Convergence analysis of multi-revolution composition time-splitting spectral methods for highly oscillatory evolution equations

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Main references

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Highly oscillatory evolution equations

Highly oscillatory evolution equation. Consider nonlinear evolution equation involving highly oscillatory linear main part

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = \tfrac{1}{\varepsilon}\,A\,u(t) + B\big(u(t)\big)\,, \quad t \in (0,T)\,, \qquad 0 < \varepsilon \ll 1\,.$$

Basic requirements.

(i) *Unitarity.* Unbounded linear operator $A : D(A) \subset X \to X$ generates unitary group $(\mathscr{E}_A(t))_{t\in\mathbb{R}}$ on underlying Banach space $(X, \|\cdot\|_X)$

$$\forall\, t \in \mathbb{R} \quad \forall\, w \in X : \qquad \big\|\mathscr{E}_A(t)\,w\big\|_X = \|w\|_X\,.$$

(ii) *Periodicity.* Associated evolution operator is periodic in time

$$\exists\, T_0 > 0 \quad \forall\, w \in X : \qquad \mathscr{E}_A(T_0)\,w = w\,.$$

Time-dependent Schrödinger equations

Application to Schrödinger equations. Consider time-dependent nonlinear Schrödinger equation for $\psi : \Omega \times (0,T) \subseteq \mathbb{R}^d \times \mathbb{R} \to \mathbb{C}$

$$\mathrm{i}\,\partial_t \psi(x,t) = \tfrac{1}{\varepsilon}\,\mathscr{A}(x)\,\psi(x,t) + \mathscr{B}\big(|\psi(x,t)|\big)\,\psi(x,t)\,, \qquad (x,t) \in \Omega \times (0,T)\,,$$

and assume that linear main part is defined by self-adjoint operator on Hilbert space.

(i) *Unitarity.* Stone's theorem ensures that evolution operator $(\mathscr{E}_{-\frac{\mathrm{i}}{\varepsilon}\mathscr{A}}(t))_{t\in\mathbb{R}}$ forms unitary group on underlying Hilbert space.

(ii) *Periodicity.* Periodicity requirement satisfied in mono-frequent case, that is, eigenvalues of $\mathscr{A}$ are integer multiples of single value.

Illustrations

Periodicity. Time-dependent Schrödinger equation with linear main part defined by self-adjoint operator satisfies additional periodicity requirement in mono-frequent case

$$\mathrm{i}\,\partial_t \psi(x,t) = \tfrac{1}{\varepsilon}\,\mathscr{A}(x)\,\psi(x,t) + \mathscr{B}\big(|\psi(x,t)|\big)\,\psi(x,t)\,, \qquad (x,t) \in \Omega \times (0,T)\,.$$

Illustrations ($d = 2$). Consider Laplacian on bounded domain (Fourier basis functions)

$$\mathscr{A} = -\Delta\,, \qquad \Omega = (-a_1, a_1) \times (-a_2, a_2) \subset \mathbb{R}^2\,,$$

$$\mathscr{A}\mathscr{F}_m = \lambda_m \mathscr{F}_m\,, \qquad m = (m_1, m_2) \in \mathbb{Z}^2\,,$$

$$\mathscr{F}_{m_\ell}(x_\ell) = \frac{1}{\sqrt{2\,a_\ell}}\,\mathrm{e}^{\mathrm{i}\,m_\ell\,\pi\,(x_\ell/a_\ell+1)}\,, \qquad x = (x_1, x_2) \in \Omega\,,$$

$$\mathscr{F}_m(x) = \mathscr{F}_{m_1}(x_1)\,\mathscr{F}_{m_2}(x_2)\,, \qquad \lambda_m = \lambda_{m_1} + \lambda_{m_2} = \pi^2\left(\frac{m_1^2}{a_1^2} + \frac{m_2^2}{a_2^2}\right),$$

$$\text{special case} \quad a_1 = \pi = a_2: \qquad T_0 = 2\pi \quad \Longrightarrow \quad \Big(\forall\, m \in \mathbb{Z}^2: \quad \mathrm{e}^{\mathrm{i}\,T_0\,\lambda_m} = 1\Big),$$

$$\text{general case} \quad \frac{a_1^2}{a_2^2} \in \mathbb{Q} \quad \Longrightarrow \quad \Big(\exists\, T_0 > 0 \quad \forall\, m \in \mathbb{Z}^2: \quad \mathrm{e}^{\mathrm{i}\,T_0\,\lambda_m} = 1\Big).$$

Similar considerations hold for additional quadratic potential (Hermite basis functions) and additional rotation term (generalised Laguerre–Fourier–Hermite basis functions).

Reformulation

Highly oscillatory evolution equation. Consider nonlinear evolution equation involving highly oscillatory linear main part

$$\frac{\mathrm{d}}{\mathrm{d}\tau}\, v(\tau) = \tfrac{1}{\varepsilon} A\, v(\tau) + B\big(v(\tau)\big), \quad \tau \in (0,T), \qquad 0 < \varepsilon \ll 1.$$

Basic requirements.

(i) *Unitarity.* Unbounded linear operator $A : D(A) \subset X \to X$ generates unitary group on underlying Banach space.

(ii) *Periodicity.* Associated evolution operator is periodic in time.

