

# A POSTERIORI ERROR CONTROL FOR EVOLUTION NONLINEAR SCHRÖDINGER EQUATIONS

IRENE KYZA

DEPARTMENT OF MATHEMATICS – UNIVERSITY OF DUNDEE



Joint work with **Theodoros Katsaounis**, KAUST, Saudi Arabia

Scottish Numerical Methods Network 2018

First Workshop: Modern numerical discretisations of PDEs and adaptivity



THE  
UNIVERSITY OF  
STRATHCLYDE  
IN GLASGOW

University of Strathclyde

30 January 2018



LONDON  
MATHEMATICAL  
SOCIETY  
EST. 1865

# Outline

- 1 Introduction
- 2 Time-discrete schemes
- 3 Fully-discrete schemes
- 4 Numerical Results
- 5 Ongoing & Future work



# The problem: $2p + 1$ NLS

$$(1) \quad \begin{cases} \partial_t u - i\alpha \Delta u = i\lambda f(u) & \text{in } \Omega \times [0, T], \\ u = 0 & \text{on } \partial\Omega \times [0, T], \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases}$$

- $\Omega$ : convex polygonal domain in  $\mathbb{R}^d$ ,  $d = 1, 2$
- $u_0 : \Omega \rightarrow \mathbb{C}$  given initial value;  $u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$
- $\alpha > 0$ ,  $\lambda \in \mathbb{R}$
- $f(u) = |u|^{2p}u$ ,  $\frac{1}{2} \leq p \leq p^*$  with  $p^* = \frac{2}{d}$
- Theory in Brezis & Gallouet, 1980; Anton, 2008

# The problem: $2p + 1$ NLS

$$(1) \quad \begin{cases} \partial_t u - i\alpha \Delta u = i\lambda f(u) & \text{in } \Omega \times [0, T], \\ u = 0 & \text{on } \partial\Omega \times [0, T], \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases}$$

- $\Omega$ : convex polygonal domain in  $\mathbb{R}^d$ ,  $d = 1, 2$
- $u_0 : \Omega \rightarrow \mathbb{C}$  given initial value;  $u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$
- $\alpha > 0$ ,  $\lambda \in \mathbb{R}$

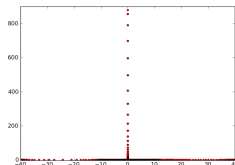
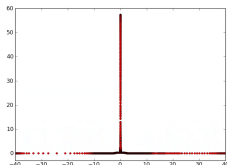
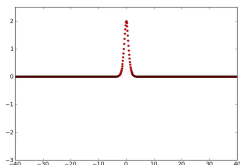
- $f(u) = |u|^{2p}u$ ,  $\frac{1}{2} \leq p \leq p^*$  with  $p^* = \frac{2}{d}$

- $p^*$ : critical exponent

- ▶ For  $\frac{1}{2} \leq p < p^*$ : (1) admits a unique solution

$$u \in C([0, T]; H_0^1(\Omega) \cap H^2(\Omega)) \cap C^1([0, T]; L^2(\Omega))$$

- ▶ For  $p = p^*$ : Solution may blowup in finite time



## The problem: $2p + 1$ NLS

$$(1) \quad \begin{cases} \partial_t u - i\alpha \Delta u = i\lambda f(u) & \text{in } \Omega \times [0, T], \\ u = 0 & \text{on } \partial\Omega \times [0, T], \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases}$$

- $f(u) = |u|^{2p}u$ ,  $\frac{1}{2} \leq p \leq p^*$  with  $p^* = \frac{2}{d}$
- $p^*$  : *critical exponent*

- Unique solution for (1) is guaranteed for  $p = p^*$  *provided*  $u_0$  is “small”  
More precisely, there exists  $B > 0$  s.t.

(1) admits a unique, global solution *provided*:  $\Gamma(u_0) := \frac{B\lambda}{\alpha(p+1)} \|u_0\|^{2p} < 1$

- 1  $\Gamma(u_0) < 1$  is automatically satisfied if  $\lambda \leq 0$  (defocusing NLS)
- 2  $\lambda > 0$  (focusing NLS): *Solution may blowup* in  $H^1$ -norm for some finite time, if  $\Gamma(u_0) \geq 1$

→ For this talk: *Assume*  $\Gamma(u_0) < 1$  for the case  $p = p^*$

**GOAL:** Derivation of *reliable & efficient approximations* to the solution  $u$  of the  $2p + 1$  NLS *without the a priori knowledge of  $u$*

- 1 Rigorous *a posteriori error control* (bounds are computable quantities decreasing with the same order as the order of the method)
- 2 Construction of *adaptive algorithms* (generation of nonuniform grids adapted to the problem)

# Existing Literature

## ○ A posteriori error control & Adaptivity:

① Adaptive algorithms *based on ad hoc mesh selection criteria* for various NLS eqs:

- ▶ Akrivis, Dougalis, Karakashian & McKinney (2003);
- ▶ Jimenez, Llorente, Mancho, Perez-Garcia & Vazquez (2003);
- ▶ Plexousakis (1996);
- ▶ Zhang, Zhang, Zhou (2006);
- ▶ ...

⇒ Numerical approximations *near blowup time*

② *No rigorous a posteriori error control*



# Existing Literature

## ○ A posteriori error control & Adaptivity:

① Adaptive algorithms *based on ad hoc mesh selection criteria* for various NLS eqs:

- ▶ Akrivis, Dougalis, Karakashian & McKinney (2003);
- ▶ Jimenez, Llorente, Mancho, Perez-Garcia & Vazquez (2003);
- ▶ Plexousakis (1996);
- ▶ Zhang, Zhang, Zhou (2006);
- ▶ ...

⇒ Numerical approximations *near blowup time*

② *No rigorous a posteriori error control*

## ○ A priori error analysis:

① **Spatial discretisation:** Finite Elements / Finite Differences

**Temporal discretisation:** Crank-Nicolson type schemes, discontinuous Galrkin, ... (Akrivis, Dougalis & Karakashian, 1991; Delfour, Fortin & Payre, 1981; Karakashian & Makridakis, 1998; ...)

② **Time-splitting spectral-type methods**

(Bao & Cai, 2014; Bao, Jin & Markowich, 2003, Thalhammer, 2012, ...)

③ **Relaxation Crank-Nicolson scheme**

(Besse, 2004; *only time discrete schemes*)

# Conservation Laws

*Choice* of the numerical scheme  $\Rightarrow$  It usually satisfies discrete analogues of:

## ○ Conservation Laws

① **Mass conservation** :  $\|u(t)\| = \|u_0\|$

② **Energy Conservation:**

$$\|\nabla u(t)\|^2 - \frac{\lambda}{\alpha(p+1)} \|u(t)\|_{L^{2p+2}}^{2p+2} = \|\nabla u_0\|^2 - \frac{\lambda}{\alpha(p+1)} \|u_0\|_{L^{2p+2}}^{2p+2}$$

•  $\|\cdot\|$ :  $L^2$ -norm in  $\Omega$ ;  $\|\cdot\|_{L^q}$ ,  $1 \leq q \leq \infty$ ,  $q \neq 2$ :  $L^q$ -norm in  $\Omega$

# Cubic NLS

- $\alpha = 1, p = 1, f(u) = |u|^2 u$

$$(2) \quad \begin{cases} \partial_t u - i\alpha \Delta u = i\lambda |u|^2 u & \text{in } \Omega \times [0, T], \\ u = 0 & \text{on } \partial\Omega \times [0, T], \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases}$$

- $U^n$  approximation (in time) of  $u(t_n)$ ,  $k$ : time-step

## 1 Crank-Nicolson method:

$$\frac{U^{n+1} - U^n}{k} + \frac{i}{2} \Delta (U^{n+1} + U^n) = \frac{i}{8} \lambda |U^{n+1} + U^n|^2 (U^{n+1} + U^n)$$

- ▶ Satisfies mass conservation

## 2 Modified Crank-Nicolson method (Delfour, Fortin & Payre, 1981):

$$\frac{U^{n+1} - U^n}{k} + \frac{i}{2} \Delta (U^{n+1} + U^n) = \frac{i}{4} \lambda (|U^{n+1}|^2 + |U^n|^2) (U^{n+1} + U^n)$$

- ▶ Satisfies energy conservation, *additionally* to mass conservation

# Crank-Nicolson schemes: Issues

## 1 Crank-Nicolson method:

$$\frac{U^{n+1} - U^n}{k} + \frac{i}{2}\Delta(U^{n+1} + U^n) = \frac{i}{8}\lambda|U^{n+1} + U^n|^2(U^{n+1} + U^n)$$

