High-order numerical schemes for computing the dynamics of nonlinear Schrödinger equation

by

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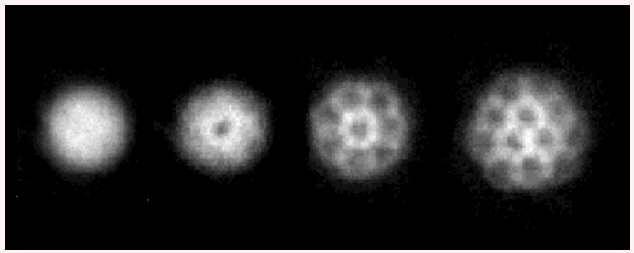
Outline of the talk

- N identical bosons
- $g = 4\pi\hbar^2 a_s/m$, where a_s denotes the s-wave scattering length of bosons.
- Confining potential $V_c(\mathbf{x}) = \frac{m}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2)$.
- The Gross-Pitaevskii equation

$$i\hbar\partial_t\varphi(\mathbf{x},t) = \frac{\delta E(\varphi)}{\delta\varphi^*} = \left[-\frac{\hbar^2}{2m}\Delta + V_c(\mathbf{x}) + Ng|\varphi|^2\right]\varphi.$$

Adding other effects

- Rotation: vortex nucleation by increasing rotation speed by Dalibard's group (2001)



$$i\hbar\partial_t\varphi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\Delta - i\hbar\boldsymbol{\Omega}\cdot(\mathbf{x}\times\nabla) + V_c(\mathbf{x}) + Ng|\varphi|^2\right]\varphi, \quad \boldsymbol{\Omega} = (0,0,\Omega)^T.$$

- Dipolar interactions: important for Chromium ^{52}Cr for example.

$$i\hbar\partial_t\varphi(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\Delta + V_c(\mathbf{x}) + Ng|\varphi|^2 + Nk\int_{\mathbb{R}^3} U(\mathbf{x}-\mathbf{x}')|\varphi(t,\mathbf{x}')|^2 d\mathbf{x}'\right]\varphi,$$

with $U(\mathbf{x}) = (1-3\cos(\text{angle}(\mathbf{x},\mathbf{e_z})))/|\mathbf{x}|^3$ and $k = \mu_0\mu_{\text{mag}}^2/2\pi$

- Stirred laser beam: add a time dependent term to the potential.
- Multi-components BEC, Rashba spin orbit coupling effect.

Nondimensionalization

Dimensionless time-dependent GPE

$$i\partial_t \varphi_j = \left(-\frac{1}{2}\Delta + V_j(\mathbf{x}) + f_j(\varphi_1, \varphi_2) - \Omega L_z\right)\varphi_j - \kappa R_j \varphi_{3-j} - \lambda \varphi_{3-j},\ j = 1, 2$$

with $\varphi_j(0, \mathbf{x}) = \varphi_{j,0}(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^d$ and

- Angular momentum $L_z = -i(x\partial_y - y\partial_x)$,
- Rashba spin orbit coupling effect $R_j = i\partial_x + (-1)^{3-j}\partial_y$,
- $f_j(\varphi_1, \varphi_2)$ and $V_{1,2}$ nonlinear effects and external potential
- λ local coupling effect

Examples:

- Quadratic confining potentials $V_j(\mathbf{x}) = \frac{1}{2}\|\gamma_j \otimes \mathbf{x}\|^2$
- Cubic nonlinearity $f_j(\varphi_1, \varphi_2) = \beta_{j1}|\varphi_1|^2 + \beta_{j2}|\varphi_2|^2$, $\beta_{11} = \beta_{22}$, $\beta_{12} = \beta_{21}$
- One component $i\partial_t \varphi = \left(-\frac{1}{2}\Delta + V + \beta|\varphi|^2 - \Omega L_z\right)\varphi$

(GPE) reads

$$i\partial_t \varphi(t,.) = \nabla_{\varphi^*(t,.)} E(\varphi(t,.)),$$

with

$$E_{\varphi_1,\varphi_2}(t) = \int_{\mathbb{R}^d} \sum_{j=1}^{2} \left(\frac{1}{2}\|\nabla\varphi_j\|^2 + V_j|\varphi_j|^2 + F_j(\varphi_1,\varphi_2) - \Omega\varphi_j^* L_z\varphi_j - \kappa\varphi_j^* R_j\varphi_{3-j} \right) - 2\lambda\,\mathrm{Re}(\varphi_1\varphi_2^*)\,d\mathbf{x},$$

where F_j is defined by $\partial_{\varphi_j^*} F_j = f_j(\varphi_1,\varphi_2)\varphi_j$, $j = 1, 2$. For the cubic nonlinearity, we have $F_j(\varphi_1,\varphi_2) = (\beta_{jj}|\varphi_j|^4 + \beta_{12}|\varphi_1|^2|\varphi_2|^2)/2$.
Then

- the equation happens to be Hamiltonian
- the energy is preserved by the dynamics: along a solution $t \mapsto \varphi(t,.)$ of (GPE), one has $E_{\varphi_1,\varphi_2}(t) = E_{\varphi_1,\varphi_2}(0)$.
- besides, the evolution preserves the total mass of the distribution:

$$N_{\varphi_1,\varphi_2}(t) = \sum_{j=1}^{2} N_{\varphi_j}(t) = \sum_{j=1}^{2} \|\varphi_j\|_2^2 = \sum_{j=1}^{2} \int_{\mathbb{R}^d} |\varphi_j|^2\,d\mathbf{x} = N_{\varphi_1,\varphi_2}(0).$$

Outline of the talk

Reference: see for example *Geometric Numerical Integration*, E. Hairer, C. Lubich & G. Wanner, Springer

We consider an arbitrary system of ODEs

$$\dot{y} = f(y) \in \mathbb{R}^n, \quad y(0) = y_0.$$

The solution if given by the *flow* F_t

$$y(t) = F_t(y_0).$$

One decompose the vector field into integrable pieces and treats them separately

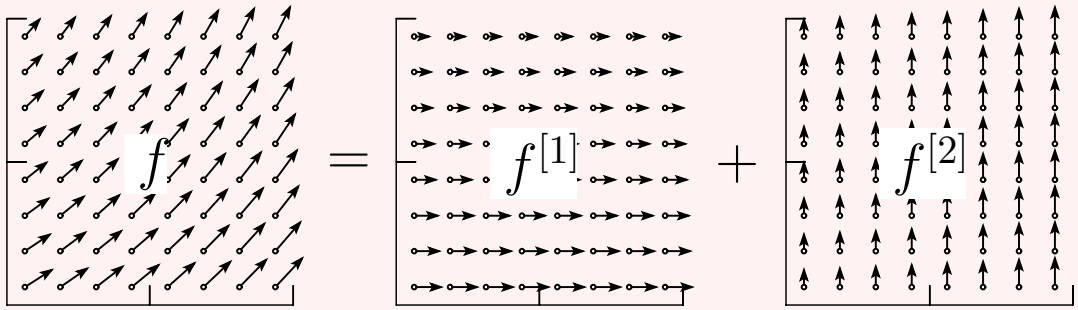


FIGURE : A splitting of a vector field

Then

$$\dot{y} = f^{[1]}(y) + f^{[2]}(y).$$

If we know the exact flows $F_t^{[i]}$ of $\dot{y} = f^{[i]}(y)$, $i = 1, 2$, then

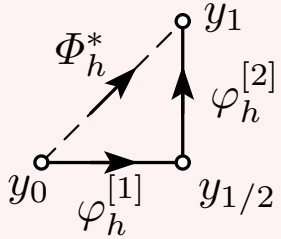
$$y_0 \xrightarrow{F_t^{[1,2]}} y_{1/2} \xrightarrow{F_t^{[1,2]}} y_{2/1}$$

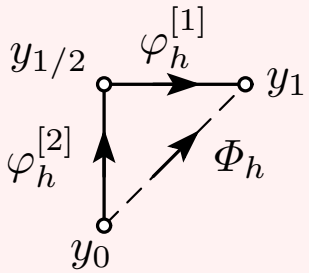
Idea for a numerical flow

$$\Phi_h : y_n \mapsto y_{n+1}$$

where $y_n \approx y(t_n)$ and $h = t_{n+1} - t_n$.

$$\Phi_h = F_h^{[2]} \circ F_h^{[1]}$$
$$\Phi_h^* = \Phi_{-h}^{-1} = F_h^{[1]} \circ F_h^{[2]}$$



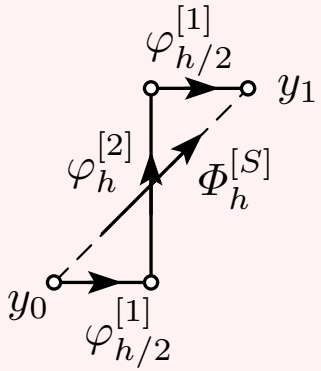


This is the *Lie-Trotter* splitting scheme.

Taylor expansion: $(F_h^{[1]} \circ F_h^{[2]})(y_0) = F_h(y_0) + \mathcal{O}(h^2)$.

We can get an higher order scheme: Strang splitting scheme

$$\Phi_h^{[S]} = F_{h/2}^{[1]} \circ F_h^{[2]} \circ F_{h/2}^{[1]},$$



If we write $F_h^{[2]} = F_{h/2}^{[2]} \circ F_{h/2}^{[2]}$, then we also have $\Phi_h^{[S]} = \Phi_{h/2} \circ \Phi_{h/2}$ and

$$\Phi_h^{[S]}(y_0) = F_h(y_0) + \mathcal{O}(h^3).$$

General Splitting Procedure: look for coefficient a_1, b_1, a_2, $\cdots$, a_m, b_m such that

$$\Psi_h = F_{b_m h}^{[2]} \circ F_{a_m h}^{[1]} \circ F_{b_{m-1} h}^{[2]} \circ \cdots \circ F_{a_2 h}^{[1]} \circ F_{b_1 h}^{[2]} \circ F_{a_1 h}^{[1]}$$

to get

$$\Psi_h(y_0) = F_h(y_0) + \mathcal{O}(h^s), \quad s > 3.$$

Example: $\partial_t \varphi = i\frac{\Delta}{2}\varphi - i|\varphi|^2\varphi$.

$$f^{[1]}(\varphi) = -i|\varphi|^2\varphi \quad \text{and} \quad f^{[2]}(\varphi) = i\frac{\Delta}{2}\varphi,$$

and

$$F_t^{[1]}(\varphi_0) = e^{-i|\varphi_0|^2}\varphi_0 \quad \text{and} \quad F_t^{[2]}(\varphi_0) = e^{i\Delta t/2}\varphi_0.$$

The usual splitting preserves mass since

$$\int_{\mathbb{R}^d} \left|F_t^{[1]}(\varphi_0)\right|^2 dx = \int_{\mathbb{R}^d} |\varphi_0|^2\, dx \quad \text{and} \quad \int_{\mathbb{R}^d} \left|F_t^{[2]}(\varphi_0)\right|^2 dx = \int_{\mathbb{R}^d} |\varphi_0|^2\, dx.$$

However, these schemes do not preserve energy.

- An important issue in the numerical time integration of (GPE) comes from the rotation term R.
- Following W. Bao, D. Marahrens, Q. Tang and Y. Zhang, (2013), we introduce new coordinates

$$A(t) = \begin{pmatrix} \cos(\Omega t) & -\sin(\Omega t) \\ \sin(\Omega t) & \cos(\Omega t) \end{pmatrix} \quad \text{or} \quad A(t) = \begin{pmatrix} \cos(\Omega t) & -\sin(\Omega t) & 0 \\ \sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$A(t)$ is orthogonal: $A(t)^{-1} = A(t)^t$.

