Defect-based local error estimators for splitting methods, with application to Schrödinger equations Part I. The linear case[1]

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Abstract

We introduce a defect correction principle for exponential operator splitting methods applied to time-dependent linear Schrödinger equations and construct a posteriori local error estimators for the Lie–Trotter and Strang splitting methods. Under natural commutator bounds on the involved operators we prove asymptotical correctness of the local error estimators, and along the way recover the known a priori convergence bounds. Numerical examples illustrate the theoretical local and global error estimates.

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1. Introduction

In this paper we derive a priori and a posteriori local error estimates for split-step time integrators applied to linear evolution equations of Schrödinger type,

$$\begin{cases} \mathrm{i}\,\partial_t \psi(x,t) = -\frac{1}{2}\,\Delta\,\psi(x,t) + V(x)\,\psi(x,t)\,, \\ \psi(x,0) = \psi_0(x)\,, \end{cases} \qquad x \in \mathbb{R}^d\,, \quad t \ge 0\,, \tag{1}$$

where we assume that the real potential $V : \mathbb{R}^d \to \mathbb{R}$ and the initial state $\psi_0 : \mathbb{R}^d \to \mathbb{C}$ are sufficiently regular. This serves as a first step towards the construction and analysis of local error estimators for nonlinear evolution equations. The choice of split-step time integrators for this problem class is motivated by their favorable performance as compared to other standard methods, which has been demonstrated for example in [1, 2]. As a prerequisite, split-step time integrators for linear evolution equations of Schrödinger type have been investigated for instance in [3, 4, 5, 6].

Our approach is conceptually rather general and not particularly focussed on (1). Thus, before studying its application to (1) in detail, we introduce and discuss it in an abstract Banach space setting. We study two situations:

- We consider the first-order Lie–Trotter splitting method for the evolutionary problem comprising three linear parts

  $$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = H\,u(t) = A\,u(t) + B\,u(t) + C\,u(t)\,, \quad t \ge 0\,, \\ u(0) = u_0\,, \end{cases} \tag{2}$$

  where $A : D(A) \subseteq \mathcal{B} \to \mathcal{B}$, $B : D(B) \subseteq \mathcal{B} \to \mathcal{B}$, $C : D(C) \subseteq \mathcal{B} \to \mathcal{B}$, and $H : D(H) \subseteq \mathcal{B} \to \mathcal{B}$ are generally unbounded linear operators on a Banach space $\mathcal{B} \supseteq D(H) \supseteq D(A) \cap D(B) \cap D(C) \neq \emptyset$. We denote the exact flow of this problem by

  $$\mathcal{E}(t) = \mathrm{e}^{tH} = \mathrm{e}^{t(A+B+C)}\,, \quad t \ge 0\,. \tag{3}$$

  The exact flow is approximated by

  $$\mathcal{S}(t) = \mathrm{e}^{tC}\,\mathrm{e}^{tB}\,\mathrm{e}^{tA} \approx \mathrm{e}^{t(A+B+C)}\,, \quad t \ge 0\,. \tag{4}$$

- We consider the second-order Strang splitting method for the evolutionary problem comprising two linear parts

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = H\, u(t) = A\, u(t) + B\, u(t)\,, \quad t \geq 0\,, \\ u(0) = u_0\,, \end{cases}$$

  with exact flow approximated by a composition of the subflows $\mathrm{e}^{tA}, \mathrm{e}^{tB}$,

$$\mathcal{S}(t) = \mathrm{e}^{tA/2}\, \mathrm{e}^{tB}\, \mathrm{e}^{tA/2} \approx \mathcal{E}(t) = \mathrm{e}^{tH} = \mathrm{e}^{t(A+B)}\,, \quad t \geq 0\,.$$

As our analysis of the Strang splitting method builds on the considerations for (4) but with $A/2$ replacing A, C, it is convenient to create a common framework for both methods. Considering (4) with $C = A$ the second order Strang splitting method reads

$$\mathcal{S}(t) = \mathrm{e}^{tA}\, \mathrm{e}^{tB}\, \mathrm{e}^{tA} \approx \mathrm{e}^{t(A+B+A)}\,, \quad t \geq 0\,. \tag{5}$$

In the context of (1) the operators A, B, C, and H generate unitary semigroups, and for this case we give a detailed analysis in Section 5.

Adaptive time stepsize selection and error control based on reliable a posteriori estimates of the local error is the key to efficient large scale computations of complex evolutionary problems. In this paper we construct local error estimators based on the defect correction principle [7] for the Lie–Trotter and Strang splitting methods. We prove that our a posteriori local error estimators are *asymptotically correct*, that is, the error of the local error estimator as compared to the exact local error operator tends to zero asymptotically faster than the error itself. Our approach is based on differential equations for the exact and numerical evolution operators. We first construct auxiliary problems of Sylvester type and define a defect of the numerical solution. An exact integral representation of the solution to a neighboring problem is subsequently evaluated by suitable numerical quadrature to construct an a posteriori local error estimator. The choice of the quadrature formulae ensures the desired order with a minimal number of defect evaluations, see Section 4 below. In this framework, we also recover the known a priori error bounds depending on the natural commutators of the involved operators, see for instance [5]. To establish convergence for concrete examples, the commutator bounds usually translate into regularity assumptions on the exact solution of equation (2).

The notion of the defect of the splitting solution has recently also been used in [8] for the purpose of a posteriori estimation of the local error in the context of spectral approximations of a linear semiclassical Schrödinger equation. In contrast, we propose an additional backsolving step and thus obtain a posteriori local error estimators which are even asymptotically correct, at some moderate additional cost.

