Three approaches for the design of adaptive time-splitting methods

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Theme

Splitting methods. Time integration of nonlinear evolution equations by exponential operator splitting methods

$$\begin{cases} u'(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \qquad t \in (0,T), \\ u(0) \text{ given}. \end{cases}$$

Linear case. For linear evolution equations, exponential operator splitting methods can be cast into general form (time grid points $0 = t_0 < \cdots < t_N \leq T$ and stepsizes $\tau_{n-1} = t_n - t_{n-1}$)

$$u'(t) = A\,u(t) + B\,u(t), \qquad t \in (0,T),$$

$$u_n = \prod_{j=1}^{s} \mathrm{e}^{b_j \tau_{n-1} B}\, \mathrm{e}^{a_j \tau_{n-1} A}\, u_{n-1} \;\approx\; u(t_n) = \mathrm{e}^{\tau_{n-1}(A+B)}\, u(t_{n-1}), \qquad n \in \{1,\dots,N\}.$$

Areas of application.

- Schrödinger equations (Quantum mechanics)
- Damped wave equations (Nonlinear acoustics)
- Parabolic equations (Pattern formation)
- Kinetic equations (Plasma physics)

Main theme

Local error control. Use of local error control to adjust time stepsize

$$\tau_{\text{optimal}} = \tau_{\text{current}} \cdot \min\left(\alpha_{\max}, \max\left(\alpha_{\min}, \sqrt[p+1]{\alpha \cdot \frac{\text{tol}}{\text{err}_{\text{local}}}}\right)\right)$$

in general enhances reliability and efficiency of time integration.

Question. How to construct estimators for local error in the context of splitting methods?

Approches. Different approaches rely on

- embedded splitting methods (with OTHMAR KOCH),
- defect-based a posteriori local error estimators (with HARALD HOFSTÄTTER, OTHMAR KOCH, WINFRIED AUZINGER),
- associated approximations with negligible additional cost (with SERGIO BLANES, FERNANDO CASAS).

Outline

Main theme. Design and theoretical analysis of local error estimators for exponential operator splitting methods.

Outline.

- Splitting methods
- Local error estimators
  - Embedded splitting methods
  - Defect-based local error estimators
  - Associated approximations
- Numerical illustrations
  - Nonlinear Schrödinger equations
  - Diffusion-reaction systems

Exponential operator splitting methods for nonlinear evolution equations

Calculus of Lie-derivatives and Gröbner–Alekseev formula

Exponential operator splitting methods

Splitting methods. For nonlinear evolution equations of form

$$\begin{cases} u'(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \quad t \in (0,T), \\ u(0) \text{ given}, \end{cases}$$

determine approximations at time grid points $0 = t_0 < \cdots < t_N \leq T$ with associated stepsizes $\tau_{n-1} = t_n - t_{n-1}$ for $n \in \{1, \dots, N\}$ by recurrence

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) \;\approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big).$$

Splitting methods rely on presumption that corresponding subproblems are solvable in accurate and efficient manner

$$v'(t) = A\big(v(t)\big), \qquad w'(t) = B\big(w(t)\big),$$
$$v(t) = \mathscr{E}_A\big(t, v(0)\big), \qquad w(t) = \mathscr{E}_B\big(t, w(0)\big).$$

High-order splitting methods are cast into following format with suitably chosen real (or complex) coefficients

$$\mathscr{S}_F(\tau,\cdot) = \mathscr{E}_B(b_s\tau,\cdot) \circ \mathscr{E}_A(a_s\tau,\cdot) \circ \cdots \circ \mathscr{E}_B(b_1\tau,\cdot) \circ \mathscr{E}_A(a_1\tau,\cdot) \;\approx\; \mathscr{E}_F(\tau,\cdot).$$

Compact formulation

Compact formulation. Calculus of Lie-derivatives permits compact formulation and reveals analogies to significantly simpler linear case

$$\begin{aligned} &\mathrm{e}^{a_1\tau D_A}\,\mathrm{e}^{b_1\tau D_B}\cdots\mathrm{e}^{a_s\tau D_A}\,\mathrm{e}^{b_s\tau D_B} \\ &\quad = \mathcal{E}_B(b_s\tau,\cdot)\circ\mathcal{E}_A(a_s\tau,\cdot)\circ\cdots\circ\mathcal{E}_B(b_1\tau,\cdot)\circ\mathcal{E}_A(a_1\tau,\cdot)\,. \end{aligned}$$

Recipe. In order to extend result for linear case to nonlinear case,

- replace operator A, B by Lie-derivatives D_A, D_B and
- reverse order of evolution operators.

