Backward error analysis for splitting methods applied to Hamiltonian PDEs.

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A first example

Focusing Schrödinger equation on $\mathbb{R}$

$$i\partial_t u(x,t) = -\Delta u(x,t) - |u(x,t)|^2 u(x,t)$$

- $\Delta = \partial_x^2$.
- Preservation of the L^2 norm $\|u(t)\|_{L^2}^2 = \|u(0)\|_{L^2}^2$.
- Preservation of the energy

$$H(u) = \int_{\mathbb{R}} |\partial_x u(x)|^2 - \frac{1}{2}|u(x)|^4 \mathrm{d}x = T(u) + P(u)$$

- Splitting schemes : For small τ,

$$\phi_H^\tau = \phi_{T+P}^\tau \simeq \phi_T^\tau \circ \phi_P^\tau, \quad \Longrightarrow \phi_H^{n\tau}(u^0) \simeq \left(\phi_T^\tau \circ \phi_P^\tau\right)^n(u^0).$$

Solitary waves

$$i\partial_t u(t,x) = -\partial_{xx} u(t,x) - |u(t,x)|^2 u(t,x), \quad u(0,x) = u^0(x), \quad x \in \mathbb{R}.$$

- Family of solutions (solitary waves)

$$u(t,x) = \rho(x-ct-x_0)\exp(i(\frac{1}{2}c(x-ct-x_0)+\theta_0))\exp(i(a+\frac{1}{4}c^2)t)$$

a, c, x_0 and θ_0 are real parameters,

$$\rho(x) = \frac{\sqrt{2a}}{\cosh(\sqrt{a}x)}.$$

- Stable solitons (orbital stability)
- Very particular solution :

$$u(t,x) = \frac{\sqrt{2}e^{it}}{\cosh(x)}.$$

Solitary waves

- Space discretization : large window $[-\pi/L, \pi/L]$ (L small). Fourier pseudo spectral methods with K equidistant points.
- First case : Explicit splitting method.

$$\phi_H^\tau = \phi_{T+P}^\tau \simeq \phi_T^\tau \circ \phi_P^\tau$$

- $K = 256$, $L = 0.11$. Courant-Friedrichs-Lewy number :

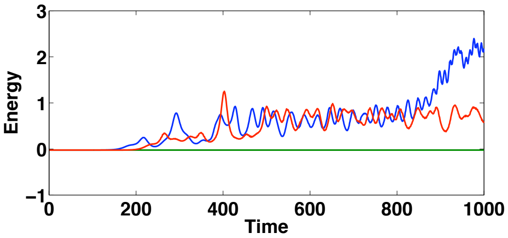
$$\mathrm{cfl} = \tau L^2 \left(\frac{K}{2}\right)^2.$$

  - $\tau = 0.1$ (cfl $= 19.8$),
  - $\tau = 0.05$ (cfl $= 9.9$),
  - $\tau = 0.01$ (cfl $= 1.9$).

Solitary waves

Evolution of the energy

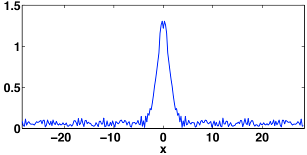
$$H(u,\bar{u}) = \int_{\mathbb{R}} |\partial_x u(x)|^2 - \frac{1}{2}|u(x)|^4 \mathrm{d}x$$

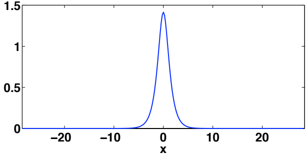


- $\tau = 0.1$ (cfl $= 19.8$) : Energy drift
- $\tau = 0.05$ (cfl $= 9.9$) : Energy drift
- $\tau = 0.01$ (cfl $= 1.9$) : No drift.

