Dynamics, numerical analysis, and some geometry

Christian Lubich
Univ. Tübingen

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Dynamics: anything that evolves in time

Numerical analysis:
construction and mathematical analysis of numerical algorithms

... and how does geometry fit in?
Introduction

*Commonplace wisdom:*  
A good algorithm should respect the structure of the problem!

*Very often:*  
“Structure” is of geometric nature.

*In this talk:*  
Numerical analysis of time-dependent problems for which geometric aspects play an important role:

**Geometric Numerical Integration**
Basic questions

- How can numerical methods be constructed that “respect the geometry” of the problem at hand?

- What are benefits of a structure-preserving algorithm, and how do they come about?
Basic questions

In this talk mainly for **Hamiltonian systems**:

- How can numerical methods be constructed that “respect the geometry” of the problem at hand?

  *relates to Hamilton–Jacobi theory*

- What are benefits of a structure-preserving algorithm, and how do they come about?

  *relates to Hamiltonian perturbation theory (KAM etc.)*
Outline

Hamiltonian systems of ordinary differential equations

Hamiltonian systems with multiple time scales

Hamiltonian partial differential equations

Dynamical low-rank approximation

Quantum dynamics
Outline

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Quantum dynamics
Hamiltonian systems

Differential equations fundamental to many branches of physics:

\[ \dot{p} = -\nabla_q H(p, q) \]
\[ \dot{q} = +\nabla_p H(p, q), \]

with Hamilton function \( H \), positions and momenta \( q(t), p(t) \in \mathbb{R}^d \)

Energy conservation: for all times \( t \),

\[ H(p(t), q(t)) = H(p(0), q(0)). \]
Numerical example with Euler methods

For a step size $h > 0$, compute $p_n \approx p(nh)$, $q_n \approx q(nh)$ for $n = 0, 1, 2, \ldots$ via

$$
\frac{p_{n+1} - p_n}{h} = -\nabla q H(p_{n+\alpha}, q_{n+\beta})
$$

$$
\frac{q_{n+1} - q_n}{h} = +\nabla p H(p_{n+\alpha}, q_{n+\beta})
$$

with $\alpha, \beta \in \{0, 1\}$.

Four methods:

- $\alpha = \beta = 0$: explicit Euler method (1768: 250 years!)
- $\alpha = \beta = 1$: implicit Euler method (1768)
- $\alpha \neq \beta$: symplectic Euler methods (ess. Hamilton, Jacobi $\sim 1840$)
Numerical example: Outer Solar System

explicit Euler, $\alpha = 0, \beta = 0$
$h = 15$

symplectic Euler, $\alpha = 0, \beta = 1$
$h = 150$

symplectic Euler, $\alpha = 1, \beta = 0$
$h = 150$

implicit Euler, $\alpha = 1, \beta = 1$
$h = 15$
“Thanks to the numerical experiments of the last two decades, we know now that the motion of the planets in the Solar System is chaotic.”

Laskar 2013
Numerical example: Outer Solar System

Figure 2.1. Numerical simulation of the outer solar system.

Projector-splitting integrator of Section 5, which is robust to small singular values and preserves both the norm and the energy of the wavefunction.

2. Hamiltonian systems of ordinary differential equations

2.1. Hamiltonian systems. Differential equations of the form (with \( \dot{=} d/dt \))

\[
\begin{align*}
\dot{p} &= q H(p, q) \\
\dot{q} &= -p H(p, q)
\end{align*}
\]

are fundamental to many branches of physics. The real-valued Hamilton function \( H \), defined on a domain of \( \mathbb{R}^d \times \mathbb{R}^d \) (the phase space), represents the total energy and \( q(t) \) and \( p(t) \) represent the positions and momenta, respectively, of a conservative system at time \( t \). The total energy is conserved:

\[ H(p(t), q(t)) = H(p(0), q(0)) \]

along every solution \( (p(t), q(t)) \) of the Hamiltonian differential equations.

Numerical example: We consider four variants of the Euler method, which for a given (small) step size \( h > 0 \) compute approximations \( p_n \approx p(nh) \) and \( q_n \approx q(nh) \) via

\[
\begin{align*}
p_{n+1} &= p_n + h \alpha q_n \\
q_{n+1} &= q_n + h \alpha p_n
\end{align*}
\]

with \( \alpha \in \{0, 1\} \). For \( \alpha = \beta = 0 \) this is the explicit Euler method, for \( \alpha = \beta = 1 \) it is the implicit Euler method. The partitioned methods with \( \alpha \neq \beta \) are known as the symplectic Euler methods. All four methods are of order \( r = 1 \), that is, the error after one step of the method is \( O(h^{r+1}) \) with \( r = 1 \).

