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 4. Modulated Fourier expansion

1. **Long-term energy preservation**
   - Construction of modulated Fourier expansion
   - Formal invariants
   - From short to long intervals
   - Several high frequencies

2. **One-dimensional wave equation**
   - Harmonic actions – long-term preservation
   - Pseudo-spectral semi-discretization
   - Full discretization
   - Long-term preservation of total energy and actions
   - Störmer–Verlet scheme – leapfrog method

Long-term energy preservation

In Lecture 3 we have seen that for highly oscillatory differential equations

$$\ddot{q} + \Omega^2 q = -\nabla U(q), \quad q = \begin{pmatrix} q_0 \\ q_1 \end{pmatrix}, \quad \Omega = \begin{pmatrix} 0 & 0 \\ 0 & \omega I \end{pmatrix}$$

we have:

for the analytic solution

- Hamiltonian $H(q, \dot{q})$ is exactly preserved (this is trivial)
- total oscillatory energy $I(q, \dot{q})$ is nearly preserved (adiabatic invariant)

for the numerical solution of exponential integrators

- Hamiltonian $H(q, \dot{q})$ is nearly preserved
- total oscillatory energy $I(q, \dot{q})$ is nearly preserved

Here, we present the idea of the proof of these statements
– using modulated Fourier expansions.

Motivation (exact solution)

Problem: $\ddot{x} + \omega^2 x = 0$

Solution: $x(t) = c_1 \mathrm{e}^{\mathrm{i}\omega t} + c_{-1} \mathrm{e}^{-\mathrm{i}\omega t}$

Problem: $\ddot{x} + \omega^2 x = -x$

Solution:
$$
\begin{aligned}
x(t) &= c_1 \mathrm{e}^{\mathrm{i}\sqrt{\omega^2+1}\, t} + c_{-1} \mathrm{e}^{-\mathrm{i}\sqrt{\omega^2+1}\, t} \\
&= \mathrm{e}^{\mathrm{i}\omega t} z^1(t) + \mathrm{e}^{-\mathrm{i}\omega t} z^{-1}(t) \\
z^1(t) &= c_1 \mathrm{e}^{\mathrm{i}\omega t\,(\sqrt{1+\omega^{-2}}-1)} = c_1 \mathrm{e}^{\mathrm{i}\,(\frac{1}{2\omega} + \mathcal{O}(\omega^{-3}))t}
\end{aligned}
$$

Problem: $\ddot{x} + \omega^2 x = g(x)$

Solution will contain terms $z^k(t)\,\mathrm{e}^{\mathrm{i}k\omega t}$ for $k \in \mathbb{Z}$ with slowly varying coefficient functions $z^k(t)$.

Sketch of the proof

for the exact solution of the highly oscillatory problem

$$\ddot{q} + \Omega^2 q = -\nabla U(q)$$

$$q(t) \approx \sum_{\mathbf{k}\in\mathbb{Z}} z^k(t)\,\mathrm{e}^{\mathrm{i}k\omega t}$$

for the numerical solution of a trigonometric integrator

$$q_{n+1} - 2\cos(h\Omega) q_n + q_{n-1} = \ldots$$

$$q_n \approx \sum_{k\in\mathbb{Z}} z^k(t)\,\mathrm{e}^{\mathrm{i}k\omega t}, \quad t = nh$$

Study of the near-preservation of the energy is in three steps:

Step 1 **Construction of the coefficient functions** as solution of a differential-algebraic system

Step 2 Find **formal invariants** of the system for the coefficient functions (close to total and oscillatory energies)

Step 3 **From short to long** time intervals concatenate estimates for short time intervals.

Step 1. Construction of the coefficient functions

Consider $\ddot{q} + \Omega^2 q = g(q) = -\nabla U(q)$ with $\Omega = \mathrm{diag}\,(0, \omega I)$ and put

$$q(t) = \begin{pmatrix} q_0(t) \\ q_1(t) \end{pmatrix} \approx \sum_{k \in \mathbb{Z}} \begin{pmatrix} z_0^k(t) \\ z_1^k(t) \end{pmatrix} \mathrm{e}^{\mathrm{i}k\omega t}$$

Inserting this ansatz into the ODE, expanding the nonlinearity into a Taylor series around $z^0(t)$, and comparing the terms with $\mathrm{e}^{\mathrm{i}k\omega t}$ yields

$$\ddot{z}_j^k + 2\mathrm{i}k\omega \dot{z}_j^k + \big(\omega_j^2 - (k\omega)^2\big) z_j^k = \sum_{s(\alpha)=k} \frac{1}{m!}\, g_j^{(m)}(z^0)(z^{\alpha_1}, \ldots, z^{\alpha_m})$$

