

# Resonances as a computational tool

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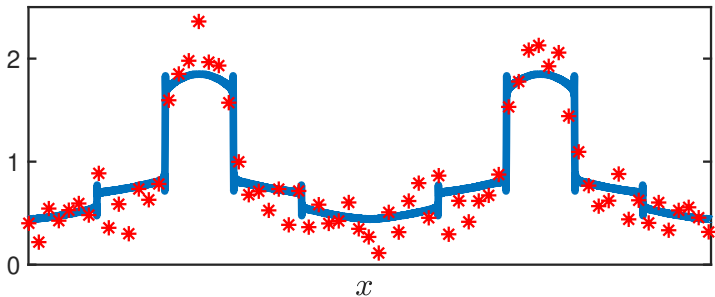
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Numerics for **non-smooth** phenomena  
in nonlinear dispersive PDEs (and beyond) ?

Talbot effect (dispersive quantisation)



blue: exact solution, red: numerical (Strang splitting)

Model problem: Korteweg–de Vries equation

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$$(S1) \quad \partial_t u + \partial_x^3 u = 0 \quad (S2) \quad \partial_t u + \frac{1}{2} \partial_x u^2 = 0$$

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Numerical approximation:  $u(0) \mapsto u^1$  (Strang)

$$u^1 = \varphi_{S1}^{\tau/2} \circ \varphi_{S2}^{\tau} \circ \varphi_{S1}^{\tau/2}(u(0))$$

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Theorem (global error): [Holden, Karlsen, Risebro, Tao '12]

$$\|u(t_n) - u^n\|_{H^1} \leq c(t_n) \tau^2 \|u\|_{L_{t_n}^\infty H^6}$$

Assumptions:

- o Burger eq is solved exactly
- o smooth solutions, e.g.,  $u \in L_{t_n}^\infty H^6$

## The Korteweg–de Vries equation

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### o Exponential integrators:

$$u(t) = e^{-t\partial_x^3} u(0) - \frac{1}{2} e^{-t\partial_x^3} \partial_x \int_0^t e^{s\partial_x^3} u^2(s) ds$$

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$$u^1 = e^{-\tau\partial_x^3} u(0) - \frac{1}{2} \tau e^{-\tau\partial_x^3} \partial_x \varphi_1(\tau\partial_x^3) (u^2(0)), \quad \varphi_1(z) = \frac{e^z - 1}{z}$$

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- Requires **smooth solutions**
- **Error analysis difficult** (at least for me): discrete Bourgain spaces

## The problem with classical methods

Structure of KdV solution: (Duhamel's formula)

$$u(t) = e^{-t\partial_x^3} u(0) - \frac{1}{2} e^{-t\partial_x^3} \partial_x \int_0^t e^{s\partial_x^3} (u^2(s)) ds \quad (\text{KdV flow})$$

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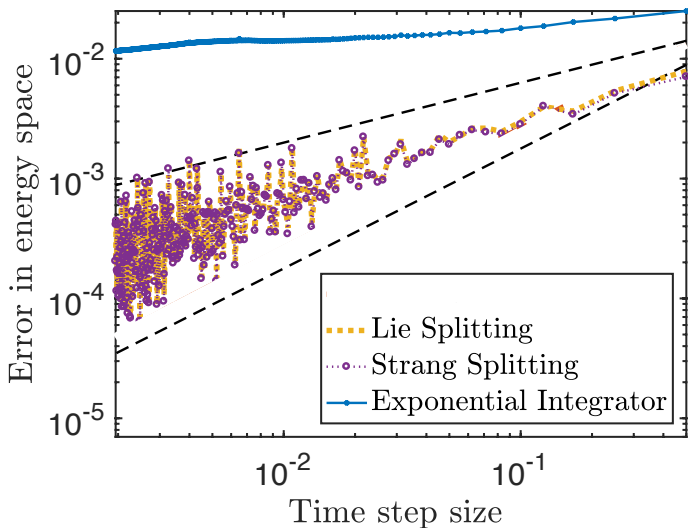
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Classical methods **linearise** frequency interactions (here  $f(u) = u^2$ )

$$\text{(splitting)} \quad e^{s\partial_x^3} f \left( e^{-s\partial_x^3} v \right) \approx f(v)$$

$$\text{(exponential)} \quad f \left( e^{-s\partial_x^3} v \right) \approx f(v)$$

Numerical experiment for 'non-smooth' data (Schrödinger with  $H^1$  data)