We apply these methods to the outer solar system, which is an \( N \)-body problem with Hamiltonian

\[
H(p, q) = \frac{1}{2} \sum_{i=0}^{N} m_i |p_i|^2 G \sum_{i=1}^{N} \sum_{j=0}^{i-1} m_i m_j |q_i - q_j|,
\]

where the symbols have their usual meaning.
Numerical example: Outer Solar System

Figure 2.2. Relative error of the Hamiltonian on the interval $0 \leq t \leq 200,000$.

Where

$$p = (p_0, \ldots, p_N),$$

$$q = (q_0, \ldots, q_N)$$

and $|\cdot|$ denotes the Euclidean norm, and the constants are taken from [HLW06, Section I.2.4]. The positions $q_i \in \mathbb{R}^3$ and momenta $p_i \in \mathbb{R}^3$ are those of the sun and the five outer planets (including Pluto).

Figure 2.1 shows the numerical solution obtained by the four versions of the Euler method on a time interval of 200,000 earth days. For the explicit Euler method the planets spiral outwards, for the implicit Euler method they spiral inwards, fall into the sun and finally are ejected. Both symplectic Euler methods show a qualitatively correct behaviour, even with a step size (in days) that is much larger than the one used for the explicit and implicit Euler methods. Figure 2.2 shows the relative error of the Hamiltonian,

$$H(p_n, q_n) - H(p_0, q_0),$$

along the numerical solution of the four versions of Euler's method on the time interval $0 \leq nh \leq 200,000$.

Whereas the size of the error increases for the explicit and implicit Euler methods, it remains bounded and small, of a size proportional to the step size $h$, for both symplectic Euler methods.

2.2. Symplecticity of the flow and symplectic integrators.

The time-$t$ flow of an ordinary differential equation $\dot{y} = f(y)$ is the map $'t$ that associates with an initial value $y_0$ at time $0$ the solution value at time $t$:

$$'t(y_0) = y(t).$$

Consider now the Hamiltonian system (2.1) or equivalently, for $y = (p, q)$,

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

with $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$.

The flow $'t$ of the Hamiltonian system is symplectic (or canonical), that is, the derivative matrix $D' t$ with respect to the initial value satisfies

$$D' t(y) > J D' t(y) = J$$

for all $y$ and $t$ for which $'t(y)$ exists. This quadratic relation is formally similar to orthogonality, with $J$ in place of the identity matrix $I$, but it is related to the preservation of areas rather than lengths in phase space.

There is also a local converse: If the flow of some differential equation is symplectic, then there exists locally a Hamilton function for which the corresponding Hamiltonian system coincides with this differential equation.

An one-step method $y_{n+1} = h(y_n)$ (with step size $h$) is scaled symplectic if the numerical flow $h$ is a symplectic map:

$$D h(y) > J D h(y) = J.$$
... and here enters Geometry:

Rewrite the Hamiltonian system for $y = (p, q)$:

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

Time-$t$ flow map $\varphi_t : y(0) \mapsto y(t)$

Characteristic property of Hamiltonian differential equations:

The flow $\varphi_t$ of the Hamiltonian system is symplectic:

$$D\varphi_t(y)^\top J D\varphi_t(y) = J$$

for all $y$ and $t$ for which $\varphi_t(y)$ exists.
Symplectic integrators

The flow $\varphi_t$ of the Hamiltonian system is symplectic:

$$D\varphi_t(y)^\top J D\varphi_t(y) = J.$$ 

A numerical one-step method (with step size $h$)

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

is called symplectic if the numerical flow $\Phi_h$ is a symplectic map:

$$D\Phi_h(y)^\top J D\Phi_h(y) = J.$$
Examples of symplectic integrators

- symplectic Euler methods \((\alpha, \beta) = (1, 0)\) or \((0, 1)\) before: de Vogelaere 1956
- variational integrators: Suris 1990, Marsden & West 2001
How does the geometry lead to improved dynamics?

Observation:
Symplectic integrators applied to Hamiltonian systems behave more favourably over long times than non-symplectic methods.