Noting that $\omega_0 = 0$, $\omega_1 = \omega$, the dominant terms give rise to

$\ddot{z}_0^0(t) = \ldots$ second order differential equation
$\dot{z}_1^{\pm 1}(t) = \ldots$ first order differential equations
$z_j^k(t) = \ldots$ algebraic relations (for the remaining pairs (j, k))

Step 2. Formal invariant

We introduce functions $y^k(t) = z^k(t)\,\mathrm{e}^{\mathrm{i}k\omega t}$ such that

$$q(t) \approx \sum_{k\in\mathbb{Z}} z^k(t)\,\mathrm{e}^{\mathrm{i}k\omega t} = \sum_{k\in\mathbb{Z}} y^k(t)$$

For the functions constructed in step 1, we have (with $\mathbf{y} = (y^k)_{k\in\mathbb{Z}}$)

$$\ddot{y}^k + \Omega^2 y^k = -\nabla_{-k}\mathcal{U}(\mathbf{y})$$

where, for $g(q) = -\nabla U(q)$,

$$\mathcal{U}(\mathbf{y}) = U(y^0) + \sum_{m\geq 1}\frac{1}{m!}\sum_{\alpha_1+\ldots+\alpha_m=0} U^{(m)}(y^0)\big(y^{\alpha_1},\ldots,y^{\alpha_m}\big)$$

With $\mathbf{y}(\lambda) = (\mathrm{e}^{\mathrm{i}k\lambda}y^k)_{k\in\mathbb{Z}}$ the expression $\mathcal{U}\big(\mathbf{y}(\lambda)\big)$ is independent of λ, so that

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\Big|_{\lambda=0}\mathcal{U}\big(\mathbf{y}(\lambda)\big) = \sum_{k\in\mathbb{Z}} \mathrm{i}k(y^k)^\top\nabla_k\mathcal{U}(\mathbf{y}) = 0$$

Step 2. Formal invariant

With this preparation we define

$$\mathcal{I}(\mathbf{y},\dot{\mathbf{y}}) = -\mathrm{i}\omega \sum_{k\in\mathbb{Z}} k (y^{-k})^\top \dot{y}^k$$

and we compute (using $\ddot{y}^k + \Omega^2 y^k = -\nabla_{-k}\mathcal{U}(\mathbf{y})$)

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{I}(\mathbf{y},\dot{\mathbf{y}}) &= -\mathrm{i}\omega \sum_{k\in\mathbb{Z}} k \Big((y^{-k})^\top \ddot{y}^k + (\dot{y}^{-k})^\top \dot{y}^k \Big) \\ &= \ \ldots \ = \mathrm{i}\omega \sum_{k\in\mathbb{Z}} k (y^{-k})^\top \nabla_{-k}\mathcal{U}(\mathbf{y}) = 0\end{aligned}$$

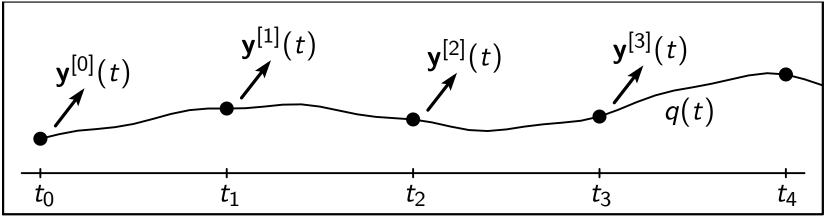
Theorem

Under the usual assumptions there exists a function $\mathcal{I}\big(\mathbf{y},\dot{\mathbf{y}}\big)$, *such that*

$$\begin{aligned}\mathcal{I}\big(\mathbf{y}(t),\dot{\mathbf{y}}(t)\big) &= \mathcal{I}\big(\mathbf{y}(0),\dot{\mathbf{y}}(0)\big) + \mathcal{O}(\omega^{-N}) \\ \mathcal{I}\big(\mathbf{y}(t),\dot{\mathbf{y}}(t)\big) &= I\big(q_1(t),\dot{q}_1(t)\big) + \mathcal{O}(\omega^{-1})\end{aligned}$$

Step 3. From short to long intervals

Consider a grid $0 = t_0 < t_1 < t_2 < \dots$ with $t_{m+1} - t_m = \mathcal{O}(1)$



On the interval $[t_m, t_{m+1}]$, consider the modulated Fourier expansion corresponding to initial values $q(t_m), \dot{q}(t_m)$, and denote the coefficient functions by $\mathbf{y}^{[m]}(t)$.