We perform the change of unknown $\varphi(t, \mathbf{x}) = \psi\left(t, A(t)\mathbf{x}\right)$.

$$\varphi \text{ solves (GPE)} \iff \psi \text{ solves (NLS)}$$

(NLS)

$$i\partial_t \psi_j = \left(-\frac{1}{2}\Delta + \tilde{V}_j(t, \tilde{\mathbf{x}}) + f_j(\psi_1, \psi_2)\right)\psi_j - \lambda\psi_{3-j}, \quad \tilde{\mathbf{x}} = A(t)\mathbf{x}$$

where

$$\tilde{V}_j(t, \tilde{\mathbf{x}}) = V_j\left(A(t)^t\tilde{\mathbf{x}}\right) \quad \text{and} \quad \psi_j(0, \tilde{\mathbf{x}}) = \psi_{j,0}(\tilde{\mathbf{x}}) = \varphi_{j,0}(\tilde{\mathbf{x}}).$$

For full GPE

- After change of unknwon, the potential is now time dependent
- If we do not perform change of unknwon, we are still interested in time dependent potential (stirred laser beam)
- The Rashba coupling term can not be eliminated by such a change of unknown. For numerical integration, we need ADI techniques.

- Problem: standard formulas are only valid for autonomous problems!
- If $X' = A(t)X$, A, X: $n \times n$ matrices: Magnus expansion
- Standard procedure: transform non-autonoumous ODE to autonomous ODE system

$$\begin{cases} x' = f(x,t), \\ x(t_0) = x_0 \end{cases} \iff \begin{cases} x' = f(x,y), \\ y' = 1, \\ x(t_0) = x_0, \\ y(t_0) = t_0 \end{cases}$$

- Drawbacks
  - Structure of the flows can be different
  - loss of efficiency

Some possible answers

- S. Blanes, F. Casas, A. Murua, 2012, "Splitting methods in the numerical integration of non-autonomous dynamical systems".
- M. Seydaoglu, S. Blanes, 2014, "High-order splitting methods for separable non-autonomous parabolic equations".

We can see our (NLS) equation as

$$i\partial_t\psi(t,\tilde{\mathbf{x}}) = \underbrace{\Big(-\frac{1}{2}\Delta + V(t,\tilde{\mathbf{x}})\Big)\psi(t,\tilde{\mathbf{x}})}_{=iL\psi} + \underbrace{\beta|\psi(t,y)|^2\psi(t,\tilde{\mathbf{x}})}_{:=iN(\psi)}.$$

or

$$i\partial_t\psi(t,\tilde{\mathbf{x}}) = \underbrace{-\frac{1}{2}\Delta\psi(t,\tilde{\mathbf{x}})}_{:=iL\psi} + \underbrace{V(t,\tilde{\mathbf{x}})\psi(t,\tilde{\mathbf{x}}) + \beta|\psi(t,y)|^2\psi(t,\tilde{\mathbf{x}})}_{:=iN(\psi)}.$$

So everything amounts to solve

$$\psi'(t) = L\psi + N(\psi(t)),$$

- Non autonomous ODE $\psi'(t) = N(t,\psi(t))$
- If we are interested in multi-component BEC with Rashba term (or rotation term without change of unknown), we need to use ADI methods. Limitation to second order methods (or use of composition methods to gain higher order).

Aim: to build high order numerical schemes based on decomposition $\psi'(t) = L\psi + N(t,\psi(t))$.

Outline of the talk

ERK methods: see M. Hochbruck and A. Ostermann, *Exponential integrators*, Acta Numer.,(2010).

We want to integrate in time

$$u'(t) = Lu(t) + N(u(t)), \quad L \in \mathbb{C}$$

Variation-of-constants formula

$$u(t_{n+1}) = e^{hL}u(t_n) + \int_0^h e^{(h-\sigma)L} N(u(t_n + \sigma))\mathrm{d}\sigma.$$

Exponential Euler method: $N(u(t_n + \sigma)) \approx N(u_n)$

$$u_{n+1} = e^{hL}u_n + h\varphi_1(hL)N(u_n)$$

with

$$\varphi_1(hL) = \frac{1}{h}\int_0^h e^{(h-\sigma)L}\mathrm{d}\sigma = \frac{e^{hL} - 1}{hL}.$$

General approach - collocation: choose collocation nodes $c_1, \cdots, c_s$

Collocation polynomial $p_n(\sigma)$ of degree $s-1$ with collocation conditions

$$p_n(c_k h) = N(u(t_n + c_k h)).$$

Note that

$$\begin{aligned} u(t_n + c_k h) &= e^{c_k L h} u(t_n) + \int_0^{c_k h} e^{(c_k h - \sigma) L} N(u(t_n + \sigma)) \mathrm{d}\sigma \\ &\approx e^{c_k L h} u(t_n) + \int_0^{c_k h} e^{(c_k h - \sigma) L} p_n(\sigma) \mathrm{d}\sigma. \end{aligned}$$

Let $u_n \approx u(t_n)$ and $u_{n,k} \approx u(t_n + c_k h)$. Then

$$u_{n,k} = e^{c_k L h} u_n + h \sum_{\ell=1}^{s} \underbrace{\left(\frac{1}{h} \int_0^{c_k h} e^{(c_k h - \sigma) L} \mathcal{L}_\ell(\sigma) \mathrm{d}\sigma \right)}_{:= a_{k,\ell}(hL)} N(u_{n,\ell}),$$

$\mathcal{L}_\ell$ Lagrange polynomial, and

$$u_{n+1} = e^{Lh} u_n + h \sum_{k=1}^{s} \underbrace{\left(\frac{1}{h} \int_0^{h} e^{(h - \sigma) L} \mathcal{L}_k(\sigma) \mathrm{d}\sigma \right)}_{:= b_k(hL)} N(u_{n,k}).$$

If $L = 0$, we recover the usual implicit Runge-Kutta scheme.

- L is not a constant: $L = \frac{i}{2}\Delta$.
- Assuming the essential of the dynamics stays in a bounded square of side of length $d > 0$, one can replace Δ with Δ_{per}.
- One has to compute the coefficients $a_{k,\ell}(ih\omega_{p,q}/2)$ and $b_k(ih\omega_{p,q}/2)$ where $\omega_{p,q} = -\left(\frac{2\pi}{d}\right)^2(p^2+q^2)$, for $(p,q) \in \mathbb{Z}^2$.

$$a_{k,\ell}(ih\omega_{p,q}/2) = \frac{1}{h}\int_0^{c_k h} e^{(c_k h-\sigma)i\omega_{p,q}/2}\mathcal{L}_\ell(\sigma)d\sigma,$$

and

$$b_k(ih\omega_{p,q}/2) = \frac{1}{h}\int_0^{h} e^{(h-\sigma)i\omega_{p,q}/2}\mathcal{L}_k(\sigma)d\sigma.$$

- Example $s = 2$, $0 \le c_1 < c_2 \le 1$,

$$a_{1,1}(ih\omega_{p,q}/2) = c_1^2\frac{e^{ic_1 h\frac{\omega_{p,q}}{2}}(1 - ic_2 h\frac{\omega_{p,q}}{2}) - 1 + ih\frac{\omega_{p,q}}{2}(c_2 - c_1)}{(c_1 - c_2)((ic_1 h\omega_{p,q}/2)^2)};$$

We assume in the following that $V(t, \mathbf{x})$ is smoothly truncated when $|x| > d/2$.
Let $\mathbb{T}_d = \mathbb{R}/(d\mathbb{Z})$.

THEOREM B-DUJARDIN-LACROIX 2015, 2016

For all $\psi_0 \in H^\sigma(\mathbb{T}_d)$, $\sigma > 1$, and all $T > 0$ such that the exact solution of (NLS) is smooth over $[0, T]$, there exists $C, h_0 > 0$ such that for all $h \in (0, h_0)$, the ERK method starting from ψ_0 is well-defined.

Moreover, we have for all $h \in (0, h_0)$ and $n \in \mathbb{N}$ such that $nh \leq T$,

$$\|\psi(t_n) - \psi_n\|_{H^\sigma(\mathbb{T}_d)} \leq Ch^s$$

If the collocation nodes are chosen to be Gauss collocation nodes, then

$$\|\psi(t_n) - \psi_n\|_{H^\sigma(\mathbb{T}_d)} \leq Ch^{2s}$$

REMARKS

- These methods never preserve neither mass nor energy.
- Methods up to order 10 can be implemented fairly easily and have reasonable computational cost.

Outline of the talk

In order to integrate in time

$$u'(t) = Lu(t) + N(u(t)),$$

- perform a change of unknown

$$v(t) = e^{-Lt}u(t) \quad \Longrightarrow \quad v'(t) = e^{-Lt}N(e^{Lt}v(t)).$$

- apply a classical s-stages implicit Runge–Kutta method with Butcher tableau given by

$$\begin{array}{c|ccc} c_1 & a_{1,1} & \cdots & a_{1,s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s,1} & \cdots & a_{s,s} \\ \hline & b_1 & \cdots & b_s \end{array}$$

$$v_{n,k} = v_n + h\sum_{\ell=1}^{s} a_{k,\ell} e^{-(t_n+c_\ell h)L} N\left(e^{(t_n+c_\ell h)L} v_{n,\ell}\right), \quad 1 \le k \le s,$$

$$v_{n+1} = v_n + h\sum_{k=1}^{s} b_k e^{-(t_n+c_k h)L} N\left(e^{(t_n+c_k h)L} v_{n,k}\right).$$

- get back to $u(t) = e^{+Lt}v(t)$ at final time $t = T$

Our equation is

$$i\partial_t\psi(t,\tilde{\mathbf{x}}) = \underbrace{-\frac{1}{2}\Delta\psi(t,\tilde{\mathbf{x}})}_{:=iL\psi} + \underbrace{V(t,\tilde{\mathbf{x}})\psi(t,\tilde{\mathbf{x}}) + \beta|\psi(t,y)|^2\psi(t,\tilde{\mathbf{x}})}_{:=iN(\psi)}.$$

- perform a change of unknown

$$v(t,\mathbf{x}) = e^{-Lt}\psi(t,\mathbf{x}) \quad \Longrightarrow \quad \partial_t v(t,\mathbf{x}) = e^{-Lt}N(t,e^{+Lt}v(t,\mathbf{x})).$$

- apply a classical RK method

Let

$$\psi_{n,k} := e^{(t_n+c_kh)L}v_{n,k} \qquad \text{and} \qquad \psi_n := e^{t_nL}v_n,$$

The Lawson method consists in solving the s nonlinear equations

$$\psi_{n,k} = e^{c_khL}\psi_n + h\sum_{\ell=1}^{s} a_{k,\ell}e^{(c_k-c_\ell)hL}N\left(t_n+c_\ell h,\psi_{n,\ell}\right),$$

and then computing ψ_{n+1} through the formula

$$\psi_{n+1} = e^{hL}\psi_n + h\sum_{k=1}^{s} b_k e^{(1-c_k)hL}N\left(t_n+c_kh,\psi_{n,k}\right).$$

Theorem B-Dujardin-Lacroix 2015

- Assume that the RK method satisfies $\sum_{k=1}^{s} b_k = 1$ and

$$\forall (k,\ell) \in \{1,\dots,s\}^2, \qquad a_{s+1-k,s+1-\ell} + a_{k,\ell} = b_\ell,$$

so that it is symmetric. Then the Lawson method is also symmetric (time reversibility).

- Assume that it satisfies the Cooper condition,

$$b_k a_{k,\ell} + b_\ell a_{\ell,k} = b_k b_\ell, \quad \forall\ 1 \le k,\ell \le s,$$

so that it preserves quadratic invariants. Then the Lawson method preserves the L^2-norm:

$$\|\psi_n\|_{L^2(\mathbb{T}_d)} = \|\psi_0\|_{L^2(\mathbb{T}_d)}, \quad \forall\ n \ge 0.$$

- Assume that the s collocation points of the RK method are Gauss points and $\psi_0 \in H^\sigma(\mathbb{T}_d)$, $\sigma > 1$, and all $T > 0$ such that the exact solution of (NLS) is smooth over $[0,T]$, there exists $C, h_0 > 0$ such that for all $h \in (0,h_0)$, the Lawson method starting from ψ_0 is well-defined.