Reformulation. Convenient to employ time scaling

$$v : [0,T] \longrightarrow X : \tau \longmapsto v(\tau),$$
$$\tau = \varepsilon t \quad \Longleftrightarrow \quad t = \tfrac{\tau}{\varepsilon},$$
$$u : \big[0, \tfrac{T}{\varepsilon}\big] \longrightarrow X : t \longmapsto u(t) = v(\varepsilon t),$$

which leads to long-term problem

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + \varepsilon\, B\big(u(t)\big), \quad t \in \big(0, \tfrac{T}{\varepsilon}\big), \qquad 0 < \varepsilon \ll 1.$$

Space and time discretisation of highly oscillatory evolution equations

Approach

Evolution operator. Consider highly oscillatory nonlinear evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + \varepsilon\, B\big(u(t)\big), \quad t \in \big(0, \tfrac{T}{\varepsilon}\big), \qquad 0 < \varepsilon \ll 1\,.$$

Employ formally linear notation for associated evolution operator

$$u(t) = \mathscr{E}_{A+\varepsilon B}(t)\, u(0)\,, \qquad t \in \big[0, \tfrac{T}{\varepsilon}\big]\,.$$

Objective. Introduce efficient space and time discretisation methods for computation of approximation to exact solution value at final time

$$u\big(\tfrac{T}{\varepsilon}\big) = \mathscr{E}_{A+\varepsilon B}\big(\tfrac{T}{\varepsilon}\big)\, u(0)\,.$$

Approach. Use approach studied in CHARTIER, MAKAZAGA, MURUA, VILLMART (2012). Employ simplifying assumption that final time is multiple of period (otherwise perform additional short time integration)

$$\text{final time } \tfrac{T}{\varepsilon} \;=\; \text{integer number} \;\times\; \text{period } T_0\,.$$

Use decomposition into equidistant subintervals

$$\text{final time } \tfrac{T}{\varepsilon} \;=\; \text{number of macro steps } N \;\times\; \text{subinterval of length } N_0\, T_0$$

with macro stepsize $H = \varepsilon N_0 > 0$ chosen such that $0 < H = \varepsilon N_0 < 1$.

Approach

Objective. Compute approximation at final time $\frac{T}{\varepsilon} = N N_0 T_0$ (recall $0 < H = \varepsilon N_0 < 1$)

$$w_N \approx \widehat{u}_N = u\left(\tfrac{T}{\varepsilon}\right) = \mathscr{E}_{A+\varepsilon B}(N N_0 T_0)\, u(0)\,.$$

Basic idea. Replace exact value at multiple of period by composition

$$\begin{aligned} u_n &= \prod_{j=1}^{r} \left(\mathscr{E}_{A-\beta_j \varepsilon N_0 B}(-T_0)\, \mathscr{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)\right) u_{n-1} \\ &\approx \widehat{u}_n = \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, \widehat{u}_{n-1}\,, \qquad n \in \{1, 2, \ldots, N\}\,. \end{aligned}$$

Suitable choice of coefficients $(\alpha_j, \beta_j)_{j=1}^{r}$ in dependence of $N_0 > 0$ leads to higher-order multi-revolution composition methods.

Remark. Solution of evolution equations with modified parameters required

$$\begin{aligned} u(t) &= \mathscr{E}_{A+\varepsilon B}(t)\, u(0)\,, & \tfrac{\mathrm{d}}{\mathrm{d}t} u(t) &= A u(t) + \varepsilon B\big(u(t)\big)\,, \\ v(t) &= \mathscr{E}_{A+\alpha_j \varepsilon N_0 B}(t)\, v(0)\,, & \tfrac{\mathrm{d}}{\mathrm{d}t} v(t) &= A v(t) + \alpha_j \varepsilon N_0 B\big(v(t)\big)\,, \\ w(t) &= \mathscr{E}_{A-\beta_j \varepsilon N_0 B}(t)\, w(0)\,, & \tfrac{\mathrm{d}}{\mathrm{d}t} w(t) &= A u(t) - \beta_j \varepsilon N_0 B\big(w(t)\big)\,. \end{aligned}$$

Approach

Objective. Compute approximation at final time $\frac{T}{\varepsilon} = N N_0 T_0$ (recall $0 < H = \varepsilon N_0 < 1$)

$$w_N \approx \widehat{u}_N = u\left(\tfrac{T}{\varepsilon}\right) = \mathscr{E}_{A+\varepsilon B}(N N_0 T_0)\, u(0)\,.$$

Basic idea. Replace exact value at multiple of period by composition

$$\begin{aligned} u_n &= \prod_{j=1}^{r} \left(\mathscr{E}_{A-\beta_j \varepsilon N_0 B}(-T_0)\, \mathscr{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)\right) u_{n-1} \\ &\approx \widehat{u}_n = \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, \widehat{u}_{n-1}\,, \qquad n \in \{1, 2, \ldots, N\}\,. \end{aligned}$$

Realisation. Realisation of multi-revolution composition method for low-dimensional time-dependent nonlinear Schrödinger equations relies on exponential operator splitting method for time discretisation combined with pseudo-spectral method for space discretisation.

Remark. Favourable behaviour of time-splitting pseudo-spectral methods for numerical solution of low-dimensional nonlinear Schrödinger equations confirmed by

- numerical comparisons (see various contributions by W. BAO and collaborators) and
- theoretical investigations (see work by CH. LUBICH and collaborators).

