mathrm{d}s} = \partial_c x^a \Omega^{cb} \partial_b F = \Omega^{ab}\partial_b F.$$

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Every function F defines a vector field X_F, its Hamiltonian vectorfield

and (almost) vice versa

Hamiltonian systems, theory

In particular, for the Hamiltonian H

$$\dot{x}^a = \Omega^{ab}\partial_b H.$$

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Immediate consequence:

$$\dot{H} = \frac{\mathrm{d}H(x(t))}{\mathrm{d}t} = \partial_a H\, \dot{x}^a = \partial_a H \Omega^{ab} \partial_b H = 0$$

Hamiltonian (energy) is conserved, a first integral of the motion

Hamiltonian systems, theory

Canonical coordinates

any $2n$ functions z^a with

$$\{z^a, z^b\} = \Omega^{ab}$$

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In terms of (q, p):
$$\{q^i, q^k\} = 0, \qquad \{q^i, p_k\} = \delta^i_k, \qquad \{p_i, p_k\} = 0.$$

Hamiltonian systems, theory

Canonical transformations

Let $\psi : M \to M$ be a map and write $y = \psi(x)$. If

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It leaves the Poisson bracket invariant

$$\{f \circ \psi, g \circ \psi\} = \{f, g\} \circ \psi.$$

Hamiltonian systems, theory

Canonical transformations

The Hamiltonian system

$$\dot{x} = \{x, H\}$$

has a solution $x(t)$ for any initial point x and any (small enough) t.

Hamiltonian systems, theory

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Define the flow map $\phi(t, x) = x(t)$ from initial point x to the point at time t.

It has the properties

$$\phi(0, x) = x \implies \frac{\partial \phi}{\partial x}(0, x) = \mathbf{1}$$

$$\frac{\partial \phi}{\partial t}(t, x) = \dot{x} = \{x, H\}(\phi(t, x))$$

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Flow property

$$\phi(t + s, x) = \phi(s, \phi(t, x))$$

Time-shift

The time-shift $\phi_t : x \mapsto \phi(t, x)$ is a canonical transformation

Proof: consider $\{f \circ \phi_t, g \circ \phi_t\}$ and $\{f, g\} \circ \phi_t$ as functions of t.

Agreement for $t = 0$.

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Compute

$$\frac{\mathrm{d}}{\mathrm{d}t} f(\phi_t(x)) = \frac{\partial f}{\partial x}\frac{\mathrm{d}}{\mathrm{d}t}\phi_t(x) = \frac{\partial f}{\partial x}\frac{\partial}{\partial t}\phi(t,x) = \{f, H\}(\phi_t(x)).$$

get

$$\frac{\mathrm{d}}{\mathrm{d}t}\{f(\phi_t(x)), g(\phi_t(x))\} = \{\frac{\mathrm{d}}{\mathrm{d}t} f(\phi_t(x)), g(\phi_t(x))\} + \{f(\phi_t(x)), \frac{\mathrm{d}}{\mathrm{d}t} g(\phi_t(x))\}$$

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or

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Hamiltonian systems, theory

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Jacobi identity

$$\frac{\mathrm{d}}{\mathrm{d}t}\{f \circ \phi_t, g \circ \phi_t\} = \{\{f, H\}, g\} + \{f, \{g, H\}\} = \{\{f, g\}, H\} = \frac{\mathrm{d}}{\mathrm{d}t}\{f, g\} \circ \phi_t$$

Symplectic integrators

Definition

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A symplectic integrator Φ_h is a canonical transformation approximating ϕ_h.

It is of order r iff
$$\Phi_h(x) - \phi_h(x) = \mathcal{O}(h^{r+1}).$$

Example: the symplectic leapfrog, Störmer-Verlet method

works for Hamiltonians of the form

$$H = \frac{1}{2}(A^{ij} p_i p_j) + V(q), \implies \dot{q}^i = A^{ij} p_j, \qquad \dot{p}_i = -\frac{\partial V}{\partial q^i} =: F_i$$

$\Phi_h : (q, p) \mapsto (q_h, p_h) =: (Q, P)$ (fixed h).