Moreover, we have for all $h \in (0,h_0)$ and $n \in \mathbb{N}$ such that $nh \le T$,

$$\|\psi(t_n) - \psi_n\|_{H^\sigma(\mathbb{T}_d)} \le Ch^{2s}$$

Outline of the talk

We want to solve

$$\psi'(t) = L\psi + N(\psi(t)) = f^{\mathsf{IM}}(t,\psi) + f^{\mathsf{EX}}(t,\psi).$$

The idea of an IMEX scheme is associate the *linear part* to an *implicit* RK scheme and the *nonlinear part* to an *explicit* RK scheme.

- The linear part should involve operators that can be efficiently inverted
- The nonlinear part involves terms such that their contribution is integrated in time at almost no cost

Two Bucher tableau ($\tilde{}$ for explicit) with same quadrature nodes c

$$\begin{array}{c|c} c & A \\ \hline & b^t \end{array} \quad \begin{array}{c|c} \tilde{c} & \tilde{A} \\ \hline & \tilde{b}^t \end{array} \quad \text{or} \quad \begin{array}{c|c|c} c & A & \tilde{A} \\ \hline & b^t & \tilde{b}^t \end{array}.$$

For efficiency reason, we consider DIRK (Diagonaly Implicit RK) for implicit part

$$K_k = \psi^n + h\sum_{\ell=1}^{k} a_{k\ell} f^{\mathsf{IM}}(t_{nl}, K_\ell) + h\sum_{\ell=1}^{k-1} \tilde{a}_{k\ell} f^{\mathsf{EX}}(t_{n\ell}, K_\ell), \quad \text{for } k = 1, \cdots, s,$$

$$\psi^{n+1} = \psi^n + h\sum_{k=1}^{s} b_k f^{\mathsf{IM}}(t_{nk}, K_k) + h\sum_{k=1}^{s} \tilde{b}_k f^{\mathsf{EX}}(t_{nk}, K_k).$$

More specifically,

$$K_k = (I - a_{kk} h L)^{-1} \left(\psi^n + h \sum_{\ell=1}^{k-1} a_{k\ell} L K_\ell + \tilde{a}_{k\ell} \tilde{K}_\ell \right)$$

$$\tilde{K}_k = f^{\mathsf{EX}}(t_n + c_k h, K_k)$$

$$\psi^{n+1} = \psi^n + h \sum_{k=1}^{s} \left(b_k L K_k + \tilde{b}_k \tilde{K}_k \right)$$

- compute a second solution $\underline{\psi}^{n+1} \neq \psi^{n+1}$ at each time step
- $\underline{\psi}_{n+1}$ has an other order of accuracy
- estimate an "optimal" time step h_n to perform the iteration from t_n to t_{n+1}.
- The computation of $\underline{\psi}^{n+1} \neq \psi^{n+1}$ should be done at very low cost.
- Use already computed stages (which are the most time consuming for RK schemes) and simply exploit different (suitable) weights for $\underline{\psi}^{n+1} \neq \Psi^{n+1}$:
  new weights $\underline{b}_i$ and $\tilde{\underline{b}}_i \longrightarrow$ embedded scheme

$$\begin{array}{c|c|c} c & A & \tilde{A} \\ \hline & b^t & \tilde{b}^t \\ & \underline{b}_i & \tilde{\underline{b}}_i \end{array}.$$

The embedded solution is given by

$$\underline{\psi}^{n+1} = \psi^n + h\sum_{k=1}^{s} \underline{b}_k f^{\mathsf{IM}}(t_{nk}, K_k) + h\sum_{k=1}^{s} \tilde{\underline{b}}_k f^{\mathsf{EX}}(t_{nk}, K_k).$$

IMEX$(q)p$, with q the order of the original scheme and p the order of the embedded one. We consider $q = p + 1$

Local error indicators $\delta^n = \delta^n(\psi^{n+1}, \underline{\psi}^{n+1})$.
Examples

$$\begin{array}{ll} L^2\text{-norm indicator} & \delta^n = \|\psi^{n+1} - \underline{\psi}^{n+1}\|_2 \\ \text{Energy indicator} & \delta^n = |E_\psi(t_{n+1}) - E_{\underline{\psi}}(t_{n+1})| \end{array}$$

Accuracy condition: $\delta^n = C(h_n)^q \leq \tau$, τ user-defined constant representing the expected accuracy.

Changing $h_n \to h_n^{\text{new}} = \alpha h_n$, one gets $\delta_n \to \alpha^q \delta_n$ and we get the control if

$$\alpha \leq \left(\frac{\tau}{\delta_n}\right)^{1/q}.$$

To avoid too many costly rejections, we accept the result of the iteration $\psi^n \to \psi^{n+1}$ if $h_n^{\text{new}} \in [c_m h_n; c_M h_n]$ ($c_m = 0.95$ and $c_M = 2$).

Summary: repeat the iteration from t_n to t_{n+1} with h_n^{new} if $h_n^{\text{new}} < c_m h_n$ or $h_n^{\text{new}} > c_M h_n$.

IMEXSP(4)3

c	A	$\tilde{A}$
	b^t	$\tilde{b}^t$
	$\underline{b}_i$	$\underline{\tilde{b}}_i$

0	0						0					
$1/2$	0	$1/2$					$1/2$	0				
$1/2$	$1/4$	$-1/4$	$1/2$				$1/4$	$1/4$	0			
1	0	1	0	0			0	-1	2	0		
1	$1/6$	0	$2/3$	$-4/3$	$3/2$		$1/6$	0	$2/3$	$1/6$	0	
1	$1/6$	0	$2/3$	$1/6$	-2	2	$1/6$	0	$2/3$	$1/6$	0	0
	$1/6$	0	$2/3$	$1/6$	-2	2	$1/6$	0	$2/3$	$1/6$	0	0
	$1/6$	0	$2/3$	$1/6$	-2	2	$1/6$	0	$2/3$	$1/12$	$1/12$	0

Outline of the talk

We compute the numerical solution to the one-dimensional cubic NLS equation

$$\partial_t \psi = \frac{i}{2}\partial_x^2 \psi + iq|\psi|^2\psi, \quad (t,x) \in [0,T] \times \mathbb{R}.$$

An exact solution for $(t,x) \in [0,T] \times \mathbb{R}$ is given by the soliton formula

$$\psi_{ex}(t,x) = \sqrt{\frac{2a}{q}}\,\mathrm{sech}\big(\sqrt{2}(\sqrt{2}x - ct)\big)\exp\left(ic\frac{\sqrt{2}x - ct}{2}\right)\exp\left(i(a + \frac{c^2}{4})t\right).$$

- periodic finite interval $(x_\ell, x_r) = (-15, 15)$
- spatial mesh size $k = \Delta x > 0$ with $k = (x_r - x_\ell)/M$ with $M = 2^P$, $P \in \mathbb{N}^*$.
- discretize the space operators using Fourier spectral approximation
- time step $h = \Delta t$, $T = 5$ and $h = T/N_T$ for some $N_T \in \mathbb{N}^\star$.
- grid points and the discrete times are

$$x_j := x_\ell + jk, \quad t_n := nh, \quad j = 0, 1, \cdots, M, \quad n = 0, 1, \cdots, N_T.$$

- ψ_j^n: approximation of $\psi(t_n, x_j)$.

We define the discrete ℓ^r norm on $\mathbb{C}^M$ as

$$\|v\|_{\ell^r} = \left(k \sum_{j=0}^{M-1} |v_j|^r \right)^{1/r}, \quad v \in \mathbb{C}^M, \ r \geq 1.$$

We consider the following errors

- Phase error

$$\mathcal{E}_{P,h} = \sup_{n \in \{0, \cdots, N\}} \left\| \psi_{ex}(t_n, \cdot) - (\psi_j^n)_j \right\|_{\ell^2},$$

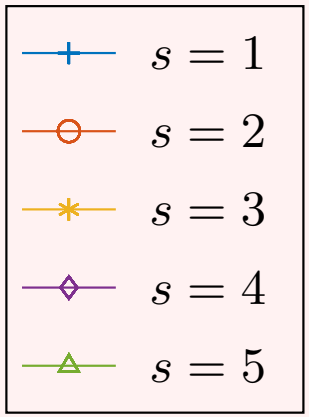
- Mass error

$$\mathcal{E}_{M,h} = \sup_{n \in \{0, \cdots, N\}} \left(\|\psi_{ex}(t_n, \cdot)\|_{\ell^2} - \left\|(\psi_j^n)_j\right\|_{\ell^2} \right) / \|\psi_{ex}(0, \cdot)\|_{\ell^2}.$$

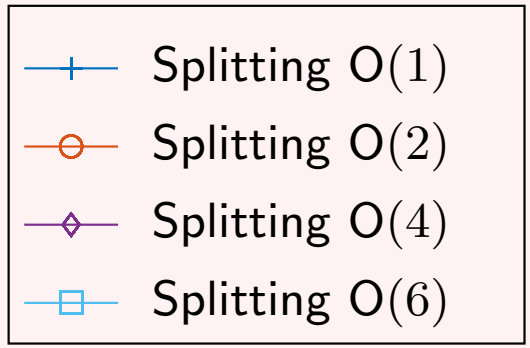
- If we define the discrete energy $E_k(v) = \frac{1}{2}\|\nabla_k v\|_{\ell^2}^2 - \frac{q}{4}\|v\|_{\ell^4}^4$, the energy error

$$\mathcal{E}_{E,h} = \sup_{n \in \{0, \cdots, N\}} \left(E_k(\psi_{ex}(t_n, \cdot)) - E_k((\psi_j^n)_j) \right) / E_k(\psi_{ex}(0, \cdot)).$$

