

Uniformly accurate methods for Klein-Gordon-Schrödinger and Klein-Gordon-Zahkarov systems

joint work with G. Kokkala and K. Schratz

Simon Baumstark | October 12, 2017



CRC 1173

Wave
phenomena

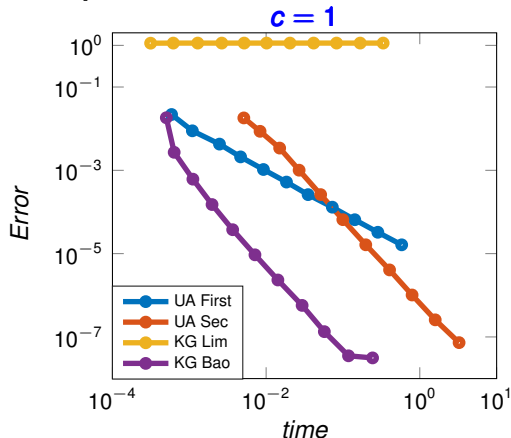
- 1 Update and introduction
- 2 Uniformly accurate scheme for the Klein-Gordon-Schrödinger system
- 3 Numerical experiments
- 4 Uniformly accurate scheme for the Klein-Gordon-Zakharov system
- 5 Outlook

Last year: UA scheme for KG equations

joint work with E. Faou and K. Schratz

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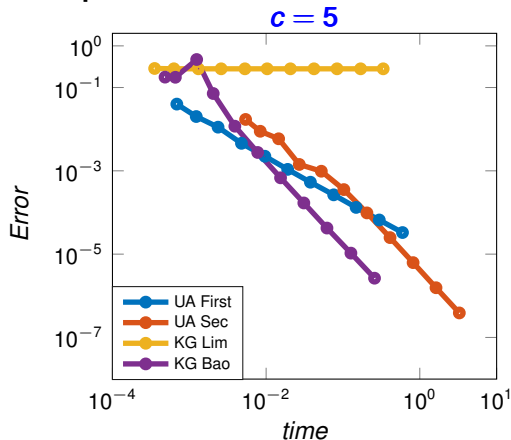
Work-precision plot:



Simulation on $x \in [0, 2\pi]$, $t \in [0, 1]$, $\tau_{ref} \approx 10^{-6}$ and $M = 256$.