Symplectic leapfrog

$$q' \leftarrow q + \frac{h}{2} A \cdot p$$
$$P \leftarrow p + hF(q')$$
$$Q \leftarrow q' + \frac{h}{2} A \cdot P$$

Symplectic integrators

Example

Symplectic leapfrog is symplectic:

Symplectic integrators

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Symplectic integrators

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Symplectic leapfrog is symplectic:

$$
\begin{aligned}
\{P, Q\} &= \{p + hF(q'), q' + \frac{h}{2}A \cdot P\} \\
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\end{aligned}
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other Poisson brackets similar

Symplectic integrators

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It is an integrator of order 2:

Symplectic integrators

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$$q(h) = q + h\dot{q} + \frac{h^2}{2}\ddot{q} + \mathcal{O}(h^3) = q + hA \cdot p + \frac{h^2}{2}A \cdot F(q) + \mathcal{O}(h^3)$$

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$$Q = q' + \frac{h}{2}A\cdot P = q + \frac{h}{2}A\cdot p + \frac{h}{2}A\cdot(p + hF(q'))$$

$$= q + hA\cdot p + \frac{h^2}{2}A\cdot F(q) + \mathcal{O}(h^3)$$

$$P = p + hF(q') = p + hF(q + \frac{h}{2}A\cdot p)$$

$$= p + hF(q) + \frac{h^2}{2}\mathrm{d}F(q)\cdot A\cdot p + \mathcal{O}(h^3)$$

Symplectic integrators

Example

Energy

$$H(P,Q) = \frac{1}{2} P \cdot A \cdot P + V(Q) = H(p,q) + \mathcal{O}(h^3)$$

is not conserved exactly.

Symplectic integrators

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General result:

Approximate symplectic integrators cannot preserve the Hamiltonian exactly.

Symplectic integrators

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is not conserved exactly.

General result:

Approximate symplectic integrators cannot preserve the Hamiltonian exactly.

If they did, they would agree with the time shift up to reparametrisation of time.

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Consider the numerical solution as the exact solution of a modified problem

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in general: given exact problem with approximate (numerical) solution

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try to find a modified vector field $\tilde{f}(x)$

$$\dot{x} = \tilde{f}(x) = f(x) + hf_2(x) + h^2 f_3(x) + \cdots$$

such that $\tilde{\phi}_h = \Phi_h$.

Theorem

Let $f(x)$ be smooth vector field and assume Φ_h admits a Taylor expansion

$$\Phi_h(x) = x + hf(x) + h^2 D_2(x) + h^3 D_3(x) + \cdots$$

then there exist unique vector fields $f_k(x)$ such that for any $N > 1$

$$\Phi_h(x) = \tilde{\phi}_{h,N}(x) + \mathcal{O}(h^{N+1}),$$

where $\tilde{\phi}_{t,N}$ is the time-shift for the truncated modified equation

$$\dot{x} = f(x) + hf_2(x) + h^2 f_3(x) + \cdots + h^{N-1} f_N(x).$$

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Proof by Taylor expansion of $\tilde{\phi}_{h,N}$ and comparing coefficients.

For symplectic leapfrog ($A = \mathbf{1}$)

$$\Phi_h \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} q + hp + \frac{h^2}{2} F(q + \frac{h}{2} p) \\ p + hF(q + \frac{h}{2} p) \end{pmatrix}$$

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gives

$$D_2 = \frac{1}{2} \begin{pmatrix} F(q) \\ \mathrm{d}F(q)p \end{pmatrix} \qquad D_3 = \frac{1}{4} \begin{pmatrix} \mathrm{d}F(q)p \\ \mathrm{d}^2 F(q)(p, p) \end{pmatrix}$$

Symplectic integrators

Backward error analysis

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and the h^2 modification of the vector field

$$f_3 = \frac{1}{12} \begin{pmatrix} -2\mathrm{d}F(q)p \\ \mathrm{d}F(q) \cdot F(q) + \mathrm{d}^2 F(q)(p, p) \end{pmatrix}$$