We focus on the linear case in this paper, as the construction and analysis of the error estimates is even more technically involved in the nonlinear case and requires to resort to the technique of Lie derivatives. This will be the subject of future work. Also, extension to higher-order splitting schemes will not be considered in this paper to keep the presentation focussed on the main ideas. Splitting the Hamiltonian operator into three parts as in (4) is a more relevant issue in the nonlinear case, for example in the presence of a rotation term in the Gross–Pitaevskii equation [1], so as a preparation we also consider the general form (2).

The present paper is organized as follows: In Section 2 we derive representations for the local error of the Lie–Trotter and Strang splitting methods in a general Banach space setting, where two versions based on either the defect or the truncation error are derived, respectively. Section 3 recovers the known a priori local error representations within the new framework as a preparation for Section 4, where we construct a posteriori local error estimators based on the former error representations, and prove their asymptotical correctness. In Section 5 we specialize our results to linear Schrödinger operators with sufficiently regular potentials and give numerical illustrations for the harmonic oscillator in 3D and a second example in 2D.

2. Local error representations

2.1. Exact and numerical evolution operator

Clearly, the exact evolution operator $\mathcal{E}$ given by (3) satisfies

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{E}(t) = \big(A + B + C\big)\,\mathcal{E}(t)\,, \quad t \geq 0\,, \\ \mathcal{E}(0) = \mathcal{I}\,. \end{cases} \tag{6}$$

Likewise, we consider the splitting operator for the numerical approximation of (3) as a continuous flow. Our formulation (4) comprises both the first order Lie–Trotter splitting method with either $C = 0$ or $C \neq 0$, and the symmetric Strang splitting method where $C = A$. Throughout, we first consider the Lie–Trotter splitting method and subsequently specialize and extend the results to the case of the Strang splitting method.

The splitting operator $\mathcal{S}$ given by (4) satisfies an initial value problem associated with a (generalized) *Sylvester equation*,

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{S}(t) = \mathcal{S}(t)A + B_C(t)\,\mathcal{S}(t) + C\,\mathcal{S}(t)\,, \quad t \geq 0\,, \\ \mathcal{S}(0) = \mathcal{I}\,. \end{cases} \tag{7}$$

Throughout we use the abbreviation

$$B_C(t) := \mathrm{e}^{tC} B\,\mathrm{e}^{-tC}\,, \tag{8}$$

and we note that

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,B_C(t) = \mathrm{e}^{tC}\,\big[C,B\big]\,\mathrm{e}^{-tC} = \big[C,B_C(t)\big]\,. \tag{9}$$

On several occasions we make use of the following solution representation for Sylvester equations related to (7): The inhomogeneous generalized Sylvester equation (for operators)

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{X}(t) = \mathcal{X}(t)A + B_C(t)\mathcal{X}(t) + C\,\mathcal{X}(t) + \mathcal{G}(t)\,, \quad t \geq 0\,, \\ \mathcal{X}(0) \text{ given}\,, \end{cases} \tag{10a}$$

admits the solution representation

$$\begin{aligned} \mathcal{X}(t) &= \mathrm{e}^{tC}\,\mathrm{e}^{tB}\,\mathcal{X}(0)\,\mathrm{e}^{tA} \\ &\qquad + \int_0^t \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\,\mathcal{G}(\tau)\,\mathrm{e}^{(t-\tau)A}\,\mathrm{d}\tau\,, \quad t \geq 0\,. \end{aligned} \tag{10b}$$

2.2. Local error, defect and truncation operators

In this section we introduce basic representations for the local error $\mathcal{S}-\mathcal{E}$ involving a defect operator and a truncation operator, respectively. These serve as a preparation for the local error expansions given in Section 3, and for the design and analysis of the a posteriori local error estimators introduced in Section 4.

The present approach is related to the integral expansion for the Strang splitting operator given in [9]. However, we pursue an alternative approach, exploiting natural representations via Sylvester equations (see (7),(10)) wherever appropriate.

Local error operator. Let

$$\mathcal{L}(t) = \mathcal{S}(t) - \mathcal{E}(t) = \mathrm{e}^{tC}\,\mathrm{e}^{tB}\,\mathrm{e}^{tA} - \mathrm{e}^{t(A+B+C)}\,, \quad t \geq 0\,. \tag{11}$$

Defect operator. We define the defect operator $\mathcal{D}$ via the relation

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{S}(t) = \big(A+B+C\big)\,\mathcal{S}(t) + \mathcal{D}(t)\,, \quad t \geq 0\,, \\ \mathcal{S}(0) = \mathcal{I}\,, \end{cases} \tag{12}$$

that is, $\mathcal{D}$ is the residual of $\mathcal{S}$ with respect to the original evolution equation (6). We have

$$\mathcal{D}(t) = \big[\mathcal{S}(t), A\big] + \big(B_C(t) - B\big)\,\mathcal{S}(t) = \big[\mathrm{e}^{tC}\mathrm{e}^{tB}, A+B\big]\,\mathrm{e}^{tA}\,, \quad t \geq 0\,, \tag{13}$$

and $\mathcal{D}(0) = 0$.

Integral representation for the local error operator (via the defect operator and the variation-of-constants formula). From (6) and (12) we obtain an initial value problem for the local error operator (11),

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}(t) = \big(A+B+C\big)\,\mathcal{L}(t) + \mathcal{D}(t)\,, \quad t \geq 0\,, \\ \mathcal{L}(0) = 0\,, \end{cases} \tag{14}$$

and the variation-of-constants formula yields the representation

$$\mathcal{L}(t) = \int_0^t \mathrm{e}^{(t-\tau)(A+B+C)}\,\mathcal{D}(\tau)\,\mathrm{d}\tau\,, \qquad t \geq 0\,, \tag{15}$$

with $\mathcal{D}$ given by (13).