Solitary waves

Profile of the solution : $|u^n(x)|$

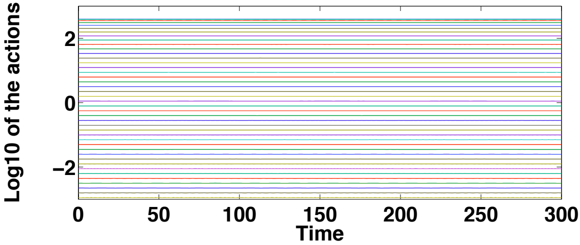




- cfl $= 19.8$ at time $t = 300$ (left)
- cfl $= 1.9$ at time $t = 10000$ (right)

Solitary waves

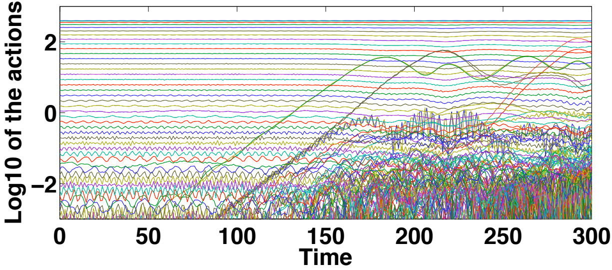
Plot of the Fourier coefficients $|\hat{u}_k(t)|^2$ for $k \in \mathbb{Z}$ in log scale.



First case : cfl $= 1.9$

Solitary waves

Plot of the Fourier coefficients $|\hat{u}_k(t)|^2$ for $k \in \mathbb{Z}$ in log scale.



Second case : cfl $= 19.8$. Leak of energy in the high modes.

Solitary waves

Same computation with the implicit-explicit integrator :

$$\phi_H^\tau = \phi_{T+P}^\tau \simeq R(i\tau\Delta) \circ \phi_P^\tau$$

with

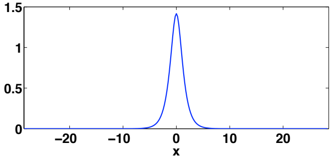
$$R(i\tau\Delta) = \frac{1 + i\tau\Delta/2}{1 - i\tau\Delta/2}$$

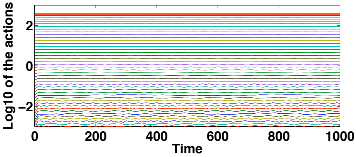
Midpoint rule applied to the free Schrödinger equation

$$i\partial_t u = -\Delta u \quad \Longrightarrow u^{n+1} = u^n + i\tau\Delta\left(\frac{u^{n+1} + u^n}{2}\right)$$

We use cfl $= 19.8$.

Solitary waves





No energy drift, preservation of the regularity, even with cfl $= 19.8$.

How to explain this ?

Backward error analysis : principles

Schrödinger systems :

$$\partial_t u = iAu + iBu$$

- A and B real operators
  (possibly unbounded, possibly nonlinear)
- Exact flow : $u(t) = \exp(it(A+B))u^0$
- Splitting methods

$$u^1 = \exp(i\tau A) \circ \exp(i\tau B)u^0 = u(\tau) + \mathcal{O}(\tau^2)$$

Global order 1, preservation of the L^2 norm

Backward error analysis : principles

Schrödinger systems :

$$\partial_t u = iAu + iBu$$

Baker-Campbell-Haussdorf formula

$$\exp(i\tau A) \circ \exp(i\tau B) = \exp(iZ(\tau))$$

$$Z(\tau) = \tau(A+B) + \tfrac{1}{2} i\tau^2 [A, B] + \cdots$$

- $[A, B] = AB - BA =: \mathrm{ad}_A(B)$
- Convergence of the series for $\tau(\|A\| + \|B\|) < 2\pi$.

Backward error analysis : principles

Nonlinear Hamiltonian systems $\dot{y} = J^{-1}\nabla H(y)$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

- $H = H_1 + H_2$. Numerical method : $\Phi^\tau = \phi^\tau_{H_1} \circ \phi^\tau_{H_2}$.
- In this situation

$$\begin{aligned} \Phi^\tau &= \exp(\tau \mathcal{L}_{H_1}) \circ \exp(\tau \mathcal{L}_{H_2}) \\ &= \exp(\tau \mathcal{L}_{H_\tau}) + \text{very small} \end{aligned}$$

with $H_\tau = H_1 + H_2 + \frac{1}{2}\tau\{H_1, H_2\} + \cdots$

- Analytic estimates : After a truncation at the order N, we have

$$\text{very small} = (C\tau N)^N \quad \text{over a compact} \quad K$$

Benettin & Giorgilli [94], Hairer & Lubich [97], Reich [99], ...
Exponential estimates on bounded set of $\mathbb{R}^n$.