How can this be explained?
Interpret the numerical method for a differential equation $\dot{y} = f(y)$ as the flow of a modified differential equation

$$\dot{\tilde{y}} = f(\tilde{y}) + hf_1(\tilde{y}) + h^2 f_2(\tilde{y}) + h^3 f_3(\tilde{y}) + \ldots$$

For a symplectic integrator applied to a Hamiltonian system, each of the perturbation terms is a Hamiltonian vector field:

$$f_j(y) = J^{-1} \nabla H_j(y)$$

Moser 1968 locally, E. Hairer 1992 globally
Rigorous backward error analysis

\[ \| \Phi_h(y_0) - \tilde{\varphi}_h(y_0) \| \leq C h e^{-c/h} \]

Benettin & Giorgilli 1994, also Hairer & L. 1997, Reich 1999

Neishtadt 1984
For a symplectic integrator, energy is conserved up to the order of the method over exponentially long times:

\[ H(y_n) - H(y_0) = O(h^r) \quad \text{for} \quad nh \leq e^{c/2h}. \]
Numerical example: Outer Solar System

Figure 2.2. Relative error of the Hamiltonian on the interval $0 \leq t \leq 200000$.

Where $p = (p_0, ..., p_N)$, $q = (q_0, ..., q_N)$, and $|\cdot|$ denotes the Euclidean norm, and the constants are taken from [HLW06, Section I.2.4]. The positions $q_i \in \mathbb{R}^3$ and momenta $p_i \in \mathbb{R}^3$ are those of the sun and the five outer planets (including Pluto).

Figure 2.1 shows the numerical solution obtained by the four versions of the Euler method on a time interval of 200 000 earth days. For the explicit Euler method the planets spiral outwards, for the implicit Euler method they spiral inwards, fall into the sun and finally are ejected. Both symplectic Euler methods show a qualitatively correct behaviour, even with a step size (in days) that is much larger than the one used for the explicit and implicit Euler methods.

Figure 2.2 shows the relative error of the Hamiltonian, $H(p_n, q_n) - H(p_0, q_0) / |H(p_0, q_0)|$, along the numerical solution of the four versions of Euler's method on the time interval $0 \leq nh \leq 200000$.

Whereas the size of the error increases for the explicit and implicit Euler methods, it remains bounded and small, of a size proportional to the step size $h$, for both symplectic Euler methods.

2.2. Symplecticity of the flow and symplectic integrators.

The time-flow of a differential equation $\dot{y} = f(y)$ is the map $'t$ that associates with an initial value $y_0$ at time 0 the solution value at time $t$: $'t(y_0) = y(t)$. Consider now the Hamiltonian system (2.1) or equivalently, for $y = (p, q)$, $\dot{y} = J_1 r H(y)$ with $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$.

The flow $'t$ of the Hamiltonian system is symplectic (or canonical), that is, the derivative matrix $D' t$ with respect to the initial value satisfies $D' t(y) > J D' t(y) = J$ for all $y$ and $t$ for which $'t(y)$ exists. This quadratic relation is formally similar to orthogonality, with $J$ in place of the identity matrix, but it is related to the preservation of areas rather than lengths in phase space.

There is also a local converse: If the flow of some differential equation is symplectic, then there exists locally a Hamilton function for which the corresponding Hamiltonian system coincides with this differential equation.

An numerical one-step method $y_{n+1} = h(y_n)$ (with step size $h$) is scaled symplectic if the numerical flow $h$ is a symplectic map: $D h(y) > J D h(y) = J$. 
Integrable and near-integrable Hamiltonian systems

Results for symplectic integrators on

- Error growth: only linearly in time.
- Near-preservation of KAM tori over exponentially long times / forever


combines backward analysis and Hamiltonian perturbation theory
Rigorous backward error analysis: once again

\[ \| \Phi_h(y_0) - \tilde{\phi}_h(y_0) \| \leq C h e^{-c/h} \]

\[ c \sim 1/\Omega \rightarrow \text{estimate meaningful only for } h\Omega \ll 1 \]
... what can be concluded when backward error analysis does not work ($h\Omega \sim 1$)?

- highly oscillatory Hamiltonian systems
- Hamiltonian PDEs: $h\Omega = \text{CFL number, typically } \approx 1$
Outline

Hamiltonian systems of ordinary differential equations

Hamiltonian systems with multiple time scales

Hamiltonian partial differential equations

Dynamical low-rank approximation

Quantum dynamics
Example: Time scales in a nonlinear oscillator chain

Figure 3.1. Chain of alternating stiff harmonic and soft anharmonic springs.