## 2 Modified Crank-Nicolson method:

$$\frac{U^{n+1} - U^n}{k} + \frac{i}{2}\Delta(U^{n+1} + U^n) = \frac{i}{4}\lambda(|U^{n+1}|^2 + |U^n|^2)(U^{n+1} + U^n)$$

⇒ Both Crank-Nicolson schemes require the solution of a *nonlinear equation at each step*

- *Computationally expensive*
- Error committed for the numerical solution of the nonlinear system at each step *should be taken into account in the a posteriori error analysis*

○ How can we avoid these difficulties? [Relaxation Crank-Nicolson scheme \(Besse, 2004\)](#)

## Relaxation Crank-Nicolson method (Besse, 2004)

- NLS:  $\partial_t u - i\alpha \Delta u = i\lambda f(u)$  in  $\Omega \times [0, T]$ ,  $f(u) = |u|^{2p} u$
- Rewrite NLS as the following system:

$$\begin{cases} \phi = |u|^{2p} & \text{in } \Omega \times (0, T], \\ \partial_t u - i\alpha \Delta u = i\lambda \phi u & \text{in } \Omega \times (0, T] \end{cases}$$

“like linear Schrödinger equation with potential  $\phi$ ”

# Relaxation Crank-Nicolson method (Besse, 2004)

○ NLS:  $\partial_t u - i\alpha \Delta u = i\lambda f(u)$  in  $\Omega \times [0, T]$ ,  $f(u) = |u|^{2p}u$

○ Rewrite NLS as the following system:

$$\begin{cases} \phi = |u|^{2p} & \text{in } \Omega \times (0, T], \\ \partial_t u - i\alpha \Delta u = i\lambda \phi u & \text{in } \Omega \times (0, T] \end{cases}$$

“like linear Schrödinger equation with potential  $\phi$ ”

○ Notation

•  $0 =: t_0 < t_1 < \dots < t_N := T$  a partition of  $[0, T]$ ,  $I_n := (t_n, t_{n+1}]$ ,

$k_n := t_{n+1} - t_n$  the variable time steps,  $k := \max_{0 \leq n \leq N-1} k_n$

•  $\bar{\partial}U^n := \frac{U^{n+1} - U^n}{k_n}$ ,  $U^{n+\frac{1}{2}} := \frac{U^{n+1} + U^n}{2}$ ,  $t_{n+\frac{1}{2}} = \frac{t_{n+1} + t_n}{2}$

○ Relaxation Crank-Nicolson method:

$$\begin{cases} \frac{k_{n-1}}{k_n + k_{n-1}} \Phi^{n+\frac{1}{2}} + \frac{k_n}{k_n + k_{n-1}} \Phi^{n-\frac{1}{2}} = |U^n|^{2p}, & 0 \leq n \leq N-1, \\ \bar{\partial}U^n - i\alpha \Delta U^{n+\frac{1}{2}} = i\lambda \Phi^{n+\frac{1}{2}} U^{n+\frac{1}{2}}, & 0 \leq n \leq N-1, \end{cases}$$

with  $k_{-1} := k_0$ ,  $\Phi^{-\frac{1}{2}} = |u_0|^{2p}$  and  $U^0 = u_0$

# Motivation behind the relaxation Crank-Nicolson method

## ○ Derivation of the first equation:

$$\phi = |u|^{2p} \rightsquigarrow \frac{k_{n-1}}{k_n + k_{n-1}} \Phi^{n+\frac{1}{2}} + \frac{k_n}{k_n + k_{n-1}} \Phi^{n-\frac{1}{2}} = |U^n|^{2p}$$

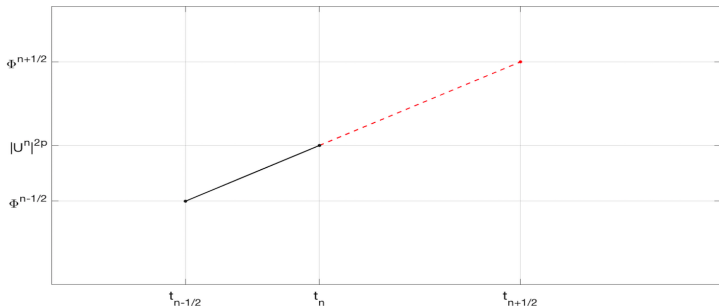
- ①  $\Phi^{n+\frac{1}{2}}$  is an approximation of  $\phi(t_{n+\frac{1}{2}}) = |u(t_{n+\frac{1}{2}})|^{2p}$

**NOTE:** If  $\Phi^{n+\frac{1}{2}} = |U^{n+\frac{1}{2}}|^{2p} \rightarrow$  Crank-Nicolson method for the  $2p + 1$  NLS

- ② How do we approximate  $\phi(t_{n+\frac{1}{2}})$ ?

At step  $n$ ,  $\Phi^{n-\frac{1}{2}}$ ,  $U^n$  are known  $\Rightarrow$  Compute  $\Phi^{n+\frac{1}{2}}$  by *linear extrapolation* between  $\Phi^{n-\frac{1}{2}}$  and  $|U^n|^{2p}$ :

$$\Phi^{n+\frac{1}{2}} := \frac{k_n + k_{n-1}}{k_{n-1}} |U^n|^{2p} - \frac{k_n}{k_{n-1}} \Phi^{n-\frac{1}{2}}$$



# Motivation behind the relaxation Crank-Nicolson method

## ○ Derivation of the first equation:

$$\phi = |u|^{2p} \rightsquigarrow \frac{k_{n-1}}{k_n + k_{n-1}} \Phi^{n+\frac{1}{2}} + \frac{k_n}{k_n + k_{n-1}} \Phi^{n-\frac{1}{2}} = |U^n|^{2p}$$

- ①  $\Phi^{n+\frac{1}{2}}$  is an approximation of  $\phi(t_{n+\frac{1}{2}}) = |u(t_{n+\frac{1}{2}})|^{2p}$

NOTE: If  $\Phi^{n+\frac{1}{2}} = |U^{n+\frac{1}{2}}|^{2p} \rightarrow$  Crank-Nicolson method for the  $2p + 1$  NLS

- ② How do we approximate  $\phi(t_{n+\frac{1}{2}})$ ?

At step  $n$ ,  $\Phi^{n-\frac{1}{2}}$ ,  $U^n$  are known  $\Rightarrow$  Compute  $\Phi^{n+\frac{1}{2}}$  by *linear extrapolation* between  $\Phi^{n-\frac{1}{2}}$  and  $|U^n|^{2p}$ :

$$\Phi^{n+\frac{1}{2}} := \frac{k_n + k_{n-1}}{k_{n-1}} |U^n|^{2p} - \frac{k_n}{k_{n-1}} \Phi^{n-\frac{1}{2}}$$

## ○ Derivation of the second equation:

$$\partial_t u - i\alpha \Delta u = i\lambda \phi u \rightsquigarrow \bar{\partial} U^n - i\alpha \Delta U^{n+\frac{1}{2}} = i\lambda \Phi^{n+\frac{1}{2}} U^{n+\frac{1}{2}}$$

- ① Apply the Crank-Nicolson method to the *linear Schrödinger equation*:

$$\partial_t u - i\alpha \Delta u = i\lambda V(x, t)u \text{ with } V(\cdot, t) := \Phi^{n+\frac{1}{2}}, t \in I_n$$



# Relaxation Crank-Nicolson method: Order of accuracy

- It is expected to be *second order accurate*

## ○ IDEA of the PROOF:

①  $\Phi^{n+\frac{1}{2}} = |u(t_{n+\frac{1}{2}})|^{2p} + \mathcal{O}(k^2), \quad 0 \leq n \leq N-1$

- ② Let  $\tilde{u}$  be the solution of

$$(3) \quad \partial_t \tilde{u} - i\alpha \Delta \tilde{u} = i\lambda \Phi^{n+\frac{1}{2}} \tilde{u} \quad \text{in } \Omega \times I_n, \quad 0 \leq n \leq N-1.$$

- We expect:  $\max_{0 \leq n \leq N} \|\tilde{u}(t_n) - U^n\| = \mathcal{O}(k^2)$  ( $\{U^n\}_{n=0}^N$  CN approximations for (3))