Classical order (dashed lines) : one and two

Nonlinear idea : KdV solution with periodic b.c.

$$u(t) = e^{-t\partial_x^3} u(0) - \frac{1}{2} e^{-t\partial_x^3} \partial_x \int_0^t \underbrace{e^{s\partial_x^3}}_{\text{red bracket}} \left( e^{-s\partial_x^3} u(0) \right)^2 ds + \int_0^t \int_0^s \dots$$

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Resonances as a computational tool:

$$\text{Osc}^{\text{KdV}}(v, t) = \partial_x \int_0^t e^{s\partial_x^3} \left( e^{-s\partial_x^3} v \right)^2 ds = \sum_{k+\ell=m} \hat{v}_k \hat{v}_\ell e^{imx} im \int_0^t e^{isR(k,\ell)} ds$$

$$R(k, \ell) = -m^3 + k^3 + \ell^3$$

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$$R(k, \ell) = -m^3 + k^3 + \ell^3 = -3k\ell m \quad (\text{factorisation of frequencies})$$

► integrate  $R(k, \ell)$  exactly + map back to physical space (numerics !)

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Scheme:

$$u^n \mapsto u^{n+1} = e^{-\tau\partial_x^3} u^n - \frac{1}{6} \left[ \partial_x^{-1} \left( e^{-\tau\partial_x^3} u^n \right)^2 - e^{-\tau\partial_x^3} \partial_x^{-1} (u^n)^2 \right]$$

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Comparison with classical methods:

Splitting method:  $R(k, \ell) \approx 0$  for all  $k, \ell \in \mathbb{Z}$

Exponential integrator:  $R(k, \ell) \approx (k + \ell)^3$  for all  $k, \ell \in \mathbb{Z}$

## Nonlinear idea (for KdV)

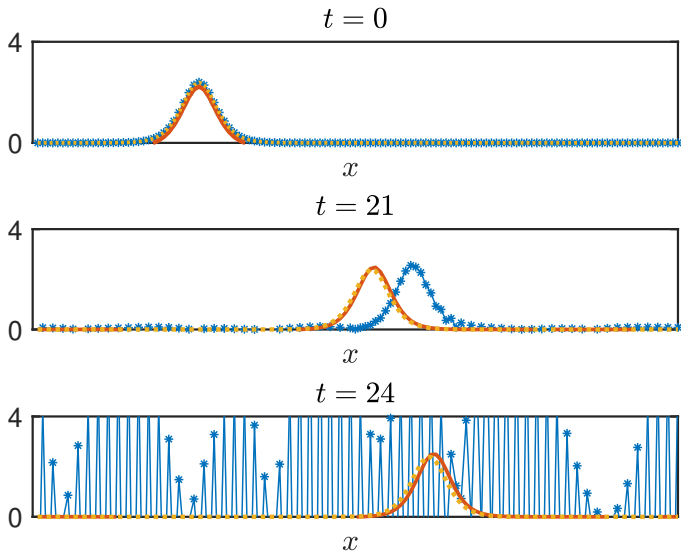


Fig.: simulation of **solitary wave solution (orange)**:  
\* **classical method**, -- **resonance based approach**

## What about a general class of (dispersive) eqs?

Dispersive PDE  $\partial_t u - i\mathcal{L}(\nabla, \frac{1}{\varepsilon})u = f(u)$  + i.c. and b.c.

Classical methods: linearise frequency interactions, e.g.,

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Nonlinear improvement:

$$e^{-i\xi\mathcal{L}} f\left(e^{i\xi\mathcal{L}} v\right) = \left[ e^{i\xi\mathcal{L}(\nabla, \frac{1}{\varepsilon})_{\text{dominant}}} f_{\text{dom}}(v) \right] f_{\text{non-oscillatory}}(v) + \text{l.o.t.}$$

Key: Choice of  $\mathcal{L}_{\text{dominant}}$ ?

