Adaptive time splitting for nonlinear Schrödinger equations in the semiclassical regime

Local error representation and a posteriori error estimator

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Workshop, Numerical Analysis of Evolution Equations

Vill, Innbruck, Austria

15.10.2014

Model Problem

As a model-problem, we consider the nonlinear Schrödinger equation

$$\begin{cases} \partial_t \psi & = F(\psi) = \frac{\mathrm{i}}{2}\varepsilon\,\Delta\psi - \frac{\mathrm{i}}{\varepsilon}\,(U + \vartheta\,|\psi|^2)\,\psi\,, \\ \psi(0) & = u\,, \end{cases} \tag{1}$$

with U as external potential and the semiclassical parameter $0 \leq \varepsilon \ll 1$, .

Applying Splitting-methods on the GPE

The right hand-side of the differential equation is split into two operators,

$$\begin{cases} \partial_t \psi(x,t) = A\,\psi(x,t) + B(\psi(x,t))\,, \\ \psi(x,0) = u(x)\,, \end{cases} \tag{2}$$

with the linear operator A and the nonlinear operator B defined as

$$A\,\psi(x,t) := \tfrac{\mathrm{i}}{2}\varepsilon \triangle \psi(x,t)\,,$$
$$B(\psi(x,t)) := -\,\tfrac{\mathrm{i}}{\varepsilon}\big(U(x) + \vartheta|\psi(x,t)|^2\big)\psi(x,t)\,.$$

Splitting solutions $\mathcal{E}_A$, $\mathcal{E}_B$

The flows $\mathcal{E}_A$ and $\mathcal{E}_B$ associated with the subproblems are

$$\partial_t\psi = \frac{\mathrm{i}}{2}\varepsilon\,\Delta\,\psi \quad \rightarrow \quad \mathcal{E}_A(t,u) = \mathrm{e}^{\mathrm{i}\frac{\varepsilon}{2}t\Delta}u\,, \tag{3a}$$

$$\partial_t\psi = -\frac{\mathrm{i}}{\varepsilon}\left(U + \vartheta\,|\psi|^2\right)\psi \quad \rightarrow \quad \mathcal{E}_B(t,u) = e^{-\mathrm{i}\frac{t}{\varepsilon}(U+\vartheta|u|^2)}u\,. \tag{3b}$$

Splitting-Methods

The numerical approximation to the exact solution of the initial problem can be found via a recurrence relation with constant step-size $t = \frac{T}{N}$ and initial value $u_0 \approx u$,

$$\begin{cases} \psi_n = \mathcal{S}(t,u) = \mathcal{E}_A(a_n t, \mathcal{E}_B(b_n t, \ldots \mathcal{E}_A(a_1 t, \mathcal{E}_B(b_1 t, u)))) \,, \\ \psi_0 = u_0 \,. \end{cases}$$

Splitting methods II

For the subsequent study the first order Lie splitting method

$$\mathcal{S}(t,u) = \mathcal{S}_{\mathrm{Lie}}(t,u) = \mathcal{E}_B(t, \mathcal{E}_A(t,u))\,, \tag{4}$$

and the two-fold symmetric second-order Strang splitting method,

$$\mathcal{S}(t,u) = \mathcal{S}_{\mathrm{Strang}}(t,u) = \mathcal{E}_A(\tfrac{1}{2}\,t, \mathcal{E}_B(t, \mathcal{E}_A(\tfrac{1}{2}\,t, u))) \tag{5}$$

will be in the focus of interest.

Strang-Splitting error expansion

Using the Gröbner-Alekseev formula, the local error

$$\mathcal{L} = \mathcal{S}(t,u) - \mathcal{E}_F(t,u)$$

for the Strang-splitting method can be written as

$$\mathcal{L}(t,u) = \mathcal{L}^{(1)} + \mathcal{L}^{(2)} = \mathcal{O}(t^3)\,, \tag{6}$$

with

$$\mathcal{L}^{(1)}(t,u) = \int_0^t \int_0^{\tau_1} \partial_2^2\, \mathcal{E}_F(t-\tau_2, \mathcal{S}(\tau_2,u))\cdot \Big(\mathcal{S}^{(1)}(\tau_2,u), \mathcal{S}^{(1)}(\tau_2,u)\Big)\Big\}\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,,$$

$$\mathcal{L}^{(2)}(t,u) = \int_0^t \int_0^{\tau_1} \partial_2\, \mathcal{E}_F(t-\tau_2, \mathcal{S}(\tau_2,u))\, \mathcal{S}^{(2)}(\tau_2,u)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,.$$