Symplectic integrators

Backward error analysis

Hence: the symplectic leapfrog method corresponds to the modified differential equation

$$\dot{q} = p - \frac{h^2}{6} \mathrm{d}F(q)p$$

$$\dot{p} = F(q) + \frac{h^2}{12} (\mathrm{d}F(q) \cdot F(q) + \mathrm{d}^2 F(q)(p, p))$$

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This is Hamiltonian for

$$\tilde{H} = \frac{1}{2}p\cdot p + V(q) - \frac{h^2}{12}\left(\mathrm{d}^2V(q)(p,p) + \mathrm{d}V(q)\cdot\mathrm{d}V(q)\right)$$

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The modified system remains Hamiltonian

Symplectic Integrators

Long-time (almost) energy conservation

Recall: numerical method Φ_h is interpreted as time-shift $\tilde{\phi}_{h,N}$ for a modified Hamiltonian for any $N > 2$

$$\tilde{H}_N = H + h^2 H_3 + h^3 H_4 + \cdots + h^{N-1} H_N$$

Consequence

$$\left.\begin{aligned} \tilde{H}_N(x_n) - \tilde{H}_N(x_0) &= \mathcal{O}(e^{-\frac{h_0}{2h}}), \\ H(x_n) - H(x_0) &= \mathcal{O}(h^2) \end{aligned}\right\} \qquad \text{for } h < h_0, t := nh \leq e^{\frac{h_0}{2h}}$$

(works for higher order methods as well)

For completely integrable systems:
$I_k(q, p)$ first integrals (action variables)

Linear growth

Let x^* be such that the 'frequencies' of the system are non-resonant, every numerical solution starting close to x^* satisfies

$$I_k(x_n) - I_k(x_0) = \mathcal{O}(h^2) \qquad \text{for } h < h_0, t := nh \leq e^{\frac{c}{h^\alpha}}$$

for some step size h_0 and constants c, α.

Also holds for perturbations of completely integrable systems.

Recall:

$$\left.\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p}(q,p), \\ \dot{p} &= -\frac{\partial H}{\partial q}(q,p) \end{aligned}\right\} \iff \dot{x} = \{x, H\} = \Omega \cdot \nabla H$$

symplectic Euler:

$$q_{n+1} = q_n + h\partial_p H(q_{n+1}, p_n)$$
$$p_{n+1} = p_n - h\partial_q H(q_{n+1}, p_n)$$

symplectic Euler:

$$q_{n+1} = q_n + h\partial_p H(q_{n+1}, p_n) \qquad \text{implicit}$$
$$p_{n+1} = p_n - h\partial_q H(q_{n+1}, p_n)$$

symplectic Euler:

$$
\begin{aligned}
q_{n+1} &= q_n + h\partial_p H(q_{n+1}, p_n) && \text{implicit} \\
p_{n+1} &= p_n - h\partial_q H(q_{n+1}, p_n) && \text{explicit}
\end{aligned}
$$

Symplectic Integrators

Other methods

symplectic Euler:

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(adjoint) symplectic Euler:

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Symplectic Integrators

Other methods

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Symplectic Integrators

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Properties

- first order accurate
- symplectic
- in general implicit

midpoint rule:

$$x_{n+1} = x_n + h\nabla H\left(\frac{x_{n+1} + x_n}{2}\right)$$

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Properties

- second order accurate
- symplectic
- implicit, (expensive)

Composition methods

Given a method Φ_h of order r, then

$$\Psi_h = \Phi_{\gamma_s h} \circ \cdots \circ \Phi_{\gamma_1 h}$$

is at least of order $r + 1$, if

$$\sum_{i=1}^{s} \gamma_i = 1, \qquad \sum_{i=1}^{s} \gamma_i^{r+1} = 0$$

When Φ_h is symplectic, then so is Ψ_h.