# Relaxation Crank-Nicolson method: Order of accuracy

- It is expected to be *second order accurate*

## ○ IDEA of the PROOF:

①  $\Phi^{n+\frac{1}{2}} = |u(t_{n+\frac{1}{2}})|^{2p} + \mathcal{O}(k^2), \quad 0 \leq n \leq N-1$

- ② Let  $\tilde{u}$  be the solution of

(3)  $\partial_t \tilde{u} - i\alpha \Delta \tilde{u} = i\lambda \Phi^{n+\frac{1}{2}} \tilde{u} \quad \text{in } \Omega \times I_n, \quad 0 \leq n \leq N-1.$

- We expect:  $\max_{0 \leq n \leq N} \|\tilde{u}(t_n) - U^n\| = \mathcal{O}(k^2)$  ( $\{U^n\}_{n=0}^N$  CN approximations for (3))

③  $\partial_t \tilde{u} - i\alpha \Delta \tilde{u} = i\lambda \left( |u(t_{n+\frac{1}{2}})|^{2p} + \mathcal{O}(k^2) \right) \tilde{u} \quad \text{in } \Omega \times I_n, \quad 0 \leq n \leq N-1$

- ④  $|z|^{2p}$ : *locally Lipschitz continuous function*

$\Rightarrow \partial_t(u - \tilde{u}) - i\alpha \Delta(u - \tilde{u}) = i\lambda |u(t)|^{2p}(u - \tilde{u}) + \mathcal{O}(k^2) \quad \text{in } \Omega \times I_n, \quad 0 \leq n \leq N-1$

- ⑤ Use the *stability of NLS*, the *continuity of  $u, \tilde{u}$*  in  $[0, T]$  and the *boundedness of  $\tilde{u}$*  to get:

$$\max_{0 \leq t \leq T} \|(u - \tilde{u})(t)\| = \mathcal{O}(k^2)$$

⑥  $\|u(t_n) - U^n\| \leq \|u(t_n) - \tilde{u}(t_n)\| + \|\tilde{u}(t_n) - U^n\|, \quad 0 \leq n \leq N$

$$\Rightarrow \max_{0 \leq n \leq N} \|u(t_n) - U^n\| = \mathcal{O}(k^2)$$

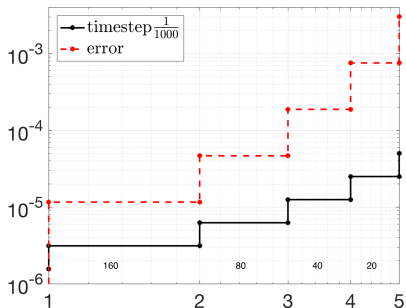
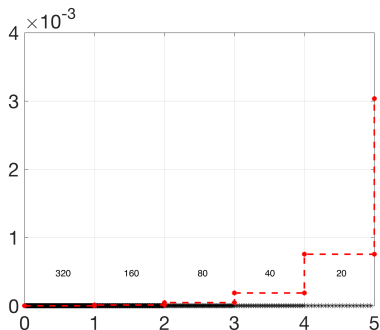
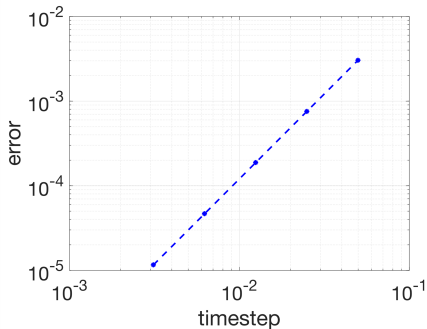
# Relaxation Crank-Nicolson method: EOC

- Numerical verification for *constant time steps*: Besse (2004)

## ○ EXAMPLE: (EOC and variable time steps)

- $d = 1$ ,  $[a, b] = [-30, 30]$ ,  $\alpha = 1$   $\lambda = 2$ ,  $p = 1$
- $u(x, t) = i \exp(i(2\omega x + t(1 - \omega^2))) / \cosh(x - x_0 - 4\omega t)$
- $x_0 = 0$ ,  $\omega = \frac{1}{4}$
- spatial discretisation: B-splines of degree 5,  $h = \frac{b-a}{M}$ ,  $M = 3000$
- $[0, T] = [0, 5]$ ,  $[0, 5] = \cup_{n=0}^4 [n, n+1]$
- In every  $[n, n+1]$  we use  $k_n = \frac{5 \times 10^{-2}}{2^{4-n}}$ ,  $n = 0, 1, 2, 3, 4$
- $E_{\text{exact}} := \max_{0 \leq n \leq N} \|u(t_n) - U^n\|$

subinterval	$k$	$E_{\text{exact}}$	EOC
[0, 1]	3.125E-03	1.1601E-05	
[1, 2]	6.250E-03	4.6623E-05	2.0068
[2, 3]	1.250E-02	1.8770E-04	2.0093
[3, 4]	2.500E-02	7.5547E-04	2.0090
[4, 5]	5.000E-02	3.0345E-03	2.0060



# Reconstruction Technique (Akrivis, Makridakis & Nochetto, 2005)

- **AIM:** Derivation of optimal order a posteriori error estimates in the  $L^\infty(L^2)$ -norm for the relaxation Crank-Nicolson scheme for the  $2p + 1$  NLS
- Relaxation Crank-Nicolson method is *second order accurate*
- $U(t) := \ell_0^n(t)U^n + \ell_1^n(t)U^{n+1}$ ,  $t \in I_n$ ,  $\ell_0^n(t) := \frac{t_{n+1} - t}{k_n}$ ,  $\ell_1^n(t) := \frac{t - t_n}{k_n}$ 
  - Using  $U$  in the a posteriori error analysis leads to suboptimal bounds (Dörfler, 1996)
  - Introduce a *reconstruction*  $\hat{U}$  of  $U$ , work with  $u - U = (u - \hat{U}) + (\hat{U} - U)$

# Reconstruction Technique (Akrivis, Makridakis & Nochetto, 2005)

- **AIM:** Derivation of optimal order a posteriori error estimates in the  $L^\infty(L^2)$ -norm for the relaxation Crank-Nicolson scheme for the  $2p + 1$  NLS
- Relaxation Crank-Nicolson method is *second order accurate*
- $U(t) := \ell_0^n(t)U^n + \ell_1^n(t)U^{n+1}$ ,  $t \in I_n$ ,  $\ell_0^n(t) := \frac{t_{n+1} - t}{k_n}$ ,  $\ell_1^n(t) := \frac{t - t_n}{k_n}$ 
  - Using  $U$  in the a posteriori error analysis leads to suboptimal bounds (Dörfler, 1996)
  - Introduce a *reconstruction*  $\hat{U}$  of  $U$ , work with  $u - U = (u - \hat{U}) + (\hat{U} - U)$

## Reconstruction Technique: Main idea

- 1 Find a *continuous projection or interpolant*  $\hat{U}$  of  $U$
- 2  $\hat{U} - U$  is of *optimal order*
- 3  $\hat{U}$  satisfies a *perturbation of the original PDE*
- 4 The perturbation term (*residual*) is a *computable quantity* or can be estimated by computable quantities of *optimal order* of accuracy
- 5 Use *PDE stability arguments* to obtain the final a posteriori estimates

# Relaxation Crank-Nicolson reconstruction & its properties

○ **The reconstruction:** For  $0 \leq n \leq N - 1$ ,

$$\hat{U}(t) := U^n + i\alpha \int_{t_n}^t \Delta U(s) ds + i\lambda \int_{t_n}^t \Phi^{n+\frac{1}{2}} U(s) ds, \quad t \in I_n$$

**NOTE:**  $\hat{U}$  coincides with the Crank-Nicolson reconstruction for

$$\partial_t u - i\alpha \Delta u = i\lambda V(x, t)u \quad \text{with } V(\cdot, t) := \Phi^{n+\frac{1}{2}}, \quad t \in I_n$$

# Relaxation Crank-Nicolson reconstruction & its properties

- **The reconstruction:** For  $0 \leq n \leq N - 1$ ,

$$\hat{U}(t) := U^n + i\alpha \int_{t_n}^t \Delta U(s) ds + i\lambda \int_{t_n}^t \Phi^{n+\frac{1}{2}} U(s) ds, \quad t \in I_n$$

**NOTE:**  $\hat{U}$  coincides with the Crank-Nicolson reconstruction for

$$\partial_t u - i\alpha \Delta u = i\lambda V(x, t)u \quad \text{with } V(\cdot, t) := \Phi^{n+\frac{1}{2}}, \quad t \in I_n$$