Strang-Splitting error expansion

$$\mathcal{L}^{(1)}(t,u) = \int_0^t \int_0^{\tau_1} \partial_2^2\, \mathcal{E}_F(t-\tau_2, \mathcal{S}(\tau_2,u)) \cdot \Big(\mathcal{S}^{(1)}(\tau_2,u), \mathcal{S}^{(1)}(\tau_2,u)\Big) \Big\}\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,,$$

$$\mathcal{L}^{(2)}(t,u) = \int_0^t \int_0^{\tau_1} \partial_2\, \mathcal{E}_F(t-\tau_2, \mathcal{S}(\tau_2,u))\, \mathcal{S}^{(2)}(\tau_2,u)\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,,$$

where

$$\mathcal{S}^{(1)}(t,u) = \tfrac{\partial}{\partial t}\mathcal{S}(t,u) - F(\mathcal{S}(t,u)) = \int_0^t s^{(1)}(t,\tau,u)\, \mathrm{d}\tau\,,$$

$$\mathcal{S}^{(2)}(t,u) = \tfrac{\partial}{\partial t}\mathcal{S}^{(1)}(t,u) - F'(\mathcal{S}(t,u))\, \mathcal{S}^{(1)}(t,u) = \int_0^t s^{(2)}(t,\tau,u)\, \mathrm{d}\tau\,.$$

Estimation of the local error

In the L_2-norm, we obtain the estimate

$$\left\|\mathcal{L}(t,u)\right\|_{L^2} \leq \ \widetilde{C} \cdot t^3 \exp\left(C\, \tfrac{t}{\varepsilon}\, \vartheta \sup_{0\leq\chi\leq\sigma\leq t} \|\mathcal{E}_F(\sigma,\mathcal{S}(\chi,u))\|^2_{H^2} \right) \cdot$$
$$\sup_{0\leq\tau\leq t} \Big(\|s^{(2)}(t,\tau,u)\|_{L^2} + \tfrac{t}{\varepsilon}\, C_U + \tfrac{t^2}{\varepsilon}\, \tilde{C}_U$$
$$+ \tfrac{t^2}{\varepsilon}\, \|u\|_{L^2} \big(\|s^{(1)}(t,\tau,u)\|_{H^2} + \tfrac{t}{\varepsilon}\, C_U \big)^2 \Big)\,, \tag{7}$$

Estimation of the local error

The dominant term in (7) is the expression $s^{(2)}$, thus

$$\begin{aligned}\left\|\mathcal{L}(t,u)\right\|_{L^2} &\approx \widetilde{C}\cdot t^3\|s^{(2)}(t,\tau,u)\|_{L^2}\\ &\leq \widetilde{C}\cdot t^3\Big(\|[B,[B,A]](u)\|_{L^2}+\|[A,[B,A]](u)\|_{L^2}\Big)+\mathcal{O}(t^3)\,,\end{aligned}$$

where

$$\begin{aligned}\|[B,[B,A]](u)\|_{L^2} &\propto \tfrac{1}{\varepsilon}\,,\\ \|[A,[B,A]](u)\|_{L^2} &\propto \varepsilon\,.\end{aligned}$$

Comparison of the asymptotic behavior

For the local error of the Strang splitting method the dominant terms are

$$\left\|\mathcal{L}_{\text{Strang}}(t,u)\right\|_{L^2} \leq t^3 \left(C_1 \tfrac{1}{\varepsilon} + C_2\,\varepsilon\right) + t^4 \left(C_3 \tfrac{1}{\varepsilon^2} + C_4\right) + \mathcal{O}(t^5)\,,$$

with $C_1(\|u\|_{H^2})$, $C_3(\|u\|_{H^2})$ and $C_2(\|u\|_{H^4})$, $C_4(\|u\|_{H^4})$.
For the Lie splitting method we have

$$\left\|\mathcal{L}_{\text{Lie}}(t,u)\right\|_{L^2} \leq C \left(t^2 + t^3 \left(\tfrac{1}{\varepsilon} + \varepsilon\right) + t^4 \left(\tfrac{1}{\varepsilon^2} + 1\right)\right) + \mathcal{O}(t^5)\,,$$

with $C(\|u\|_{H^2})$.

Numerical results I

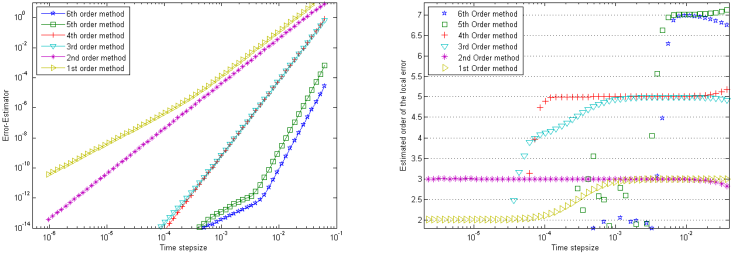


Figure: t - **dependence of the local error**.
Left: Estimated local error with respect to t. Right: Estimated order of the method.