New approach of BEA

$$\partial_t u = iAu + iBu$$

- Problem : $A = -\Delta$ is not bounded.
- Linear case : the BCH does not converge
- Nonlinear case : estimate in a Banach space under assumptions on a much smaller space.

$$\|\phi^{\tau}_{H_1} \circ \phi^{\tau}_{H_2}(y) - \phi^{\tau}_{H_\tau}(y)\|_{L_2} = \mathcal{O}(\tau^N C(\|y\|_{H^{2N}})).$$

A priori bound of the numerical solution in all the H^s.
Not true in general.

New approach of BEA

$$\exp(i\tau A) \circ \exp(i\tau B) = \exp(iZ_0) \circ \exp(i\tau B) = \exp(iZ(\tau))??$$

- $Z_0 = \tau A = \mathrm{diag}(\lambda_k)$ bounded but not small.
- Explicit integrators : $\lambda_k = \tau |k|^2$ in Fourier.
- implicit-explicit integrators : $\lambda_k = 2\arctan(h|k|^2/2)$

$$\frac{1+ix}{1-ix} = \exp(2i\arctan(x)).$$

$$R(-i\tau\Delta) = \frac{1 - i\tau\Delta/2}{1 + i\tau\Delta/2} = \exp(2i\arctan(-\tau\Delta/2)) =: \exp(iZ_0).$$

New approach of BEA

Find $Z(t)$ such that

$$\forall\, t \in [0,\tau], \quad \exp(iZ_0)\circ\exp(itB) = \exp(iZ(t)), \quad Z(0) = Z_0.$$

Equation

$$Z'(t) = (\mathrm{d}\exp_{iZ(t)})^{-1}\exp(-iZ(t))B = \sum_{n\geq 0}\frac{B_n}{n!}\mathrm{ad}^n_{iZ(t)}(B).$$

- B_n Bernoulli numbers. $\displaystyle\sum_{n=0}^{\infty}\frac{B_n}{n!}x^n = \frac{x}{e^x-1}.$
- Expansion : $Z(t) = Z_0 + tZ_1 + \cdots$
- Second term :

$$Z_1 = \sum_{n\geq 0}\frac{B_n}{n!}i^k\mathrm{ad}^n_{Z_0}(B).$$

Nonlinear case : $\mathrm{ad}_H(K) = \{H,K\}$ (Hamiltonian).

Linear Schrödinger equation

$$\partial_t u(t,x) = -i\Delta u(t,x) + iV(x)u(t,x), \quad u(0,x) = u_0(x).$$

- $x \in \mathbb{T}^d$. In Fourier $A = -\Delta = \mathrm{diag}(|k|^2)$. $B = (\widehat{V}_{k-\ell})_{k,\ell\in\mathbb{Z}^d}$.
- $Z_0 = \mathrm{diag}(\lambda_k)$ with $\lambda_k = \tau|k|^2$ or $\lambda_k = 2\arctan(\tau|k|^2/2)$.

$$\begin{aligned} \left(\mathrm{ad}_{Z_0} W\right)_{k\ell} &= \left((Z_0)_{kk} - (Z_0)_{\ell\ell}\right) W_{k\ell}, \\ &= (\lambda_k - \lambda_\ell) W_{k\ell}. \end{aligned}$$

- $(Z_1)_{k\ell} = B_{k\ell} \frac{i(\lambda_k - \lambda_\ell)}{\exp(i(\lambda_k - \lambda_\ell)) - 1}$ well defined for $|\lambda_k - \lambda_\ell| < 2\pi$

Modified energy

Theorem (Debussche & Faou 2008)

For the implicit-explicit integrator, there exists a symmetric operator $S(\tau)$ such that for all $\tau \leq \tau_0$

$$R(-i\tau\Delta)\exp(i\tau V) = \exp(i\tau S(\tau))$$

Moreover

$$S(\tau) = \frac{2}{\tau}\arctan(-\tau\Delta/2) + \tilde{V}(\tau)$$

- $\tilde{V}(\tau)$ modified (bounded and smooth) potential
- $\langle u|S(\tau)|u\rangle$ invariant of the numerical scheme
- No residual term.
- Backward error analysis result.
- Same result for explicit splitting with CFL.