- **Properties:**

①  $\hat{U}$  is a *time-continuous function*

②  $\hat{U}(t_n) = U(t_n) = U^n, \quad 0 \leq n \leq N$

③  $\partial_t \hat{U} - i\alpha \Delta \hat{U} = i\lambda f(\hat{U}) + \hat{r}, \quad t \in I_n$  with

$$\hat{r} = -i\alpha \Delta(\hat{U} - U) - i\lambda(f(\hat{U}) - f(U)) - i\lambda(|U|^{2p} - \Phi^{n+\frac{1}{2}})U$$

④  $(\hat{U} - U)(t) = -\frac{i}{2}(t - t_n)(t_{n+1} - t)(\alpha \Delta + \lambda \Phi^{n+\frac{1}{2}})\bar{\partial} U^n, \quad t \in I_n$   
 $\Rightarrow \hat{r}$  is expected to be *second order accurate* in time (provided  $U^n$  are second order approximations to  $u(t_n)$ )



# Variational formulations & Error equation

## ○ Variational formulations:

$$\begin{cases} \langle \partial_t u(t), v \rangle + i\alpha \langle \nabla u(t), \nabla v \rangle = i\lambda \langle f(u(t)), v \rangle, & \forall v \in H_0^1(\Omega), t \in [0, T] \\ u(\cdot, 0) = u_0 & \text{in } \Omega. \end{cases}$$

$$\begin{cases} \langle \partial_t \hat{U}(t), v \rangle + i\alpha \langle \nabla \hat{U}(t), \nabla v \rangle = i\lambda \langle f(\hat{U}(t)), v \rangle + \langle \hat{r}(t), v \rangle, & \forall v \in H_0^1(\Omega), t \in I_n \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases}$$

○ Error equation: Let  $\hat{e} := u - \hat{U}$ . Then,  $\hat{e}(0) = 0$  and for  $t \in I_n$ ,

$$(4) \quad \langle \hat{e}_t(t), v \rangle + i\alpha \langle \nabla \hat{e}(t), \nabla v \rangle = i\lambda \langle f(u(t)) - f(\hat{U}(t)), v \rangle - \langle \hat{r}(t), v \rangle, \quad \forall v \in H_0^1(\Omega)$$

# Variational formulations & Error equation

## ○ Variational formulations:

$$\begin{cases} \langle \partial_t u(t), v \rangle + i\alpha \langle \nabla u(t), \nabla v \rangle = i\lambda \langle f(u(t)), v \rangle, & \forall v \in H_0^1(\Omega), t \in [0, T] \\ u(\cdot, 0) = u_0 & \text{in } \Omega. \end{cases}$$

$$\begin{cases} \langle \partial_t \hat{U}(t), v \rangle + i\alpha \langle \nabla \hat{U}(t), \nabla v \rangle = i\lambda \langle f(\hat{U}(t)), v \rangle + \langle \hat{r}(t), v \rangle, & \forall v \in H_0^1(\Omega), t \in I_n \\ u(\cdot, 0) = u_0 & \text{in } \Omega, \end{cases}$$

○ **Error equation:** Let  $\hat{e} := u - \hat{U}$ . Then,  $\hat{e}(0) = 0$  and for  $t \in I_n$ ,

$$(4) \quad \langle \hat{e}_t(t), v \rangle + i\alpha \langle \nabla \hat{e}(t), \nabla v \rangle = i\lambda \langle f(u(t)) - f(\hat{U}(t)), v \rangle - \langle \hat{r}(t), v \rangle, \quad \forall v \in H_0^1(\Omega)$$

① If  $f$  was linear  $\Rightarrow f(u) - f(\hat{U}) = f(\hat{e}) \Rightarrow$  A posteriori error estimate is obtained *directly* using the stability of the original PDE  
(Katsaounis, K., 2015: A posteriori error estimates for the linear Schrödinger equation)

② Set  $v = \hat{e}$  in (4) and then take real parts to obtain:

$$\frac{1}{2} \frac{d}{dt} \|\hat{e}(t)\|^2 = \lambda \operatorname{Rei} \langle f(u) - f(\hat{U}), \hat{e} \rangle(t) - \operatorname{Re} \langle \hat{r}, \hat{e} \rangle(t), \quad t \in I_n$$

③ **RECALL:**  $f(z) = |z|^{2p} z$

Q: How do we handle  $\operatorname{Rei} \langle f(u) - f(\hat{U}), \hat{e} \rangle(t)$ ?

# Main Ingredients

(I) **Mean Value Theorem:** For  $t \in [0, T]$ ,

$$f(u) - f(\hat{U}) = D_{\hat{e}}f(w), \quad w = su + (1-s)\hat{U}, \quad s(t) \in [0, 1]$$

$$(II) \quad (a+b)^q \leq \gamma(q)(a^q + b^q), \quad a, b \geq 0, \quad \gamma(q) := \begin{cases} 2^{q-1}, & q \geq 1 \\ 1, & 0 \leq q \leq 1, \end{cases}$$

$$(III) \quad \text{Gagliardo-Nirenberg inequality: } \|v\|_{L^{2p+2}} \leq \beta \|\nabla v\|^\zeta \|v\|^{1-\zeta}, \quad \zeta := \frac{pd}{2(p+1)}$$

(IV) **Conservation Laws:** For  $t \in [0, T]$ ,

▶ **Mass Conservation:**  $\|u(t)\| = \|u_0\|$

▶ **Energy Conservation:**  $\|\nabla u(t)\|^2 - \|\nabla u_0\|^2 = \frac{\lambda}{p+1} (\|u(t)\|_{L^{2p+2}}^{2p+2} - \|u_0\|_{L^{2p+2}}^{2p+2})$

○ (I)+(II)  $\Rightarrow$

$$(5) \quad |\operatorname{Rei}\langle f(u) - f(\hat{U}), \hat{e} \rangle(t)| \leq 2^{2p} p \left( \|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} + \|\hat{U}(t)\|_{L^\infty}^{2p} \|\hat{e}(t)\|^2 \right)$$

# Estimation of $\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2}$

- 1 Gagliardo-Nirenberg inequality  $\Rightarrow$

$$(6) \quad \|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \|\nabla \hat{e}(t)\|^{pd} \|\hat{e}(t)\|^{p(2-d)} \|\hat{e}(t)\|^2, \quad B := \beta^{2p+2}$$

- 2 Since  $p(2-d) \geq 0$  for  $d = 1, 2$ :

$$(7) \quad \begin{aligned} \|\hat{e}(t)\|^{p(2-d)} &\leq \left( \|u(t)\| + \|\hat{U}(t)\| \right)^{p(2-d)} \\ &\leq \gamma(p(2-d)) \left( \|u(t)\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)} \right) \end{aligned}$$

- 3 Mass conservation  $\Rightarrow$

$$(8) \quad \|\hat{e}(t)\|^{p(2-d)} \leq \gamma(p(2-d)) \left( \|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)} \right)$$

- 4 Use (8) in (6) to obtain:

$$(9) \quad \|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \gamma(p(2-d)) \left( \|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)} \right) \|\nabla \hat{e}(t)\|^{pd} \|\hat{e}(t)\|^2$$

# Estimation of $\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2}$

- 1 Gagliardo-Nirenberg inequality  $\Rightarrow$

$$(6) \quad \|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \|\nabla \hat{e}(t)\|^{pd} \|\hat{e}(t)\|^{p(2-d)} \|\hat{e}(t)\|^2, \quad B := \beta^{2p+2}$$

- 2 Since  $p(2-d) \geq 0$  for  $d = 1, 2$ :

$$(7) \quad \begin{aligned} \|\hat{e}(t)\|^{p(2-d)} &\leq \left( \|u(t)\| + \|\hat{U}(t)\| \right)^{p(2-d)} \\ &\leq \gamma(p(2-d)) \left( \|u(t)\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)} \right) \end{aligned}$$

- 3 Mass conservation  $\Rightarrow$

$$(8) \quad \|\hat{e}(t)\|^{p(2-d)} \leq \gamma(p(2-d)) \left( \|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)} \right)$$

- 4 Use (8) in (6) to obtain:

$$(9) \quad \|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \gamma(p(2-d)) \left( \|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)} \right) \|\nabla \hat{e}(t)\|^{pd} \|\hat{e}(t)\|^2$$