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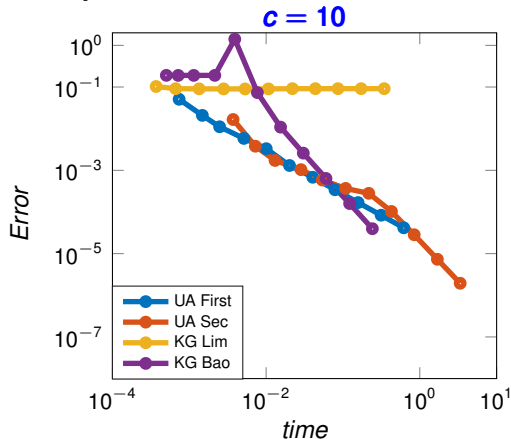
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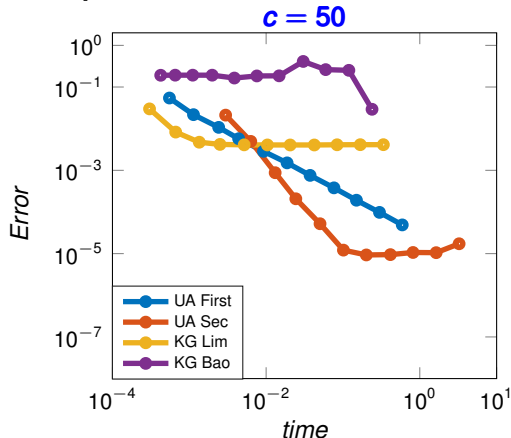
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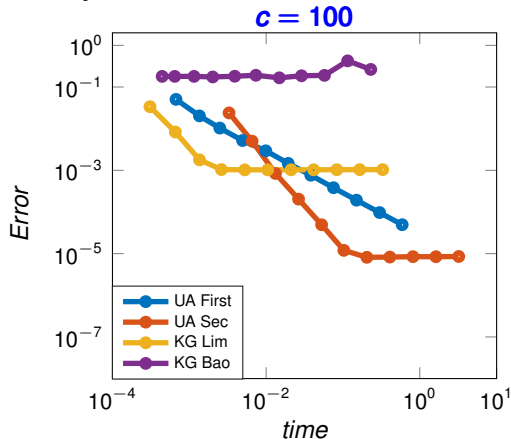
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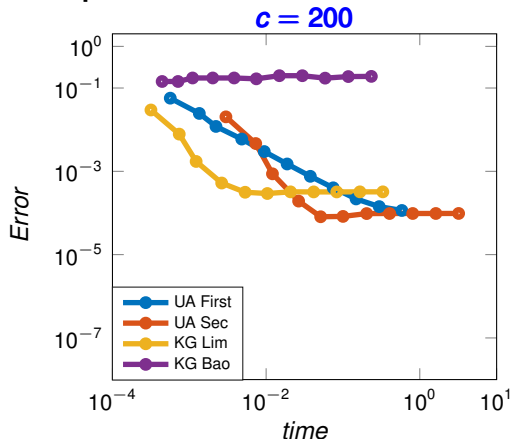
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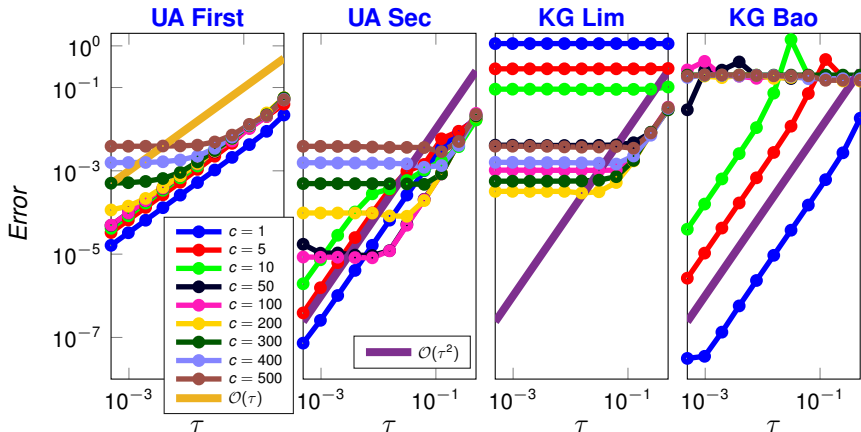
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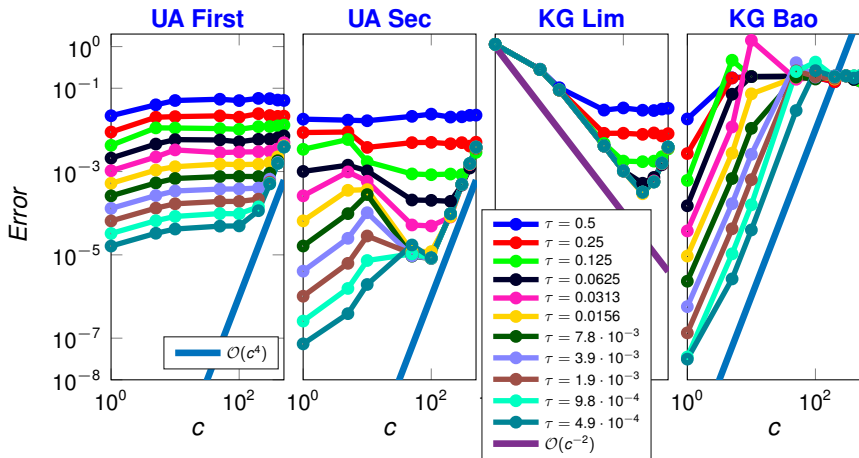
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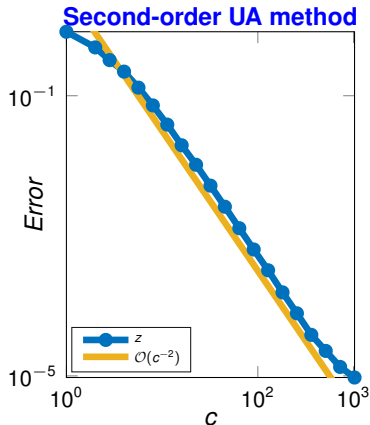
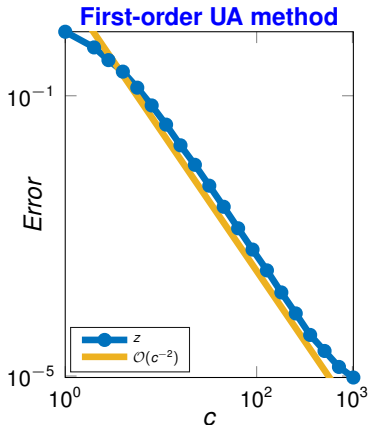
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■ Limit convergence:



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Model problem

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with initial conditions

$$z(0, x) = z_0(x), \quad \partial_t z(0, x) = c^2 z_1(x), \quad n(0, x) = n_0(x),$$

and periodic boundary conditions.

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- **Numerical Challenge:**

Highly oscillatory (non-relativistic) limit regime, i.e. $c \gg 1$.

- **Goal:** Search numerical approx. $z^n \approx z(t_n)$, $n^n \approx n(t_n)$ with $t_n = n\tau$.

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- Here: Gautschi-type method by Bao/Dong/Zhao (2013):
Exponential wave integrator pseudospectral (EWI-PS) method

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Exponential wave integrator pseudospectral (EWI-PS) method

Idea: Discretize Duhamel's formula (variation of constants formula).

Gautschi-type methods

- KGS equation $(\langle \nabla \rangle_c := \sqrt{-\Delta + c^2})$:

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- Duhamel's formula ($\bullet := c \langle \nabla \rangle_c \tau$):

$$z(t_n + \tau) = \cos(\bullet)z(t_n) + \tau \operatorname{sinc}(\bullet)z'(t_n) + c^2 \int_0^\tau \frac{\sin(c \langle \nabla \rangle_c (\tau - s))}{c \langle \nabla \rangle_c} |n(t_n + s)|^2 ds,$$

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- Problem: large derivative $\partial_t z = \mathcal{O}(c^2)$.

- Gautschi-type method applied to KGS system at $t_n = 0.6$:

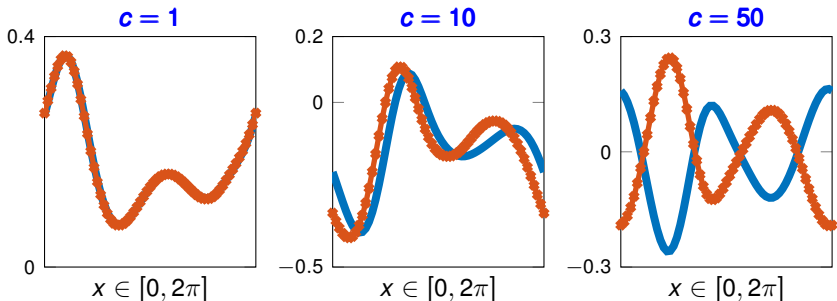


Figure: **blue line:** reference solution of z ($\tau_{\text{ref}} \approx 10^{-5}$),
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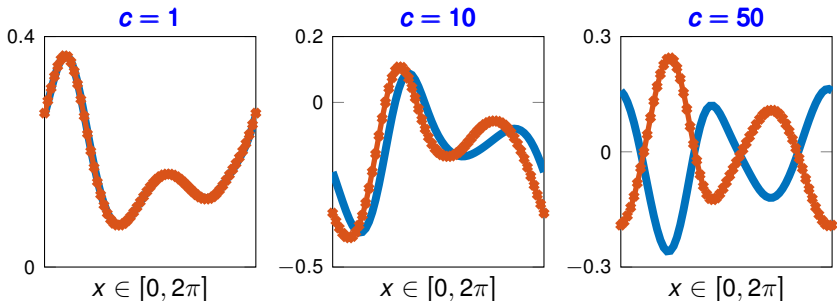


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Problem: Time step restriction for large c !