Modified energy

$$S(\tau) = \frac{2}{\tau}\arctan(-\tau\Delta/2) + \tilde{V}(\tau)$$

We have for the numerical solution u^n :

$$\langle u^n | S(\tau) | u^n \rangle = \langle u^0 | S(\tau) | u^0 \rangle$$

Corollary

for all n we have

$$\sum_{|k| \leq 1/\sqrt{\tau}} |k|^2 |u_k^n|^2 + \frac{1}{\tau} \sum_{|k| > 1/\sqrt{\tau}} |u_k^n|^2 \leq C_0 \|u^0\|_{H^1}^2 .$$

- Fully discrete system : aliasing problems
- Under CFL conditions : H^1 bounds of the solution independent on K.

Cubic nonlinear Schrödinger equation

$$i\partial_t u = -\Delta u + |u|^2 u = \frac{\partial H}{\partial \bar{u}}(u,\bar{u})$$

Wave function $u(t,x) \in \mathbb{C}$, $x \in \mathbb{T}$.

- Hamiltonian

$$H(u,\bar{u}) = \int_{\mathbb{T}} (|\nabla u|^2 + \frac{1}{2}|u|^4) \mathrm{d}x.$$

- Decomposition $u = \sum_{k\in\mathbb{Z}} u_k e^{ikx}$,

$$\begin{aligned} H(u,\bar{u}) &= T(u,\bar{u}) + P(u,\bar{u}) \\ &= \sum_{k\in\mathbb{Z}} |k|^2 \| u_k|^2 + \frac{1}{2} \sum_{k+m-\ell-j=0} u_k u_m \bar{u}_\ell \bar{u}_j. \end{aligned}$$

Cubic nonlinear Schrödinger equation

- Hamiltonian system : for all $k \in \mathbb{Z}$,

$$\dot{u}_k = -i|k|^2 u_k - i \sum_{k=k-\ell+m} u_k \bar{u}_\ell u_m.$$

- $A = -\Delta$, $B = P$ Polynomial Hamiltonian P

$$P = \frac{1}{2} \sum_{k+m-\ell-j=0} u_k u_m \bar{u}_\ell \bar{u}_j$$

Action of $Z_0 = \sum_k \lambda_k |u_k|^2$:

$$\{Z_0, u_k u_m \bar{u}_\ell \bar{u}_j\} = i\Omega_{km\ell j} u_k u_m \bar{u}_\ell \bar{u}_j$$

where

$$\Omega_{km\ell j} = \lambda_k + \lambda_m - \lambda_\ell - \lambda_j$$

Modified energy

First term :

$$Z_1 = \frac{1}{2} \sum_{k+m-\ell-j=0} \left(\frac{i\Omega_{km\ell j}}{e^{i\Omega_{km\ell j}} - 1} \right) u_k u_m \bar{u}_\ell \bar{u}_j$$

- Z_1 : Control of the small denominator at the order 4.
- Z_2 : defined similarly, but of degree 6.
- Construction of Z_n : $\lambda_k \leq \frac{2\pi}{n+1}$.
- In general : CFL condition $\tau|k|^2 \leq \frac{2\pi}{n+1}$ or $\tau|k|^2 \leq 2\tan(\frac{\pi}{n+1})$

Modified flow

Theorem (Faou & Grébert 2009)

There exists a polynomial Hamiltonian H_τ such that for all $u \in B_M = \{\, u \in \ell^1 \mid \|u\|_{\ell^1} \leq M \,\}$, we have

$$\|\phi_P^\tau \circ \phi_{Z_0}^1(u) - \phi_{H_\tau}^\tau(u)\|_{\ell^1} \leq \tau^{N+1}(CN)^N.$$