\* NOTE: If  $d = 3 \Rightarrow p(2-d) < 0$  and (6) *fails*

# Estimation of the nonlinear term: Final steps

- 1 Substitute (9) into (5) ( $|\operatorname{Re} i \langle f(u) - f(\hat{U}), \hat{e} \rangle(t)| \leq 2^{2p} \rho (\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} + \|\hat{U}(t)\|_{L^\infty}^{2p} \|\hat{e}(t)\|^2)$ ) to obtain:

$$|\lambda \operatorname{Re} i \langle f(u) - f(\hat{U}), \hat{e} \rangle(t)| \leq A \left( (\|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)}) \|\nabla \hat{e}(t)\|^{pd} + \|\hat{U}(t)\|_{L^\infty}^{2p} \right) \|\hat{e}(t)\|^2$$

A: *explicitly known constant*

# Estimation of the nonlinear term: Final steps

- 1 Substitute (9) into (5) ( $|\operatorname{Re} i \langle f(u) - f(\hat{U}), \hat{e} \rangle(t)| \leq 2^{2p} \rho (\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} + \|\hat{U}(t)\|_{L^\infty}^{2p} \|\hat{e}(t)\|^2)$ ) to obtain:

$$|\lambda \operatorname{Re} i \langle f(u) - f(\hat{U}), \hat{e} \rangle(t)| \leq A \left( (\|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)}) \|\nabla \hat{e}(t)\|^{pd} + \|\hat{U}(t)\|_{L^\infty}^{2p} \right) \|\hat{e}(t)\|^2$$

A: *explicitly known constant*

- 2 Recall that:

$$\frac{1}{2} \frac{d}{dt} \|\hat{e}(t)\|^2 = \lambda \operatorname{Re} i \langle f(u) - f(\hat{U}), \hat{e} \rangle(t) - \operatorname{Re} \langle \hat{r}, \hat{e} \rangle(t), \quad t \in I_n$$

- 3 Thus, for  $t \in I_n$ :

$$\frac{d}{dt} \|\hat{e}(t)\| \leq A \left( (\|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)}) \|\nabla \hat{e}(t)\|^{pd} + \|\hat{U}(t)\|_{L^\infty}^{2p} \right) \|\hat{e}(t)\| + \|\hat{r}(t)\|$$

$\Rightarrow$  Gronwall's inequality  $\rightsquigarrow$  A posteriori error bound for  $\hat{e}$  in the  $L^\infty(L^2)$ -norm as long as we can estimate  $\|\nabla \hat{e}(t)\|^{pd}$  a posteriori

How do we estimate  $\|\nabla \hat{e}(t)\|^{pd}$  a posteriori?

## Estimation of $\|\nabla \hat{e}(t)\|^{pd}$

- $pd \geq 0 \Rightarrow \|\nabla \hat{e}(t)\|^{pd} \leq \gamma(pd) \left( \|\nabla \hat{U}(t)\|^{pd} + \|\nabla u(t)\|^{pd} \right)$
- A posteriori bound for  $\|\nabla u(t)\|$ :

**LEMMA:** There exists  $G(u_0)$  *explicitly computable* (and depending also on  $\lambda, \alpha, p, d$ ) such that

$$\|\nabla u(t)\| \leq G(u_0), \quad t \in [0, T].$$



# Estimation of $\|\nabla \hat{e}(t)\|^{pd}$

- $pd \geq 0 \Rightarrow \|\nabla \hat{e}(t)\|^{pd} \leq \gamma(pd) \left( \|\nabla \hat{U}(t)\|^{pd} + \|\nabla u(t)\|^{pd} \right)$
- A posteriori bound for  $\|\nabla u(t)\|$ :

**LEMMA:** There exists  $G(u_0)$  *explicitly computable* (and depending also on  $\lambda, \alpha, p, d$ ) such that

$$\|\nabla u(t)\| \leq G(u_0), \quad t \in [0, T].$$

\* The proof is technical and uses the Gagliardo-Nirenberg inequality, and mass & energy conservation for the continuous problem.

\* For  $p = p^* = \frac{2}{d}$ ,  $G(u_0) \sim \frac{1}{1 - \Gamma(u_0)} \Rightarrow G(u_0) \rightarrow \infty$  as  $\Gamma(u_0) \rightarrow 1$

# The main theorem

○ Let

$$\mathcal{H}(\hat{U}, u_0; t) := A\left(\gamma(pd) \left(\|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)}\right) \left(G(u_0)^{pd} + \|\nabla \hat{U}(t)\|^{pd}\right) + \|\hat{U}(t)\|_{L^\infty}^{2p}\right)$$

Then

$$\frac{d}{dt} \|\hat{e}(t)\| \leq \mathcal{H}(\hat{U}, u_0; t) \|\hat{e}(t)\| + \|\hat{r}(t)\|, \quad t \in I_n$$

○ **RECALL:**  $\hat{r} = -i\alpha\Delta(\hat{U} - U) - i\lambda(f(\hat{U}) - f(U)) - i\lambda(|U|^{2p} - \Phi^{n+\frac{1}{2}})U$

# The main theorem

○ Let

$$\mathcal{H}(\hat{U}, u_0; t) := A\left(\gamma(pd)\left(\|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)}\right)\left(G(u_0)^{pd} + \|\nabla\hat{U}(t)\|^{pd}\right) + \|\hat{U}(t)\|_{L^\infty}^{2p}\right)$$

Then 
$$\frac{d}{dt}\|\hat{e}(t)\| \leq \mathcal{H}(\hat{U}, u_0; t)\|\hat{e}(t)\| + \|\hat{r}(t)\|, \quad t \in I_n$$

○ **RECALL:**  $\hat{r} = -i\alpha\Delta(\hat{U} - U) - i\lambda(f(\hat{U}) - f(U)) - i\lambda(|U|^{2p} - \Phi^{n+\frac{1}{2}})U$

○ Gronwall's inequality gives:

**THEOREM** (a posteriori error estimate in  $L^\infty(L^2)$ ):

$$\|(u - \hat{U})(t)\| \leq \exp\left(\int_0^t \mathcal{H}(\hat{U}, u_0; s) ds\right) \int_0^t \|\hat{r}(s)\| ds, \quad t \in [0, T]$$

- Is the estimate sharp for the non blowup cases?
- What is the behaviour of  $\exp\left(\int_0^t \mathcal{H}(\hat{U}, u_0; s) ds\right)$ ?
  - ① It tends to  $\infty$  *exponentially fast* if  $p = p^* = \frac{2}{d}$  and  $\Gamma(u_0) \rightarrow 1$
  - ② What happens in other cases?  $\rightsquigarrow$  *Numerical experiments*

# The main theorem

○ Let

$$\mathcal{H}(\hat{U}, u_0; t) := A\left(\gamma(pd)\left(\|u_0\|^{p(2-d)} + \|\hat{U}(t)\|^{p(2-d)}\right)\left(G(u_0)^{pd} + \|\nabla\hat{U}(t)\|^{pd}\right) + \|\hat{U}(t)\|_{L^\infty}^{2p}\right)$$

Then 
$$\frac{d}{dt}\|\hat{e}(t)\| \leq \mathcal{H}(\hat{U}, u_0; t)\|\hat{e}(t)\| + \|\hat{r}(t)\|, \quad t \in I_n$$

○ **RECALL:**  $\hat{r} = -i\alpha\Delta(\hat{U} - U) - i\lambda(f(\hat{U}) - f(U)) - i\lambda(|U|^{2p} - \Phi^{n+\frac{1}{2}})U$

○ Gronwall's inequality gives:

**THEOREM** (a posteriori error estimate in  $L^\infty(L^2)$ ):

$$\|(u - \hat{U})(t)\| \leq \exp\left(\int_0^t \mathcal{H}(\hat{U}, u_0; s) ds\right) \int_0^t \|\hat{r}(s)\| ds, =: \mathcal{E}(t)^{1/p} \quad t \in [0, T]$$

- Is the estimate sharp for the non blowup cases?
- What is the behaviour of  $\exp\left(\int_0^t \mathcal{H}(\hat{U}, u_0; s) ds\right)$ ?
  - ① It tends to  $\infty$  *exponentially fast* if  $p = p^* = \frac{2}{d}$  and  $\Gamma(u_0) \rightarrow 1$
  - ② What happens in other cases?  $\rightsquigarrow$  *Numerical experiments*

# An improved estimate for $d = 1$

①  $\|\hat{e}(t)\| \leq \mathcal{E}(t)^{1/p}$

② Go back to  $\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \|\nabla \hat{e}(t)\|^{pd} \|\hat{e}(t)\|^{p(2-d)} \|\hat{e}(t)\|$