Truncation operator. We define the truncation operator $\mathcal{T}$ via the relation

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{E}(t) = \mathcal{E}(t)A + B_C(t)\,\mathcal{E}(t) + C\,\mathcal{E}(t) + \mathcal{T}(t)\,, \quad t \geq 0\,, \\ \mathcal{E}(0) = \mathcal{I}\,, \end{cases} \tag{16}$$

that is, $\mathcal{T}$ is the residual of $\mathcal{E}$ with respect to the homogeneous Sylvester equation (7). We have

$$\begin{aligned} \mathcal{T}(t) &= \big[A, \mathcal{E}(t)\big] + \big(B - B_C(t)\big)\,\mathcal{E}(t) \\ &= \big(A + B - B_C(t)\big)\,\mathcal{E}(t) - \mathcal{E}(t)A\,, \quad t \geq 0\,, \end{aligned} \tag{17}$$

and $\mathcal{T}(0) = 0$.

Note that the defect operator $\mathcal{D}$ from (13) is an a posteriori approximation for the unknown quantity $-\mathcal{T}$.

Integral representation for the local error operator (via the truncation operator and the solution of the Sylvester equation). From (7) and (16) we obtain an initial value problem for the local error operator (11),

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}(t) = \mathcal{L}(t)A + B_C(t)\,\mathcal{L}(t) + C\,\mathcal{L}(t) - \mathcal{T}(t)\,, \quad t \geq 0\,, \\ \mathcal{L}(0) = 0\,, \end{cases} \tag{18}$$

alternatively to (14). From (10) we obtain

$$\mathcal{L}(t) = -\int_0^t \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\,\mathcal{T}(\tau)\,\mathrm{e}^{(t-\tau)A}\,\mathrm{d}\tau\,, \qquad t \geq 0\,, \tag{19}$$

alternatively to (15), with $\mathcal{T}$ given by (17).

Our design of an a posteriori local error estimator aims for replacing the integral representation (15) or (19), respectively, by a sufficiently accurate, computable approximation. Section 4 is devoted to this topic.

3. A priori local error expansions

In this section, the local error operator $\mathcal{L}$ is expanded via a sequence of differential equations, in a way that its dependence on problem data, in particular commutators involving A, B and C, can be explicitly inferred from the resulting integral representations. As a by-product, a priori local error bounds as for example given in [5], are recovered in a natural way, i.e.,

$$\mathcal{L}(t) = \mathcal{O}\big(t^{p+1}\big)$$

with $p = 1$ for the Lie–Trotter splitting method and $p = 2$ for the Strang splitting method ($C = A$), respectively.

We derive several versions of such local error expansions, involving (i) the defect operator $\mathcal{D}$, and (ii) the truncation operator $\mathcal{T}$, respectively.

3.1. Expansions involving defect operator

Expansion of the defect operator via differential equations — Lie–Trotter splitting method. As the defect $\mathcal{D}$ is defined in terms of the splitting operator $\mathcal{S}$, see (13), it turns out to be most natural to expand $\mathcal{D}$ by means of a differential equation of Sylvester type analogous to (7). Thus we consider

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{D}(t) = \mathcal{D}(t)A + B_C(t)\,\mathcal{D}(t) + C\,\mathcal{D}(t) + \mathcal{R}_{\mathcal{D}}(t)\,, \quad t \geq 0\,, \\ \mathcal{D}(0) = 0\,, \end{cases} \tag{20}$$

that is, $\mathcal{R}_{\mathcal{D}}$ is the residual of $\mathcal{D}$ with respect to the homogeneous Sylvester equation. To recast $\mathcal{R}_{\mathcal{D}}$ we differentiate (13), and a straightforward calculation yields

$$\begin{aligned}\mathcal{R}_{\mathcal{D}}(t) &= \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{D}(t) - \big(\mathcal{D}(t)A + B_C(t)\,\mathcal{D}(t) + C\,\mathcal{D}(t)\big)\\ &= \big[B_C(t) + C, A + B\big]\,\mathcal{S}(t)\,, \quad t \geq 0\,.\end{aligned}$$

Thus, we have

$$\mathcal{R}_{\mathcal{D}}(t) = \mathcal{K}_1(t)\,\mathcal{S}(t)\,, \quad \mathcal{K}_1(t) = \big[B_C(t) + C, A + B\big]\,, \quad t \geq 0\,. \tag{21}$$

In this way we obtain an integral representation for the defect operator,

$$\mathcal{D}(t) = \int_0^t \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\,\mathcal{R}_{\mathcal{D}}(\tau)\,\mathrm{e}^{(t-\tau)A}\,\mathrm{d}\tau\,, \quad t \geq 0\,, \tag{22}$$

and the requirement $\mathcal{L}(t) = \mathcal{O}\big(t^{p+1}\big)$ or $\mathcal{D}(t) = \mathcal{O}\big(t^{p}\big)$, respectively, reduces to

$$\mathcal{R}_{\mathcal{D}}(t) = \mathcal{O}\big(t^{p-1}\big)\,.$$

These considerations lead to the following result.