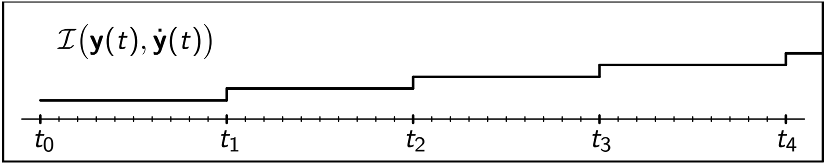
On the whole interval $t \geq 0$, consider $\mathbf{y}(t)$ defined by

$$\mathbf{y}(t) = \mathbf{y}^{[m]}(t) \quad \text{for} \quad t \in [t_m, t_{m+1}]$$

Note that $\mathbf{y}(t)$ has jump discontinuities of size $\mathcal{O}(\omega^{-N})$ at t_m.

Consequence. The invariant $\mathcal{I}\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big)$ has jump discontinuities of size $\mathcal{O}(\omega^{-N})$ at t_m.

Step 3. From short to long intervals



The near invariant $\mathcal{I}\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big)$ has

- jump discontinuities of size $\mathcal{O}(\omega^{-N})$ at t_m,
- slope of size $\mathcal{O}(\omega^{-N})$ in between.

This implies that

$$\big|\mathcal{I}\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big) - \mathcal{I}\big(\mathbf{y}(0), \dot{\mathbf{y}}(0)\big)\big| \le C\, t\, \omega^{-N}$$

Since $\mathcal{I}\big(\mathbf{y}(t), \dot{\mathbf{y}}(t)\big)$ is close to $I\big(q_1(t), \dot{q}_1(t)\big)$, this proves that

$$I\big(q_1(t), \dot{q}_1(t)\big) = I\big(q_1(0), \dot{q}_1(0)\big) + \mathcal{O}(\omega^{-1}) + \mathcal{O}(t\, \omega^{-N})$$

Extensions

- **several high frequencies**
  resonant frequencies
- **infinitely many high frequencies**
  semi-linear wave equation, Schrödinger equation
- **one state-dependent high frequency**
  semi-linear wave equation with slowly varying wave speed;
  charged particle dynamics in a non-constant strong magnetic field

Contributors (2000 – 2018):

Ch. Lubich, E. H., D. Cohen, L. Gauckler, D. Weiss, ...

Several high frequencies

We consider the problem $\ddot{q} + \Omega^2 q = -\nabla U(q)$ where

$$q = \begin{pmatrix} q_0 \\ q_1 \\ \vdots \\ q_\ell \end{pmatrix} \qquad \Omega = \begin{pmatrix} 0 & & & \\ & \omega_1 & & \\ & & \ddots & \\ & & & \omega_\ell \end{pmatrix}$$

It is Hamiltonian with $(\omega_0 = 0)$

$$H(q, \dot{q}) = \frac{1}{2} \sum_{j=0}^{\ell} \Big(\|\dot{q}_j\|^2 + \omega_j^2 \|q_j\|^2 \Big) + U(q)$$

We assume that the ω_j are well separated, i.e.,

$$\omega_j = \frac{\lambda_j}{\varepsilon}, \qquad 0 < \lambda_1 < \lambda_2 < \ldots < \lambda_\ell, \quad 0 < \varepsilon \ll 1$$

Modulated Fourier expansion: what is different?

ω is a vector, and k becomes a multi-index:

$$q(t) = \sum_{k\in\mathcal{N}} e^{\mathrm{i}\,k\cdot\omega\, t} z^k(t)$$

where $\quad k\cdot\omega = k_1\omega_1 + \ldots + k_\ell\omega_\ell .$

The functions $e^{\mathrm{i}\,k\cdot\omega\, t}$ are not always independent.

Resonance module:

$$\mathcal{M} := \{ k \in \mathbb{Z}^\ell \,;\; k_1\lambda_1 + \ldots + k_\ell\lambda_\ell = 0 \}$$

From every equivalence class $[k] := k + \mathcal{M}$ we choose a representative such that $|k| = |k_1| + \ldots + |k_\ell|$ is minimal.
The set of these representatives is denoted by $\mathcal{N}$,

$$\mathcal{N} = \mathbb{Z}^\ell / \mathcal{M}$$

The proof of the long-time behaviour is the same, but more technical.