Approach

Approach. Compute approximation at final time $\frac{T}{\varepsilon} = N N_0 T_0$ (recall $0 < H = \varepsilon N_0 < 1$)

$$w_N \approx \widehat{u}_N = u\big(\tfrac{T}{\varepsilon}\big) = \mathscr{E}_{A+\varepsilon B}(N N_0 T_0)\, u(0)\,.$$

Step 1. Replace exact value at multiple of period by composition (macro stepsize $H = \varepsilon N_0$)

$$\prod_{j=1}^{r} \big(\mathscr{E}_{A-\beta_j \varepsilon N_0 B}(-T_0)\, \mathscr{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)\big)\, v \approx \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, v\,.$$

Step 2. Apply time-splitting method (micro time stepsize $h = \frac{T_0}{K}$)

$$\prod_{k=1}^{K} \prod_{\ell=1}^{s} \Big(\mathscr{E}_{\gamma B}\big(b_\ell \tfrac{T_0}{K}\big)\, \mathscr{E}_A\big(a_\ell \tfrac{T_0}{K}\big)\Big)\, v \approx \mathscr{E}_{A+\gamma B}(T_0)\, v\,.$$

Step 3. Apply pseudo-spectral method (projection, quadrature approximation)

$$\mathscr{E}_A(t)\, \mathscr{Q}_M v \approx \mathscr{E}_A(t)\, v\,.$$

For Fourier spectral method discrete solution given by (1D)

$$\sum_{m=-\frac{M}{2}}^{\frac{M}{2}-1} \sum_{k=1}^{M} \omega_k\, v(\xi_k)\, \overline{\mathscr{F}_m(\xi_k)}\, \mathrm{e}^{-\mathrm{i}\lambda_m t}\, \mathscr{F}_m \approx \sum_{m\in\mathbb{Z}} \int_\Omega v(x)\, \overline{\mathscr{F}_m(x)}\, \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}\lambda_m t}\, \mathscr{F}_m\,.$$

Full discretisation

Multi-revolution composition time-splitting pseudo-spectral method. Resulting fully discrete solution with macro stepsize $H = \varepsilon N_0$ and micro time stepsize $h = \frac{T_0}{K}$ given by

$$w_n = \prod_{j=1}^{r} \left(\prod_{k=1}^{K} \prod_{\ell=1}^{s} \left(\mathcal{E}_{-\beta_j HB}(-b_\ell h)\, \mathcal{E}_A(-a_\ell h)\, \mathcal{Q}_M \right) \prod_{k=1}^{K} \prod_{\ell=1}^{s} \left(\mathcal{E}_{\alpha_j HB}(b_\ell h)\, \mathcal{E}_A(a_\ell h)\, \mathcal{Q}_M \right) \right) w_{n-1}$$

$$\approx \widehat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0)\, \widehat{u}_{n-1}\,, \qquad n \in \{1, 2, \ldots, N\}\,.$$

Examples. First-order composition method and first-order Lie–Trotter splitting method

$$w_n = \prod_{k=1}^{K} \left(\mathcal{E}_{HB}(h)\, \mathcal{E}_A(h)\, \mathcal{Q}_M \right) w_{n-1}\,.$$

Second-order composition method and second-order Strang splitting method

$$\alpha_1 = \tfrac{1}{2}\left(1 + \tfrac{1}{N_0}\right), \qquad \beta_1 = \tfrac{1}{2}\left(1 - \tfrac{1}{N_0}\right),$$

$$w_n = \prod_{k=1}^{K} \left(\mathcal{E}_{-\beta_1 HB}\left(-\tfrac{h}{2}\right) \mathcal{E}_A(-h)\, \mathcal{Q}_M\, \mathcal{E}_{-\beta_1 HB}\left(-\tfrac{h}{2}\right) \right) \prod_{k=1}^{K} \left(\mathcal{E}_{\alpha_1 HB}\left(\tfrac{h}{2}\right) \mathcal{E}_A(h)\, \mathcal{Q}_M\, \mathcal{E}_{\alpha_1 HB}\left(\tfrac{h}{2}\right) \right) w_{n-1}\,.$$

Computational cost

Computational cost. Realisation of r-stage multi-revolution composition method based on s-stage time-splitting pseudo-spectral method requires $N \times 2r \times Ks$ spectral transforms (macro stepsize $H = \varepsilon N_0$, micro stepsize $h = \frac{T_0}{K}$)

$$w_n = \prod_{j=1}^{r} \left(\prod_{k=1}^{K} \prod_{\ell=1}^{s} \left(\mathcal{E}_{-\beta_j HB}(-b_\ell h)\, \mathcal{E}_A(-a_\ell h)\, \mathcal{Q}_M \right) \prod_{k=1}^{K} \prod_{\ell=1}^{s} \left(\mathcal{E}_{\alpha_j HB}(b_\ell h)\, \mathcal{E}_A(a_\ell h)\, \mathcal{Q}_M \right) \right) w_{n-1}$$

$$\approx \widehat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0)\, \widehat{u}_{n-1}, \qquad n \in \{1, 2, \ldots, N\}.$$

Sole application of s-stage time-splitting pseudo-spectral method with time stepsize $h = \frac{T_0}{K}$ requires in total $N \times N_0 \times Ks$ spectral transforms.