Example methods ($p = 1, 2$)

Low-order methods.

- First-order Lie–Trotter splitting method

$$a_1 = 1 = b_1 \,, \qquad \mathscr{S}_F(\tau, \cdot) = \mathrm{e}^{\tau D_B} \, \mathrm{e}^{\tau D_A} \,.$$

- Second-order Strang splitting method

$$a_1 = \tfrac{1}{2} = a_2 \,, \qquad b_1 = 1 \,, \qquad b_2 = 0 \,,$$
$$\mathscr{S}_F(\tau, \cdot) = \mathrm{e}^{\frac{1}{2}\tau D_A} \, \mathrm{e}^{\tau D_B} \, \mathrm{e}^{\frac{1}{2}\tau D_A} \,.$$

Example methods ($p = 4$)

Higher-order methods.

- Symmetric fourth-order splitting method by Blanes, Moan (2002)

$$a_1 = 0\,, \qquad a_2 = 0.245298957184271 = a_7\,,$$
$$a_3 = 0.604872665711080 = a_6\,, \qquad a_4 = \tfrac{1}{2} - (a_2 + a_3) = a_5\,,$$
$$b_1 = 0.0829844064174052 = b_7\,, \qquad b_2 = 0.396309801498368 = b_6\,,$$
$$b_3 = -0.0390563049223486 = b_5\,, \qquad b_4 = 1 - 2\,(b_1 + b_2 + b_3)\,.$$

  Stability ensured for evolution equations of Schrödinger type.

- Symmetric fourth-order splitting method by Yoshida ($s = 4$, complex variant of famous scheme)

$$\alpha = 0.324396404020171182976156 - 0.134586272490806696789444\,\mathrm{i}\,,$$
$$\beta = 0.351207191959657634047688 + 0.269172544981613393578885\,\mathrm{i}\,,$$
$$a_1 = \tfrac{1}{2}\,\alpha\,, \qquad a_2 = \tfrac{1}{2}\,(\alpha + \beta) = a_3\,, \qquad a_4 = a_1\,,$$
$$b_1 = \alpha = b_3\,, \qquad b_2 = \beta\,, \qquad b_4 = 0\,.$$

  Stability ensured for evolution equations of parabolic type, since $\Re(a_j), \Re(b_j) \geq 0$ for $j \in \{1, \ldots, 4\}$.

Approaches for design and analysis of local error estimators

Local error estimators

Approaches. Study different approaches for design and theoretical analysis of local error estimators for splitting methods.

- Embedded splitting methods

  O. Koch, Ch. Neuhauser, M. Th. *Embedded exponential operator splitting methods for the time integration of nonlinear evolution equations* (2013).

- A posteriori local error estimators

  W. Auzinger, O. Koch, M. Th. *Defect-based local error estimators for splitting methods, with application to Schrödinger equations. Part I. The linear case* (2012).

  W. Auzinger, O. Koch, M. Th. *Defect-based local error estimators for splitting methods, with application to Schrödinger equations. Part II. Higher-order methods for linear problems* (2014).

  W. Auzinger, H. Hofstätter, O. Koch, M. Th. *Defect-based local error estimators for splitting methods, with application to Schrödinger equations. Part III. The nonlinear case* (2015).

- Approximations with negligible additional cost (recent work with Sergio and Fernando)

Simplification. Specify local error estimators for first time step ($\tau > 0$).

Embedded splitting methods

Examples and theoretical basis

Embedded splitting methods

Heuristic approach. Consider splitting method of nonstiff order p

$$u_1 = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\tau D_A}\,\mathrm{e}^{b_{s+1-j}\tau D_B}\,u_0\,.$$

Design related splitting method of nonstiff order $\widehat{p}$ such that certain coefficients coincide

$$\widehat{u}_1 = \prod_{j=1}^{\widehat{s}} \mathrm{e}^{\widehat{a}_{s+1-j}\tau D_A}\,\mathrm{e}^{\widehat{b}_{s+1-j}\tau D_B}\,u_0\,.$$

Use difference between two approximations as local error estimator

$$\mathrm{err}_{\mathrm{local}} = \big\| u_1 - \widehat{u}_1 \big\|_X\,.$$

Remark. Approach in spirit of *embedded Runge-Kutta methods* (but with higher cost).