▶ For  $d = 2$ ,  $\|\hat{e}(t)\|^{p(2-d)} = 1$

▶ For  $d = 1$ , instead of using  $\|\hat{e}(t)\|^p \leq \gamma(p)(\|u_0\|^p + \|\hat{U}(t)\|^p)$  (triangular inequality), use  $\|\hat{e}(t)\|^p \leq \mathcal{E}(t)$  to get

$$\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \|\nabla \hat{e}(t)\|^p \mathcal{E}(t) \|\hat{e}(t)\|^2$$

③ Estimate  $\|\nabla \hat{e}(t)\|^p$  as before

④ Use Gronwall's inequality to obtain

# An improved estimate for $d = 1$

- 1  $\|\hat{e}(t)\| \leq \mathcal{E}(t)^{1/p}$
- 2 Go back to  $\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \|\nabla \hat{e}(t)\|^{pd} \|\hat{e}(t)\|^{p(2-d)} \|\hat{e}(t)\|$ 
  - ▶ For  $d = 2$ ,  $\|\hat{e}(t)\|^{p(2-d)} = 1$
  - ▶ For  $d = 1$ , instead of using  $\|\hat{e}(t)\|^p \leq \gamma(p)(\|u_0\|^p + \|\hat{U}(t)\|^p)$  (triangular inequality), use  $\|\hat{e}(t)\|^p \leq \mathcal{E}(t)$  to get

$$\|\hat{e}(t)\|_{L^{2p+2}}^{2p+2} \leq B \|\nabla \hat{e}(t)\|^p \mathcal{E}(t) \|\hat{e}(t)\|^2$$

- 3 Estimate  $\|\nabla \hat{e}(t)\|^p$  as before
- 4 Use Gronwall's inequality to obtain

**THEOREM** (improved a posteriori error estimate in  $L^\infty(L^2)$  for  $d = 1$ ):

$$\|(u - \hat{U})(t)\| \leq \exp\left(\int_0^t \mathcal{K}(\hat{U}, u_0; s) ds\right) \int_0^t \|\hat{r}(s)\| ds, \quad t \in [0, T],$$

$$\text{with } \mathcal{K}(\hat{U}, u_0; t) := A \left( \mathcal{E}(t) \left( G(u_0)^p + \|\nabla \hat{U}(t)\|^p \right) + \|\hat{U}(t)\|_{L^\infty}^{2p} \right)$$

\* Since  $\mathcal{E}(T) \rightarrow 0$  as  $k \rightarrow 0$ , we expect  $\int_0^T \mathcal{K}(\hat{U}, u_0; s) ds \rightarrow \int_0^T \|u(s)\|_{L^\infty}^{2p} ds$  as  $k \rightarrow 0$

# Modified relaxation Crank-Nicolson-Galerkin method

## ○ SPATIAL DISCRETISATION: FINITE ELEMENTS

- $\{\mathcal{T}_n\}_{n=0}^N$  family of triangulations of  $\Omega$
- Finite element spaces:  $\mathbb{V}^n := \{V_n \in H_0^1(\Omega) : \forall K \in \mathcal{T}_n, V_n|_K \in \mathbb{P}^r\}$ 
  - ▶  $\mathbb{V}^n$  are allowed to change from one time step to another

# Modified relaxation Crank-Nicolson-Galerkin method

## ○ SPATIAL DISCRETISATION: FINITE ELEMENTS

- $\{\mathcal{T}_n\}_{n=0}^N$  family of triangulations of  $\Omega$
- Finite element spaces:  $\mathbb{V}^n := \{V_n \in H_0^1(\Omega) : \forall K \in \mathcal{T}_n, V_n|_K \in \mathbb{P}^r\}$ 
  - ▶  $\mathbb{V}^n$  are allowed to change from one time step to another

○ Modified relaxation Crank-Nicolson-Galerkin method: Seek approximations  $U^n \in \mathbb{V}^n$  to  $u(t_n)$  such that for  $0 \leq n \leq N-1$ :

$$\begin{cases} \frac{k_{n-1}}{k_n + k_{n-1}} \Phi^{n+\frac{1}{2}} + \frac{k_n}{k_n + k_{n-1}} \mathcal{P}^{n+1} \Phi^{n-\frac{1}{2}} = \mathcal{P}^{n+1} (|U^n|^{2p}), \\ \frac{U^{n+1} - \mathcal{P}^{n+1} U^n}{k_n} - i\alpha \frac{\Delta^{n+1} U^{n+1} + \mathcal{P}^{n+1} \Delta^n U^n}{2} = i\lambda \mathcal{P}^{n+1} \left( \Phi^{n+\frac{1}{2}} U^{n+\frac{1}{2}} \right), \end{cases}$$

with  $\Phi^{-\frac{1}{2}} = \mathcal{P}^0 (|u_0|^{2p})$ ,  $U^0 = \mathcal{P}^0 u_0$

- $\mathcal{P}^n : L^2(\Omega) \rightarrow \mathbb{V}^n$  is the  $L^2$ -projection onto  $\mathbb{V}^n$ :  
 $\langle \mathcal{P}^n v, V_n \rangle = \langle v, V_n \rangle, \forall V_n \in \mathbb{V}^n, v \in L^2(\Omega)$
- $-\Delta^n : H_0^1(\Omega) \rightarrow \mathbb{V}^n$  is the discrete laplacian onto  $\mathbb{V}^n$ :  
 $\langle -\Delta^n v, V_n \rangle = \langle \nabla v, \nabla V_n \rangle, \forall V_n \in \mathbb{V}^n, v \in H_0^1(\Omega)$



# Time–Space reconstruction

ELLIPTIC RECONSTRUCTION (Makridakis & Nochetto, 2006):

$$\langle \nabla \mathcal{R}^n V_n, \nabla \varphi \rangle = \langle -\Delta^n V_n, \varphi \rangle, \quad \forall \varphi \in H_0^1(\Omega)$$

SPACE RECONSTRUCTION:

$$U(t) = \ell_0^n(t)U^n + \ell_1^n(t)U^{n+1} \Rightarrow \omega(t) := \ell_0^n(t)\mathcal{R}^n U^n + \ell_1^n(t)\mathcal{R}^{n+1}U^{n+1}, \quad t \in I_n$$

TIME – SPACE RECONSTRUCTION:

$$\begin{aligned} \hat{U}(t) := & \mathcal{R}^n U^n + \frac{t - t_n}{k_n} (\mathcal{R}^{n+1} \mathcal{P}^{n+1} U^n - \mathcal{R}^n U^n) + i\alpha \int_{t_n}^t \mathcal{R}^{n+1} \Theta(s) ds \\ & + i\lambda \int_{t_n}^t \mathcal{R}^{n+1} \mathcal{P}^{n+1} \left( \Phi^{n+\frac{1}{2}} U(s) \right) ds, \quad t \in I_n, \end{aligned}$$

$$\Theta(t) := \ell_0^n(t)\mathcal{P}^{n+1}\Delta^n U^n + \ell_1^n(t)\Delta^{n+1}U^{n+1}, \quad t \in I_n;$$

○ PROPERTIES:

- 1  $\hat{U}$  is a **time-continuous function** and satisfies  $\hat{U}(t_n) = \mathcal{R}^n U^n$ ,  $0 \leq n \leq N$
- 2  $\hat{U}$  satisfies a **perturbation of the original P.D.E.**
- 3  $\hat{U} - \omega$  is **second order accurate in time**

## A posteriori error estimates for the fully discrete scheme: The idea

- Let  $e := u - U$ . Write  $e = \epsilon + \sigma + \hat{\rho}$  with  $\epsilon := \omega - U$ ,  $\sigma := \hat{U} - \omega$ ,  $\hat{\rho} := u - \hat{U}$   
Then

$$\max_{0 \leq t \leq t_m} \|e(t)\| \leq \max_{0 \leq t \leq t_m} \|\epsilon(t)\| + \max_{0 \leq t \leq t_m} \|\sigma(t)\| + \max_{0 \leq t \leq t_m} \|\hat{\rho}(t)\|$$