Lecture 5. Highly oscillatory systems

1. **Long-term energy preservation**
   - Construction of modulated Fourier expansion
   - Formal invariants
   - From short to long intervals
   - Several high frequencies

2. **One-dimensional wave equation**
   - Harmonic actions – long-term preservation
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One-dimensional wave equation

We consider

$$\partial_t^2 u - \partial_x^2 u + \rho\, u + g(u) = 0$$

Domain: $-\pi \le x \le \pi$ and $t \ge 0$

Nonlinearity: smooth and $g(0) = g'(0) = 0$

Boundary conditions: periodic

Initial data: small in the Sobolev norm

$$\Big(\big\| u(\cdot,0) \big\|_{s+1}^2 + \big\| \partial_t u(\cdot,0) \big\|_s^2 \Big)^{1/2} \le \varepsilon$$

Exactly conserved quantities

Total energy (potential $U(u) = \int g(u)\, du$)

$$H(t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \Big(\tfrac{1}{2} \Big((\partial_t u)^2 + (\partial_x u)^2 + \rho\, u^2 \Big) + U(u) \Big)\, dx$$

Momentum

$$K(t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \partial_x u \; \partial_t u \, dx$$

Aim of the talk

discuss the long-time conservation of energy and momentum by numerical discretizations

Harmonic actions

In terms of the Fourier coefficients

$$u(x,t) = \sum_{j=-\infty}^{\infty} u_j(t) e^{\mathrm{i}jx}, \quad \partial_t u(x,t) = \sum_{j=-\infty}^{\infty} v_j(t) e^{\mathrm{i}jx}$$

the wave equation becomes with $\omega_j = \sqrt{j^2 + \rho}$

$$\partial_t^2 u_j + \omega_j^2 u_j + \mathcal{F}_j g(u) = 0 \qquad \text{for} \quad j \in \mathbb{Z}$$

Harmonic actions

$$I_j(t) = \frac{\omega_j}{2} |u_j(t)|^2 + \frac{1}{2\omega_j} |v_j(t)|^2$$

Preservation properties for the exact solution

Total energy and **momentum** are exactly conserved.

Harmonic actions $I_j(t) = \frac{\omega_j}{2}|u_j(t)|^2 + \frac{1}{2\omega_j}|v_j(t)|^2$

Assumptions:

a) Non-resonance condition of the form: for given N and $\varepsilon > 0$ there exists $\sigma > 0$ such that $(\cdots) \le C\varepsilon^N$

b) Initial data: $\big\|u(\cdot,0)\big\|_{s+1}^2 + \big\|\partial_t u(\cdot,0)\big\|_s^2 \le \varepsilon^2$

$$\|v\|_s = \Big(\sum_{j=-\infty}^{\infty} \omega_j^{2s}|v_j|^2\Big)^{1/2}$$

Bambusi (2003) shows that the non-resonance condition is satisfied for almost all ρ satisfying $0 < \rho_0 \le \rho \le \rho_1$.

Theorem (A)

Under the above assumptions, for $s \geq \sigma + 1$,

$$\sum_{\ell=0}^{\infty} \omega_\ell^{2s+1} \frac{|I_\ell(t) - I_\ell(0)|}{\varepsilon^2} \leq C\,\varepsilon \quad \text{for} \quad 0 \leq t \leq \varepsilon^{-N+1}$$

This is closely related to results by
Bambusi (2003) and by Bourgain (1996).

Corollary (spatial regularity)

For $t \leq \varepsilon^{-N+1}$, *we have*

$$\big\|u(\cdot,t)\big\|_{s+1}^2 + \big\|\partial_t u(\cdot,t)\big\|_s^2 \leq \varepsilon^2(1 + C\varepsilon)$$

Example

$$\partial_t^2 u - \partial_x^2 u + \rho\, u + g(u) = 0$$

Equation: $\rho = 0.5$ and $g(u) = -u^2$

Boundary conditions: periodic

Initial data: $\varepsilon = 0.1$

$$u(x,0) = \Big(\frac{x}{\pi} - 1\Big)^3 \Big(\frac{x}{\pi} + 1\Big)^2 \varepsilon$$

$$\partial_t u(x,0) = 0.1 \cdot \frac{x}{\pi}\Big(\frac{x}{\pi} - 1\Big)\Big(\frac{x}{\pi} + 1\Big)^2 \varepsilon$$

which are in H^{s+1} and H^s, respectively, for $s < 2$.