In general, N is given by the CFL condition. $\|u\|_{\ell^1} := \sum_{k\in\mathbb{Z}} |u_k|$.

$$H_\tau(u,\bar{u}) = \sum_{k\in\mathbb{Z}} \frac{1}{\tau}\lambda_k |u_k|^2 + \frac{1}{2} \sum_{k+m-\ell-j=0} \frac{i\Omega_{km\ell j}}{e^{i\Omega_{km\ell j}} - 1} u_k u_m \bar{u}_\ell \bar{u}_j + \mathcal{O}(\tau)$$

CFL conditions

Splitting or implicit explicit method : CFL condition

For cubic NLS : cfl numbers

τ^{N+1}	x	$2\arctan(x/2)$
τ^2	3.14	∞
τ^3	2.10	3.46
τ^4	1.57	2.00
τ^5	1.27	1.45
τ^6	1.05	1.15
τ^7	0.90	0.96
τ^8	0.80	0.83
τ^9	0.70	0.73
τ^{10}	0.63	0.65

Fully discrete case

The discretized Hamiltonian writes (in dimension 1)

$$\sum_{k\in B_K} |k|^2 |u_k|^2 + \frac{1}{2} \sum_{\substack{k,m,\ell,j\in B_K^4 \\ k+m-\ell-j\in K\mathbb{Z}}} u_k u_m \bar{u}_\ell \bar{u}_j .$$

where $B_K = \{ j \in \mathbb{Z} \mid -\frac{K}{2} \leq j \leq \frac{K}{2} - 1 \}$.
Modified Hamiltonian for the explicit splitting with CFL ($\lambda_k = \tau |k|^2$).

$$H_\tau(u,\bar{u}) = \sum_{k\in B_K} |k|^2 |u_k|^2 + \frac{1}{2} \sum_{\substack{k,m,\ell,j\in B_K^4 \\ k+m-\ell-j\in K\mathbb{Z}}} \frac{i\Omega_{km\ell j}}{e^{i\Omega_{km\ell j}} - 1} u_k u_m \bar{u}_\ell \bar{u}_j + \mathcal{O}(\tau)$$

No aliasing problems in the Wiener algebra ℓ^1.

Fully discrete solution

- If $u^{K,n}$ is the polynomial fully discrete solution : Preservation of the modified energy as long as the solution remains bounded in ℓ^1.
- In dimension 1 : $\|u\|_{\ell^1} \leq \|u\|_{H^1}$.
  Global existence of H^1 small solutions of NLS.
  Discrete analog :

Theorem (dimension 1)

There exists ϵ_0 *such that if* $\epsilon < \epsilon_0$ *and* $\|u^{K,0}\|_{H^1} \leq \epsilon$, *then*

$$\forall\, n\tau \leq C_N \tau^{-N} \qquad \|u^{K,n}\|_{H^1} \leq C\epsilon$$

where C *does not depend on* K.

Quasiperiodic solutions ?

Defocusing NLS on $\mathbb{T}^2$

$$i\partial_t u = -\Delta u + |u|^2 u$$

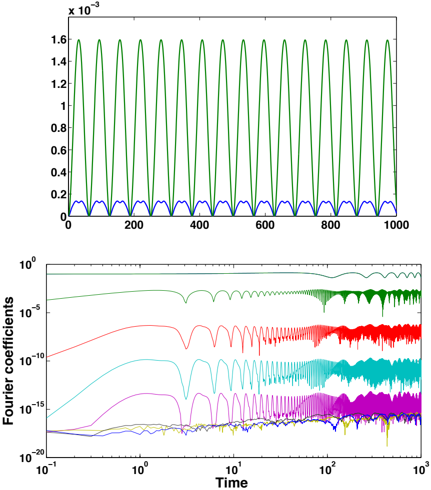
- Bourgain (1996), Wang (2010) : *There are many quasiperiodic solutions.*
- Colliander, Keel, Stafilani, Takaoka, Tao (2008) : *For all ϵ, M, $s > 1$, there exist a solution with*

$$\|u(0)\|_{H^s} < \epsilon \quad \text{and} \quad t > 0 \quad \text{s.t.} \quad \|u(t)\|_{H^s} > M$$

Let us try

$$u(0) = \frac{\epsilon}{\beta + \cos(y) - \sin(x)}$$

Quasiperiodic solutions ?