Example (Schrödinger equations)

Example. Favourable scheme ($p = 4$, BLANES & MOAN) and embedded scheme ($\widehat{p} = 3$, KOCH & TH.).

j	a_j	j	b_j
1	0	1,7	0.0829844064174052
2,7	0.245298957184271	2,6	0.396309801498368
3,6	0.604872665711080	3,5	$-$0.0390563049223486
4,5	$1/2-(a_2+a_3)$	4	$1-2\,(b_1+b_2+b_3)$

j	$\widehat{a}_j$	j	$\widehat{b}_j$
1	a_1	1	b_1
2	a_2	2	b_2
3	a_3	3	b_3
4	a_4	4	b_4
5	0.3752162693236828	5	0.4463374354420499
6	1.4878666594737946	6	$-$0.0060995324486253
7	$-$1.3630829287974774	7	0

Example (Parabolic equations)

Example. Complex scheme ($p = 4$, Yoshida) and embedded scheme ($\widehat{p} = 3$, Koch & Th.).

j	a_j
1	0
2,4	0.3243964040201712 + 0.1345862724908067 i
3	0.3512071919596576 − 0.2691725449816134 i

j	b_j
1,4	0.1621982020100856 + 0.0672931362454034 i
2,3	0.3378017979899144 − 0.0672931362454034 i

j	$\widehat{a}_j$
1	a_1
2	0.4157701540561051 + 0.2129482257474245 i
3	0.3855092282056243 − 0.1105557092016989 i
4	0.1987206177382706 − 0.1023925165457255 i

j	$\widehat{b}_j$
1	b_1
2	0.4052251807333103 + 0.1988642124619028 i
3	0.4325766172566041 − 0.2661573487073062 i
4	0

Theoretical justification

Theoretical justification. Consider high-order splitting methods and employ local error representations that are suitable for nonlinear evolution equations involving unbounded operators.

Theorem (Th. 2008, Th. 2012, Koch & Neuhauser & Th. 2013)

A splitting method of nonstiff order p admits the (formal) expansion

$$\mathscr{L}_F(t,v) = \sum_{k=1}^{p} \sum_{\substack{\mu\in\mathbb{N}^k \\ |\mu|\le p-k}} \frac{1}{\mu!}\, t^{k+|\mu|}\, C_{k\mu} \prod_{\ell=1}^{k} ad_{D_A}^{\mu_\ell}(D_B)\, \mathrm{e}^{tD_A}\, v + R_{p+1}(t,v)\,,$$

$$C_{k\mu} = \sum_{\lambda\in\Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell}\, c_{\lambda_\ell}^{\mu_\ell} - \prod_{\ell=1}^{k} \frac{1}{\mu_\ell+\cdots+\mu_k+k-\ell+1}\,.$$

Main tools. Calculus of Lie derivatives, Gröbner–Alekseev formula.

Remark. Further considerations show that resulting (redundant) stiff order conditions $C_{k\mu}=0$ coincide with nonstiff order conditions.

Theoretical justification

Remarks.

- Application of local error representation to different classes of (non)linear evolution equations such as Schrödinger equations or diffusion-reaction systems requires characterisation of domains of iterated Lie-commutators (regularity and consistency requirements).
- In connection with Schrödinger equations, it is often justified to assume that exact solution is regular. For linear equations versus nonlinear equations, the regularity requirements are

$$D = H^{p}(\Omega)\,, \qquad D = H^{2p}(\Omega)\,.$$

- For sufficiently regular solutions (bounded in D), above local error representation implies

$$\mathscr{L}_F(\tau, v) = \mathscr{S}_F(\tau, v) - \mathscr{E}_F(\tau, v) = \mathscr{O}\big(\tau^{p+1}\big)\,.$$

  Provided that $\widehat{p} > p$, this justifies use of local error estimator

$$\mathrm{err}_{\mathrm{local}} = \big\| u_1 - \widehat{u}_1 \big\|_X = \mathscr{O}\big(\tau^{p+1}\big)\,.$$

Global error estimate (Full discretisations)

Discretisation. Full discretisation of nonlinear Schrödinger equations (GPE) by high-order variable stepsize time-splitting methods combined with pseudo-spectral methods (Fourier, Sine, Hermite).

Theorem (Th. 2012)

Provided that exact solution remains bounded in fractional power space X_β defined by principal linear part for $\beta \geq p$, global error estimate holds

$$\big\| u_{NM} - u(t_N) \big\|_X \leq C \Big(\big\| u_0 - u(0) \big\|_X + \tau_{\max}^p + M^{-q} \Big).$$

Extensions.