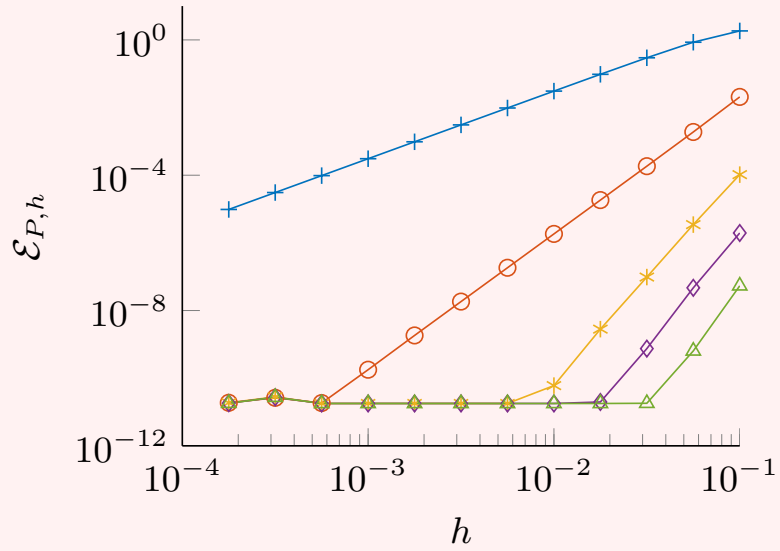
Legends



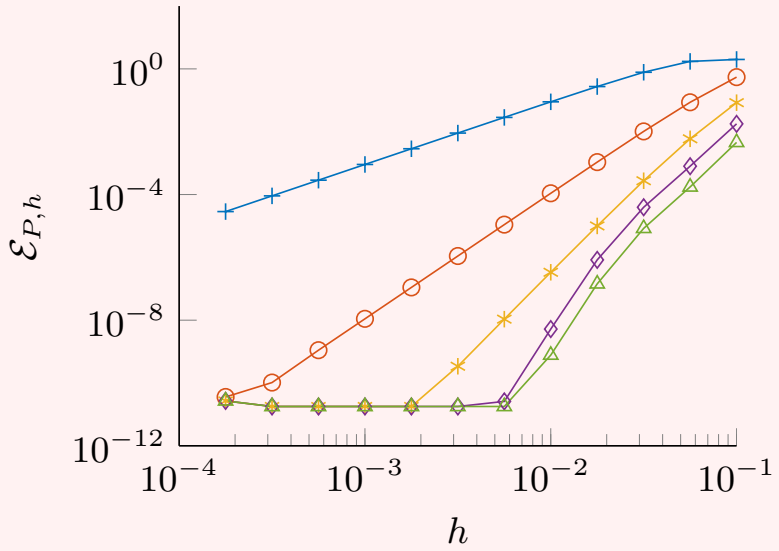
ERK and Lawson methods
order h^s



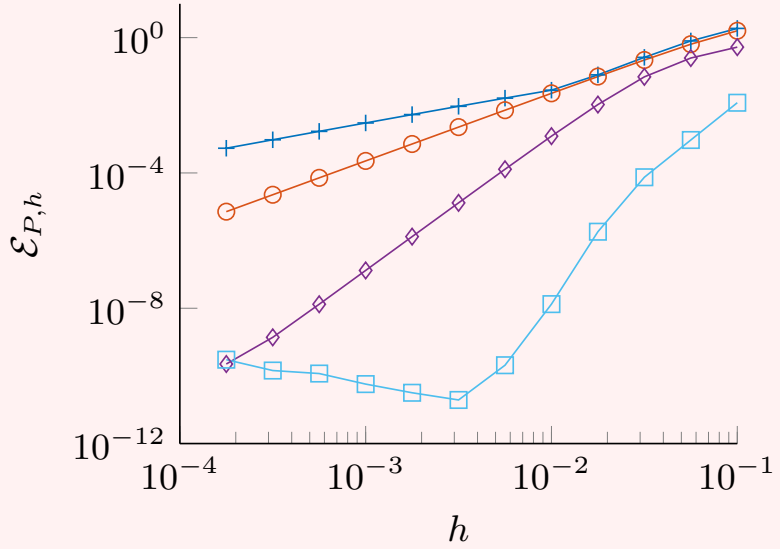
Splitting schemes



Gauss-ERK

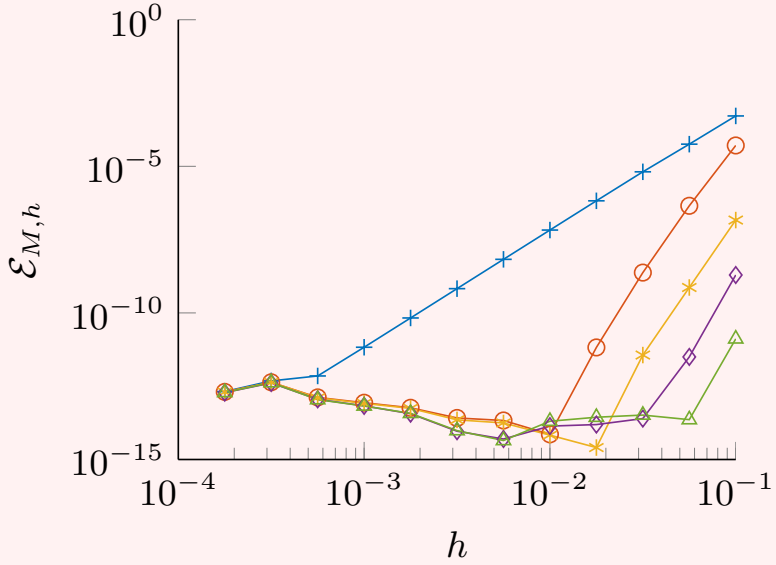


Gauss-Lawson

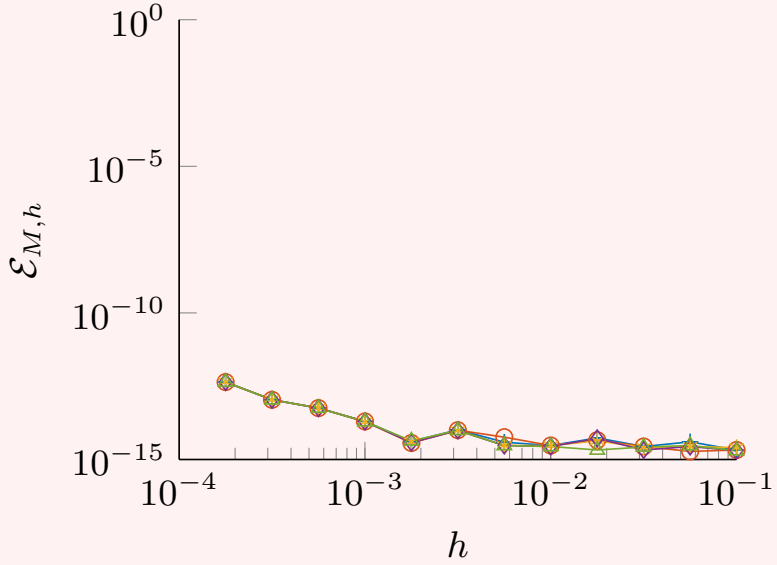


Splitting

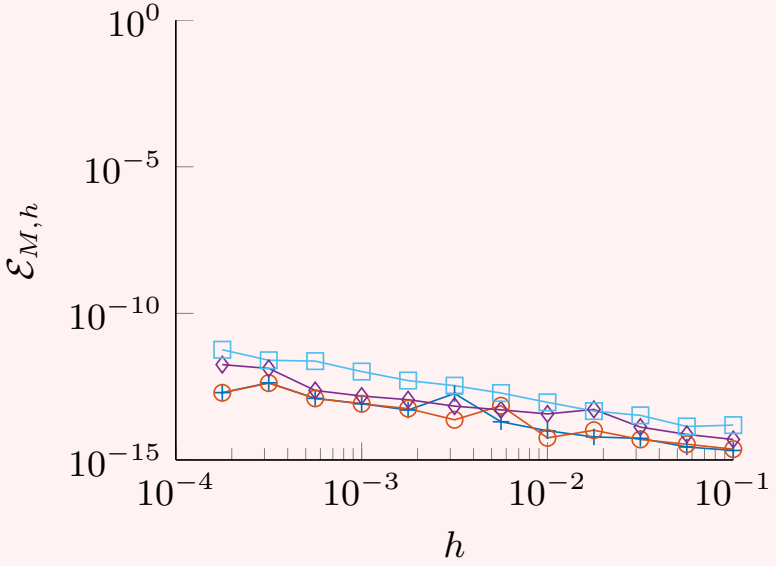
Evolution of $\mathcal{E}_{P,h}$ error w.r.t h



Gauss-ERK

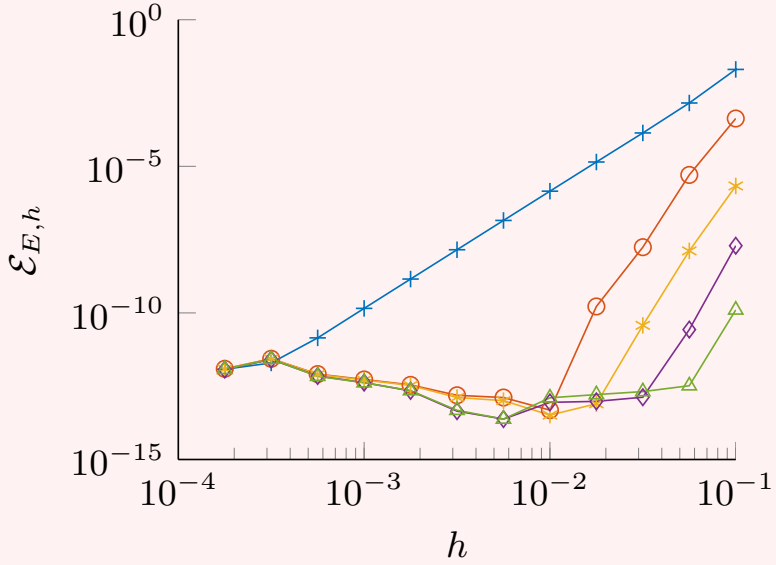


Gauss-Lawson

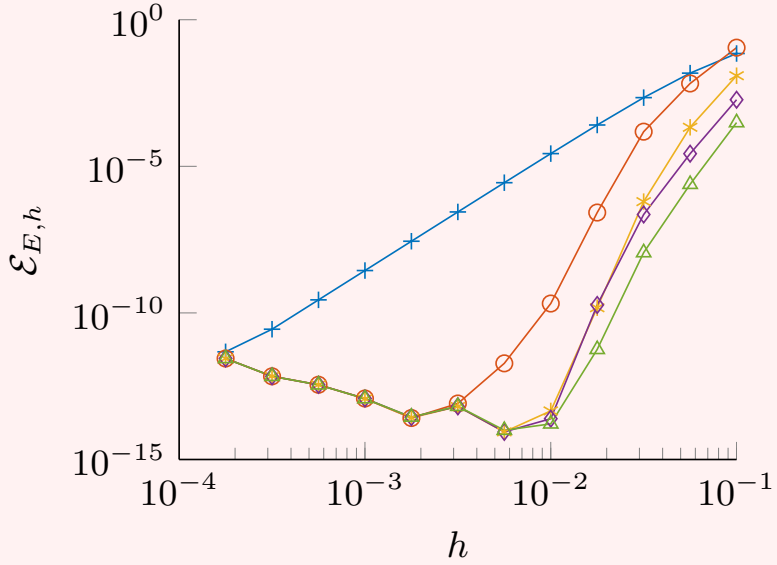


Splitting

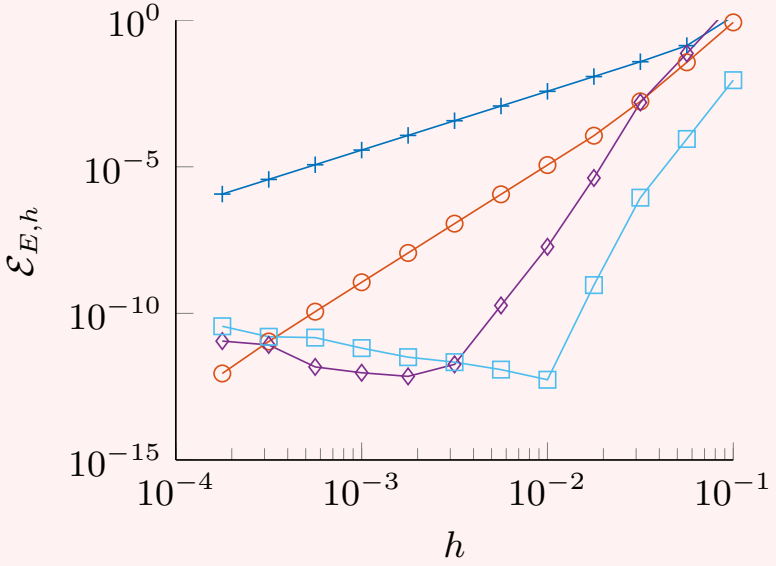
Evolution of $\mathcal{E}_{M,h}$ error w.r.t h