Resonances as a  
computational tool

Equation ( $\mathcal{L}, f$ )  
(classical numerics)

Resonances<sup>a</sup>  $R(k)$   
(LAHACODE method)

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

$$-2k^2 + 2k(\ell + m) + 2\ell m$$

KdV  $\partial_t u + \partial_x^3 u = \partial_x(u^2)$

$$3k\ell(k + \ell)$$

KG  $\varepsilon^2 \partial_t^2 u - \Delta u + \varepsilon^{-2} u = |u|^2 u$   $\sum_{\lambda=\pm 2,4} e^{it\lambda \frac{1}{\varepsilon^2}} u_{\text{non-oscillatory}}^\lambda$

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Resonances as a  
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Example: cubic NLS  $i\partial_t u = -\Delta u + |u|^2 u$  with  $x \in \mathbb{T}^d$

$$\int_0^t e^{-i\xi\Delta} f \left( e^{i\xi\Delta} v \right) d\xi = \sum_{k=k_1-k_2+k_3 \in \mathbb{Z}^d} \hat{v}_{k_1} \bar{\hat{v}}_{k_2} \hat{v}_{k_3} e^{ikx} \cdot \int_0^t e^{i(k^2 - k_1^2 + k_2^2 - k_3^2)\xi} d\xi$$

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Q: Dominant part in  $R(k_1, k_2, k_3) = 2k_2^2 + 2k_1k_3 - 2k_2(k_1 + k_3)$  ?

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Q: Dominant part in  $R(k_1, k_2, k_3) = 2k_2^2 + 2k_1k_3 - 2k_2(k_1 + k_3)$

## Numerical example: Talbot effect

Cubic Schrödinger equation with **step function initial value**

For times  $t = \pi\mathbb{Q}$ : We observe **quantisation**

Analysis for linear dispersive eqs: K. Oskolkov, P. Olver, ...  
for 1d, periodic cubic Schrödinger eq: M.B. Erdogan, N. Tzirakis

## A lot of Questions

### Bottleneck of resonances as a computational tool

Equation  $(\mathcal{L}, f)$

(classical numerics)

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Resonances<sup>a</sup>  $R(k)$

(LAHACODE method)

$$-2k^2 + 2k(\ell + m) + 2\ell m$$

$$3k\ell(k + \ell)$$

$$\sum_{\lambda=\pm 2,4} e^{it\lambda \frac{1}{\varepsilon^2}} u^\lambda_{\text{non-oscillatory}}$$

Q1 : Can we find an **overarching algorithm** ?

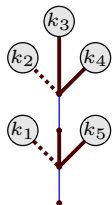
Q2 : Error estimates at **low regularity** ?

Q3 : More **general class of equations** ?

Q4 : **Structure preservation, long time scales, ...** ?

## Part 1 : Overarching algorithm

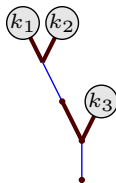
[Bruned–S, Forum of Mathematics Pi '22]



Framework for periodic dispersive pdes

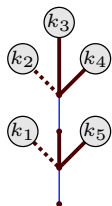
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via decorated trees



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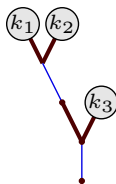
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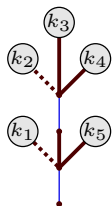


Difficulty: control of frequency interactions

$$u(t) = e^{it\mathcal{L}} u_0 + e^{it\mathcal{L}} \int_0^t e^{-i\xi_1 \mathcal{L}} f(e^{i\xi_1 \mathcal{L}} u_0) d\xi_1$$

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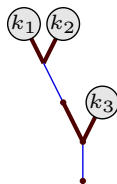
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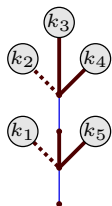
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$$+ e^{it\mathcal{L}} \int_0^t e^{-i\xi_1 \mathcal{L}} \left[ f'(e^{i\xi_1 \mathcal{L}} u_0) e^{i\xi_1 \mathcal{L}} \int_0^{\xi_1} e^{-i\xi_2 \mathcal{L}} f(e^{i\xi_2 \mathcal{L}} u_0) d\xi_2 \right] d\xi_1 + \dots$$



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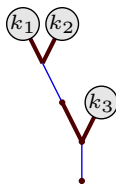
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Difficulty: control of frequency interactions

$$u(t) = e^{it\mathcal{L}} u_0 + e^{it\mathcal{L}} \int_0^t e^{-i\xi_1\mathcal{L}} f(e^{i\xi_1\mathcal{L}} u_0) d\xi_1 \\ + e^{it\mathcal{L}} \int_0^t e^{-i\xi_1\mathcal{L}} \left[ f'(e^{i\xi_1\mathcal{L}} u_0) e^{i\xi_1\mathcal{L}} \int_0^{\xi_1} e^{-i\xi_2\mathcal{L}} f(e^{i\xi_2\mathcal{L}} u_0) d\xi_2 \right] d\xi_1 + \dots$$