## A posteriori error estimates for the fully discrete scheme: The idea

- Let  $\mathbf{e} := \mathbf{u} - \mathbf{U}$ . Write  $\mathbf{e} = \boldsymbol{\epsilon} + \boldsymbol{\sigma} + \hat{\boldsymbol{\rho}}$  with  $\boldsymbol{\epsilon} := \boldsymbol{\omega} - \mathbf{U}$ ,  $\boldsymbol{\sigma} := \hat{\mathbf{U}} - \boldsymbol{\omega}$ ,  $\hat{\boldsymbol{\rho}} := \mathbf{u} - \hat{\mathbf{U}}$   
Then

$$\max_{0 \leq t \leq t_m} \|\mathbf{e}(t)\| \leq \max_{0 \leq t \leq t_m} \|\boldsymbol{\epsilon}(t)\| + \max_{0 \leq t \leq t_m} \|\boldsymbol{\sigma}(t)\| + \max_{0 \leq t \leq t_m} \|\hat{\boldsymbol{\rho}}(t)\|$$

- 1  $\boldsymbol{\epsilon} := \boldsymbol{\omega} - \mathbf{U}$  the *elliptic error*,  $\max_{0 \leq t \leq t_m} \|\boldsymbol{\epsilon}(t)\| \leq C_2 \mathcal{E}_m^{\mathbb{S},0}$ 
  - ▶ The error  $\boldsymbol{\epsilon}$  is estimated *a posteriori* via *elliptic residual-type error estimators*
- 2  $\boldsymbol{\sigma} := \hat{\mathbf{U}} - \boldsymbol{\omega}$  the *error due to the time reconstruction*,  $\max_{0 \leq t \leq t_m} \|\boldsymbol{\sigma}(t)\| \leq \mathcal{E}_m^{\mathbb{T},0}$ 

( $\boldsymbol{\sigma}$  is handled similarly to the difference between  $\mathbf{U}$  and the reconstruction in the time-discrete case)

## A posteriori error estimates for the fully discrete scheme: The idea

- Let  $e := u - U$ . Write  $e = \epsilon + \sigma + \hat{\rho}$  with  $\epsilon := \omega - U$ ,  $\sigma := \hat{U} - \omega$ ,  $\hat{\rho} := u - \hat{U}$   
Then

$$\max_{0 \leq t \leq t_m} \|e(t)\| \leq \max_{0 \leq t \leq t_m} \|\epsilon(t)\| + \max_{0 \leq t \leq t_m} \|\sigma(t)\| + \max_{0 \leq t \leq t_m} \|\hat{\rho}(t)\|$$

- 1  $\epsilon := \omega - U$  the *elliptic error*,  $\max_{0 \leq t \leq t_m} \|\epsilon(t)\| \leq C_2 \mathcal{E}_m^{S,0}$ 
  - ▶ The error  $\epsilon$  is estimated *a posteriori* via *elliptic residual-type error estimators*
- 2  $\sigma := \hat{U} - \omega$  the *error due to the time reconstruction*,  $\max_{0 \leq t \leq t_m} \|\sigma(t)\| \leq \mathcal{E}_m^{T,0}$ 

( $\sigma$  is handled similarly to the difference between  $U$  and the reconstruction in the time-discrete case)
- 3  $\hat{\rho} := u - \hat{U}$  the *main error*  
 $\hat{\rho}$  is handled as in the *time-discrete cases*  
... but with arguments more technically involved!

# A posteriori estimates for the fully discrete scheme

**THEOREM** (a posteriori error estimate in  $L^\infty(L^2)$ ): For  $1 \leq m \leq N$ :

$$\max_{0 \leq t \leq t_m} \|(u - U)(t)\| \leq C_2 \mathcal{E}_m^{S,0} + \mathcal{E}_m^{T,0} + \exp\left(\int_0^{t_m} \mathcal{N}(U, u_0; t) dt\right) \times \\ \left(\|u_0 - U^0\| + C_2 \eta_{2, \mathbb{V}^0}(U^0) + \mathcal{E}_m^{T,1} + \mathcal{E}_m^{T,2} + C_2(\mathcal{E}_m^{S,1} + \mathcal{E}_m^{S,2}) + \widehat{C}_2 \mathcal{E}_m^{S,3} + \mathcal{E}_m^C + \mathcal{E}_m^D\right)$$

- $\mathcal{N}(U, u_0; t)$  is the *fully discrete analogue* of  $\mathcal{H}(\hat{U}, u_0; t)$  in the time discrete scheme
- $\mathcal{E}_m^{T,0}, \mathcal{E}_m^{T,1}, \mathcal{E}_m^{T,2}$ : **time-estimators**,  $\mathcal{E}_m^{S,0}, \mathcal{E}_m^{S,1}, \mathcal{E}_m^{S,2}, \mathcal{E}_m^{S,3}$ : **space-estimators**
- $\mathcal{E}_m^C$ : **coarsening estimator**,  $\mathcal{E}_m^D$ : **linearisation estimator**
- $\eta_{2, \mathbb{V}^n}(V^n) := \left\{ \sum_{K \in \mathcal{T}_n} \left( \|h_K^2(\Delta - \Delta^n)V^n\|_{L^2(K)}^2 + \|h_K^{\frac{3}{2}} J[\nabla V^n]\|_{L^2(\partial K)}^2 \right) \right\}^{\frac{1}{2}}$ ,  $0 \leq n \leq N$

**THEOREM** (improved a posteriori error estimate in  $L^\infty(L^2)$  for  $d = 1$ ): For  $1 \leq m \leq N$ :

$$\max_{0 \leq t \leq t_m} \|(u - U)(t)\| \leq C_2 \mathcal{E}_m^{S,0} + \mathcal{E}_m^{T,0} + \exp\left(\int_0^{t_m} \mathcal{M}(U, u_0; t) dt\right) \times \\ \left(\|u_0 - U^0\| + C_2 \eta_{2, \mathbb{V}^0}(U^0) + \mathcal{E}_m^{T,1} + \mathcal{E}_m^{T,2} + C_2(\mathcal{E}_m^{S,1} + \mathcal{E}_m^{S,2}) + \widehat{C}_2 \mathcal{E}_m^{S,3} + \mathcal{E}_m^C + \mathcal{E}_m^D\right)$$

- $\mathcal{M}(U, u_0; t)$  is the *fully discrete analogue* of  $\mathcal{K}(\hat{U}, u_0; t)$  in the time discrete scheme

# Explicit form of the estimators

## ○ TIME ESTIMATORS:

$$\mathcal{E}_m^{T,0} := \max_{1 \leq n \leq m} \frac{k_{n-1}^2}{8} \left[ \|\tilde{\delta}W^n\| + C_2 \eta_{2,\mathbb{V}^n}(\tilde{\delta}W^n) \right], \quad \tilde{\delta}W^{n+1} := i\alpha \partial_t \Theta(t) + i\lambda \mathcal{P}^{n+1} \left( \Phi^{n+\frac{1}{2}} \bar{\delta}U^n \right)$$

$$\mathcal{E}_m^{T,1} := \sum_{n=1}^m \frac{\alpha k_{n-1}^3}{12} \|\Delta^n \tilde{\delta}W^n\|, \quad \mathcal{E}_m^{T,2} := \sum_{n=1}^m \frac{k_n^3}{6} \mathcal{L}_{31}^n$$

$$\mathcal{L}_{31}^n := (\rho + \frac{1}{2}) \left( \varepsilon_n^{T,\infty} + \varepsilon_n^{S,\infty} + \max \left\{ \|U^{n-1}\|_{L^\infty}, \|U^n\|_{L^\infty} \right\} \right)^{2\rho} \left( \|\tilde{\delta}W^n\| + C_2 \eta_{2,\mathbb{V}^n}(\tilde{\delta}W^n) \right)$$

$$\varepsilon_n^{T,\infty} := \frac{k_{n-1}^2}{8} \left[ \|\tilde{\delta}W^n\|_{L^\infty} + C_\infty (\ln \underline{h}_n)^2 \eta_{\infty,\mathbb{V}^n}(\tilde{\delta}W^n) \right]$$

$$\varepsilon_n^{S,\infty} := \max \left\{ (\ln \underline{h}_n)^2 \eta_{\infty,\mathbb{V}^n}(U^n), (\ln \underline{h}_{n-1})^2 \eta_{\infty,\mathbb{V}^{n-1}}(U^{n-1}) \right\}$$