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Multiscale expansion yields **decoupled free Schrödinger limit system**

$$\begin{aligned}\partial_t u_\infty(t, x) &= -\frac{i}{2} \Delta u_\infty(t, x), & u_\infty(0) &= z_0 - iz_1, \\ \partial_t n_\infty(t, x) &= i \Delta n_\infty(t, x), & n_\infty(0) &= n_0,\end{aligned}$$

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Advantage:

Non-oscillatory limit system can be solved exactly in Fourier space!

■ Limit approximation vs. reference solution at $t_n = 0.7$:

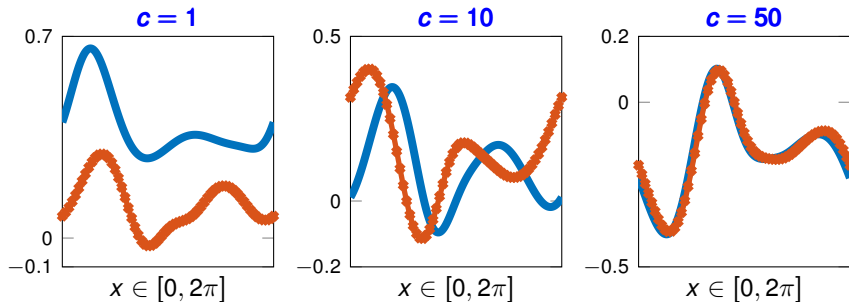


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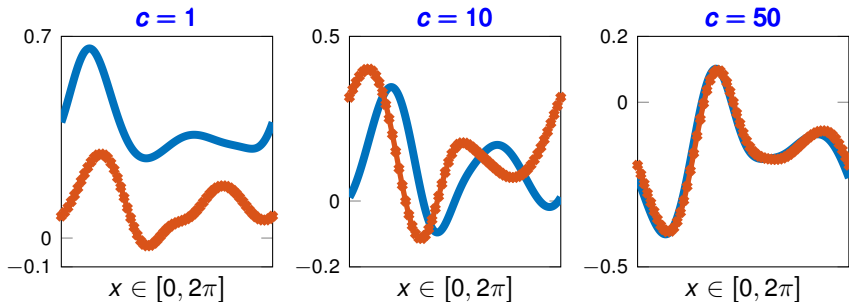


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Problem: Good approximation only for $c \gg 1$!

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Other UA scheme:

Bao/Zhao 2013: only linear convergence rate $\mathcal{O}(\tau)$ for all $c \in [1, \infty)$

Uniformly accurate scheme

- KGS as first-order system in time with $z = \frac{1}{2}(u + \bar{u})$

$$i\partial_t u = -c\langle\nabla\rangle_c u + c\langle\nabla\rangle_c^{-1}|n|^2,$$

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- \mathcal{A}_c and $c\langle\nabla\rangle_c^{-1}$ are uniformly bounded in c :

$$\|\mathcal{A}_c u\|_r^2 \leq \frac{1}{2}\|u\|_{r+2}^2, \quad \|c\langle\nabla\rangle_c^{-1} u\|_r \leq \|u\|_r.$$

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Advantage:

All operators uniformly bounded in $c \rightsquigarrow \partial_t u_*$ uniformly bounded in $c!$

Uniformly accurate scheme

A first-order UA scheme

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- Duhamel's formula yields

$$u_*(t_n + \tau) = e^{i\tau \mathcal{A}_c} u_*(t_n) - ic \langle \nabla \rangle_c^{-1} e^{i\tau \mathcal{A}_c} \int_0^\tau e^{-is \mathcal{A}_c} e^{-ic^2(t_n+s)} |n(t_n + s)|^2 ds,$$

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- We obtain:

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- Now we integrate the highly-oscillatory phases $e^{\pm ic^2(t_n+s)}$ exactly.

- Yields **first-order UA scheme**:

$$u_*^{n+1} = e^{i\tau A_c} u_*^n - i\tau e^{-ic^2 t_n} \varphi_1(-i\tau c^2) c \langle \nabla \rangle_c^{-1} e^{i\tau A_c} |n^n|^2,$$

$$n^{n+1} = e^{i\tau \Delta} n^n + \frac{i}{2} \tau e^{i\tau \Delta} \left[e^{ic^2 t_n} \varphi_1(ic^2 \tau) u_*^n n^n + e^{-ic^2 t_n} \varphi_1(-ic^2 \tau) \overline{u_*^n} n^n \right]$$

with

$$u_*^0 = z_0 - ic^{-1} \langle \nabla \rangle_c^{-1} z_1,$$

$$n^0 = n_0,$$

and $\varphi_1(x) := \frac{e^x - 1}{x}$.