Conclusion. For smaller value of decisive parameter $0 < \varepsilon \ll 1$, which corresponds to larger final time $\frac{T}{\varepsilon} = N N_0 T_0 \gg 1$, reasonable assumption $0 < H = \varepsilon N_0 < 1$ with $N_0 \gg 1$ implies

$$N \times 2r \times Ks \ll N \times N_0 \times Ks.$$

Numerical illustrations. Numerical illustrations for cubic Schrödinger equation given in CHARTIER, MAKAZAGA, MURUA, VILLMART (2012) confirm that second- and fourth-order multi-revolution composition methods combined with second-order Strang time-splitting Fourier pseudo-spectral method are superior in efficiency compared to sole application of time-splitting method for long-term integration (in regime $0 < \varepsilon \ll 1$, $\frac{T}{\varepsilon} = N N_0 T_0 \gg 1$).

Convergence analysis

Convergence analysis

Situation. Consider multi-revolution composition time-splitting pseudo-spectral method in regime $0 < \varepsilon \ll 1$ ($\frac{T}{\varepsilon} = N N_0 T_0 \gg 1$, macro stepsize $H = \varepsilon N_0$, micro stepsize $h = \frac{T_0}{K}$)

$$w_n = \prod_{j=1}^{r} \left(\prod_{k=1}^{K} \prod_{\ell=1}^{s} \left(\mathcal{E}_{-\beta_j HB}(-b_\ell h)\, \mathcal{E}_A(-a_\ell h)\, \mathcal{Q}_M \right) \prod_{k=1}^{K} \prod_{\ell=1}^{s} \left(\mathcal{E}_{\alpha_j HB}(b_\ell h)\, \mathcal{E}_A(a_\ell h)\, \mathcal{Q}_M \right) \right) w_{n-1}$$

$$\approx \widehat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0)\, \widehat{u}_{n-1}, \qquad n \in \{1, 2, \ldots, N\}.$$

Aim. For evolution equation with regular solution analyse stability and error behaviour of full discretisation based on

- multi-revolution composition method of order P
- time-splitting method of order p
- pseudo-spectral method

and deduce convergence estimate of form

$$\text{global error} = \mathcal{O}\left(H^P\right) + \mathcal{O}\left(h^p\right) + \mathcal{O}\left(M^{-\rho}\right).$$

Stability and error analysis of multi-revolution composition methods

Stability analysis

Objective. Stability analysis of multi-revolution composition method

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + \varepsilon\, B\big(u(t)\big), \quad t \in \big(0, \frac{T}{\varepsilon}\big), \\ u(0) = u_0\,, \end{cases} \qquad 0 < \varepsilon \ll 1\,,$$

$$u_{n+1} = \prod_{j=1}^{r} \big(\mathscr{E}_{A-\beta_j \varepsilon N_0 B}(-T_0)\, \mathscr{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)\big)\, u_n$$

$$\approx\ \widehat{u}_{n+1} = \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, \widehat{u}_n\,, \qquad n \in \{0, 1, \ldots, N-1\}\,.$$

Stability. Due to unitarity of evolution operator associated with nonlinear time-dependent Schrödinger equation involving real-valued potential and real parameter $\gamma \in \mathbb{R}$

$$\mathrm{i}\, \partial_t \psi(x,t) = -\Delta \psi(x,t) + V(x)\, \psi(x,t) + \gamma\, \mathscr{B}\big(|\psi(x,t)|\big)\, \psi(x,t)\,, \qquad (x,t) \in \Omega \times \mathbb{R},$$
$$\|\psi(\cdot,t)\|_{L^2} = \|\psi(\cdot,0)\|_{L^2}\,, \qquad t \in \mathbb{R},$$

stability of multi-revolution composition method in Lebesgue-space $X = L^2(\Omega, \mathbb{C})$ is evident

$$\|u_{n+1}\|_X = \|u_n\|_X\,, \qquad n \in \{0, 1, \ldots, N-1\}\,.$$

Remark. Stability in Sobolev-space of higher degree is more involved task.

Objective

Objective. Error analysis of multi-revolution composition method applied to highly oscillatory evolution equation

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t} u(t) = A\,u(t) + \varepsilon\, B\big(u(t)\big), \quad t \in \big(0, \frac{T}{\varepsilon}\big), \\ u(0) = u_0\,, \end{cases} \qquad 0 < \varepsilon \ll 1\,,$$

$$u_{n+1} = \prod_{j=1}^{r} \big(\mathscr{E}_{A-\beta_j \varepsilon N_0 B}(-T_0)\, \mathscr{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)\big)\, u_n$$

$$\approx \widehat{u}_{n+1} = \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, \widehat{u}_n\,, \qquad n \in \{0, 1, \ldots, N-1\}\,.$$

Approach. Employ stepwise expansion of solution value $\mathscr{E}_{A+\gamma B}(t)\, v$ based on variation-of-constants formula and specify remainder terms.

First step. As first step provide rigorous analysis for linear case with bounded operator B.

Remark. Error analysis given in Chartier, Makazaga, Murua, Villmart (2012) relies on infinite Taylor series expansions of $\mathscr{E}_{A+\gamma B}(t)$. Presence of unbounded operators A, B requires to adapt strategies for deducing error estimates for multi-revolution composition methods.