Idea (tree series): 
$$\hat{u}_k(t) = \sum_{T \in \mathcal{V}_k^p} \frac{\Upsilon^f(T)}{S(T)} (\mathcal{I}_p T)(t, u_0) + \mathcal{O}(t^{p+1})$$

$(\mathcal{I}_p = \mathcal{I}_{t, \xi_1, \dots, \xi_p}$  integral operator,  $T$  trees with leaf decoration  $k_\ell$ )

## Part 1 : Overarching algorithm

[Bruned–S, Forum of Mathematics Pi '22]

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Discretisation operator  $\mathcal{I}_p \approx \mathcal{I}_p^d$  (in spirit of **resonance approach**)

$$\mathcal{I}_p^{(d)} = \left( \hat{\mathcal{I}}_p^{(d)} \otimes A_p^{(d)} \right) \Delta \quad (\text{Birkhoff-type factorisation})$$

structure close to SPDEs with **Regularity Structures** [M. Hairer 2014]

## Part 2 : Sharp error estimates in low regularity spaces

[Ostermann–Rousset–S, JEMS, FoCM '22]

**Continuous level:** Strichartz estimates (Ginibre–Velo, Keel–Tao)

$$\|e^{it\Delta}v\|_{L_t^p L_x^q(\mathbb{R}^d)} \leq C_{d,q,p} \|v\|_{L_x^2(\mathbb{R}^d)} \quad 2 \leq p, q \leq \infty, \frac{2}{p} + \frac{d}{q} = \frac{d}{2}, (p, q, d) \neq (2, \infty, 2)$$

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Finite dimensional (discrete) counterpart ?

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Finite dimensional (discrete) counterpart ?

**Ignat–Zuazua:**  $L^2$  error estimates for cubic NLS:  $u \in H^2(\mathbb{R}^d)$ ,  $d \leq 3$

**Theorem** (Ostermann–Rousset–S): For every  $(p, q)$  admissible ( $p > 2$ )  $\exists C > 0$  s.t. for  $K = \tau^{-\alpha/2}$  with  $\|F\|_{l_\tau^p L^q} = (\tau \sum_{k \in \mathbb{Z}} \|F_k\|_{L^q}^p)^{1/p}$  and  $\alpha \geq 1$

$$\|e^{it_n \Delta} \Pi_K v\|_{l_\tau^p L_x^q(\mathbb{R}^d)} \leq c_{d,q,p} \tau^{p(1-\alpha)} \|v\|_{L_x^2(\mathbb{R}^d)} \quad (\text{discrete } t_n = n\tau)$$

$L^2$  error estimates for  $u \in H^\sigma, \sigma > 0$  ( $u \xrightarrow{p} u_{\Pi_K} \xrightarrow{t_n} u_{\Pi_K}^n$ )

$$\|u(t_n) - u_{\Pi_K}^n\|_{L^2(\mathbb{R}^d)} \leq \tau^\delta c(T, \|u\|_{H^\sigma(\mathbb{R}^d)}), \quad \delta = \delta(d, \sigma, \alpha)$$

( $\mathbb{T}, \mathbb{T}^2$ : discrete Bourgain  $\|\Pi_K u_n\|_{l_\tau^4 L^4(\mathbb{T})} \lesssim (K\tau^{1/2})^{1/2} \|u_n\|_{X_\tau^{0, \frac{3}{8}}}$ )

### Part 3 : Non periodic b.c., general class of equations

[Rousset–S, Li–Ma–S, SIAM J. Numer. Anal. '21, '22]

#### Model problem:

$$\partial_t u + \mathcal{L}u = f(u, \bar{u}) \quad (t, x) \in \mathbb{R} \times \Omega \subset \mathbb{R}^d$$

- $\mathcal{L}$  generates contractive  $\mathcal{C}_0$  semigroup on  $X$
- $-\mathcal{L} + \overline{\mathcal{L}}$  generates unitary group on  $X$
- $f(u, \bar{u}) = \mathcal{B}(F(u) \cdot G(\bar{u}))$ ,  $F, G : \mathbb{C} \rightarrow \mathbb{C}^J$  smooth,  $\mathcal{B}$  linear

Ex.: NLS, Ginzburg-Landau, (half-)wave, Navier–Stokes, etc.