Lemma 1 (Local error expansion via defect, Lie–Trotter). *The local error* $\mathcal{L}$ (11) *satisfies* (14)*,*

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}(t) = \big(A + B + C\big)\,\mathcal{L}(t) + \mathcal{D}(t)\,, \quad t \geq 0\,,\\ \mathcal{L}(0) = 0\,. \end{cases}$$

Here, the defect operator $\mathcal{D}$*, see* (12), (13)*, is the solution of* (20)*,*

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{D}(t) = \mathcal{D}(t)A + B_C(t)\,\mathcal{D}(t) + C\,\mathcal{D}(t) + \mathcal{R}_{\mathcal{D}}(t)\,, \quad t \geq 0\,,\\ \mathcal{D}(0) = 0\,, \end{cases}$$

where $\mathcal{R}_{\mathcal{D}}$ *is given by* (21)*,*

$$\mathcal{R}_{\mathcal{D}}(t) = \mathcal{K}_1(t)\,\mathcal{S}(t)\,, \quad \mathcal{K}_1(t) = \big[B_C(t) + C, A + B\big]\,, \quad t \geq 0\,. \tag{23}$$

Due to $\mathcal{D}(0) = 0$ *we also have* $\mathcal{L}'(0) = 0$*. This yields the integral representation*

$$\begin{aligned}\mathcal{L}(t) = \int_0^t \int_0^{\tau_1} &\mathrm{e}^{(t-\tau_1)(A+B+C)}\,\mathrm{e}^{\tau_1 C}\,\mathrm{e}^{(\tau_1-\tau_2)B}\,\mathrm{e}^{-\tau_2 C}\\ &\times \big[B_C(\tau_2) + C, A + B\big]\,\mathrm{e}^{\tau_2 C}\,\mathrm{e}^{\tau_2 B}\,\mathrm{e}^{\tau_1 A}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,, \quad t \geq 0\,.\end{aligned} \tag{24}$$

For $C = 0$, (23) specializes to

$$\mathcal{R}_{\mathcal{D}}(t) = \mathcal{K}_1(t)\,\mathcal{S}(t)\,, \quad \mathcal{K}_1(t) = \big[B, A\big]\,, \quad t \geq 0\,. \tag{25}$$

Provided that the integrand in (24) remains bounded (on a suitable domain), $\mathcal{L}(t) = \mathcal{O}\big(t^2\big)$ readily follows.

Further expansion — Strang splitting method. For the Strang splitting method ($C = A$) we obtain from (21)

$$\mathcal{R}_{\mathcal{D}}(t) = \mathcal{K}_1(t)\,\mathcal{S}(t)\,, \quad \mathcal{K}_1(t) = \big[A + B_A(t), A + B\big]\,, \quad t \geq 0\,. \tag{26}$$

Using $\mathcal{K}_1(0) = 0$ a straightforward expansion yields

$$\mathcal{K}_1(t) = \int_0^t \tfrac{\mathrm{d}}{\mathrm{d}\tau}\,\mathcal{K}_1(\tau)\,\mathrm{d}\tau\,, \qquad t \geq 0\,,$$

with (see (9))

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{K}_1(t) = \big[\tfrac{\mathrm{d}}{\mathrm{d}t}B_A(t), A + B\big] = \big[\mathrm{e}^{tA}\,\big[A, B\big]\,\mathrm{e}^{-tA}, A + B\big]\,, \tag{27}$$

whence

$$\mathcal{K}_1(t) = \int_0^t \big[\mathrm{e}^{\tau A}\,\big[A, B\big]\,\mathrm{e}^{-\tau A}, A + B\big]\,\mathrm{d}\tau\,, \quad t \geq 0\,. \tag{28}$$

This yields the following version of Lemma 1 for the case of the Strang splitting method.

Lemma 2 (Local error expansion via defect, Strang). *The local error* $\mathcal{L}$ (11) *satisfies* (14) *with* $C = A$*,*

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}(t) = \big(A + B + A\big)\,\mathcal{L}(t) + \mathcal{D}(t)\,, \quad t \geq 0\,, \\ \mathcal{L}(0) = 0\,. \end{cases}$$

Here, the defect operator $\mathcal{D}$*, see* (12), (13), *is the solution of* (20) *with* $C = A$*,*

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{D}(t) = \mathcal{D}(t)A + B_A(t)\,\mathcal{D}(t) + A\,\mathcal{D}(t) + \mathcal{R}_{\mathcal{D}}(t)\,, \quad t \geq 0\,, \\ \mathcal{D}(0) = 0\,, \end{cases}$$

where $\mathcal{R}_{\mathcal{D}}$ is given by (26),(28),

$$\mathcal{R}_{\mathcal{D}}(t) = \mathcal{K}_1(t)\,\mathcal{S}(t)\,, \quad \mathcal{K}_1(t) = \int_0^t \big[\mathrm{e}^{\tau A}\,\big[A,B\big]\,\mathrm{e}^{-\tau A}, A+B\big]\,\mathrm{d}\tau\,, \quad t \geq 0\,. \tag{29}$$

Due to $\mathcal{D}(0) = 0$ we also have $\mathcal{L}'(0) = 0$. Moreover, from $\mathcal{K}_1(0) = 0$ we also have $\mathcal{D}'(0) = \mathcal{L}''(0) = 0$. This yields the integral representation

$$\begin{aligned} \mathcal{L}(t) = \int_0^t \int_0^{\tau_1} \int_0^{\tau_2} & \mathrm{e}^{(t-\tau_1)(A+B+A)}\,\mathrm{e}^{\tau_1 A}\,\mathrm{e}^{(\tau_1-\tau_2)B}\,\mathrm{e}^{-\tau_2 A} \\ & \times \big[[A, B_A(\tau_3)], A+B\big]\,\mathrm{e}^{\tau_2 A}\,\mathrm{e}^{\tau_2 B}\,\mathrm{e}^{\tau_1 A}\,\mathrm{d}\tau_3\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,, \quad t \geq 0\,. \end{aligned} \tag{30}$$

As expected, for the Strang splitting method it follows $\mathcal{L}(t) = \mathcal{O}\big(t^3\big)$, provided that the integrands remain bounded on a suitable domain.