Error analysis (Linear case, $P = 1$)

Aim. For multi-revolution composition method applied to linear evolution equation deduce expansion with respect to $H = \varepsilon N_0$ (initial step)

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + \varepsilon\, B\, u(t), \quad t \in \left(0, \tfrac{T}{\varepsilon}\right), \qquad 0 < \varepsilon \ll 1,$$

$$u_1 = \prod_{j=1}^{r} \left(\mathscr{E}_{A-\beta_j \varepsilon N_0 B}(-T_0)\, \mathscr{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)\right) u_0 \;\approx\; \widehat{u}_1 = \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, u_0,$$

$$u_1 - \widehat{u}_1 = \mathscr{O}\left(H^{P+1}\right).$$

Special case. Focus on simple approximation

$$P = 1: \qquad u_1 - \widehat{u}_1 = \mathscr{E}_{A+\varepsilon N_0 B}(T_0)\, u_0 - \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, u_0 = \mathscr{O}\left(H^{P+1}\right).$$

Fundamental tool. Employ linear variation-of-constants formula and use periodicity $\mathscr{E}_A(T_0) = I$ (evolution operator near-identity map, smooth dependence on parameter)

$$u(t) = \mathscr{E}_{A+\varepsilon B}(t)\, u_0 = \mathscr{E}_A(t)\, u_0 + \varepsilon \int_0^t \mathscr{E}_A(t-\tau)\, B\, \mathscr{E}_{A+\varepsilon B}(\tau)\, u_0\, \mathrm{d}\tau, \qquad t \in \left[0, \tfrac{T}{\varepsilon}\right],$$

$$\mathscr{E}_{A+\varepsilon B}(n T_0) = I + \varepsilon \int_0^{n T_0} \mathscr{E}_A(-\tau)\, B\, \mathscr{E}_{A+\varepsilon B}(\tau)\, \mathrm{d}\tau, \qquad n \in \mathbb{Z}.$$

Explanation (Linear case, $P = 1$)

Explanation. Repeated application of linear variation-of-constants formula and periodicity requirement $\mathscr{E}_A(T_0) = I$ leads to expansion of exact value involving T_0-periodic integrand (remainder bounded in underlying function space)

$$\begin{aligned}\mathscr{E}_{A+\varepsilon B}(N_0 T_0) &= I + \varepsilon \int_0^{N_0 T_0} \mathscr{E}_A(-\tau)\, B\, \mathscr{E}_{A+\varepsilon B}(\tau)\, \mathrm{d}\tau \\ &= I + \varepsilon \int_0^{N_0 T_0} \mathscr{E}_A(-\tau)\, B\, \mathscr{E}_A(\tau)\, \mathrm{d}\tau + \varepsilon^2 \int_0^{N_0 T_0} \int_0^{\tau} \mathscr{E}_A(-\tau)\, B\, \mathscr{E}_A(\tau-\sigma)\, B\, \mathscr{E}_{A+\varepsilon B}(\sigma)\, \mathrm{d}\sigma\, \mathrm{d}\tau\,, \\ &= I + \varepsilon \int_0^{N_0 T_0} f(\tau)\, \mathrm{d}\tau + \mathscr{O}\big(H^2\big), \qquad f(\tau + T_0) = f(\tau)\,, \qquad H = \varepsilon N_0\,.\end{aligned}$$

Decomposition of interval $[0, N_0 T_0]$ and suitable integral transformation permits reduction to primary interval $[0, T_0]$

$$\begin{aligned}\mathscr{E}_{A+\varepsilon B}(N_0 T_0) &= I + \varepsilon \sum_{\ell=1}^{N_0} \int_0^{T_0} f(\tau + (\ell-1) T_0)\, \mathrm{d}\tau + \mathscr{O}\big(H^2\big) \\ &= I + \varepsilon N_0 \int_0^{T_0} f(\tau)\, \mathrm{d}\tau + \mathscr{O}\big(H^2\big) = \mathscr{E}_{A+\varepsilon N_0 B}(T_0) + \mathscr{O}\big(H^2\big)\,.\end{aligned}$$

Suggests to consider first-order multi-revolution composition method (leading terms of expansions coincide) and proves error relation

$$P = 1: \qquad u_1 - \widehat{u}_1 = \mathscr{E}_{A+\varepsilon N_0 B}(T_0)\, u_0 - \mathscr{E}_{A+\varepsilon B}(N_0 T_0)\, u_0 = \mathscr{O}\big(H^{P+1}\big), \qquad H = \varepsilon N_0\,.$$

Error analysis (Linear case)

Extension. Consider multi-revolution composition method of classical order $P \in \mathbb{N}_{\geq 1}$.

- Derivatives of evolution operator with respect to decisive parameter satisfy bound

$$\|\partial_\varepsilon^k \mathcal{E}_{A+\varepsilon B}(t)\, v\|_X \leq \left(\|B\|_{X\leftarrow X}\, |t|\right)^k \|v\|_X\,, \qquad t \in \mathbb{R}, \quad k \in \mathbb{N}, \quad v \in X\,.$$

- Employ Taylor series expansions of exact and numerical evolution operator with respect to decisive parameter.
- Validity of order conditions ensures that dominant terms in expansions cancel.
- Suitable estimation of remainder yields error estimate.

Lemma

$$\Big\| \prod_{j=1}^{r} \left(\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0)\, \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)\right) v - \mathcal{E}_{A+\varepsilon B}(N_0 T_0)\, v \Big\|_X$$
$$\leq \frac{C}{(P+1)!}\, \|B\|_{X\leftarrow X}^{P+1}\, T_0^{P+1}\, H^{P+1}\, \|v\|_X\,, \qquad v \in X\,.$$

Remark. Rigorous extension to nonlinear problems more involved.