First-order UA scheme

Asymptotic convergence to the limit scheme

First-order UA scheme

Asymptotic convergence to the limit scheme

- Iteration scheme for the limit system

$$u_{\infty}^{n+1} = e^{-\frac{i\tau}{2}\Delta} u_{\infty}^n,$$

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Asymptotic convergence to the limit scheme

- Iteration scheme for the limit system

$$u_{\infty}^{n+1} = e^{-\frac{i\tau}{2}\Delta} u_{\infty}^n,$$

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- First-order uniformly accurate scheme

$$u_*^{n+1} = e^{i\tau\mathcal{A}_c} u_*^n - i\tau e^{-ic^2 t_n} \varphi_1(-i\tau c^2) c \langle \nabla \rangle_c^{-1} e^{i\tau\mathcal{A}_c} |n^n|^2,$$

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With $\|\mathcal{A}_c + \frac{1}{2}\Delta\|_r = \mathcal{O}(c^{-2})$

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With $\| \tau \varphi_1(ic^2 \tau) \|_r = \mathcal{O}(c^{-2})$, for $l \neq 0$

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$$u_*^{n+1} = e^{-\frac{i\tau}{2}\Delta} u_*^n + \mathcal{O}(c^{-2}),$$

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Theorem (Convergence bound for the first-order UA scheme)

Fix $r > d/2$ and assume that

$$\sup_{0 \leq t \leq T} \|u_*(t)\|_{r+2} + \|n_*(t)\|_{r+2} \leq M.$$

For u_* defined in the first-order scheme we set

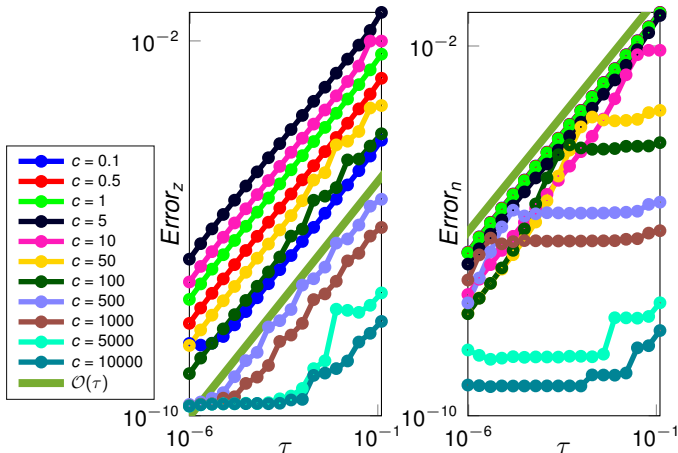
$$z^n := \frac{1}{2} \left(e^{ic^2 t_n} u_*^n + e^{-ic^2 t_n} \overline{u_*^n} \right).$$

Then, there exists a $T_r > 0$ and $\tau_0 > 0$ such that for $\tau \leq \tau_0$ and $t_n \leq T_r$ we have for all $c > 0$ that

$$\|z(t_n) - z^n\|_r + \|n(t_n) - n^n\|_r \leq \tau K_{r,t_n,M},$$

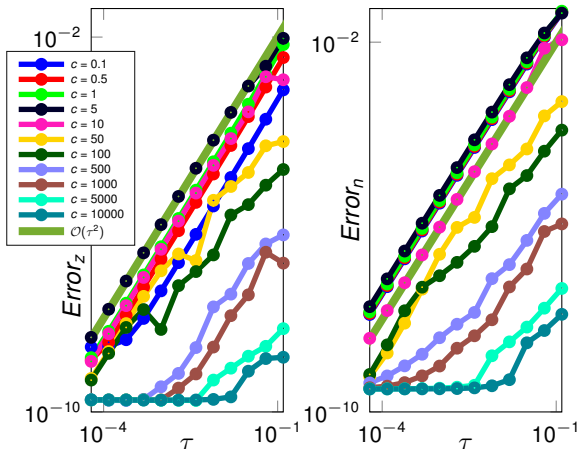
where the constant $K_{r,t_n,M}$ can be chosen independently of c .