3.2. Expansions involving truncation operator

Expansion of the truncation operator by differential equations — Lie–Trotter splitting method. As the truncation operator $\mathcal{T}$ is given in terms of the exact evolution operator $\mathcal{E}$, it is natural to consider the initial value problem

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{T}(t) = \big(A+B+C\big)\,\mathcal{T}(t) + \mathcal{R}_{\mathcal{T}}(t)\,, \quad t \geq 0\,, \\ \mathcal{T}(0) = 0\,, \end{cases} \tag{31}$$

that is, $\mathcal{R}_{\mathcal{T}}$ is the residual of $\mathcal{T}$ with respect to the homogeneous evolution equation. To recast $\mathcal{R}_{\mathcal{T}}$ we differentiate (17), and a straightforward calculation yields

$$\mathcal{R}_{\mathcal{T}}(t) = \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{T}(t) - \big(A+B+C\big)\mathcal{T}(t) = \big[A+B, B_C(t)+C\big]\,\mathcal{E}(t)\,, \quad t \geq 0\,.$$

Thus, with $\mathcal{K}_1$ from (21), we have

$$\mathcal{R}_{\mathcal{T}}(t) = -\mathcal{K}_1(t)\,\mathcal{E}(t)\,, \quad \mathcal{K}_1(t) = \big[B_C(t)+C, A+B\big]\,, \quad t \geq 0\,. \tag{32}$$

In this way we obtain an integral representation for the truncation operator,

$$\mathcal{T}(t) = \int_0^t \mathrm{e}^{(t-\tau)(A+B+C)}\,\mathcal{R}_{\mathcal{T}}(\tau)\,\mathrm{d}\tau\,, \quad t \geq 0\,, \tag{33}$$

and the requirement $\mathcal{L}(t) = \mathcal{O}\big(t^{p+1}\big)$ or $\mathcal{T}(t) = \mathcal{O}\big(t^p\big)$, respectively, reduces to

$$\mathcal{R}_{\mathcal{T}}(t) = \mathcal{O}\big(t^{p-1}\big)\,.$$

These considerations lead to the following result.

Lemma 3 (Local error expansion via truncation, Lie–Trotter). *The local error* $\mathcal{L}$ (11) *satisfies* (18),

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}(t) = \mathcal{L}(t)A + B_C(t)\,\mathcal{L}(t) + C\,\mathcal{L}(t) - \mathcal{T}(t)\,, \quad t \geq 0\,, \\ \mathcal{L}(0) = 0\,. \end{cases}$$

Here, the truncation operator $\mathcal{T}$*, see* (16), (17)*, is the solution of* (31),

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{T}(t) = \big(A + B + C\big)\,\mathcal{T}(t) + \mathcal{R}_{\mathcal{T}}(t)\,, \quad t \geq 0\,, \\ \mathcal{T}(0) = 0\,, \end{cases}$$

where $\mathcal{R}_{\mathcal{T}}$ *is given by* (32),

$$\mathcal{R}_{\mathcal{T}}(t) = -\mathcal{K}_1(t)\,\mathcal{E}(t)\,, \quad \mathcal{K}_1(t) = \big[B_C(t) + C, A + B\big]\,, \quad t \geq 0\,. \tag{34}$$

Due to $\mathcal{T}(0) = 0$ *we also have* $\mathcal{L}'(0) = 0$*. This yields the integral representation*

$$\begin{aligned} \mathcal{L}(t) = \int_0^t \int_0^{\tau_1} &\mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau_1)B}\,\mathrm{e}^{-\tau_1 C}\,\mathrm{e}^{(\tau_1-\tau_2)(A+B+C)}\,\big[B_C(\tau_2) + C, A + B\big] \\ &\times \mathrm{e}^{\tau_2(A+B+C)}\,\mathrm{e}^{(t-\tau_1)A}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,, \quad t \geq 0\,. \end{aligned}$$

For $C = 0$, in particular, (34) specializes to

$$\mathcal{R}_{\mathcal{T}}(t) = -\mathcal{K}_1(t)\,\mathcal{E}(t)\,, \quad \mathcal{K}_1(t) = \big[B, A\big]\,, \quad t \geq 0\,. \tag{35}$$

Again, we obtain the expected result $\mathcal{L}(t) = \mathcal{O}\big(t^2\big)$ for the Lie–Trotter splitting method, provided that the integrand remains bounded on a suitable domain.

Further expansion — Strang splitting method. For the case of the Strang splitting method ($C = A$), we obtain the following version of Lemma 3.

Lemma 4 (Local error expansion via truncation, Strang). *The local error* $\mathcal{L}$ (11) *satisfies* (18) *with* $C = A$,

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{L}(t) = \mathcal{L}(t)A + B_A(t)\,\mathcal{L}(t) + A\,\mathcal{L}(t) - \mathcal{T}(t)\,, \quad t \geq 0\,, \\ \mathcal{L}(0) = 0\,. \end{cases}$$

Here, the truncation operator $\mathcal{T}$, see (16), (17), is the solution of (31) with $C = A$,

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{T}(t) = \big(A + B + A\big)\,\mathcal{T}(t) + \mathcal{R}_{\mathcal{T}}(t)\,, \quad t \geq 0\,, \\ \mathcal{T}(0) = 0\,, \end{cases}$$

where $\mathcal{R}_{\mathcal{T}}$ is given by (28), (32)

$$\mathcal{R}_{\mathcal{T}}(t) = -\mathcal{K}_1(t)\,\mathcal{E}(t)\,, \quad \mathcal{K}_1(t) = \int_0^t \big[\mathrm{e}^{\tau A}\,\big[A, B\big]\,\mathrm{e}^{-\tau A}, A + B\big]\,\mathrm{d}\tau\,, \quad t \geq 0\,. \tag{36}$$