Total energy : bold black line

Harmonic actions: alternatively in blue and red

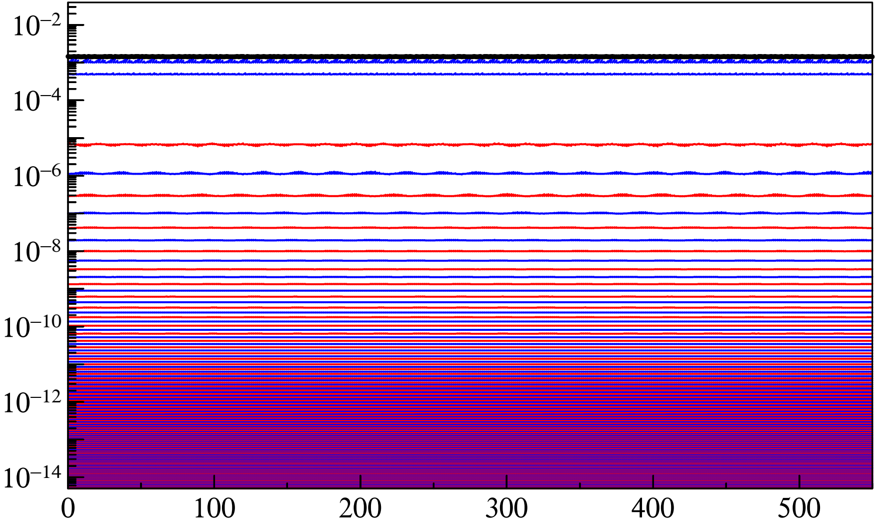
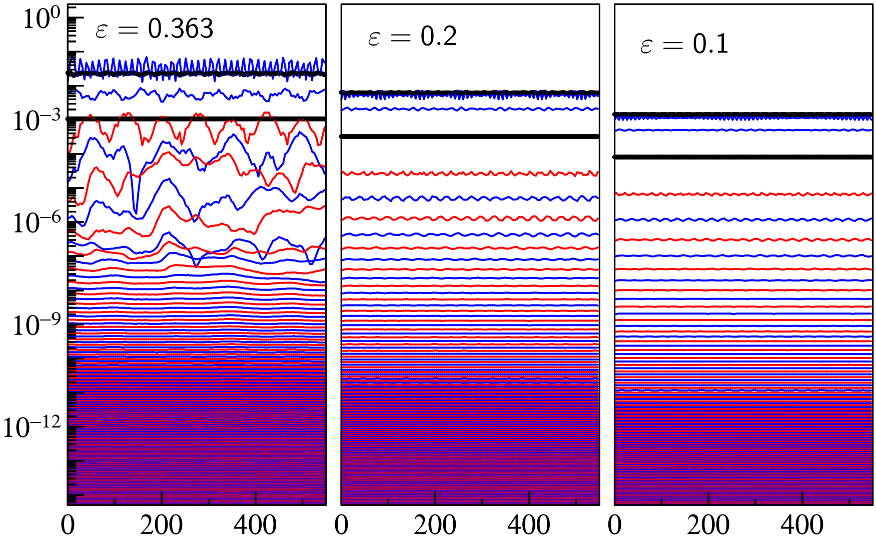


Illustration of the condition on initial data

Blow-up for $\varepsilon \geq 0.364$



Pseudo-spectral semi-discretization

We consider equidistant collocation points in space

$$x_k = k\pi/M \quad \text{for} \quad k = -M, \ldots, M-1$$

and an approximation by the trigonometric polynomial

$$u^M(x,t) = \sum_{|j|\le M}{}' q_j(t)\mathrm{e}^{\mathrm{i}jx}$$

The $2M$-periodic sequence $q = (q_j)$ satisfies

$$\frac{d^2 q_j}{dt^2} + \omega_j^2 q_j = f_j(q) \qquad \text{with} \qquad f(q) = -\mathcal{F}_{2M}\, g(\mathcal{F}_{2M}^{-1} q)$$

where $\mathcal{F}_{2M}$ stands for the discrete Fourier transform

$$\big(\mathcal{F}_{2M} w\big)_j = \frac{1}{2M} \sum_{k=-M}^{M-1} w_k \mathrm{e}^{-\mathrm{i}jx_k}, \qquad \big(\mathcal{F}_{2M}^{-1} q\big)_k = \sum_{l=-M}^{M-1} q_l \mathrm{e}^{\mathrm{i}kx_l}$$

Hamiltonian structure of the semi-discretization

Pseudo-spectral discretization is an ODE with Hamiltonian

$$
\begin{aligned}
H_M(p,q) &= \frac{1}{2}\sum_{|j|\le M}{}' \Big(|p_j|^2 + \omega_j^2 |q_j|^2 \Big) + V(q) \\
V(q) &= \frac{1}{2M}\sum_{k=-M}^{M-1} U\big((\mathcal{F}_{2M}^{-1} q)_k \big)
\end{aligned}
$$

which is exactly preserved by the semi-discrete solution.