Definition

The adjoint Φ_h^* of a method Φ_h is defined by

$$x_1 = \Phi_h^*(x_0) \iff x_0 = \Phi_{-h}(x_1)$$

Composition with adjoint

If Φ_h is a (symplectic) method order 1, then

$$\Phi_{h/2}^* \circ \Phi_{h/2}$$

is a (symplectic) method of order 2

more general results exist.

Symplectic Integrators

Other methods

Example: for $H = \frac{1}{2}p^2 + V(q)$ and Φ_h symplectic Euler

$$\begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \overset{\Phi_{h/2}}{\longmapsto} \begin{pmatrix} q_{\frac{1}{2}} \\ p_{\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} q_0 + \frac{h}{2} p_0 \\ p_0 - \frac{h}{2} \partial_q V(q_{\frac{1}{2}}) \end{pmatrix}$$

Symplectic Integrators

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$$\begin{pmatrix} q_{\frac{1}{2}} \\ p_{\frac{1}{2}} \end{pmatrix} \overset{\Phi^*_{h/2}}{\longmapsto} \begin{pmatrix} q_1 \\ p_1 \end{pmatrix} = \begin{pmatrix} q_{\frac{1}{2}} + \frac{h}{2} p_1 \\ p_{\frac{1}{2}} - \frac{h}{2}\partial_q V(q_{\frac{1}{2}}) \end{pmatrix}$$

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symplectic leap-frog

Runge-Kutta methods

Properties:

- symplectic RK methods are necessarily implicit
- A-stable
- s-stage method has maximal order $2s$
- preserve all linear symmetries
- preserve quadratic integrals

Splitting methods

If $H = H_1 + H_2$ with symplectic integrators Φ_h^1 and Φ_h^2 for H_1 and H_2 then

$$\Psi_h = \Phi^1_{\frac{h}{2}} \circ \Phi^2_h \circ \Phi^1_{\frac{h}{2}}$$

is a symplectic integrator for H .

Symplectic integrators

When to use

- Symplectic integrators preserve phase space structures
- fixed points
- invariant tori (KAM) and their neighbourhoods
- invariant sets
- in general: phase portraits
- not for highly accurate computation of one orbit

Variational Integrators

Another point of view: Hamilton's principle in configuration space

$$\delta \int_{t_0}^{t_1} L(q, \dot{q})\,\mathrm{d}t = 0, \qquad q(t_0) = q_0, q(t_1) = q_1 \text{ fixed.}$$

yields Lagrangian equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.$$

Variational Integrators

Define the momenta by Legendre transform

$$p = \frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \implies \dot{q} = \dot{q}(q, p)$$

then obtain a Hamiltonian system for $H = p\dot{q} - L$.

Variational Integrators

For a solution $q(t)$ define the function

$$S(q_0, q_1) = \int_{t_0}^{t_1} L(q, \dot{q}) \, \mathrm{d}t.$$

then

$$\begin{aligned} \mathrm{d}S &= \frac{\partial L}{\partial \dot{q}}(q_0, \dot{q}_0)\mathrm{d}q_0 + \frac{\partial L}{\partial \dot{q}}(q_1, \dot{q}_1)\mathrm{d}q_1 \\ &= p_0 \mathrm{d}q_0 - p_1 \mathrm{d}q_1 \end{aligned}$$

Variational Integrators

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Consequence

The map $(q_0, p_0) \mapsto (q_1, p_1)$ is symplectic with generating function S.

Idea

Take q_0 and q_1 close and derive a discrete evolution by discretising Hamilton's principle directly.

Idea

Take q_0 and q_1 close and derive a discrete evolution by discretising Hamilton's principle directly.

$$S_h(\{q_i\}_{i=0:N}) = \sum_{i=0}^{N-1} L_h(q_i, q_{i+1})$$

with

$$L_h(q_i, q_{i+1}) \approx \int_{t_n}^{t_{n+1}} L_h(q(t), \dot{q}(t))\,\mathrm{d}t$$

Fixing q_0 and q_N and extremising

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yields

Discrete Lagrange equations

$$0 = \frac{\partial S_h}{\partial q_i} = \partial_2 L_h(q_{i-1}, q_i) + \partial_1 L_h(q_i, q_{i+1}), \qquad 0 < i < N. \qquad (\star)$$

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3-term recurrence for determining $\{q_i\}_{i=0:N}$ from (q_0, q_1).