Order plot: First-order UA scheme:



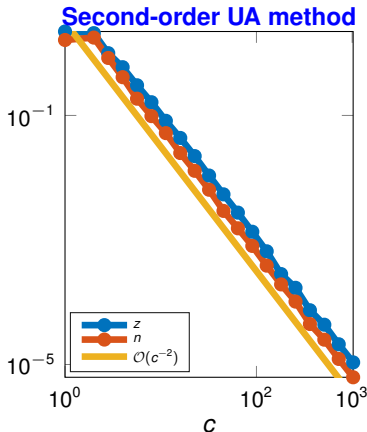
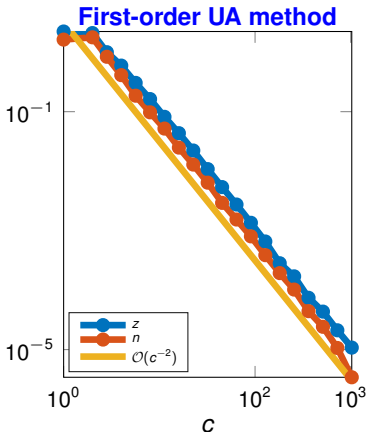
Simulation on $x \in [0, 2\pi]$, $t \in [0, 0.125]$, $\tau_{ref} \approx 10^{-7}$ and $M = 256$.

Order plot: Second-order UA scheme:



Simulation on $x \in [0, 2\pi]$, $t \in [0, 0.125]$, $\tau_{ref} \approx 10^{-7}$ and $M = 256$.

- Limit approximation:



Simulation on $x \in [0, 2\pi]$, $t \in [0, 1]$, $\tau_{ref} \approx 10^{-6}$ and $M = 256$.

Work in progress

Model problem

Consider the **Klein-Gordon-Zakharov (KGZ) system**:

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$$\begin{aligned}c^{-2}\partial_{tt}z - \Delta z + c^2z &= -nz, \\ \alpha^{-2}\partial_{tt}n - \Delta n &= \Delta|z|^2\end{aligned}$$

with initial conditions

$$\begin{aligned}z(0) &= z_0, & \partial_t z(0) &= c^2 z_1, \\ n(0) &= n_0, & \partial_t n(0) &= \alpha n_1,\end{aligned}$$

in the **non-singular limit regime**, i.e. $\alpha = \gamma c, \gamma \in \mathbb{R}_+$.

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- **Derivation:** We want to follow the procedure for the KGS system analogously

The twisting

KGZ as **first-order system in time** with $z = \frac{1}{2} (u + \bar{u})$ and $n = \Re(h)$

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$$i\partial_t h = -\alpha\langle\nabla\rangle_0 h - \frac{1}{4}\alpha\langle\nabla\rangle_0 |u + \bar{u}|^2.$$

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$$u_* = e^{-ic^2 t} u, \quad h_* = e^{-i\alpha\langle\nabla\rangle_0 t} h$$

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■ First-order system in u_* , h_*

$$i\partial_t u_* = \mathcal{A}_c u_* - \frac{1}{2}c\langle\nabla\rangle_c^{-1}\Re(e^{i\alpha\langle\nabla\rangle_0 t} h_*)(u_* + e^{-2ic^2 t} \bar{u}_*)$$

$$i\partial_t h_* = -\frac{\alpha}{4}\langle\nabla\rangle_0 e^{-i\alpha\langle\nabla\rangle_0 t} (2|u_*|^2 + e^{2ic^2 t} u_*^2 + e^{-2ic^2 t} \bar{u}_*^2)$$

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■ Integrating:

$$h_*(t_n + \tau) = h(t_n) + \frac{i\alpha}{4} \langle \nabla \rangle_0 \int_0^\tau e^{-i\alpha \langle \nabla \rangle_0 (t_n + s)} \left(2|u_*(t_n + s)|^2 + e^{2ic^2 (t_n + s)} u_*^2(t_n + s) + c.c. \right) ds$$