The coupling potential $U$ is assumed smooth with derivatives bounded independently of the small parameter $\varepsilon$. On eliminating the momenta $p_j = \dot{q}_j$, the Hamilton equations become the system of second-order differential equations

$$\ddot{q}_j + \frac{\omega_j^2}{\varepsilon^2} q_j = r_j U(q), \quad j = 0, \ldots, m,$$

where $r_j$ denotes the gradient with respect to $q_j$, and where $\omega_0 = 0$. We are interested in the behaviour of the system for initial values with an oscillatory energy that is bounded independently of $\varepsilon$:

$$H^!(p(0), q(0)) \leq \text{Const}.$$
Highly oscillatory Hamiltonian systems

\[ H(p, q) = H_\omega(p, q) + H_{\text{slow}}(p, q), \]

where the oscillatory and slow-motion energies are given by

\[ H_\omega(p, q) = \sum_{j=1}^{m} \frac{1}{2} \left( |p_j|^2 + \omega_j^2 |q_j|^2 \right), \quad H_{\text{slow}}(p, q) = \frac{1}{2} |p_0|^2 + U(q) \]

for \( p = (p_0, p_1, \ldots, p_m) \) and \( q = (q_0, q_1, \ldots, q_m) \),

with high frequencies

\[ \omega_j \geq \varepsilon^{-1}, \quad 0 < \varepsilon \ll 1. \]
Example: Time scales in a nonlinear oscillator chain

Here we consider a related class of oscillatory Hamiltonian systems for which the long-time behaviour is by now quite well understood analytically both for the continuous problem and its numerical discretizations, and which show interesting behaviour on several time scales. The considered multiscale Hamiltonian systems couple high-frequency harmonic oscillators with a Hamiltonian of slow motion. An illustrative example of such a Hamiltonian is provided by a Fermi–Pasta–Ulam type system of point masses interconnected by stiff harmonic and soft anharmonic springs, as shown in Figure 3.1; see [GGMV92] and [HLW06, Section I.5].

The general setting is as follows: For positions $q = (q_0, q_1, \ldots, q_m)$ and momenta $p = (p_0, p_1, \ldots, p_m)$ with $p_j$, $q_j$ $\in \mathbb{R}^d$, let the Hamilton function be given by

$$H(p, q) = H^! (p, q) + H_{\text{slow}} (p, q),$$

where the oscillatory and slow-motion energies are given by

$$H^! (p, q) = \frac{1}{2} \sum_{j=1}^m (|p_j|^2 + |q_j|^2),
$$

$$H_{\text{slow}} (p, q) = \frac{1}{2} |p_0|^2 + U(q),$$

with high frequencies $\omega_j$.

The coupling potential $U$ is assumed smooth with derivatives bounded independently of the small parameter $\varepsilon$. On eliminating the momenta $p_j = \dot{q}_j$, the Hamilton equations become the system of second-order differential equations

$$\ddot{q}_j + \omega_j^2 q_j = r_j U(q), j = 0, \ldots, m,$$

where $r_j$ denotes the gradient with respect to $q_j$, and where $\omega_0 = 0$. We are interested in the behaviour of the system for initial values with an oscillatory energy that is bounded independently of $\varepsilon$:

$$H^! (p(0), q(0)) \leq \text{Const}.$$

This system shows different behaviour on different time scales:

1. Almost-harmonic motion of the fast variables $(p_j, q_j)$ ($j \neq 0$) on timescale $\varepsilon$;
2. Motion of the slow variables $(p_0, q_0)$ on timescale $\varepsilon^0$;
3. Energy exchange between the harmonic oscillators with the same frequency on the timescale $\varepsilon$;
4. Energy exchange between the harmonic oscillators corresponding to frequencies in 1:2 or 1:3 resonance on the timescales $\varepsilon^2$ or $\varepsilon^3$, respectively;
5. Near-preservation of the $j$th oscillatory energy $E_j = \frac{1}{2} (|p_j|^2 + |q_j|^2)$ for non-resonant frequency $\omega_j$ beyond the timescale $\varepsilon^N$ for arbitrary $N$. 


Long-time behaviour: theory

Two different approaches:

(NF) Canonical coordinate transformations of Hamiltonian perturbation theory to a normal form, from which long-time behaviour can be read off (e.g. Benettin & Giorgilli 1989).

(MFE) Modulated Fourier expansions in time: embed the original system in a high-dimensional system of modulation equations which has a Lagrangian/Hamiltonian structure with invariance properties (Hairer & L. since 2000, with Cohen and Gauckler).

MFE approach transfers to numerical discretizations.
Modulated Fourier expansion

Technique for analysing weakly nonlinear systems over long times:

- **Solution approximation over short time (MFE)**

\[ q_j(t) \approx \sum_k z_j^k(t) e^{i(k \cdot \omega)t} \]

with slowly varying modulation functions \( z_j^k \)

- **Lagrange structure and invariance properties** of the modulation system: then use Noether’s theorem (1918)

→ long-time results on energy and adiabatic invariants for continuous and discrete weakly nonlinear oscillatory systems
“This report is intended to be the first one in a series dealing with the behavior of certain nonlinear physical systems where the non-linearity is introduced as a perturbation to a primarily linear problem. The behavior of the systems is to be studied for times which are long compared to the characteristic periods of the corresponding linear problem.”