Numerical results II

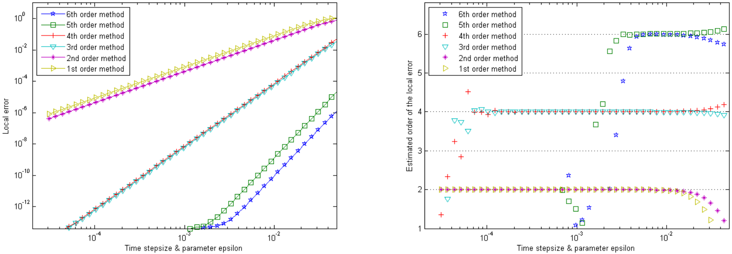


Figure: $(t = \varepsilon)$ - **dependence of the local error**.
Left: Estimated local error with respect to t and ε.
Right: Estimated order of the method.

A posteriori local error estimator

We have constructed an a posteriori local error estimator,

$$\mathcal{P}(t,u) = \tfrac{1}{p+1}\, t\, \mathcal{S}^{(1)}(t,u) \approx \mathcal{L}(t,u), \tag{8}$$

for which we want to analyze its deviation from the local error, which is expected to be

$$\mathcal{P}(t,u) - \mathcal{L}(t,u) = \mathcal{O}(t^{p+2})\,.$$

Comparison of the obtained defect estimations

For the deviation of the local error estimator, we have found estimates for the dominant terms. For the Lie splitting method,

$$\|\mathcal{P}_{\text{Lie}}(t,u) - \mathcal{L}_{\text{Lie}}(t,u)\|_{L^2} \leq t^3 \left(C_1 \tfrac{1}{\varepsilon} + C_2\,\varepsilon\right) + t^4 \left(C_3 \tfrac{1}{\varepsilon^2} + C_4\right) + \mathcal{O}(t^5)\,,$$

with $C_1(\|u\|_{H^2})$, $C_3(\|u\|_{H^2})$ and $C_2(\|u\|_{H^4})$, $C_4(\|u\|_{H^4})$.
For the Strang splitting method,

$$\|\mathcal{P}_{\text{Strang}}(t,u) - \mathcal{L}_{\text{Strang}}(t,u)\|_{L^2} \leq t^4 \left(C_1 + C_2\,\varepsilon^2\right) + C_3\,t^5 \left(\tfrac{1}{\varepsilon} + \varepsilon + \varepsilon^3\right) + \mathcal{O}(t^6)\,,$$

with $C_1(\|u\|_{H^4})$ and $C_2(\|u\|_{H^6})$, $C_3(\|u\|_{H^6})$.

Numerical results I

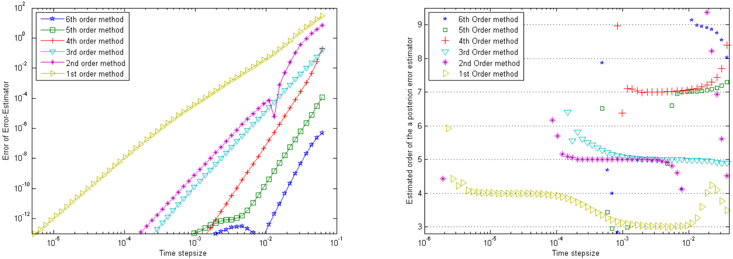
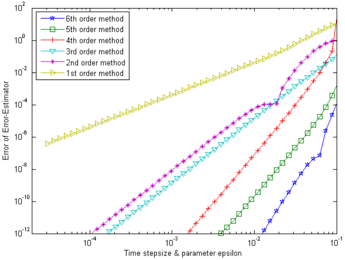


Figure: $(t = \varepsilon)$ - **dependence of the a posteriori error estimator**.
Left: Estimated defect of the error estimator with respect to t.
Right: Estimated order of the method.

Numerical results II



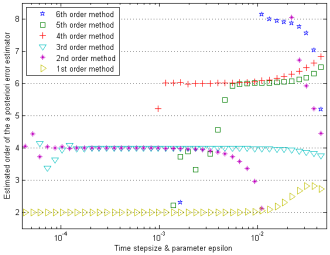


Figure: $(t = \varepsilon)$ - **dependence of the a posteriori error estimator**.
Left: Estimated defect of the error estimator with respect to t and ε.
Right: Estimated order of the method.

Open tasks

- Extension to higher order splitting methods
- Consider other nonlinearities of the form $f(|\psi|^2)$ as $\frac{|\psi|^2}{1+|\psi|^2}$ or $\Delta^{-1}|\psi|^2$.
- Extend the estimates depending on t and ε to splitting methods with three or more subproblems as in

$$i\varepsilon\partial_t u = \big(-\tfrac{\varepsilon}{2}\Delta + V + f(|u|^2) + \varepsilon\tau \arg(u)\big)\, u\,.$$

References

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- Descombes, S., Thalhammer, M., 2012. The Lie-Trotter splitting for nonlinear evolutionary problems with critical parameters. A compact local error representation and application to nonlinear Schrödinger equations in the semi-classical regime. IMA J. Numer. Anal. 33, 722–745.
- Auzinger, W., Kassebacher, T., Koch, O., Thalhammer, M., 2014. Adaptive splitting methods for nonlinear Schrödinger equations in the semiclassical regime. ASC Report No. 27/2014, Institute for Analysis and Scientific Computing, Vienna University of Technology.

Questions?