Gauss-ERK

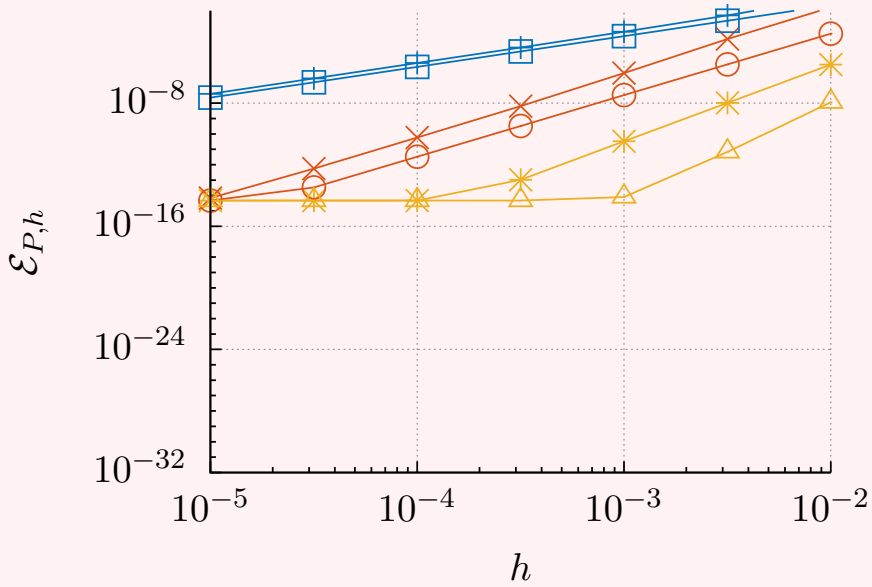


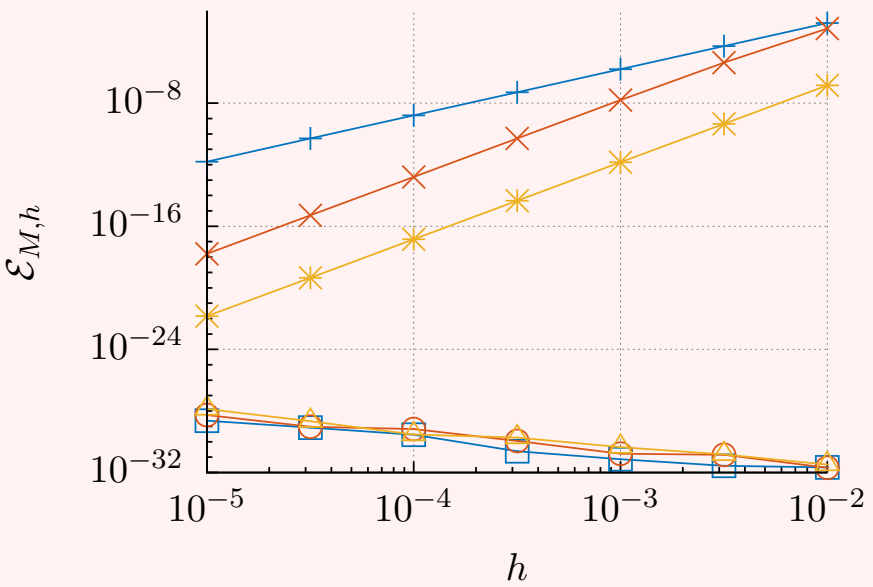
Gauss-Lawson

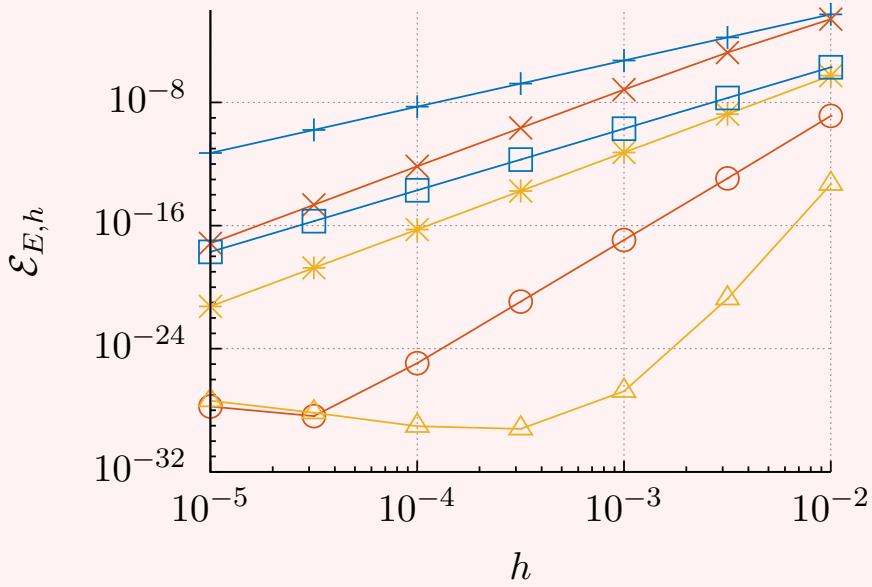


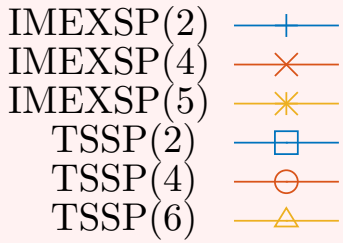
Splitting

Evolution of $\mathcal{E}_{E,h}$ error w.r.t h


10^{-8}
10^{-16}
10^{-24}
10^{-32}
$\mathcal{E}_{P,h}$
10^{-5}
10^{-4}
10^{-3}
10^{-2}
h


10^{-8}
10^{-16}
10^{-24}
10^{-32}
$\mathcal{E}_{M,h}$
10^{-5}
10^{-4}
10^{-3}
10^{-2}
h


10^{-8}
10^{-16}
10^{-24}
10^{-32}
$\mathcal{E}_{E,h}$
10^{-5}
10^{-4}
10^{-3}
10^{-2}
h


IMEXSP(2)
IMEXSP(4)
IMEXSP(5)
TSSP(2)
TSSP(4)
TSSP(6)

$$i\partial_t\psi = -\partial_x^2\psi + V\psi + G_1|\psi|^2\psi + G_2|\psi|^4\psi, \quad t > 0, x \in \mathbb{R},$$

with $V(t,x) = \frac{x}{2}\omega^2\cos(\omega t + \beta_0)$.
The exact solution is

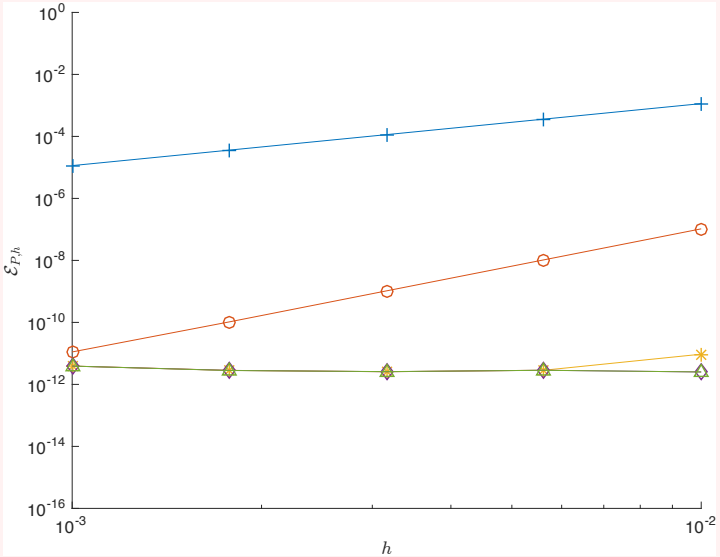
$$\psi_{\text{ex}}(t,x) = \eta\frac{\exp\left(i\left(-\frac{\omega}{2}x\sin(\omega t+\beta_0) - \frac{\omega^2}{8}t + \frac{\omega}{16}\sin(2\omega t + 2\beta_0) - E_c t\right)\right)}{\left(\sqrt{1-b}\cosh(2\sqrt{-E_c}(x - \cos(\omega t + \beta_0))) + 1\right)^{1/2}}.$$

We choose

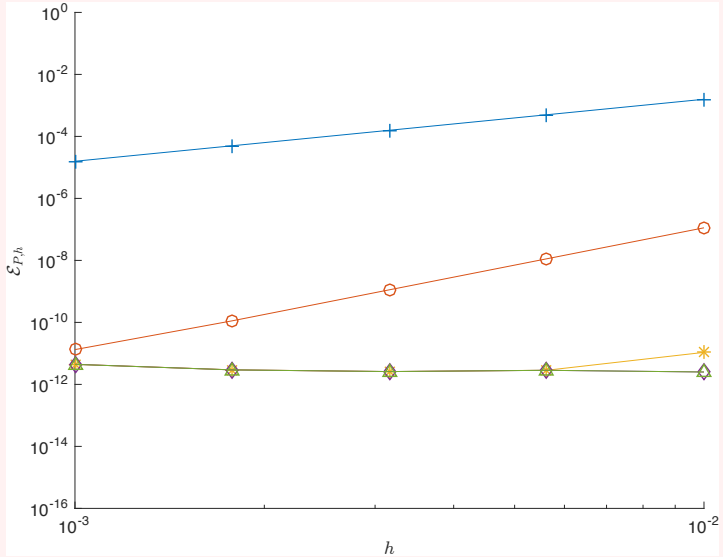
$$G_1 = -2, G_2 = 1/2, \omega = 2, E_c = -1, \beta_0 = 0, \eta = \sqrt{\frac{4E_c}{G_1}}, b = -16\frac{E_c G_2}{3G_1^2}.$$

The numerical parameters are

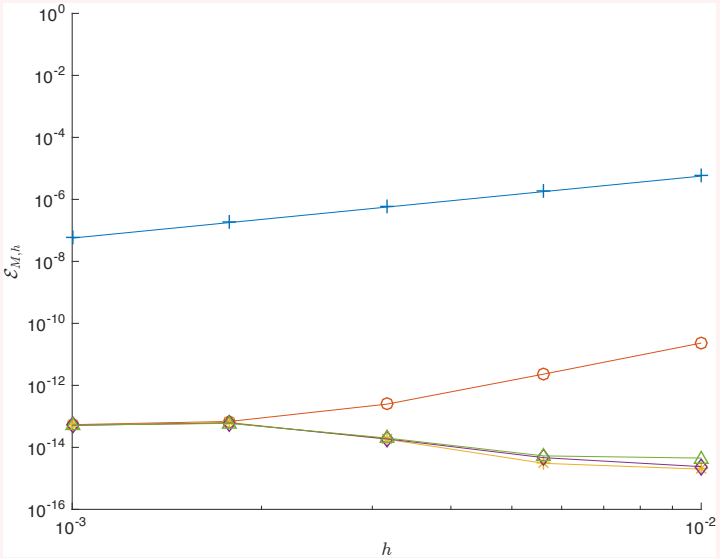
$$Tf = 10, \quad x \in (-30, 30), \quad N = 2^{10}$$