Comments.

- Total energy of the wave equation is not exactly preserved.
- The momentum of the wave equation $K(p,q) = -\sum_{|j|\le M}{}'' i\, j\, q_{-j} p_j$ is no longer exactly preserved.
- We consider the harmonic actions $I_j(p,q) = \frac{\omega_j}{2}\, |q_j|^2 + \frac{1}{2\omega_j}\, |p_j|^2$

Theorem (B)

Under the assumptions of Theorem (A) we have, for $0 \le t \le \varepsilon^{-N+1}$,

$$\sum_{\ell=0}^{M} \omega_\ell^{2s+1} \frac{|I_\ell(t) - I_\ell(0)|}{\varepsilon^2} \le C\,\varepsilon$$

$$\frac{|H(t) - H(0)|}{\varepsilon^2} \le C\,\varepsilon\, M^{-s-1}$$

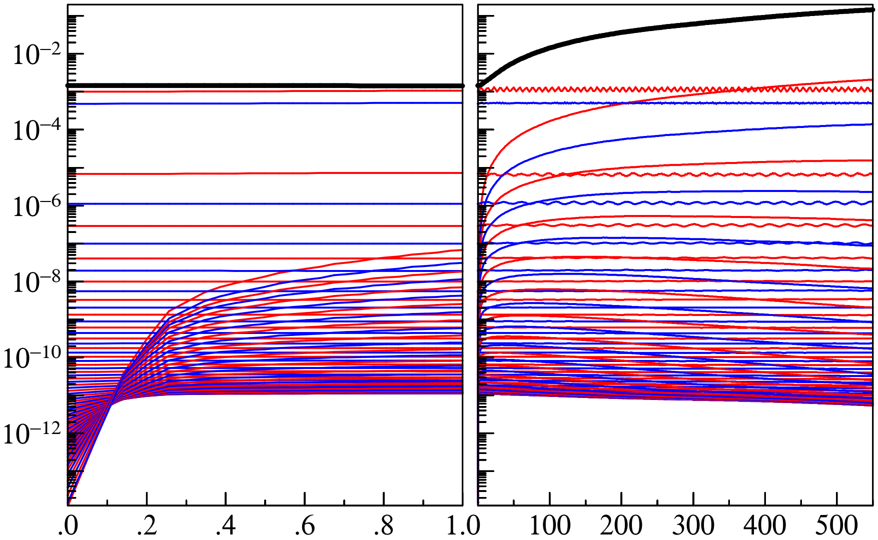
$$\frac{|K(t) - K(0)|}{\varepsilon^2} \le C\,t\,\varepsilon\, M^{-s-1}$$

The first estimate implies long-time regularity of the solution of the semi-discretization

$$\left\| u^M(\cdot, t) \right\|_{s+1}^2 + \left\| v^M(\cdot, t) \right\|_s^2 \le \varepsilon^2 (1 + C\varepsilon)$$

Explicit Runge-Kutta method (DOPRI5), $2M = 2^7$

$Atol = 10^{-5}$, $Rtol = 10^{-4}$, 32 735 accepted steps



Full discretization (trigonometric integrator)

To the semi-discretized system $\frac{d^2q}{dt^2} + \Omega^2 q = f(q)$ we apply

$$q^{n+1} - 2\cos(h\Omega)\, q^n + q^{n-1} = h^2\, \Psi\, f(\Phi q^n)$$

where $\Psi = \psi(h\Omega)$ and $\Phi = \phi(h\Omega)$. The filter functions are assumed to satisfy the symplecticty condition

$$\psi(\xi) = \mathrm{sinc}\,(\xi)\, \phi(\xi)$$

The velocity approximation p^n is given by

$$2h\, \mathrm{sinc}\,(h\Omega)\, p^n = q^{n+1} - q^{n-1}$$

Aim: explain the long-time behaviour of this method

Assumptions for long-term energy preservation

a) Non-resonance condition of the form: for given N and $\varepsilon > 0$ there exists $\sigma > 0$ such that $(\cdots) \leq C\varepsilon^N$. This is stronger than in the analytic case.