- Time-dependent Gross–Pitaevskii equations with additional rotation term, see Hofstätter, Koch, Th. (2014).
- Multi-revolution composition time-splitting pseudo-spectral methods for highly oscillatory problems (with Chartier, Méhats).

Associated approximations with negligible additional computational cost

Examples and theoretical basis

Novel approach

Approach. Consider nonlinear evolution equation

$$\begin{cases} u'(t) = A\big(u(t)\big) + B\big(u(t)\big), & t \in (0,T), \\ u(0) = u_0. \end{cases}$$

Realise higher-order splitting method in straightforward manner

$$\begin{aligned} & u = u_n \\ & \text{for } j = 1 : s \\ & \qquad u = \mathscr{E}_A(a_j \tau_n, u) \qquad \text{Solution of subproblem } u'(t) = A\big(u(t)\big) \\ & \qquad u = \mathscr{E}_B(b_j \tau_n, u) \qquad \text{Solution of subproblem } u'(t) = B\big(u(t)\big) \\ & \text{end} \\ & u_{n+1} = u \end{aligned}$$

Use suitable linear combination of intermediate values to compute associated approximation that serves as local error estimator.

Novel approach

Schrödinger equations. Consider splitting method by Blanes, Moan

$$p = 4\,, \qquad s = 7\,.$$

Associated third-order approximation obtained by certain linear combination of intermediate values yields local error estimator

$$
\begin{array}{ll}
u = u_n & u_{\text{Estimator}} = \alpha_0\, u \\
\text{for } j = 1 : s & \\
\quad u = \mathcal{E}_A(a_j \tau_n, u) & u_{\text{Estimator}} = u_{\text{Estimator}} + \alpha_{2j-1}\, u \\
\quad u = \mathcal{E}_B(b_j \tau_n, u) & u_{\text{Estimator}} = u_{\text{Estimator}} + \alpha_{2j}\, u \\
\text{end} & \\
u_{n+1} = u & \text{Local error estimator} = u - u_{\text{Estimator}}
\end{array}
$$

Parabolic equations. Consider instead splitting method by Yoshida with complex coefficients and melt two subsequent time steps ($p = 4$, $s = 7$).

Novel approach

Benefit. Compared to approaches based on embedded splitting methods or defect-based local error estimators, novel approach leads to local error estimators with negligible additional computational cost.

Open questions.

- Provide coefficients for favourable higher-order splitting methods.
- Numerical tests confirm stability of associated approximations. Rigorous argument?

Numerical examples

Local error control

Local error control. Use of local error control to adjust time stepsize

$$\tau_{\text{optimal}} = \tau_{\text{current}} \cdot \min\left(\alpha_{\max}, \max\left(\alpha_{\min}, \sqrt[p+1]{\alpha \cdot \frac{\text{tol}}{\text{err}_{\text{local}}}}\right)\right),$$

$$\alpha_{\max} = 1.5\,, \qquad \alpha_{\min} = 0.2\,, \qquad \alpha = 0.25\,,$$

enhances reliability and efficiency of time integration.

Illustration (Schrödinger equation)

Test equation (see Bao et al.). Consider nonlinear Schrödinger equation under harmonic potential ($d = 1$, $\omega = 2$, $\vartheta = 1$)

$$\mathrm{i}\,\partial_t \psi(x,t) = \Big(-\tfrac{1}{2}\,\varepsilon\,\Delta + \tfrac{1}{\varepsilon}\,U(x) + \tfrac{1}{\varepsilon}\,\vartheta\,\big|\psi(x,t)\big|^2 \Big)\,\psi(x,t)\,.$$

Small value of (semi-classical) parameter $\varepsilon > 0$ causes high oscillations in initial condition and solution

$$\psi(x,0) = \varrho_0(x)\,\mathrm{e}^{\mathrm{i}\,\frac{1}{\varepsilon}\,\sigma_0(x)}\,, \qquad \varrho_0(x) = \mathrm{e}^{-x^2}\,, \qquad \sigma_0(x) = -\ln\big(\mathrm{e}^{x} + \mathrm{e}^{-x}\big)\,.$$

Use Fourier spectral space discretisation combined with fourth-order time-splitting method by Blanes & Moan ($x \in [-8,8]$, $M = 8192$, $t \in [0,3]$).

Illustration (Solution behaviour for $\varepsilon = 10^{-2}$)

First observation. Even a simple local error control for second-order Strang splitting method based on first-order Lie–Trotter splitting method is useful to enhance reliability! See Movie.