Convergence result

Convergence result (Linear case)

Convergence analysis. For evolution equation with regular solution analyse stability and error behaviour of full discretisation based on

- multi-revolution composition method of order P
- time-splitting method of order p
- pseudo-spectral method

and deduce convergence estimate of form

$$\text{global error} = \mathcal{O}\big(H^P\big) + \mathcal{O}\big(h^p\big) + \mathcal{O}\big(M^{-\rho}\big).$$

Dependence on macro and micro stepsizes. Above considerations explain dependence of global error on macro stepsize. Dependence on micro stepsize and superconvergent behaviour of symmetric versus non-symmetric time-splitting methods explained in CHARTIER, MÉHATS, TH., ZHANG (2015). Illustration by numerical examples.

Convergence result (Linear case)

Theorem (Global error estimate)

Assume that the unbounded linear operator A satisfies the stated requirements and that the linear operator B is bounded. For the full discretisation of the linear Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = A\,u(t) + \varepsilon\,Bu(t)\,, \quad t \in \big(0, \tfrac{T}{\varepsilon}\big]\,, \qquad 0 < \varepsilon \ll 1\,,$$

combine a multi-revolution composition method of nonstiff order $P \in \mathbb{N}_{\geq 1}$, applied with macro stepsize H, a time-splitting method of nonstiff order $p \in \mathbb{N}_{\geq 1}$, applied with micro time stepsize h, and a pseudo-spectral method applied with M_0^d basis functions. Under the assumption that the exact solution remains bounded in the fractional power space X_ϑ for some $\vartheta \geq \frac{p}{2}$, the global error estimate

$$\|u_{MN} - u\big(\tfrac{T}{\varepsilon}\big)\|_X \leq \|u_0 - u(0)\|_X + CH^P + CM_0^{-\rho} + \begin{cases} C\big(h^{2\vartheta} + Hh^p\big) & \text{if splitting non-symmetric,} \\ C\big(h^{2\vartheta} + \varepsilon h^p\big) & \text{if splitting symmetric,} \end{cases}$$

is valid with $\rho = \rho(\vartheta) > 0$ depending on the considered pseudo-spectral method and $C > 0$ depending in particular on upper bounds for $\max\{\|u(t)\|_{X_\vartheta} : 0 \leq t \leq \frac{T}{\varepsilon}\}$, where $\frac{T}{\varepsilon} = NN_0T_0$.

Numerical illustrations

Illustrations

Model problem. Consider time-dependent nonlinear Schrödinger equation with regular solution ($d = 1$, $T_0 = 2\pi$)

$$\mathrm{i}\,\partial_t \psi(x,t) = -\partial_{xx}\psi(x,t) + \varepsilon\, V(x)\,|\psi(x,t)|^2 \psi(x,t)\,,$$

$$V(x) = 2\cos(2x)\,, \quad \psi(x,0) = \cos(x) + \sin(x)\,, \qquad (x,t) \in (-\pi,\pi) \times \left(0, \tfrac{T}{\varepsilon}\right].$$

Space discretisation. Apply Fourier pseudo-spectral method for space discretisation (spatial error for $M = 256$ basis functions insigificant).

Illustrations.

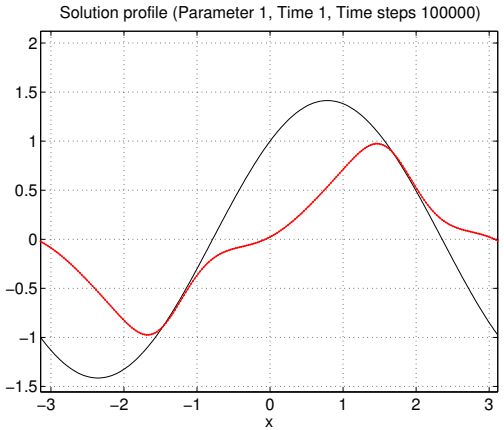
- Solution behaviour in dependence of decisive parameter
- Error behaviour of time-splitting methods
- Error behaviour of multi-revolution composition time-splitting methods

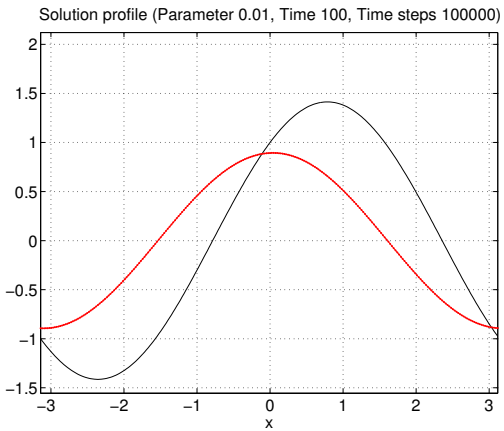
Solution behaviour

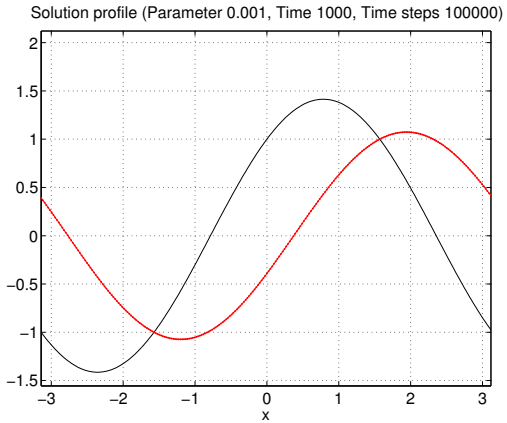
Solution behaviour. Illustrate behaviour of solution to nonlinear Schrödinger equation in dependence of decisive parameter (real part, $T = 1$). Apply Strang-splitting method with time stepsize Δt (verify result for refined time stepsize)