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#### Resonance based approach:

$$u^{\ell+1} = e^{\tau\mathcal{L}} \left( u^\ell + \tau \mathcal{B} \left( F(u^\ell) \cdot \varphi_1(\tau(-\mathcal{L} + \bar{\mathcal{L}})) G(\bar{u}^\ell) \right) \right)$$



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Convergence\* :  $\|u(t_n) - u^n\|_X \leq c\tau$  if  $\|\mathcal{C}[f, \mathcal{L}](u, \bar{u})\|_{L_{t \leq t_n}^\infty X} < \infty$

$$\mathcal{C}[f, \mathcal{L}](v, w) = -\mathcal{L}f(v, w) + D_1 f(v, w) \cdot \mathcal{L}v + D_2 f(v, w) \cdot \mathcal{L}w$$

\*improves classical convergence results (if  $\mathcal{L}$  satisfies Leibniz rule)

Part 4: What about structure preservation, long time scales, etc. ?

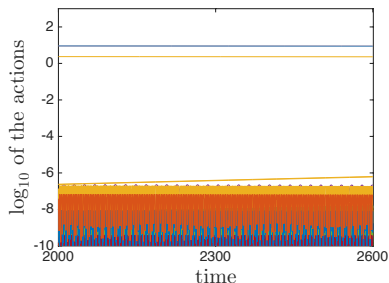
**Problem:** numerical resonances (= purely discrete artifact) trigger non-physical energy shift from low to high modes (even for  $C^\infty$  data)

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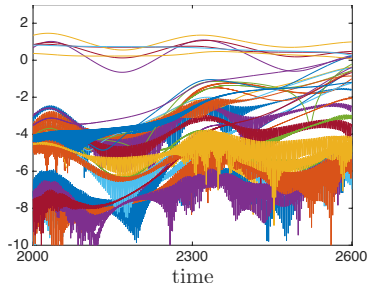
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Splitting method:



non-resonant  
( $\Delta t = 0.315$ )



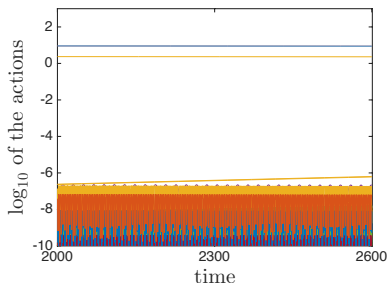
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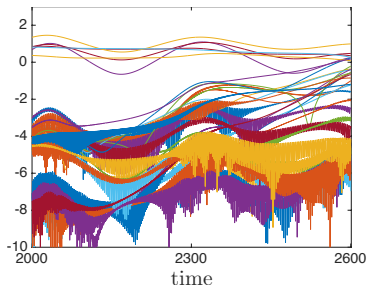
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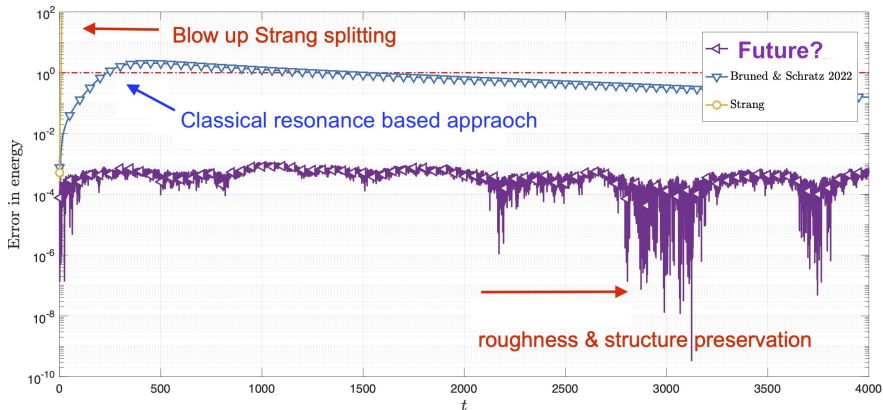


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## Part 4: What about structure preservation, long time scales, etc. ?

... gets even worse for rough data !

Example: cubic NLS on  $\mathbb{T}$  with  $\mathcal{O}(1)$  rough data



[Alama Bronsard–Bruned–Maierhofer–Schratz, arXiv:2305.16737]

## Still a lot of open Questions

Q1 : Structure preservation for rough data?

Q2 : Non-smooth phenomena on long time scales

(e.g., blow up, growth of Sobolev norms, wave turbulence, ... ) ?

How far can we actually go at the discrete level :  
down with regularity and up in time scales ?