Due to $\mathcal{T}(0) = 0$ we also have $\mathcal{L}'(0) = 0$. Moreover, from $\mathcal{K}_1(0) = 0$ we also have $\mathcal{D}'(0) = \mathcal{L}''(0) = 0$. This yields the integral representation

$$\begin{aligned} \mathcal{L}(t) = \int_0^t \int_0^{\tau_1} \int_0^{\tau_2} & \mathrm{e}^{tA}\,\mathrm{e}^{(t-\tau_1)B}\,\mathrm{e}^{-\tau_1 A}\,\mathrm{e}^{(\tau_1-\tau_2)(A+B+A)} \\ & \times \big[\big[A, B_A(\tau_3)\big], A + B\big]\,\mathrm{e}^{\tau_2(A+B+A)}\mathrm{e}^{(t-\tau_1)A}\,\mathrm{d}\tau_3\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,, \quad t \geq 0\,. \end{aligned}$$

Provided that the integrand is bounded on a suitably chosen domain, we again conclude $\mathcal{L}(t) = \mathcal{O}\big(t^3\big)$.

4. A posteriori local error estimators

In the following, we construct and analyze a posteriori local error estimators for the Lie–Trotter and Strang splitting methods based on the previous local error representations.

4.1. Construction

Our defect-based local error estimators for the Lie–Trotter and Strang splitting methods rely on quadrature approximations of the integral representation (19) for $\mathcal{L}$, but with the truncation operator replaced by the negative defect operator, $\mathcal{T} \approx -\mathcal{D}$. In terms of differential equations, we thus proceed from equation (18) for $\mathcal{L}$ and replace the inhomogeneity $-\mathcal{T}$ by its approximation[2] $\mathcal{D}$. This defines an approximation $\widetilde{\mathcal{L}}$ for the local error operator $\mathcal{L}$ as the solution of the Sylvester equation

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,\widetilde{\mathcal{L}}(t) = \widetilde{\mathcal{L}}(t)A + B_C(t)\,\widetilde{\mathcal{L}}(t) + C\,\widetilde{\mathcal{L}}(t) + \mathcal{D}(t)\,, \quad t \geq 0\,, \\ \widetilde{\mathcal{L}}(0) = 0\,. \end{cases} \tag{37}$$

[2] This is equivalent to approximating (14) by the corresponding Sylvester equation.

An integral representation for $\widetilde{\mathcal{L}}$ is obtained from (10), and for practical evaluation this is subsequently replaced by an appropriate quadrature approximation. This defines the computable a posteriori error estimator $\mathcal{P}$:

$$\begin{aligned} &\mathcal{P}(t) = \text{quadrature approximation for } \widetilde{\mathcal{L}}(t), \\ &\text{where } \ \widetilde{\mathcal{L}}(t) = \int_0^t \underbrace{\mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\,\mathcal{D}(\tau)\,\mathrm{e}^{(t-\tau)A}}_{=:\,\mathcal{F}(\tau;t)}\,\mathrm{d}\tau\,, \quad t \geq 0\,. \end{aligned} \tag{38}$$

Quadrature defining $\mathcal{P}$ for the Lie–Trotter splitting method. For the Lie–Trotter splitting method we apply the second-order trapezoidal rule

$$\int_0^t \mathcal{F}(\tau;t)\,\mathrm{d}\tau \approx t\,\big(\tfrac{1}{2}\,\mathcal{F}(0;t) + \tfrac{1}{2}\,\mathcal{F}(t;t)\big) \tag{39}$$

to the integral in (38), and obtain due to (13) and $\mathcal{D}(0) = 0$ (see Lemma 1)

$$\mathcal{P}(t) = \tfrac{1}{2}\,t\,\mathcal{F}(t;t) = \tfrac{1}{2}\,t\,\mathcal{D}(t) = \tfrac{1}{2}\,t\,\big(\mathrm{e}^{tC}\,\mathrm{e}^{tB}(A+B) - (A+B)\,\mathrm{e}^{tC}\,\mathrm{e}^{tB}\big)\,\mathrm{e}^{tA}\,.$$

This choice of the quadrature formula ensures that the desired order two is obtained with a single defect evaluation. In particular, for $C = 0$ we have

$$\mathcal{P}(t) = \tfrac{1}{2}\,t\,\big(\mathrm{e}^{tB}A - A\,\mathrm{e}^{tB}\big)\,\mathrm{e}^{tA}\,, \quad t \geq 0\,. \tag{40}$$

Quadrature defining $\mathcal{P}$ for the Strang splitting method. For the Strang splitting method we apply the third-order Hermite quadrature rule

$$\int_0^t \mathcal{F}(\tau;t)\,\mathrm{d}\tau \approx t\,\big(\tfrac{2}{3}\,\mathcal{F}(0;t) + \tfrac{1}{6}\,t\,\partial_\tau\mathcal{F}(0;t) + \tfrac{1}{3}\,\mathcal{F}(t;t)\big) \tag{41}$$

to the integral in (38), and obtain due to (13) and $\mathcal{D}(0) = \mathcal{D}'(0) = 0$ (see Lemma 2)

$$\mathcal{P}(t) = \tfrac{1}{3}\,t\,\mathcal{F}(t;t) = \tfrac{1}{3}\,t\,\mathcal{D}(t) = \tfrac{1}{3}\,t\,\big(\mathrm{e}^{tA}\,\mathrm{e}^{tB}(A+B) - (A+B)\,\mathrm{e}^{tA}\,\mathrm{e}^{tB}\big)\,\mathrm{e}^{tA}\,. \tag{42}$$

Again, this choice of the quadrature formula ensures that the desired order three is obtained with a single defect evaluation.