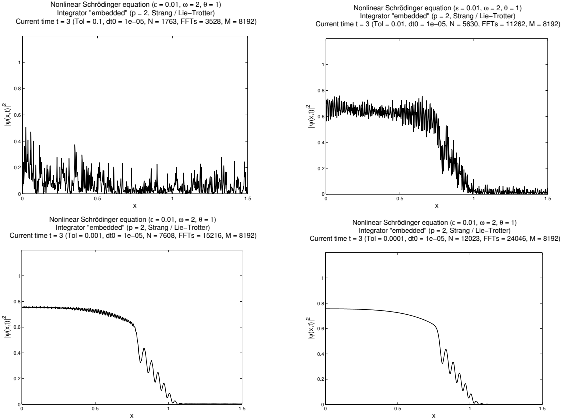


Illustration (Global error)

Expectation. Use of higher-order methods will enhance efficiency.

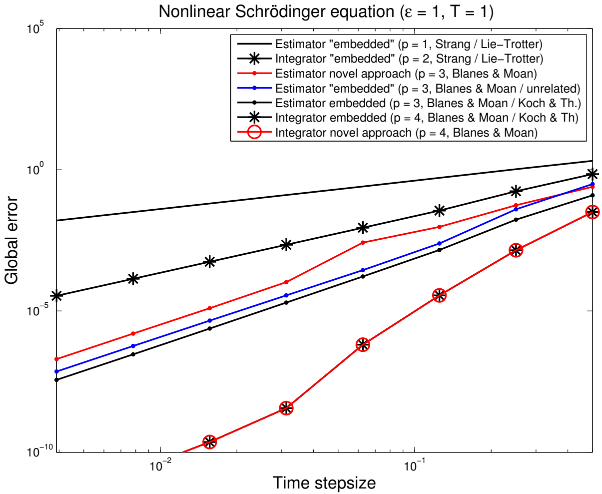
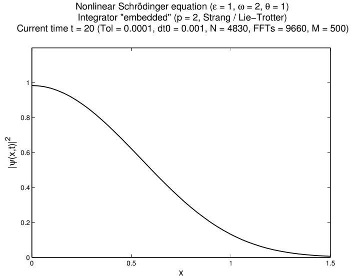


Illustration ($\varepsilon = 1$)

Comparison. Compare approach based on embedded splitting methods with novel approach. Obtain expected results for $\varepsilon = 1$, $T = 10$, $\mathrm{Tol} = 10^{-4}$.

- Higher-order method superior to low-order method (e.g. with respect to number of FFT transforms).



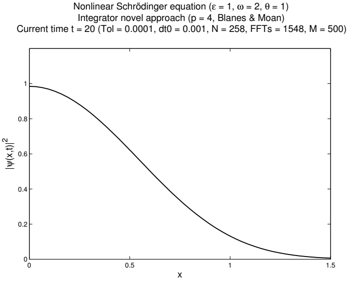
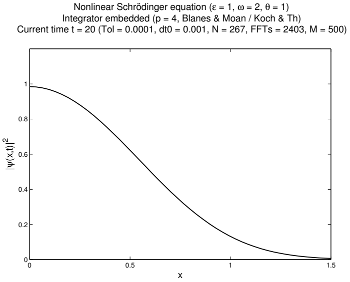


Illustration ($\varepsilon = 1$)

Comparison. Compare approach based on embedded splitting methods with novel approach. Obtain expected results for $\varepsilon = 1$, $T = 10$, $\mathrm{Tol} = 10^{-4}$.

- Good performance of novel approach in comparison with embedded method (e.g. with respect to number of FFT transforms).



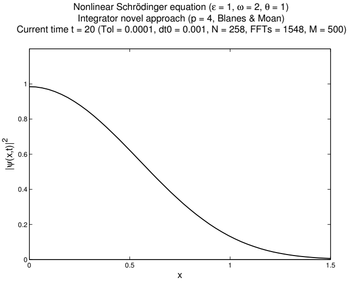


Illustration ($\varepsilon = 1$)

Best performance. Observe best performance for novel approach (FFTs).