$$\varepsilon = 1\,,\ \frac{T}{\varepsilon} = 1\,,\ \Delta t = 10^{-5}\,, \qquad \varepsilon = 10^{-1}\,,\ \frac{T}{\varepsilon} = 10\,,\ \Delta t = 10^{-4}\,,$$

$$\varepsilon = 10^{-2}\,,\ \frac{T}{\varepsilon} = 100\,,\ \Delta t = 10^{-3}\,, \qquad \varepsilon = 10^{-3}\,,\ \frac{T}{\varepsilon} = 1000\,,\ \Delta t = 10^{-2}\,.$$







Time-splitting methods

Error behaviour. Analyse error behaviour of sole application of first-order Lie–Trotter splitting method ($p = 1$), second-order Strang splitting method ($p = 2$), and fourth-order splitting method by Yoshida ($p = 4$) for time integration of nonlinear Schrödinger equation

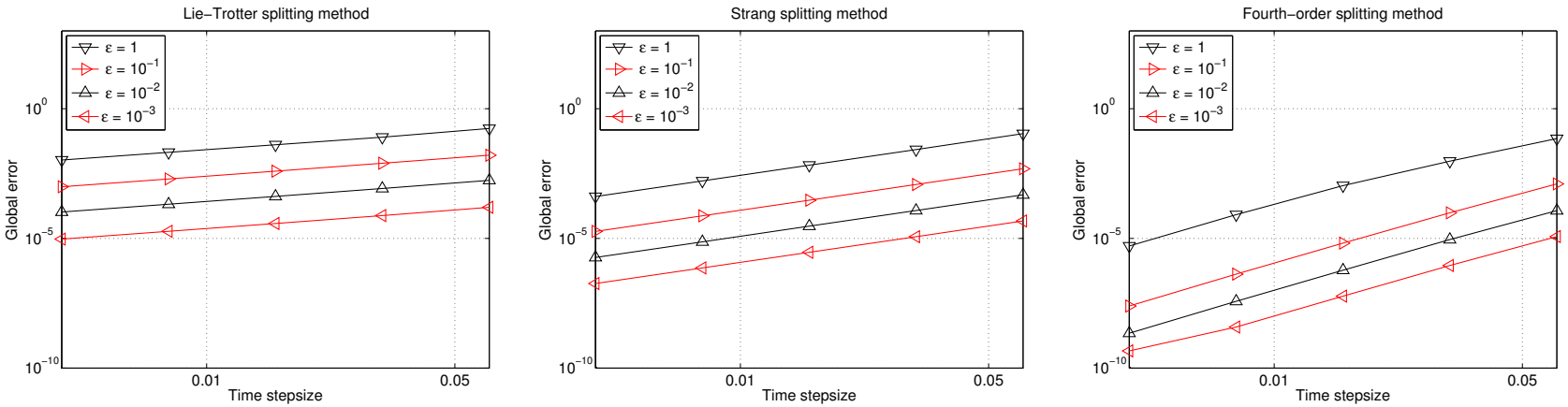
$$\mathrm{i}\,\partial_t \psi(x,t) = -\partial_{xx}\psi(x,t) + \varepsilon\, V(x)\,|\psi(x,t)|^2 \psi(x,t)\,,$$

$$V(x) = 2\cos(2x)\,, \quad \psi(x,0) = \cos(x) + \sin(x)\,, \qquad (x,t) \in (-\pi,\pi) \times \left(0, \tfrac{T}{\varepsilon}\right].$$

Numerical results. Numerical results confirm error relation for regular solution

$$\text{global error at final time } \frac{T}{\varepsilon} = \mathcal{O}\big(\varepsilon h^p\big), \qquad \frac{T}{\varepsilon} = N\Delta t\,,$$

see theoretical error estimate deduced in Chartier, Méhats, Th., Zhang (2014).



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Numerical results. Numerical results confirm error relation for regular solutions

$$\text{global error at final time } \tfrac{T}{\varepsilon}: \qquad \mathrm{err}_\varepsilon = \mathcal{O}\big(\varepsilon h^p\big), \qquad \tfrac{T}{\varepsilon} = Nh,$$

see theoretical error estimate deduced in Chartier, Méhats, Th., Zhang (2014).