For practical evaluation, the operator $\mathcal{P}$ is applied to the starting value u_0 of the current splitting step with time stepsize Δt, i.e., we compute

$$\mathcal{P}(\Delta t)u_0 \quad \text{with } \ \mathcal{P} \ \text{ from (40) or (42), respectively.} \tag{43}$$

4.2. Analysis of asymptotical correctness

Our aim is to show that $\mathcal{P}$ is an asymptotically correct local error estimator, i.e., its deviation satisfies

$$\big(\mathcal{P}-\mathcal{L}\big)(t)=\mathcal{O}\big(t^{p+2}\big)\,,\quad t\geq 0\,,$$

with $p=1$ for the Lie–Trotter splitting method and $p=2$ for the Strang splitting method, respectively. With

$$\big(\mathcal{P}-\mathcal{L}\big)(t)=\big(\mathcal{P}-\widetilde{\mathcal{L}}\big)(t)+\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)\,,\quad t\geq 0\,,$$

estimation of the deviation $\mathcal{P}-\mathcal{L}$ of the local error estimate $\mathcal{P}$ is done below in two steps:

- Estimation of the deviation $\widetilde{\mathcal{L}}-\mathcal{L}$. Taking the difference of (37) and (18) we see that $\widetilde{\mathcal{L}}-\mathcal{L}$ is the solution of the Sylvester equation

$$\begin{cases}\frac{\mathrm{d}}{\mathrm{d}t}\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)=\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)A+B_C(t)\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)\\ \qquad\qquad\qquad +\,C\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)+\big(\mathcal{D}+\mathcal{T}\big)(t)\,,\quad t\geq 0\,,\\ \big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(0)=0\,.\end{cases}\tag{44}$$

  Thus, estimation of $\widetilde{\mathcal{L}}-\mathcal{L}$ essentially reduces to estimating $\mathcal{D}+\mathcal{T}$, the error of the approximation $\mathcal{D}\approx-\mathcal{T}$.

- Estimation of the quadrature error $\mathcal{P}-\widetilde{\mathcal{L}}$, see (38)–(42).

In the sequel, these steps are elaborated in detail.

4.2.1. Analysis of the deviation $\widetilde{\mathcal{L}}-\mathcal{L}$

Here our aim is to show that

$$\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)=\mathcal{O}\big(t^{p+2}\big)\,,\quad t\geq 0\,,$$

which, due to (44), reduces to the requirement

$$\big(\mathcal{D}+\mathcal{T}\big)(t)=\mathcal{O}\big(t^{p+1}\big)\,,\quad t\geq 0\,.$$

As a first step, via the differential equations for $\mathcal{D}$ and $\mathcal{T}$, see (20)–(22) and (31)–(33), we obtain[3]

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}\big(\mathcal{D}+\mathcal{T}\big)(t) &= \mathcal{D}(t)A + B_C(t)\,\mathcal{D}(t) + C\,\mathcal{D}(t) + \big(A+B+C\big)\,\mathcal{T}(t) \\ &\qquad + \mathcal{R}_{\mathcal{D}}(t) + \mathcal{R}_{\mathcal{T}}(t) \\ &= \big(A+B+C\big)\,\big(\mathcal{D}+\mathcal{T}\big)(t) + \big[\mathcal{D}(t),A\big] + \big(B-B_C(t)\big)\,\mathcal{D}(t) \\ &\qquad + \mathcal{K}_1(t)\,\mathcal{S}(t) - \mathcal{K}_1(t)\,\mathcal{E}(t) \\ &= \big(A+B+C\big)\,\big(\mathcal{D}+\mathcal{T}\big)(t) + \mathcal{K}_1(t)\,\mathcal{L}(t) + \mathcal{D}_1(t)\,, \quad t \geq 0\,,\end{aligned}$$

with $\mathcal{K}_1$ from (21), and denoting

$$\mathcal{D}_1(t) = \big[\mathcal{D}(t),A\big] + \big(B-B_C(t)\big)\,\mathcal{D}(t)\,, \quad t \geq 0\,. \tag{45}$$

Thus we obtain an initial value problem for $\mathcal{D}+\mathcal{T}$,

$$\begin{cases} \tfrac{\mathrm{d}}{\mathrm{d}t}\big(\mathcal{D}+\mathcal{T}\big)(t) = \big(A+B+C\big)\,\big(\mathcal{D}+\mathcal{T}\big)(t) \\ \qquad\qquad + \mathcal{K}_1(t)\,\mathcal{L}(t) + \mathcal{D}_1(t)\,, \quad t \geq 0\,, \\ \big(\mathcal{D}+\mathcal{T}\big)(0) = 0\,. \end{cases} \tag{46}$$

It remains to show that the inhomogeneity in (46), is $\mathcal{O}\big(t^p\big)$. For the first contribution $\mathcal{K}_1(t)\,\mathcal{L}(t)$, this is straightforward from (21) together with the appropriate local error estimates. It remains to show that $\mathcal{D}_1$ from (45) satisfies

$$\mathcal{D}_1(t) = \mathcal{O}\big(t^p\big)\,, \quad t \geq 0\,.$$

For this purpose, we derive yet another differential equation. Aiming at a Sylvester equation for $\mathcal{D}_1$, we separately consider the two contributions on the right-hand side to (45).