Variational Integrators

Discrete equations

Introduce discrete momenta by

$$p_i = -\partial_1 L_h(q_i, q_{i+1}) \implies q_{i+1} = q_{i+1}(q_i, p_i)$$

and use $(\star)$ to get

$$p_{i+1} = -\partial_1 L_h(q_{i+1}, q_{i+2}) = \partial_2 L_h(q_i, q_{i+1})$$

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Discrete Hamilton equations

$$\Phi_h : (q_i, p_i) \mapsto (q_i, q_{i+1}) \mapsto (q_{i+1}, p_{i+1})$$

is a symplectic integrator.

The discretisation of L determines the properties of Φ_h.

Variational Integrators

Example

Define $L_h(q_i, q_{i+1})$ by approximating

$$q(t) \approx \frac{1}{h}\left((t - t_i)q_{i+1} + (t_{i+1} - t)q_i\right)$$

and using the trapezoidal rule

$$\int_{t_i}^{t_{i+1}} L(q(t), \dot{q}(t))\,\mathrm{d}t \approx L_h(q_i, q_{i+1})$$
$$= \frac{h}{2}\left(L(q_i, \frac{q_{i+1} - q_i}{h}) + L(q_{i+1}, \frac{q_{i+1} - q_i}{h})\right)$$

Variational Integrators

Example

For a mechanical system $L(q, \dot{q}) = \frac{1}{2}\dot{q}^2 - V(q)$

$$L_h(q_i, q_{i+1}) = \frac{(q_{i+1} - q_i)^2}{2h} - \frac{h}{2}\left(V(q_i) + V(q_{i+1})\right)$$

Variational Integrators

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Exercise: Show that this yields the (symplectic) method

$$v_{i+\frac{1}{2}} = p_i + \frac{h}{2}F_i$$
$$q_{i+1} = q_i + hv_{i+\frac{1}{2}}$$
$$p_{i+1} = v_{i+\frac{1}{2}} + \frac{h}{2}F_{i+1}$$

Compare with SLF.

Infinite dimensional systems

General equations

PDE for a function $f(t,x)$

$$\dot{f} = F(f', f)$$

Numerical approximation

- method of lines discretisation (semi-discretisation):

$$x \to x_i, \qquad f(t,x) \to f_i(t) = f(t,x_i), \qquad f'(t,x) \to \sum_s \alpha_s f_{i+s}$$

$$\dot{f} = F(f', f) \to \dot{f}_i = F(f_{i+s}),$$

- simultaneous space-time discretisations (e.g., method of characteristics)

Infinite dimensional systems

Equations with structure

With additional structures

- discretise the primary structures
  Poisson bracket, Hamiltonian, action

Infinite dimensional systems

Equations with structure

With additional structures

- discretise the primary structures
  Poisson bracket, Hamiltonian, action
- derive discretised equations with structure
  Hamiltonian eq'ns, variational eq'ns

Infinite dimensional systems

Equations with structure

With additional structures

- discretise the primary structures
  Poisson bracket, Hamiltonian, action
- derive discretised equations with structure
  Hamiltonian eq'ns, variational eq'ns
- use structure preserving algorithms

Infinite dimensional systems

Example, KdV

KdV equation, Hamiltonian equation with

$$H = \frac{1}{2\pi}\int_0^{2\pi} \frac{1}{6}u^3 - \frac{1}{2}u_x^2 \,\mathrm{d}x$$

and

$$\{F, G\} = \frac{1}{2\pi}\int_0^{2\pi} \frac{\delta F}{\delta u}\frac{\mathrm{d}}{\mathrm{d}x}\frac{\delta G}{\delta u}\,\mathrm{d}x$$