Drawback! Number of time steps N increases in dependence of parameter!

h	N	$\mathrm{err}_{10^{-1}}$	p	N	$\mathrm{err}_{10^{-2}}$	p	N	$\mathrm{err}_{10^{-3}}$	p
$6.2\cdot10^{-2}$	160	$1.2\cdot10^{-3}$		1600	$1.1\cdot10^{-4}$		16000	$1.1\cdot10^{-5}$	
$3.1\cdot10^{-2}$	320	$9.6\cdot10^{-5}$	3.7	3200	$9.0\cdot10^{-6}$	3.7	32000	$8.9\cdot10^{-7}$	3.7
$1.5\cdot10^{-2}$	640	$6.5\cdot10^{-6}$	3.8	6400	$5.9\cdot10^{-7}$	3.9	64000	$5.9\cdot10^{-8}$	3.9
$7.8\cdot10^{-3}$	1280	$4.1\cdot10^{-7}$	3.9	12800	$3.7\cdot10^{-8}$	3.9	128000	$3.8\cdot10^{-9}$	3.9
$3.9\cdot10^{-3}$	2560	$2.4\cdot10^{-8}$	4.0	25600	$2.2\cdot10^{-9}$	4.0	256000	$4.5\cdot10^{-10}$	3.0

Global errors of fourth-order splitting method by Yoshida for $\varepsilon = 10^{-1}, 10^{-2}, 10^{-3}$

Multi-revolution composition time-splitting methods

Error behaviour (Composition). Study error behaviour of second-order multi-revolution composition method ($P = 2$) for time integration of nonlinear Schrödinger equation

$$\mathrm{i}\,\partial_t \psi(x,t) = -\partial_{xx}\psi(x,t) + \varepsilon\, V(x)\,|\psi(x,t)|^2 \psi(x,t)\,,$$

$$V(x) = 2\cos(2x)\,, \quad \psi(x,0) = \cos(x) + \sin(x)\,, \qquad (x,t) \in (-\pi,\pi) \times \left(0, \tfrac{T}{\varepsilon}\right].$$

Numerical results. Numerical results confirm error relation for regular solutions (if micro stepsize $h = \frac{T_0}{K}$ sufficiently small)

$$\text{global error at final time } \tfrac{T}{\varepsilon} = \mathcal{O}\big(H^P\big)\,, \qquad \tfrac{T}{\varepsilon} = N\,N_0\,T_0\,, \qquad H = \varepsilon N_0\,,$$

see theoretical error estimate deduced in Chartier, Méhats, Th., Zhang (2015).

N	1000	500	250	125
N_0	2	4	8	16
H	$2\cdot10^{-3}$	$4\cdot10^{-3}$	$8\cdot10^{-3}$	$16\cdot10^{-3}$
error	$6.58\cdot10^{-7}$	$3.31\cdot10^{-6}$	$1.39\cdot10^{-5}$	$5.64\cdot10^{-5}$
P		2.33	2.07	2.01

Global errors of second-order multi-revolution composition method for $\varepsilon = 10^{-3}$ and $T = 4\pi$.
Error of time-splitting method insignificant for $p = 4$, $K = 10^3$.
Reference solution computed for refined macro stepsize $H = 10^{-3}$ ($N = 2000$, $N_0 = 1$).

Multi-revolution composition time-splitting methods

Error behaviour (Splitting). Study error behaviour of multi-revolution composition method ($P = 2$) combined with symmetric second-order Strang splitting method ($p = 2$) for time integration of nonlinear Schrödinger equation

$$\mathrm{i}\,\partial_t \psi(x,t) = -\partial_{xx}\psi(x,t) + \varepsilon\, V(x)\,|\psi(x,t)|^2 \psi(x,t)\,,$$

$$V(x) = 2\cos(2x)\,, \quad \psi(x,0) = \cos(x) + \sin(x)\,, \qquad (x,t) \in (-\pi,\pi) \times \left(0, \tfrac{T}{\varepsilon}\right].$$

Numerical results. Numerical results confirm error relation for regular solutions (if macro stepsize $H = \varepsilon N_0$ sufficiently small)

$$\text{global error at final time } \tfrac{T}{\varepsilon} = \mathcal{O}\big(\varepsilon h^p\big)\,, \qquad \tfrac{T}{\varepsilon} = N N_0 T_0\,, \qquad h = \tfrac{T_0}{K}\,,$$

see theoretical error estimate deduced in Chartier, Méhats, Th., Zhang (2015).

h	$3.9\cdot10^{-1}$	$1.9\cdot10^{-1}$	$9.8\cdot10^{-2}$	$4.9\cdot10^{-2}$	$2.4\cdot10^{-2}$
error(ε)	$2.23\cdot10^{-2}$	$6.85\cdot10^{-3}$	$1.46\cdot10^{-3}$	$3.61\cdot10^{-4}$	$9.34\cdot10^{-5}$
error(2ε)	$4.46\cdot10^{-2}$	$1.37\cdot10^{-2}$	$2.93\cdot10^{-3}$	$7.22\cdot10^{-4}$	$1.86\cdot10^{-4}$
$\frac{\text{error}(2\varepsilon)}{\text{error}(\varepsilon)}$	2.00	2.00	2.00	2.00	2.00
p		1.70	2.22	2.01	1.95

Global errors at $T = 4\pi$ for symmetric second-order splitting, where $\varepsilon = 10^{-3}$, $N = 2000$, $N_0 = 1$ and $2\varepsilon = 2\cdot10^{-3}$, $N = 1000$, $N_0 = 1$, respectively. Error of composition method insignificant for $P = 2$. Reference solution computed by fourth-order splitting method.

Conclusions and future work

Conclusions. Multi-revolution compositon methods combined with time-splitting pseudo-spectral methods for highly oscillatory evolution equations.

- Rigorous convergence analysis completed for linear case.
- Superconvergent behaviour of symmetric splitting methods explained for nonlinear case.

Future work. Treatment of Dirac equation in non-relativistic regime.

Thank you!