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■ Taylor expansion and integrating the high oscillatory phases exactly

$$h_*^{n+1} = h_*^n + \frac{i\alpha}{4} \langle \nabla \rangle_0 e^{-i\alpha \langle \nabla \rangle_0 t_n} \left[2\tau \varphi_1(-i\alpha \langle \nabla \rangle_0 \tau) |u_*^n|^2 + e^{2ic^2 t_n} \tau \varphi_1(i(-\alpha \langle \nabla \rangle_0 + 2c^2)\tau) (u_*^n)^2 + c.c. \right]$$

$$h_*^{n+1} = h_*^n + \frac{i\alpha}{2} \langle \nabla \rangle_0 e^{-i\alpha \langle \nabla \rangle_0 t_n} \tau \varphi_1(-i\alpha \langle \nabla \rangle_0 \tau) |u_*^n|^2$$
$$+ \frac{i\alpha}{4} \langle \nabla \rangle_0 e^{-i\alpha \langle \nabla \rangle_0 t_n} \left(e^{2ic^2 t_n} \tau \varphi_1(i(-\alpha \langle \nabla \rangle_0 + 2c^2)\tau) (u_*^n)^2 + c.c. \right)$$

$$\begin{aligned}
 h_*^{n+1} = h_*^n &+ \underbrace{\frac{i\alpha}{2} \langle \nabla \rangle_0 e^{-i\alpha \langle \nabla \rangle_0 t_n} \mathcal{T} \varphi_1(-i\alpha \langle \nabla \rangle_0 \mathcal{T})}_{=: h} |u_*^n|^2 \\
 &+ \frac{i\alpha}{4} \langle \nabla \rangle_0 e^{-i\alpha \langle \nabla \rangle_0 t_n} \left(e^{2ic^2 t_n} \mathcal{T} \varphi_1(i(-\alpha \langle \nabla \rangle_0 + 2c^2) \mathcal{T}) (u_*^n)^2 + c.c. \right)
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 \end{aligned}$$

- For l_1 we have

$$l_1 = \frac{i\alpha}{2} \langle \nabla \rangle_0 e^{-i\alpha \langle \nabla \rangle_0 t_n} \tau \frac{e^{-i\alpha \langle \nabla \rangle_0 \tau} - 1}{-i\alpha \langle \nabla \rangle_0 \tau}$$

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 &= \frac{1}{2} \left(e^{-i\alpha \langle \nabla \rangle_0 t_n} - e^{-i\alpha \langle \nabla \rangle_0 t_{n+1}} \right)
 \end{aligned}$$

First-order uniformly accurate scheme

$$\begin{aligned}
 u_*^{n+1} &= e^{-i\mathcal{A}_c\tau} u_*(t_n) + \frac{i}{2} c \langle \nabla \rangle_c^{-1} e^{i\tau\mathcal{A}_c} [I_1^n - I_2^n], \\
 h_*^{n+1} &= h_*^n + \frac{1}{2} (e^{-i\alpha\langle \nabla \rangle_0 t_n} - e^{-i\alpha\langle \nabla \rangle_0 t_{n+1}}) |u_*^n|^2 \\
 &\quad + \frac{1}{4} \langle \nabla \rangle_0 \frac{e^{-i(\alpha\langle \nabla \rangle_0 + 2c^2)\tau} - 1}{-(\langle \nabla \rangle_0 + 2c\gamma^{-1})} e^{-i(\alpha\langle \nabla \rangle_0 + 2c^2)t_n} u_*^{n2} \\
 &\quad + \frac{1}{4} \langle \nabla \rangle_0 \frac{e^{i(-\alpha\langle \nabla \rangle_0 + 2c^2)\tau} - 1}{-\langle \nabla \rangle_0 + 2c\gamma^{-1}} e^{i(-\alpha\langle \nabla \rangle_0 + 2c^2)t_n} (u_*^n)^2,
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with

$$\begin{aligned}
 I_1^n &= \frac{1}{2} \left[e^{i\alpha\langle \nabla \rangle_0 t_n} \tau \varphi_1(i\alpha\langle \nabla \rangle_0 \tau) + e^{-i\alpha\langle \nabla \rangle_0 t_n} \tau \varphi_1(-i\alpha\langle \nabla \rangle_0 \tau) \right] \Re(h_*^n) (u_*^n + e^{-2ic^2 t} \overline{u_*^n}), \\
 I_2^n &= \frac{1}{2i} \left[e^{i\alpha\langle \nabla \rangle_0 t_n} \tau \varphi_1(i\alpha\langle \nabla \rangle_0 \tau) - e^{-i\alpha\langle \nabla \rangle_0 t_n} \tau \varphi_1(-i\alpha\langle \nabla \rangle_0 \tau) \right] \Im(h_*^n) (u_*^n + e^{-2ic^2 t} \overline{u_*^n}).
 \end{aligned}$$