Small quasiperiodic solutions are *generic* ?

Energy cascade

Can we observe energy exchanges ?
For small initial data, we have for $t < T/\epsilon^2$

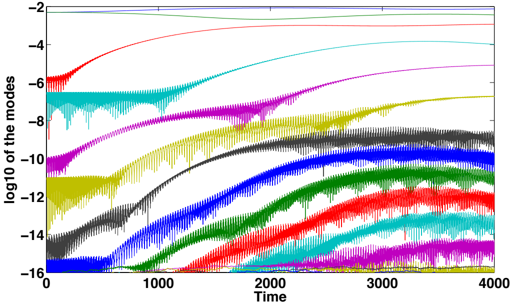
$$u(t) \simeq \sum_{j \in \mathbb{Z}^2} a_j(\epsilon^2 t) e^{ij\cdot x - it|j|^2} + \mathcal{O}(\epsilon^2)$$

where (normal forms/geometric optic/WKB/MFE)

$$\dot{a}_j = \sum_{\substack{j=k-\ell+m \\ |j|^2=|k|^2-|\ell|^2+|m|^2}} a_k \bar{a}_\ell a_m$$

Possible resonances between the modes (frequencies rectangles)

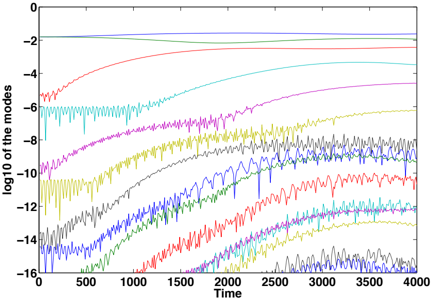
Energy cascade



$$u(0) = \epsilon(1 + e^{ix} + e^{-ix} + e^{iy} + e^{-iy})$$

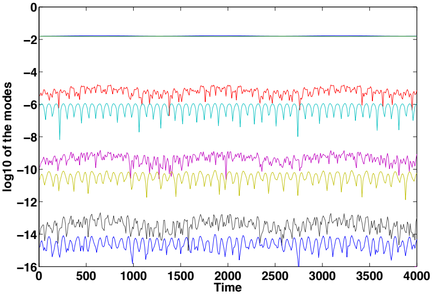
Energy transfer to the high modes (Proof : Carles & Faou 2010)

Simulating energy cascades



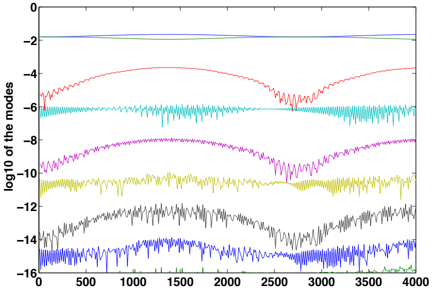
Computation with an explicit splitting algorithm
$\lambda_k = \tau |k|^2$, $\tau = 0.1$, grid 128×128.

Simulating energy cascades



Computation with an implicit-explicit splitting algorithm
$\lambda_k = 2\arctan(\tau|k|^2/2)$, $\tau = 0.1$, grid 128×128.

Simulating energy cascades



Computation with an implicit-explicit splitting algorithm
$\lambda_k = 2\arctan(\tau|k|^2/2)$, $\tau = 0.05$, grid 128×128.

Simulating energy cascades

Problem : Modified energy + geometric optic :
Numerical resonant system

$$\dot{a}_j = \sum_{\substack{j=k-\ell+m \\ \lambda_j=\lambda_k-\lambda_\ell+\lambda_m}} a_k \bar{a}_\ell a_m$$

Implicit schemes destroy the resonances.