b) Numerical non-resonance condition

$$|\sin(h\omega_j)| \geq h\varepsilon^{1/2} \quad \text{for} \quad |j| \leq M$$

c) Symplecticity condition

$$\psi(\xi) = \mathrm{sinc}\,(\xi)\,\varphi(\xi)$$

d) Small initial data:

$$\|q(0)\|_{s+1}^2 + \|p(0)\|_s^2 \leq \varepsilon^2, \quad s \geq \sigma + 1$$

Theorem (C)

Under the above assumptions we have for the trigonometric integrator, on an interval of length $0 \le t_n = nh \le \varepsilon^{-N+1}$,

$$\sum_{\ell=0}^{M} \omega_\ell^{2s+1} \frac{|I_\ell(p^n,q^n) - I_\ell(p^0,q^0)|}{\varepsilon^2} \le C\,\varepsilon$$

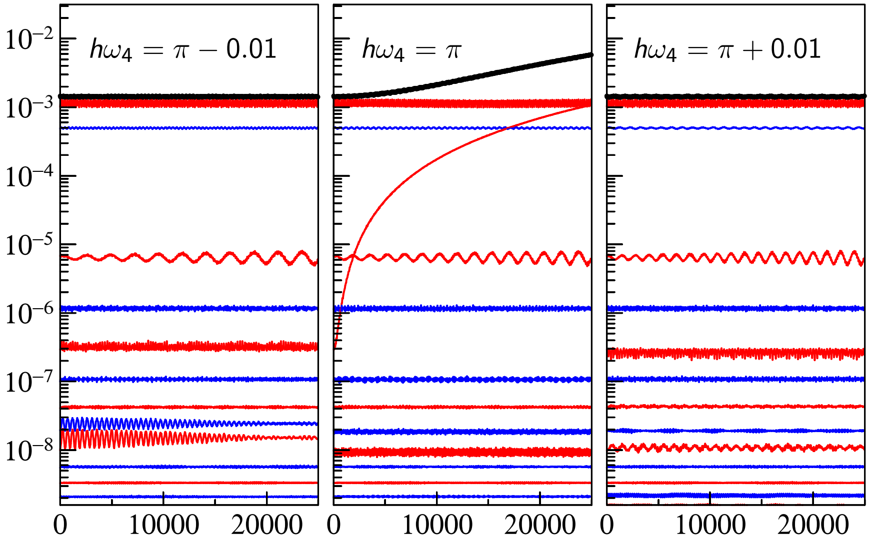
$$\frac{|H_M(p^n,q^n) - H_M(p^0,q^0)|}{\varepsilon^2} \le C\,\varepsilon$$

$$\frac{|K(p^n,q^n) - K(p^0,q^0)|}{\varepsilon^2} \le C(\varepsilon + M^{-s} + t\,\varepsilon\, M^{-s+1})$$

The first estimate implies boundedness over long times of the numerical solution (full discretization)

$$\|q^n\|_{s+1}^2 + \|p^n\|_s^2 \le \varepsilon^2(1 + C\varepsilon)$$

Numerical non-resonance condition, $\psi = \mathrm{sinc}\,,\ \phi = 1$



Störmer–Verlet as trigonometric integrator

For $\ddot{q} + \Omega^2 q = g(q)$ we consider the **Störmer–Verlet method**

$$\begin{aligned} q^{n+1} - 2q^n + q^{n-1} &= -(h\Omega)^2 q^n + h^2 g(q^n) \\ q^{n+1} - q^{n-1} &= 2h\, p^n \end{aligned}$$

and write it as **trigonometric integrator**

$$\begin{aligned} \widetilde{q}^{\,n+1} - 2\cos(h\widetilde{\Omega})\,\widetilde{q}^{\,n} + \widetilde{q}^{\,n-1} &= h^2 \Psi g(\Phi \widetilde{q}^{\,n}) \\ \widetilde{q}^{\,n+1} - \widetilde{q}^{\,n-1} &= 2h\,\mathrm{sinc}\,(h\widetilde{\Omega})\,\widetilde{p}^{\,n} \end{aligned}$$

where $\Psi = \psi(h\widetilde{\Omega})$, $\Phi = \phi(h\widetilde{\Omega})$ with $\psi = \mathrm{sinc}\,$, $\phi = 1$, and

$$I - \frac{1}{2}(h\Omega)^2 = \cos(h\widetilde{\Omega}) \quad \text{or equiv.} \quad \sin\Big(\frac{h\widetilde{\Omega}}{2}\Big) = \frac{h\Omega}{2}$$

$$\widetilde{q}^{\,n} = \mathrm{sinc}\,(h\widetilde{\Omega})\, q^n \quad \text{and} \quad \widetilde{p}^{\,n} = p^n$$