First-order uniformly accurate scheme

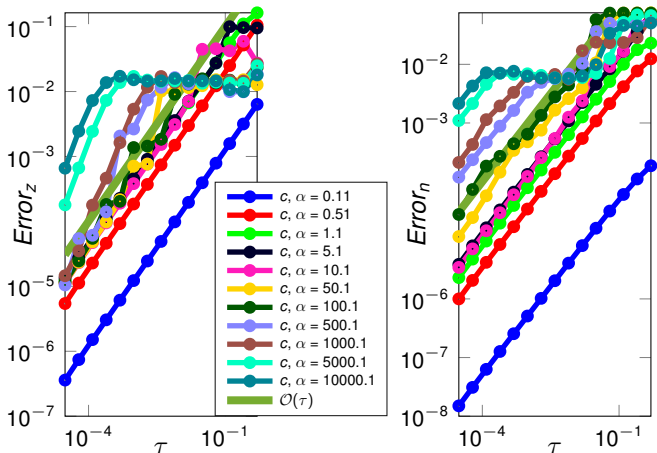
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 \end{aligned}$$

First numerical experiments ($\gamma = 1$)

Order plot:



Simulation on $x \in [0, 2\pi]$, $t \in [0, 1]$, $\tau_{ref} \approx 10^{-6}$ and $M = 256$.

Questions:

- Right twisting of h ?
- Right calculation of the UA scheme?
- Convergence to the numerical scheme of the limit system?

Remark

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- Derivation of the schemes for the KGZ equation also works for $z \in \mathbb{C}$, i.e. $z = \frac{1}{2}(u + \bar{v})$.

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- Generalization to **higher order schemes**:
Insert Duhamel's formula for $u_*(t_n + s)$ into $u_*(t_n + \tau)$ and go on analogously to the derivation of the first-order scheme.

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- Derivation of the schemes for the KGZ equation also works for $z \in \mathbb{C}$, i.e. $z = \frac{1}{2}(u + \bar{v})$.
- Generalization to **higher order schemes**:
Insert Duhamel's formula for $u_*(t_n + s)$ into $u_*(t_n + \tau)$ and go on analogously to the derivation of the first-order scheme.
- For KGS also the second-order schemes converge in the limit to the corresponding second-order numerical method for the limit equation.

- Work-precision plots for KGS and KGZ.
- Error analysis of the first-order scheme for the KGZ system.

- Construct higher-order methods for the KGZ system.
- Error analysis of the higher-order methods.

- Can we twist (KG, KGS, KGZ) such that $\partial_{tt}u_{**} = \mathcal{O}(1)$?

- 1 W. Bao, X. Dong, X. Zhao: *An exponential wave integrator pseudospectral method for the Klein-Gordon-Zakharov system*, SIAM J. Sci. Comput., 35:A2903-A2927 (2013)
- 2 W. Bao, X. Zhao: *A uniformly accurate (UA) multiscale time integrator Fourier pseudospectral method for the Klein-Gordon-Schrödinger equations in the nonrelativistic limit regime*, Numer. Math., 135:A2903-A2927 (2013)
- 3 S.B., E. Faou, K. Schratz: *Uniformly accurate exponential-type integrators for KG equations with asymptotic convergence to classical splitting schemes in the nonlinear Schrödinger limit*, to appear in Math. Comp. (2017), <http://arxiv.org/abs/1606.04652>
- 4 S.B., G. Kokkala, K. Schratz: *Asymptotic consistent exponential-type integrators for Klein-Gordon-Schrodinger systems from relativistic to non-relativistic regimes*, submitted (2017)
- 5 M. Hochbruck and C. Lubich: *A Gautschi-type method for oscillatory second-order differential equations*, Numer. Math., 83:403–426 (1999)