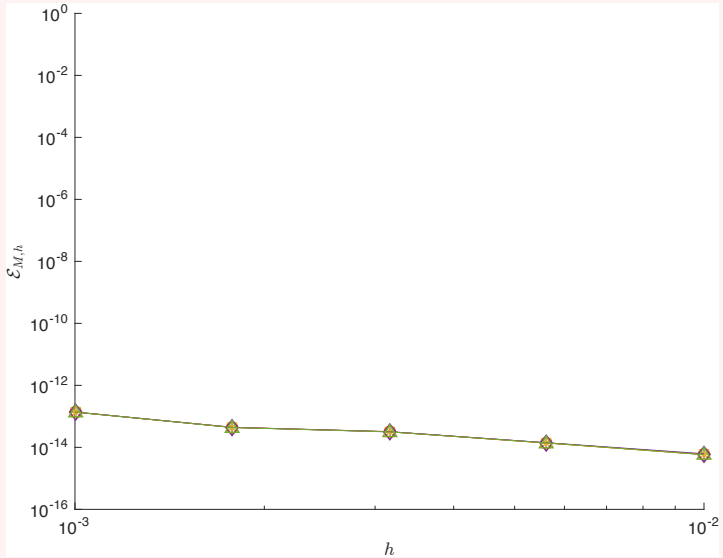
$\mathcal{E}_{P,h}$ Gauss-ERK



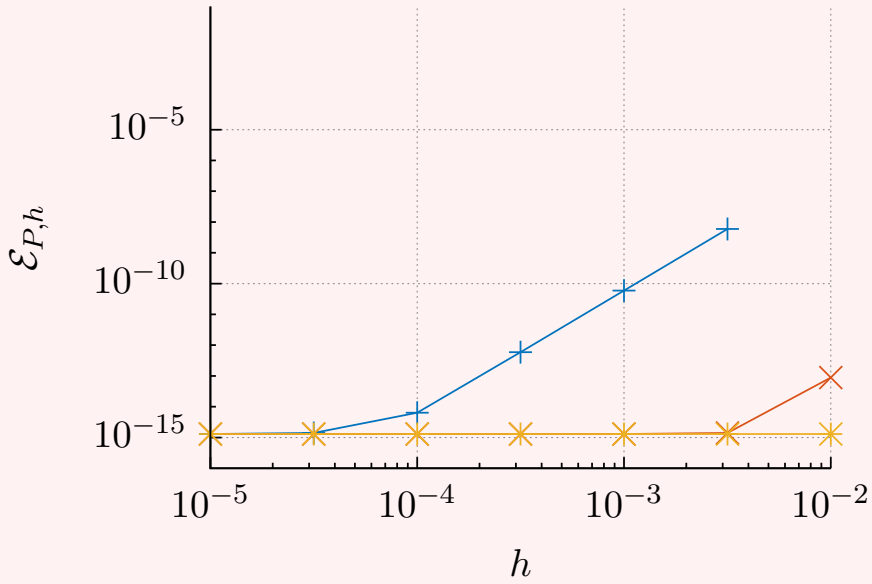
$\mathcal{E}_{P,h}$ Gauss-Lawson

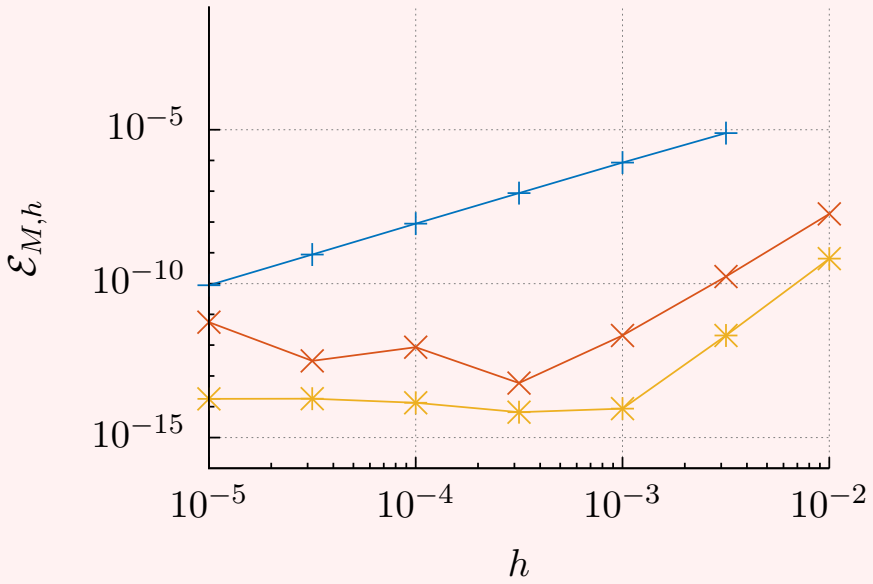


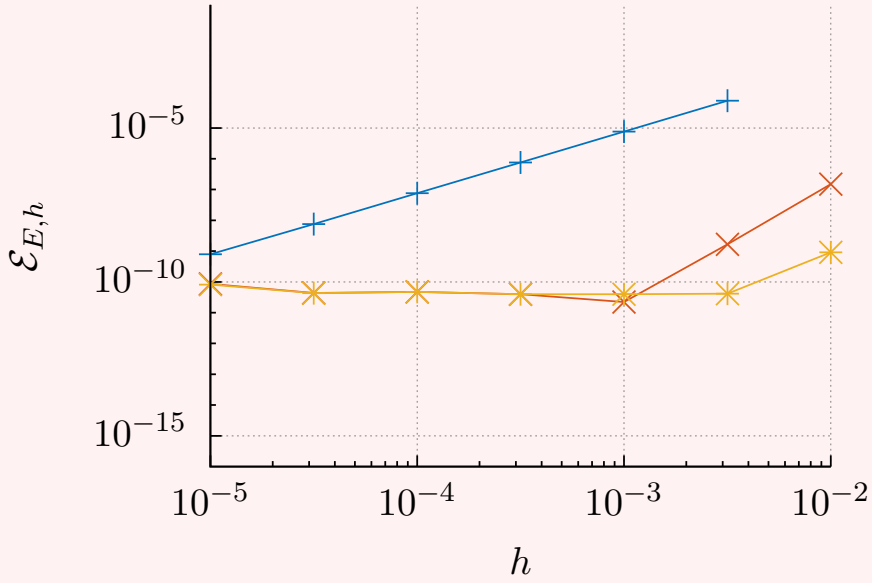
$\mathcal{E}_{M,h}$ Gauss-ERK



$\mathcal{E}_{M,h}$ Gauss-Lawson

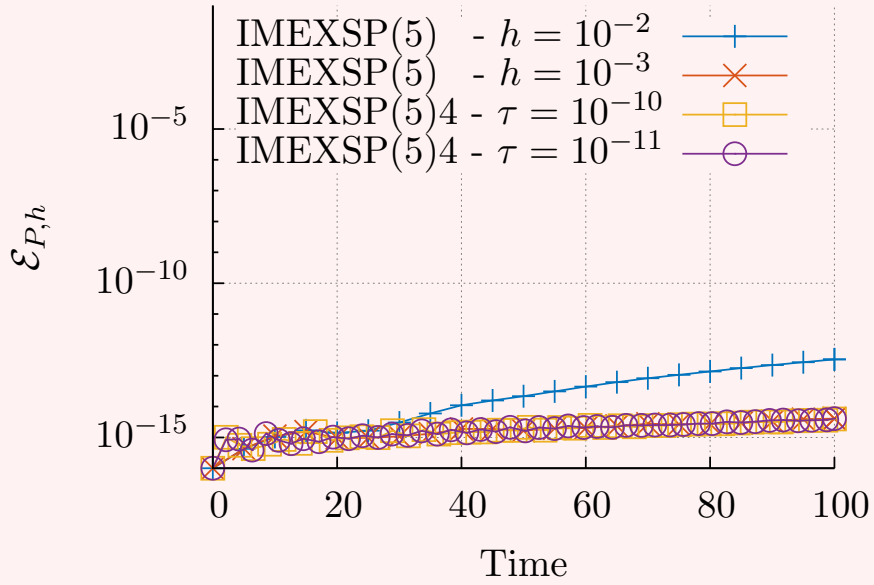

$\mathcal{E}_{P,h}$
10^{-5}
10^{-10}
10^{-15}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
h

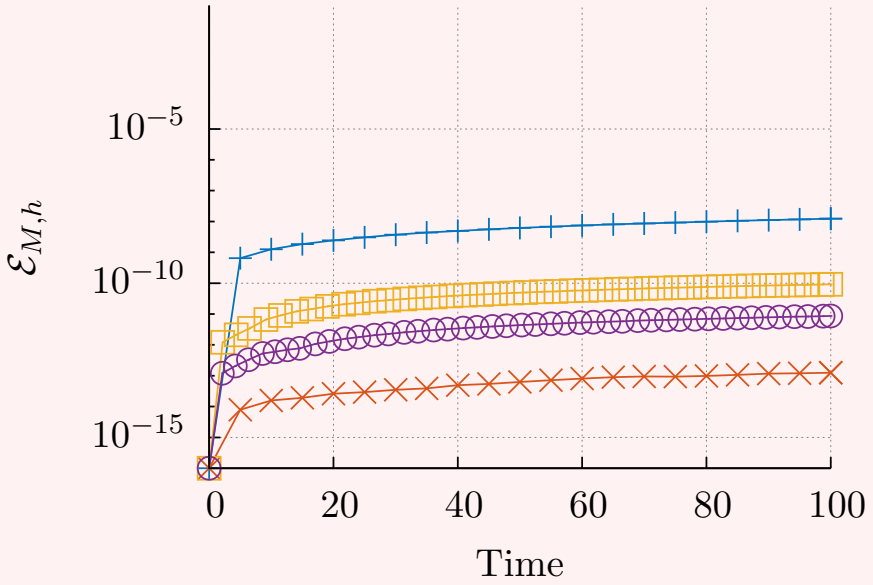

$\mathcal{E}_{M,h}$
10^{-5}
10^{-10}
10^{-15}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
h

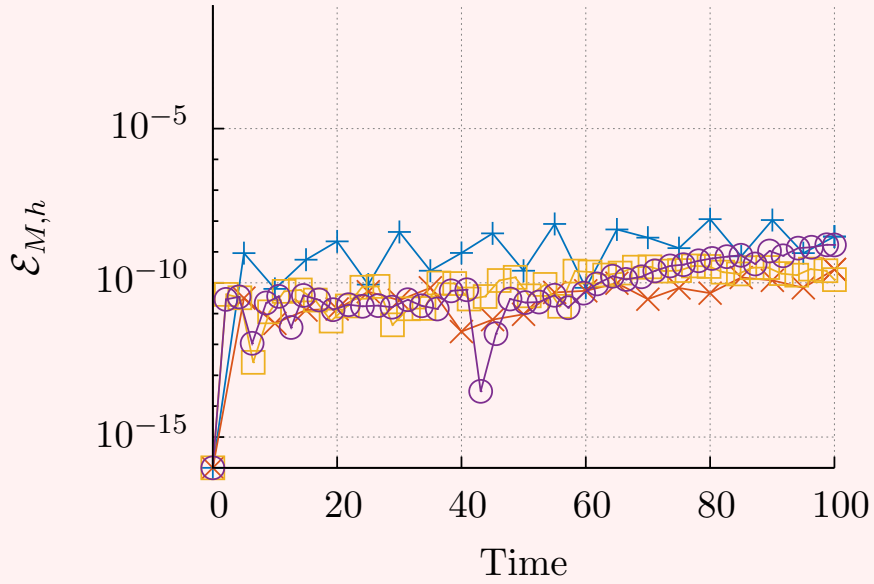

$\mathcal{E}_{E,h}$
10^{-5}
10^{-10}
10^{-15}
10^{-5}
10^{-4}
10^{-3}
10^{-2}
h

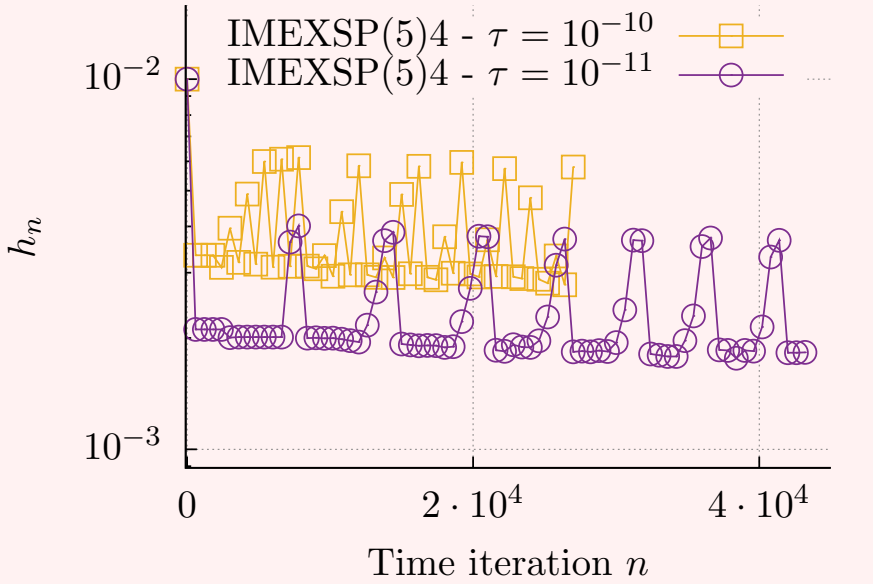

IMEXSP(2)
IMEXSP(4)
IMEXSP(5)

1D simulations - variable time step









We can reproduce the same experiments in 2D with soliton: the results are completely similar.