Fermi, Pasta & Ulam 1955

... which is just what modulated Fourier expansions are good for.
Outline

Hamiltonian systems of ordinary differential equations

Hamiltonian systems with multiple time scales

Hamiltonian partial differential equations

Dynamical low-rank approximation

Quantum dynamics
What are their benefits?

What about long-time near-conservation of energy?

Obstructions:

- Backward analysis does not work for CFL numbers near 1.
- Even for small CFL numbers, the numerical method will nearly preserve the Hamilton function of the spatially discretized system, not that of the PDE.

Nevertheless...
Mode energies in a nonlinear wave equation \( u_{tt} - u_{xx} + \frac{1}{2} u = u^2 \) with periodic b.c., only first Fourier mode excited initially

Stability of plane waves under nonlinear perturbations?

can be rigorously explained using modulated Fourier expansions. Gauckler, Hairer, L. & Weiss 2012, Gauckler & Weiss 2017
Some further results

Numerical long-time near-conservation of energy in the weakly nonlinear regime:

- nonlinearly perturbed wave equation in 1D
  Cohen, Hairer, L. 2008 via MFE
- nonlinear Schrödinger equation in 1D
  Faou 2011 via modified BEE, Gauckler 2016 via MFE
- NLS with a convolution potential in any dimension
  Gauckler & L. 2010 via MFE

Numerical orbital stability results for NLS:

- ground state: Bambusi, Faou & Grébert 2013 via mod. BEE
- plane waves: Faou, Gauckler & L. 2014 via MFE
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Low-rank approximation: data compression and model reduction

HUGE time-dependent matrices $A(t) \in \mathbb{R}^{m \times n}$, given explicitly or unknown solution of matrix ODE $\dot{A} = F(A)$

Approximate by low-rank matrices: use SVD-like decomposition

$$A(t) \approx Y(t) = U(t)S(t)V(t)^T,$$

where $U(t) \in \mathbb{R}^{m \times r}$, $V(t) \in \mathbb{R}^{n \times r}$ have orthonormal columns, $S(t) \in \mathbb{R}^{r \times r}$ is invertible.

$$\text{rank } r \ll m, n$$
Dynamical low-rank approximation

Low-rank manifold $\mathcal{M} = \{ Y \in \mathbb{R}^{m \times n} : \text{rank } Y = r \}$
Orthogonal projection onto the tangent space at $Y \in \mathcal{M}$: $P_Y$

Dynamical low-rank approximation: find $Y(t) \in \mathcal{M}$ from ODE

$$\dot{Y} = P_Y F(Y), \quad Y(0) \in \mathcal{M}.$$ 

Project the vector field onto the tangent space of the approximation manifold

Dirac 1930, quantum physics: time-dependent variational principle
\[ \dot{Y} = P_Y F(Y) \]
Small singular values: high curvature

\[ \dot{Y} = P_Y F(Y) \] yields ODEs for the factors of \( Y = USV^T \).

However, the ODEs for \( U, S, V \) are a pain to integrate numerically: they contain \( S^{-1} \) as factor, \( S \) is typically ill-conditioned.

**Geometric obstruction:** with \( \sigma_r = \) smallest nonzero singular value,

\[
\frac{1}{\sigma_r} \sim \text{curvature of } \mathcal{M} \text{ at } Y
\]

Is tangent space projection a reasonable approach for a manifold with high curvature?
Ruled surface
Split the tangent space projection, which at $Y = USV^\top$ is an alternating sum of three subprojections:

$$P_Y Z = ZVV^\top - UU^\top ZVV^\top + UU^\top Z.$$ 

Splitting integrator:

- updates the factorization $Y_n = U_n S_n V_n^\top$ from $n$ to $n + 1$.
- alternates between solving differential equations for slim matrices ($US$, $S$, $VS^\top$) and orthogonal decompositions.

---

L. & Oseledets 2014
Robustness to small singular values

The projector-splitting integrator
- reproduces rank-\(r\) matrices exactly.
- admits convergent error bounds that are independent of the singular values.

Why so robust?
In each substep of the algorithm, the approximation moves along a flat subspace of the manifold \(\mathcal{M}\) of rank-\(r\) matrices. In this way, the high curvature due to small singular values does no harm.

Kieri, L. & Walach 2016
Ruled surface
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Numerical approximation in quantum dynamics combines

- Hamiltonian PDEs and
- dynamical low-rank approximation of tensors and tensor networks

→ Hamiltonian PDEs on low-rank tensor manifolds
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