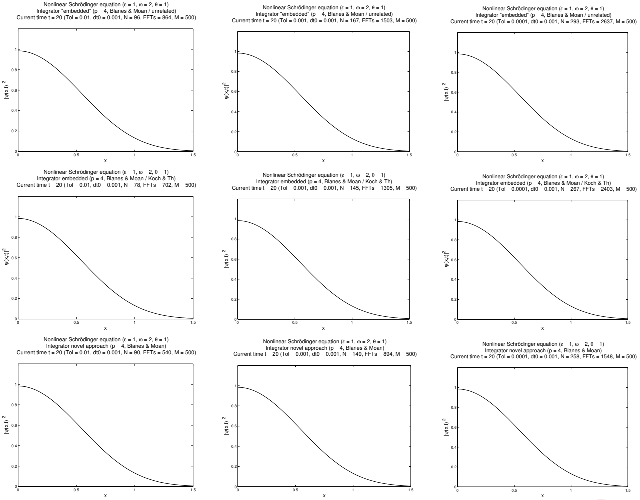


Illustration ($\varepsilon = 10^{-2}$)

Observation. Time integration of test equation for $\varepsilon = 10^{-2}$ is delicate task. Number of time steps does not necessarily increase for smaller tolerances. Influence of choice of initial time stepsize? Improvement of local error control in this situation?

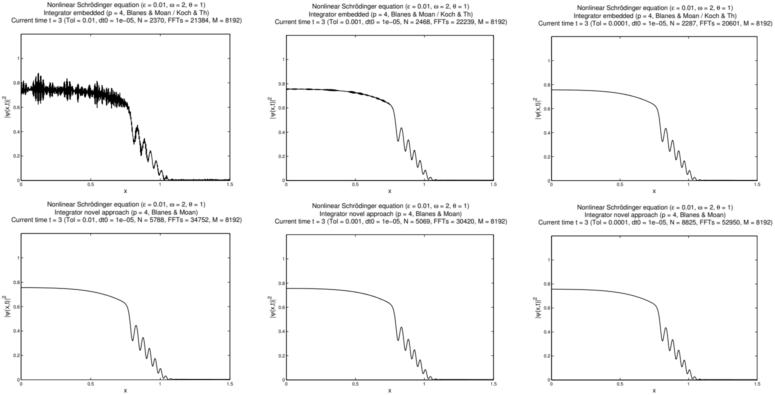


Illustration (Gray–Scott equations)

Test equation . Consider system of diffusion–reaction equations ($d = 2$)

$$\begin{cases} \partial_t u(x,t) = \big(D_u \Delta - \alpha\big)\, u(x,t) - u(x,t)\,\big(v(x,t)\big)^2 + \alpha\,, \\ \partial_t v(x,t) = \big(D_v \Delta - \beta\big)\, v(x,t) + u(x,t)\,\big(v(x,t)\big)^2\,. \end{cases}$$

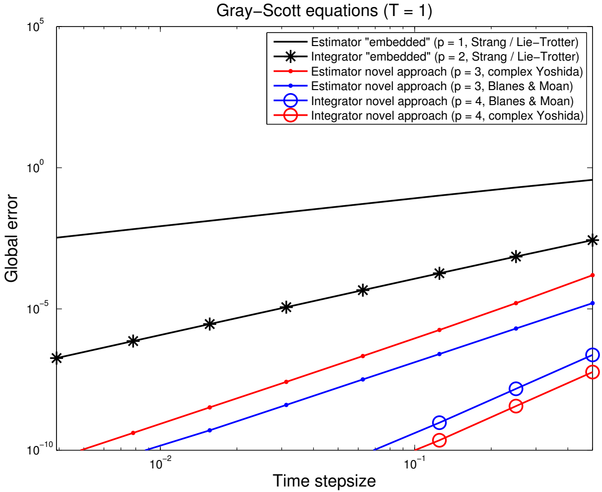
Special choice of parameters causes formation of patterns over long times

$$D_u = 2\,D_v = 0.16\,, \qquad f = 0.035\,, \qquad k = 0.06\,, \qquad \alpha = f\,, \qquad \beta = f + k\,,$$

see also NICOLAS P. ROUGIER. Use Fourier spectral space discretisation combined with fourth-order complex time-splitting method by YOSHIDA ($x \in [-75, 75]$, $M = 150 \times 150$).

Movie
Formation of patterns

Illustration (Global error)



Conclusions and future work

Conclusions.

- Adaptivity in time essential for reliable and efficient numerical simulations.
- Novel approach for time-splitting methods provides local error estimators with negligible additional cost.

Open questions.

- Theoretical understanding of novel local error estimators (favourable stability behaviour). Design of higher-order schemes.
- Detailed study of local error control for semi-classical Schrödinger equation to understand unexpected behaviour.

Thank you!