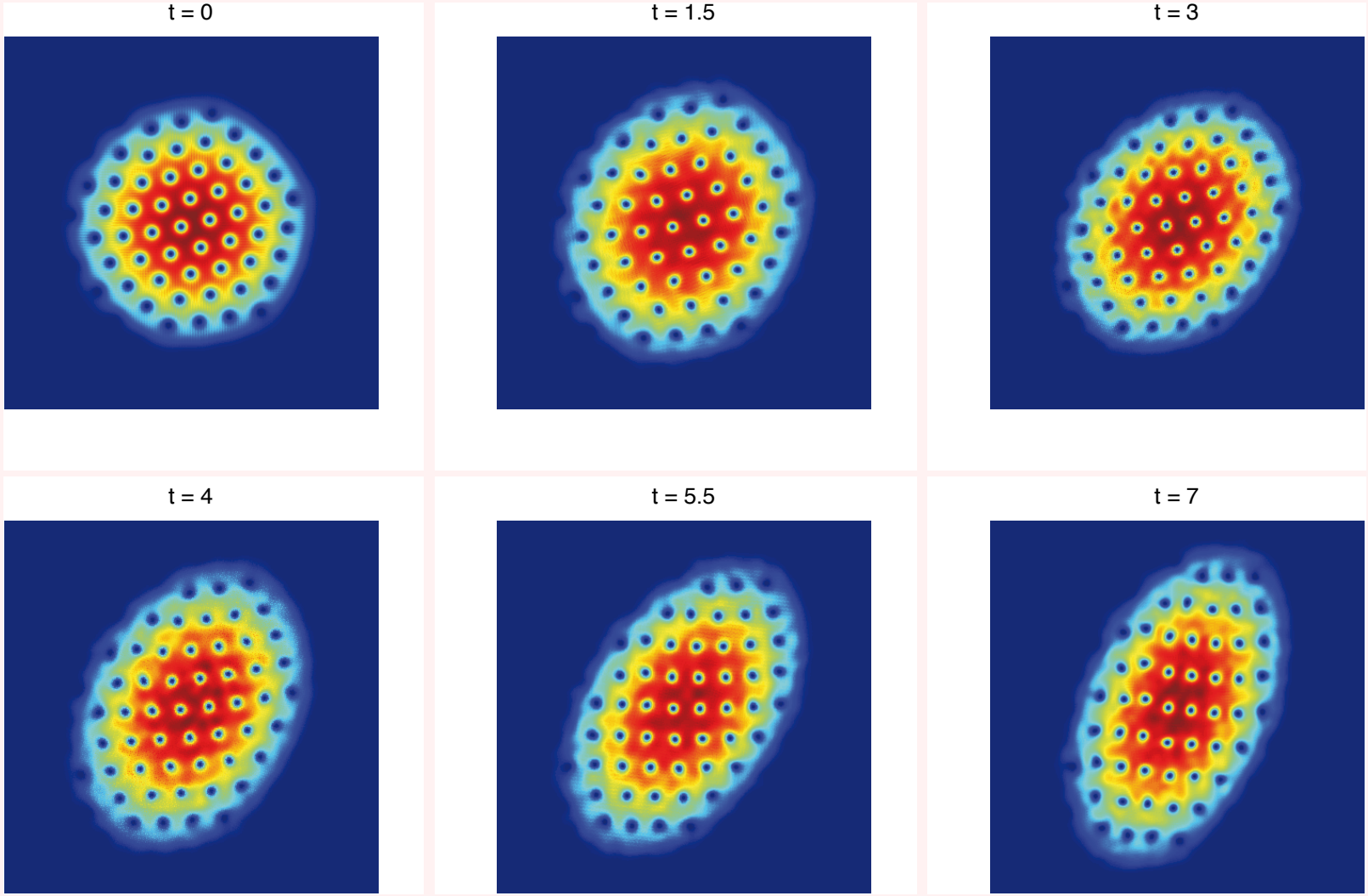
We present here a comparison of a BEC simulation realized in W. Bao, D. Marahrens, Q. Tang and Y. Zhang, (2013).

DIMENSIONLESS TIME-DEPENDENT GPE WITH ROTATING TERM

$$i\partial_t \varphi(\mathbf{x},t) = \left(-\frac{1}{2}\Delta + V_c(\mathbf{x}) + \beta|\varphi(\mathbf{x},t)|^2 - \Omega L_z\right)\varphi(\mathbf{x},t),\ \varphi(0,\mathbf{x}) = \varphi_0(\mathbf{x}),$$

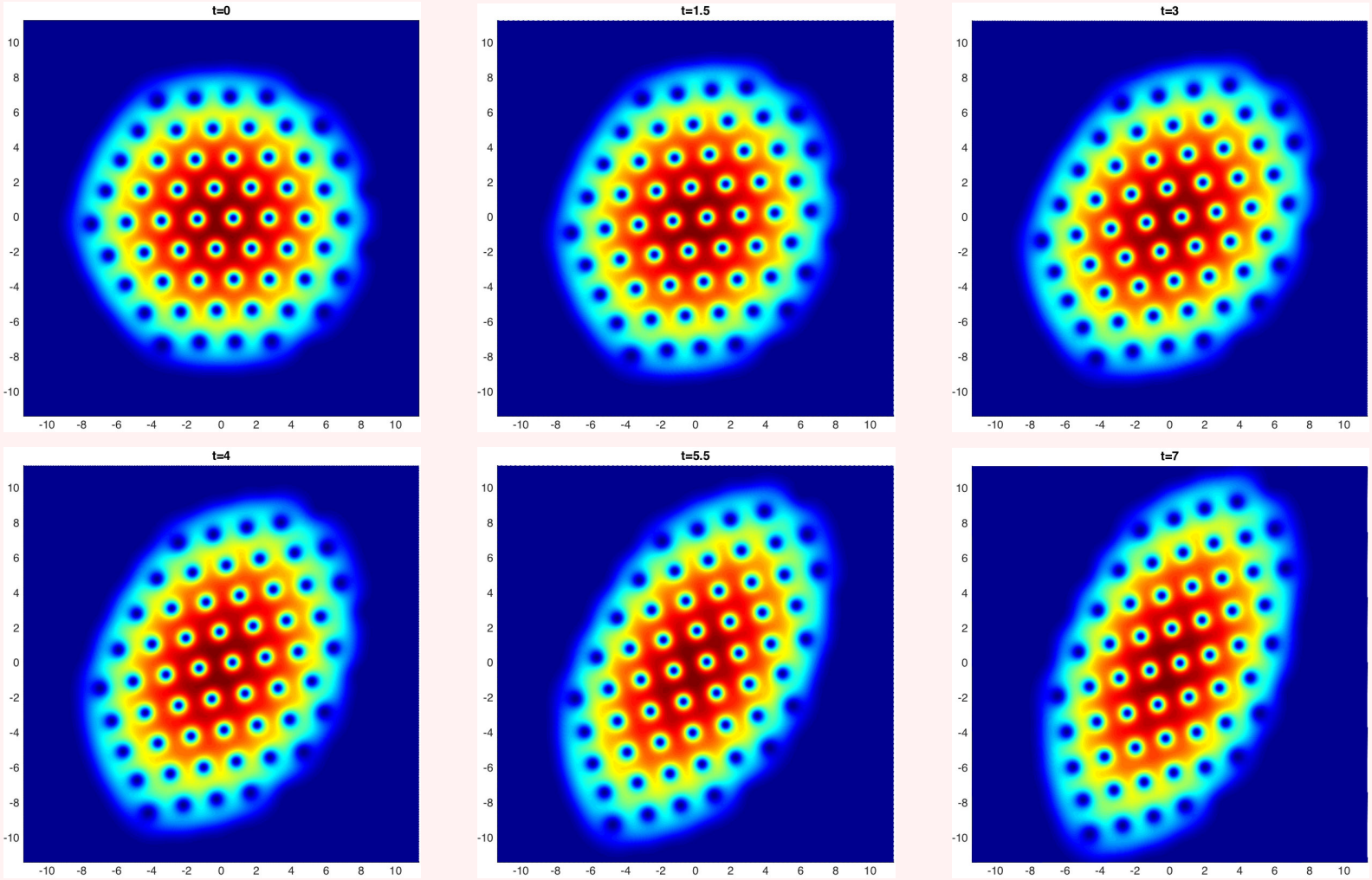
Parameters

- $\beta = 1000$, $\Omega = 0.9$, $\gamma_x = 1.05$ and $\gamma_y = 0.95$
- The computational domain is $(-16,16)^2$ with $2^9 = 512$ Fourier modes in each direction.
- $T = 7$
- Usual splitting scheme of order 2 with $h = 10^{-4}$ for Bao, Marahrens, Tang and Zhang
- Gauss-ERK method of order 6 with $h = 10^{-3}$.



Contour plots of the density function $|\varphi(t, \mathbf{x})|^2$ in a rotating BEC.

Result of Bao, Marahrens, Tang and Zhang



Contour plots of the density function $|\varphi(t, \mathbf{x})|^2$ in a rotating BEC.

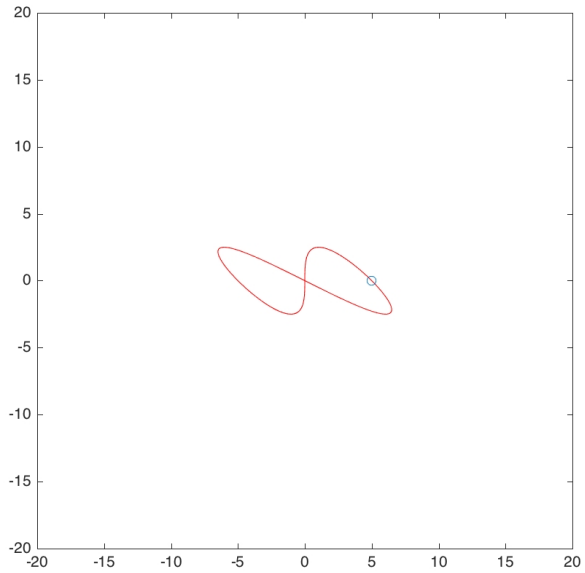
Drag a laser beam into a BEC at rest (without rotation)

$$i\partial_t \varphi(\mathbf{x},t) = \left(-\frac{1}{2}\Delta + V(t,\mathbf{x}) + \beta|\varphi(\mathbf{x},t)|^2\right)\varphi(\mathbf{x},t),\ \ \varphi(0,\mathbf{x}) = \varphi_0(\mathbf{x}),$$

$$V(t,\mathbf{x}) = \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2) + V_0 e^{-\frac{(x-x(t))^2 + (y-y(t))^2}{d}}$$

$$x(t) = 4\cos(\mu t)(1-\sin(\mu t))$$
$$y(t) = 4\cos(\mu t)\sin(\mu t)$$

$$\gamma_x = \gamma_y = 1, \quad \mu = 0.74, \quad d = 0.3,$$
$$V_0 = 100.$$



Use of Gauss-ERK method of order 2 with $h = 2 \cdot 10^{-3}$, $T_f = 15$, $x \in (-20, 20)^2$, grid 512×512.