Infinite dimensional systems

Example, KdV

Functions on the circle:

$$x_i = \frac{2\pi}{N} i = i\Delta, \quad f_i = f(x_i), \quad f_0 = f_N$$

local functionals

$$F(u) = \frac{1}{2\pi}\int_0^{2\pi} f(u, u_x, \ldots)\,\mathrm{d}x \to F(u_i)$$

functional derivative

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon} F(u+\epsilon h)|_{\epsilon=0} = \frac{1}{2\pi}\int_0^{2\pi} \frac{\delta F}{\delta u} h\,\mathrm{d}x \to \frac{\mathrm{d}}{\mathrm{d}\epsilon} F(u_i+\epsilon h_i)|_{\epsilon=0} = \sum_i \frac{\partial F}{\partial u_i} h_i$$

Infinite dimensional systems

Example, KdV

Discrete Poisson bracket:

$$\{f,g\} \to \{\, (f_i),(g_i)\} = \frac{N}{2}\sum_{i=0}^{N-1} f_i\,(g_{i+1} - g_{i-1}) = f^t \Omega g$$

with

$$\Omega = \frac{N}{2}\begin{pmatrix} 0 & 1 & & -1 \\ -1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ 1 & & -1 & 0 \end{pmatrix}$$

Infinite dimensional systems

Example, KdV

discrete Hamiltonian

$$H = \frac{1}{N} \sum_{i=0}^{N-1} \left[\frac{1}{6} u_i^3 - \frac{1}{2} \left(\frac{u_{i+1} - u_i}{\Delta} \right)^2 \right]$$

and discrete equations

$$\dot{u}_i = \{u_i, H\} = \frac{N}{2} \left(\frac{\partial H}{\partial u_{i+1}} - \frac{\partial H}{\partial u_{i-1}} \right)$$

Infinite dimensional systems

Example, NLS

Lagrangian for NLS

$$L = \int \mathrm{i}(\bar{\psi}\dot{\psi} - \psi\dot{\bar{\psi}}) - \psi_x\bar{\psi}_x - \frac{\kappa}{2}|\psi|^4 \,\mathrm{d}x$$

discrete version

$$L_\Delta = \Delta \sum_k \mathrm{i}(\bar{\psi}_k\dot{\psi}_k - \psi_k\dot{\bar{\psi}}_k) - \frac{1}{\Delta^2}(\psi_{k+1} - \psi_k)(\bar{\psi}_{k+1} - \bar{\psi}_k) - \frac{\kappa}{2}|\psi_k|^4$$

momenta

$$\pi_k = \frac{\partial L_\Delta}{\partial \dot{\psi}_k} = \mathrm{i}\Delta\bar{\psi}_k \implies \{\psi_k, \bar{\psi}_l\} = -\frac{\mathrm{i}}{\Delta}\delta_{kl}$$

Infinite dimensional systems

Example, NLS

discrete Hamiltonian

$$H_\Delta = \sum_k \pi_k \psi_k + \bar{\pi}_k \bar{\psi}_k - L_\Delta$$
$$= \sum_k \frac{1}{\Delta}(\psi_{k+1} - \psi_k)(\bar{\psi}_{k+1} - \bar{\psi}_k) + \frac{\kappa}{2}\Delta|\psi_k|^4$$

discrete Hamiltonian eq'ns

$$\dot{\psi}_k = \{\psi_k, H_\Delta\}$$

Infinite dimensional systems

Example, NLS

Ablowitz-Ladik discretisation

$$H_\Delta = \Delta \sum_k \frac{1}{\Delta^2}(\psi_{k+1}\bar{\psi}_k + \bar{\psi}_{k+1}\psi_k) - \frac{1}{\Delta^4}\log(1 + \Delta^2|\psi_k|^2)$$

deformed non-standard Poisson bracket

$$\{\psi_k, \bar{\psi}_l\} = 2\mathrm{i}\delta_{kl}(1 + \Delta^2|\psi_k|^2)$$

also gives a discretised version of NLS

$$\mathrm{i}\dot{\psi}_k + \frac{1}{\Delta^2}(\psi_{k+1} - 2\psi_k + \psi_{k-1}) + |\psi_k|^2(\psi_{k+1} + \psi_{k-1})$$

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