Application of results for exponential integrators

- analytical non-resonance condition for $\widetilde{\omega}_j$
- numerical non-resonance condition OK: $h\omega_M < 2$
- symplecticity condition OK: $\psi = \mathrm{sinc}\,,\ \phi = 1$
- smallness of initial data

We have for example

$$\sum_{\ell=0}^{\infty} \widetilde{\omega}_\ell^{2s+1}\, \frac{|\widetilde{I}_\ell(p^n,q^n) - \widetilde{I}_\ell(p^0,q^0)|}{\varepsilon^2} \le C\,\varepsilon$$

where $\quad \widetilde{I}_\ell(p^n,q^n) = \dfrac{\widetilde{\omega}_\ell}{2}\,\mathrm{sinc}^{\,2}(h\widetilde{\omega}_\ell)\,|q_\ell^n|^2 + \dfrac{1}{2\widetilde{\omega}_\ell}\,|p_\ell^n|^2$

Since

$$\widetilde{I}_\ell(p^n, q^n) = \frac{\omega_\ell}{\widetilde{\omega}_\ell}\Big(I_\ell(p^n, q^n) - \gamma(h\omega_\ell)\frac{\omega_\ell}{2}|q_\ell|^2\Big)$$

with $\gamma(h\omega) = \dfrac{(h\omega)^2}{4} < 1$ we have:

Theorem (Störmer–Verlet)

Under the above assumptions we have for the Störmer–Verlet integrator, on an interval of length $0 \le t_n = nh \le \varepsilon^{-N+1}$,

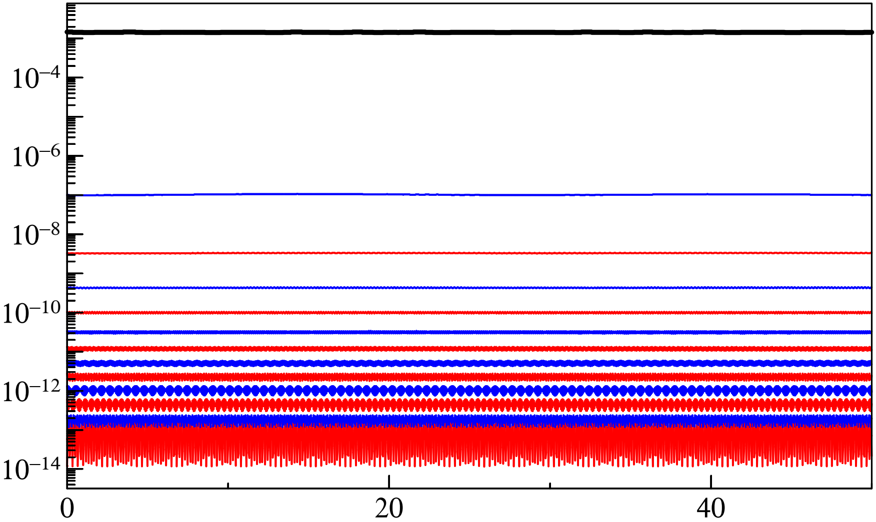
$$\sum_{\ell=0}^{\infty} \omega_\ell^{2s-1} \frac{|I_\ell(p^n, q^n) - I_\ell(p^0, q^0)|}{\varepsilon^2} \le C\,(\varepsilon + h^2)$$

$$\frac{|H_M(p^n, q^n) - H_M(p^0, q^0)|}{\varepsilon^2} \le C\,(\varepsilon + h^2)$$

$$\frac{|K(p^n, q^n) - K(p^0, q^0)|}{\varepsilon^2} \le C(\varepsilon + h^2 + M^{-s} + t\,\varepsilon\, M^{-s+1})$$

Illustration: CFL number ≈ 1.92

every fifth harmonic action is drawn



References

for analytical solution

Long-time analysis of nonlinearly perturbed wave equations via modulated Fourier expansions.
Arch. Ration. Mech. Anal. 187 (2008) 341–368

for pseudo-spectral semi-discretization

Spectral semi-discretizations of weakly nonlinear wave equations over long times.
Found. Comput. Math. 8 (2008) 319–334

for full discretization

Conservation of energy, momentum and actions in numerical discretizations of nonlinear wave equations.
Numerische Mathematik 110 (2008) 113–143