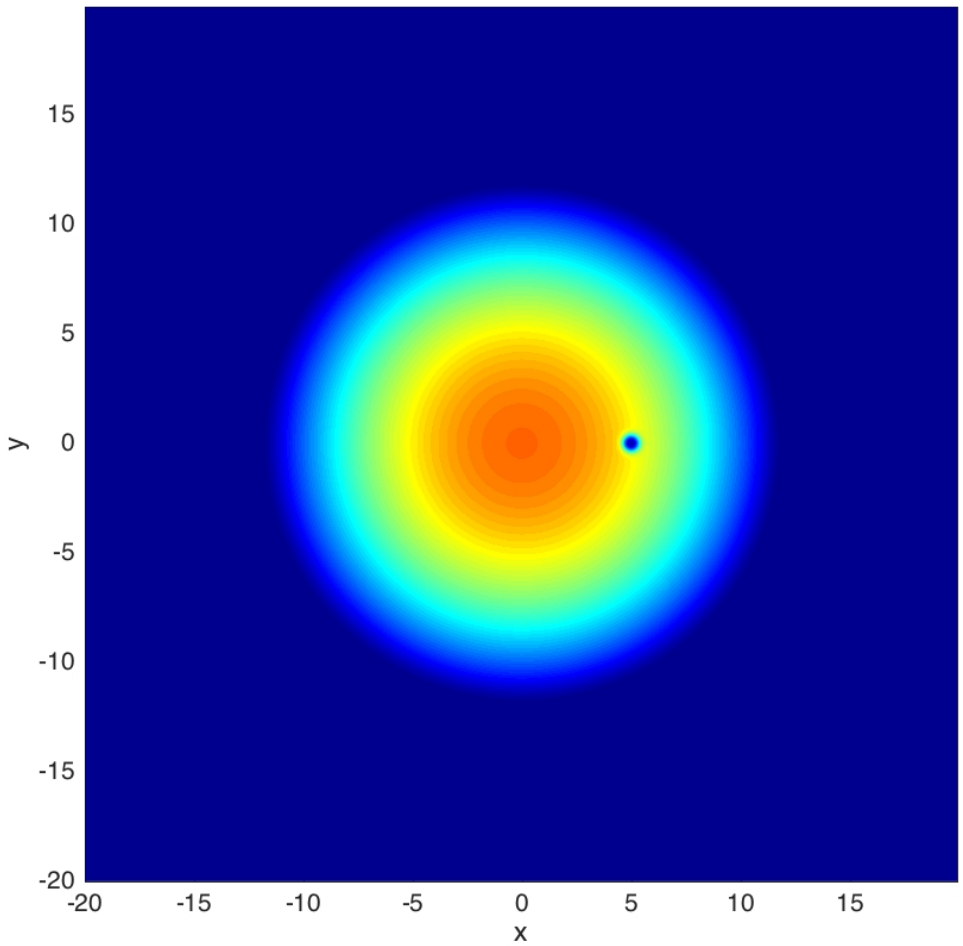
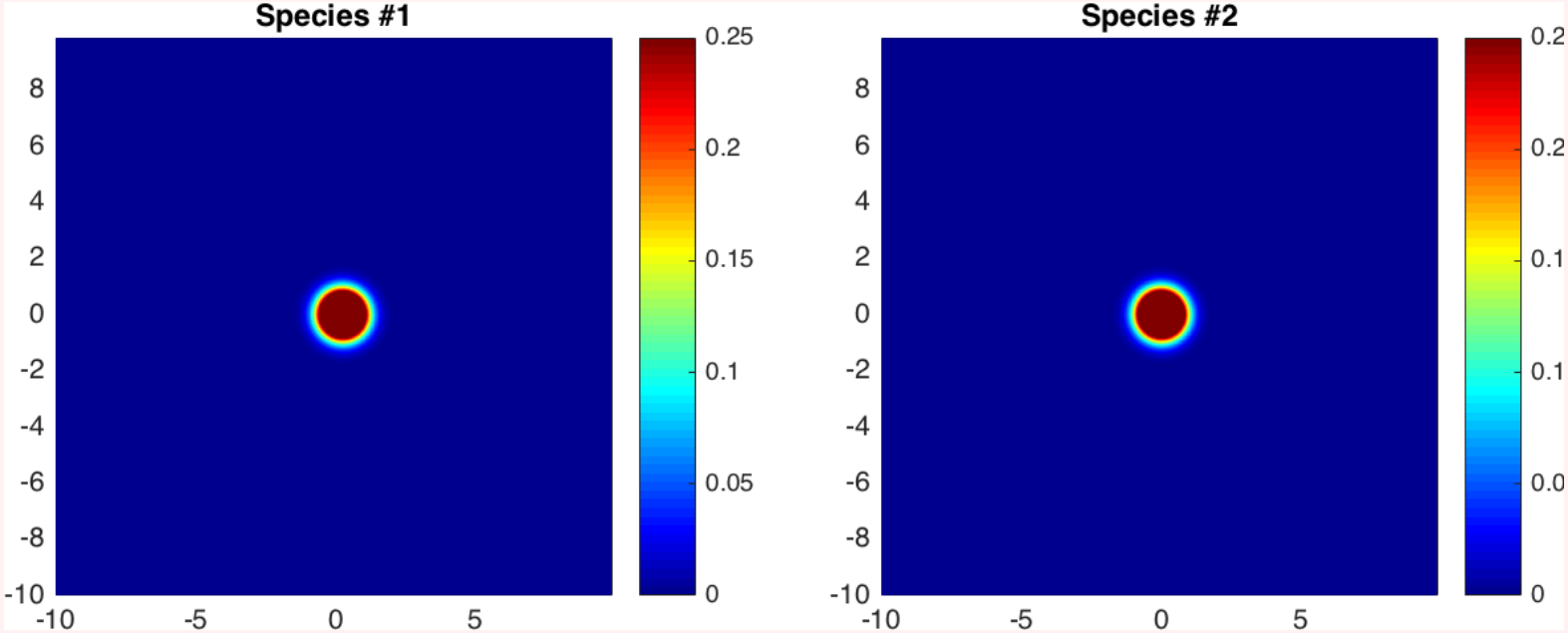


Figure : Stirred laser beam

We consider
$$\begin{cases} i\partial_t \psi_1(t,\mathbf{x}) = \left[-\frac{\Delta}{2} + V(\mathbf{x}) + \alpha_{11}|\psi_1|^2 + \alpha_{12}|\psi_2|^2 - \Omega L_z\right]\psi_1, \\ i\partial_t \psi_2(t,\mathbf{x}) = \left[-\frac{\Delta}{2} + V(\mathbf{x}) + \alpha_{12}|\psi_1|^2 + \alpha_{22}|\psi_2|^2 - \Omega L_z\right]\psi_2, \end{cases}$$

with $\Omega = 1/2$, $\gamma_x = \gamma_y = 1$, $\alpha_{11} = \alpha_{22} = 1$ and $\alpha_{12} = 5$.

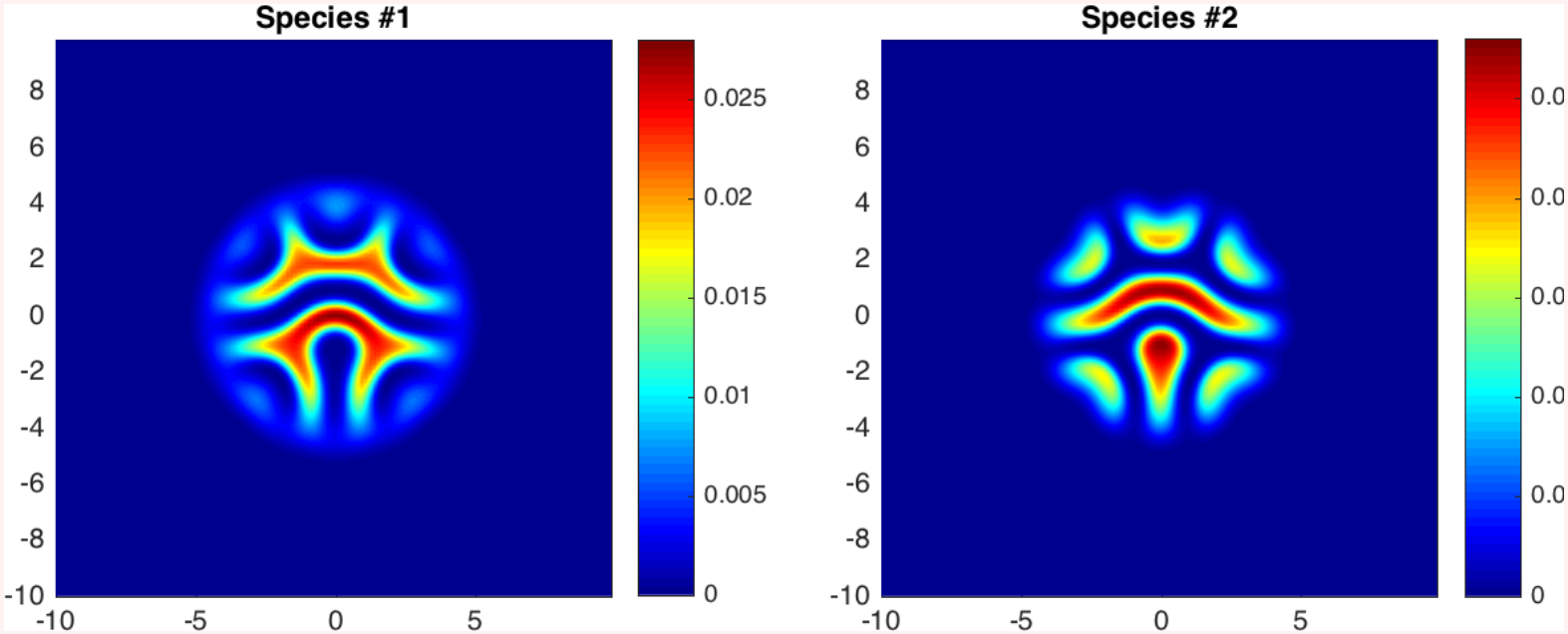
- $(x, y) \in (-10, 10)^2$, with a grid of 128×128 nodes,
- $T = 10$ and $h = 2 \cdot 10^{-3}$.
- $\psi_1(0, x) = e^{-x^2-y^2+5ix}$, $\psi_2(0, x) = e^{-x^2-y^2}$



$$\begin{cases} i\partial_t\psi_1(t,\mathbf{x}) = \left[-\dfrac{\Delta}{2} + V(\mathbf{x}) + \alpha_{11}|\psi_1|^2 + \alpha_{12}|\psi_2|^2 - \Omega L_z\right]\psi_1 - \kappa(i\partial_x + \partial_y)\psi_2, \\ i\partial_t\psi_2(t,\mathbf{x}) = \left[-\dfrac{\Delta}{2} + V(\mathbf{x}) + \alpha_{12}|\psi_1|^2 + \alpha_{22}|\psi_2|^2 - \Omega L_z\right]\psi_2 - \kappa(i\partial_x - \partial_y)\psi_1, \end{cases}$$

with $\Omega = 1/2$, $\gamma_x = \gamma_y = 1.2$, $\alpha_{11} = \alpha_{22} = 400$, $\alpha_{12} = 800$, $\kappa = 1.75$.

- $(x, y) \in (-10, 10)^2$, with a grid of 128×128 nodes,
- $T = 20$ and $h = 2 \cdot 10^{-3}$.



- We derive three RK type schemes for (NLS) eqs: ERK, Lawson and IMEX
- ERK and Lawson schemes are proven to be convergent to order s
- ERK and Lawson schemes are of order $2s$ for Gauss collocation points
- Lawson scheme preserves mass if coefficients of RK method satistify Cooper condition
- ERK, Lawson and IMEX methods are efficient even for nonautonomous systems
- Variable time step