## ○ SPACE ESTIMATORS:

$$\mathcal{E}_m^{S,0} := \max_{0 \leq n \leq m} \eta_{2,\mathbb{V}^n}(U^n), \quad \mathcal{E}_m^{S,1} := \sum_{n=1}^m \frac{k_{n-1}^2}{4} \eta_{2,\mathbb{V}^n}(\tilde{\delta}W^n), \quad \mathcal{E}_m^{S,3} := \sum_{n=1}^m k_{n-1} \eta_{2,\hat{\mathbb{V}}^n} \left( \frac{U^n}{k_{n-1}}, \frac{U^{n-1}}{k_{n-1}} \right)$$

$$\mathcal{E}_m^{S,0} := \sum_{n=1}^m \mathcal{L}_{32}^n \max \left\{ \eta_{2,\mathbb{V}^n}(U^n), \eta_{2,\mathbb{V}^{n-1}}(U^{n-1}) \right\}, \quad \mathcal{L}_{32}^n := (2\rho + 1) \left( C_\infty \varepsilon_n^{S,\infty} + \max \left\{ \|U^n\|_{L^\infty}, \|U^{n-1}\|_{L^\infty} \right\} \right)^{2\rho}$$

## ○ COARSENING & LINEARISATION ESTIMATORS:

$$\mathcal{E}_m^C := \sum_{n=0}^{m-1} \int_{I_n} \|(I - \mathcal{P}^{n+1}) \left( \frac{U^n}{k_n} + i\alpha \ell_0^n(t) \Delta^n U^n \right)\| dt, \quad \mathcal{E}_m^D := \sum_{n=0}^{m-1} \int_{I_n} \left\| \left( f(U) - \mathcal{P}^{n+1} \left( \Phi^{n+\frac{1}{2}} U \right) \right) (t) \right\| dt$$

$$\eta_{\infty,\mathbb{V}^n}(V^n) := \max_{K \in \mathcal{T}_n} \left\{ \|h_K^2 (\Delta - \Delta^n) V^n\|_{L^\infty(K)} + \|h_K J[\nabla V^n]\|_{L^\infty(\partial K)} \right\}, \quad \underline{h}_n := \min_{K \in \mathcal{T}_n} h_K$$

$$\eta_{2,\hat{\mathbb{V}}^n}(V^n, V^{n-1}) := \left\{ \sum_{K \in \hat{\mathcal{T}}_n} \left( \|h_K^2 [(\Delta - \Delta^n) V^n - (\Delta - \Delta^{n-1}) V^{n-1}]\|_{L^2(K)}^2 + \|h_K^{\frac{3}{2}} J[\nabla V^n - \nabla V^{n-1}]\|_{L^2(\hat{\mathcal{S}}_K^n)}^2 \right) \right\}^{\frac{1}{2}}$$

# A numerical implementation

## ○ EXAMPLE: Exact solution

- $d = 1$ ,  $[a, b] = [-30, 30]$ ,  $T = 1$ ,  $\alpha = 1$   $\lambda = 2$ ,  $p = 1$
- uniform grids, B-splines of degree  $r$ ,  $h = \frac{b-a}{M}$ ,  $k \sim h^{\frac{r+1}{2}}$
- $u(x, t) = i \exp(i(2\omega x + t(1 - \omega^2))) / \cosh(x - x_0 - 4\omega t)$
- $x_0 = 0$ ,  $\omega = \frac{1}{4}$

# A numerical implementation

## ○ EXAMPLE: Exact solution

- $d = 1$ ,  $[a, b] = [-30, 30]$ ,  $T = 1$ ,  $\alpha = 1$ ,  $\lambda = 2$ ,  $p = 1$
- uniform grids, B-splines of degree  $r$ ,  $h = \frac{b-a}{M}$ ,  $k \sim h^{\frac{r+1}{2}}$
- $u(x, t) = i \exp(i(2\omega x + t(1 - \omega^2))) / \cosh(x - x_0 - 4\omega t)$
- $x_0 = 0$ ,  $\omega = \frac{1}{4}$

## ○ Behaviour of the exponential terms:

Let  $\mathcal{E}_N^{\mathcal{M}} := \sum_{n=0}^{N-1} \int_{I_n} \mathcal{M}(U, u_0; t) dt$  and  $\mathcal{E}_N^{\mathcal{N}} := \sum_{n=0}^{N-1} \int_{I_n} \mathcal{N}(U, u_0; t) dt$

	$r = 1(\text{linear})$		$r = 2(\text{quadratic})$		$r = 3(\text{cubic})$	
$M$	$\mathcal{E}_N^{\mathcal{M}}$	$\mathcal{E}_N^{\mathcal{N}}$	$\mathcal{E}_N^{\mathcal{M}}$	$\mathcal{E}_N^{\mathcal{N}}$	$\mathcal{E}_N^{\mathcal{M}}$	$\mathcal{E}_N^{\mathcal{N}}$
2400	7.847	17.423	7.820	2.233	7.820	1.164
3600	7.831	9.757	7.817	1.613	7.817	1.071
4800	7.825	6.737	7.816	1.382	7.816	1.040
6000	7.821	5.187	7.815	1.267	7.815	1.025
7200	7.820	4.263	7.814	1.201	7.815	1.018
8400	7.818	3.658	7.813	1.158	7.815	1.013
9600	7.818	3.234	7.813	1.128	7.815	1.010

- As resolution increases,  $\mathcal{E}_N^{\mathcal{N}} \rightarrow \int \|u(t)\|_{L^\infty}^{2p} dt = 1$ , for this example



# EOC of the estimators for quadratic splines ( $r = 2$ )

$M$	$\varepsilon_N^{S,0}$	EOC	$\varepsilon_N^{S,1}$	EOC	$\varepsilon_N^{S,2}$	EOC	$\varepsilon_N^{S,3}$	EOC
2400	1.3817E-05	-	2.64149E-07	-	4.1466E-05	-	2.5055E-05	-
3600	4.0936E-06	3.0001	4.25720E-08	4.5018	1.2283E-05	3.0007	7.4230E-06	3.0003
4800	1.7270E-06	3.0000	1.16949E-08	4.4912	5.1813E-06	3.0003	3.1315E-06	3.0001
6000	8.8421E-07	3.0000	4.28570E-09	4.4988	2.6527E-06	3.0002	1.6033E-06	3.0001
7200	5.1169E-07	3.0000	1.88822E-09	4.4956	1.5351E-06	3.0001	9.2783E-07	3.0000
8400	3.2223E-07	3.0000	9.44191E-10	4.4960	9.6671E-07	3.0001	5.8429E-07	3.0000
9600	2.1587E-07	3.0000	5.20390E-10	4.4615	6.4762E-07	3.0000	3.9142E-07	3.0000

$k-1$	$\varepsilon_N^{T,0}$	EOC	$\varepsilon_N^{T,1}$	EOC	$\varepsilon_N^{T,2}$	EOC
252	8.2786E-06	-	3.1156E-04	-	1.6442E-05	-
464	2.4426E-06	2.0055	9.2190E-05	2.0007	4.8667E-06	2.0002
715	1.0288E-06	2.0032	3.8879E-05	2.0003	2.0526E-06	2.0001
1000	5.2600E-07	2.0021	1.9891E-05	2.0000	1.0501E-06	2.0000
1314	3.0466E-07	2.0016	1.1528E-05	1.9993	6.0850E-07	2.0000
1656	1.9182E-07	2.0012	7.2678E-06	1.9957	3.8324E-07	2.0000
2023	1.2854E-07	2.0010	4.8767E-06	1.9943	2.5686E-07	2.0000

$\varepsilon^{Total}$	Error	$\varepsilon^{Total} / \text{Error}$
4.1688E-04	1.6587E-05	25.13
1.2334E-04	4.9118E-06	25.11
5.2012E-05	2.0186E-06	25.77
2.6612E-05	1.0202E-06	26.09
1.5418E-05	5.8838E-07	26.20
9.7171E-06	3.7056E-07	26.22
6.5176E-06	2.4818E-07	26.26

# Reference and Ongoing & Future Work

- More details on the analysis can be found in:  
Th. Katsaounis, I.K., *A posteriori error analysis for evolution nonlinear Schrödinger equations up to the critical exponent, under minor revision in SIAM J. Numer. Anal.*, [arXiv:1601.02430](https://arxiv.org/abs/1601.02430)
- Ongoing & Future Work:
  - 1 Numerical implementation for  $d = 2$
  - 2 Construction of adaptive algorithm, *based on the a posteriori error estimators*
  - 3 Extension of the results for  $d = 3$  (other Sobolev embedding inequalities)
  - 4 Blowup cases????
    - ▶ Local a posteriori estimates for the  $2d$  cubic NLS:  
I.K., PhD Thesis, University of Crete, 2009
    - ▶ Strichartz Estimates
  - 5 Higher order time-discretisations

**Thank you very much!**