- First, again with the help of equation (20) for $\mathcal{D}$, a short calculation yields

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}\big[\mathcal{D}(t),A\big] &= \big[\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}(t),A\big] \\ &= \big[\mathcal{D}(t)A + \big(B_C(t)+C\big)\,\mathcal{D}(t) + \mathcal{R}_{\mathcal{D}}(t),A\big] \\ &= \big[\mathcal{D}(t),A\big]\,A + (B_C(t)+C)\,\big[\mathcal{D}(t),A\big] \\ &\qquad + \big[B_C(t)+C,A\big]\,\mathcal{D}(t) + \big[\mathcal{R}_{\mathcal{D}}(t),A\big]\,, \quad t \geq 0\,.\end{aligned}$$

[3] Alternatively, we could work with a Sylvester equation for $\mathcal{D}+\mathcal{T}$, but this makes no essential difference in the subsequent analysis.

- In a similar manner, using (9) we obtain

$$\begin{aligned}
&\tfrac{\mathrm{d}}{\mathrm{d}t}\big(\big(B-B_C(t)\big)\,\mathcal{D}(t)\big)\\
&\qquad = \mathrm{e}^{tC}\,\big[C,B\big]\,\mathrm{e}^{-tC}\,\mathcal{D}(t) + \big(B-B_C(t)\big)\,\tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathcal{D}(t)\\
&\qquad = \mathrm{e}^{tC}\,\big[C,B\big]\,\mathrm{e}^{-tC}\,\mathcal{D}(t)\\
&\qquad\qquad + \big(B-B_C(t)\big)\big(\mathcal{D}(t)A + \big(B_C(t)+C\big)\,\mathcal{D}(t) + \mathcal{R}_{\mathcal{D}}(t)\big)\\
&\qquad = \big(B-B_C(t)\big)\,\mathcal{D}(t)A + \big(B_C(t)+C\big)\,\big(B-B_C(t)\big)\,\mathcal{D}(t)\\
&\qquad\qquad + \big[B_C(t)+C,B\big]\,\mathcal{D}(t) + \big(B-B_C(t)\big)\,\mathcal{R}_{\mathcal{D}}(t)\,, \quad t\geq 0\,.
\end{aligned}$$

Summing up these contributions yields

$$\begin{aligned}
\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}_1(t) &= \mathcal{D}_1(t)A + B_C(t)\,\mathcal{D}_1(t) + C\,\mathcal{D}_1(t)\\
&\qquad + \big[\mathcal{R}_{\mathcal{D}}(t),A\big] + \big(B-B_C(t)\big)\,\mathcal{R}_{\mathcal{D}}(t) + \mathcal{K}_1(t)\,\mathcal{D}(t)\,, \quad t\geq 0\,,
\end{aligned}$$

with $\mathcal{R}_{\mathcal{D}}$ and $\mathcal{K}_1$ from (21). Thus, denoting

$$\mathcal{R}_{\mathcal{D},1}(t) = \big[\mathcal{R}_{\mathcal{D}}(t),A\big] + \big(B-B_C(t)\big)\,\mathcal{R}_{\mathcal{D}}(t)\,, \quad t\geq 0\,, \tag{47}$$

we obtain

$$\begin{aligned}
\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}_1(t) &= \mathcal{D}_1(t)A + B_C(t)\,\mathcal{D}_1(t) + C\,\mathcal{D}_1(t)\\
&\qquad + \mathcal{K}_1(t)\,\mathcal{D}(t) + \mathcal{R}_{\mathcal{D},1}(t)\,, \quad t\geq 0\,.
\end{aligned} \tag{48}$$

The inhomogeneity in (48) can be expressed in a more elementary way. We write

$$\mathcal{K}_1(t)\,\mathcal{D}(t) + \mathcal{R}_{\mathcal{D},1}(t) = 2\,\mathcal{K}_1(t)\,\mathcal{D}(t) + \big(\mathcal{R}_{\mathcal{D},1}(t) - \mathcal{K}_1(t)\,\mathcal{D}(t)\big)\,.$$

With $\mathcal{R}_{\mathcal{D},1}$ defined in (47), the relation $\mathcal{D}(t) = \big[\mathcal{S}(t),A\big] + \big(B-B_C(t)\big)\,\mathcal{S}(t)$ and $\mathcal{R}_{\mathcal{D}}(t) = \mathcal{K}_1(t)\,\mathcal{S}(t)$ (see (13),(21)), a short calculation yields

$$\begin{aligned}
\mathcal{R}_{\mathcal{D},1}(t) - \mathcal{K}_1(t)\,\mathcal{D}(t) &= \big[\mathcal{K}_1(t)\,\mathcal{S}(t),A\big] + \big(B-B_C(t)\big)\,\mathcal{K}_1(t)\,\mathcal{S}(t)\\
&\qquad - \mathcal{K}_1(t)\,\big[\mathcal{S}(t),A\big] - \mathcal{K}_1(t)\,\big(B-B_C(t)\big)\,\mathcal{S}(t)\\
&= [\mathcal{K}_1(t),A]\,\mathcal{S}(t) + [(B-B_C(t)),\mathcal{K}_1(t)]\,\mathcal{S}(t)\\
&= [\mathcal{K}_1(t),A+(B_C(t)-B)]\,\mathcal{S}(t).
\end{aligned}$$

Thus, we obtain the following initial value problem of Sylvester type for $\mathcal{D}_1$ (recall that $\mathcal{D}(0) = 0$, see (15), and thus $\mathcal{D}_1(t) = 0$, see (45)),

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}_1(t) = \mathcal{D}_1(t)A + B_C(t)\,\mathcal{D}_1(t) + C\,\mathcal{D}_1(t) \\ \qquad\qquad + 2\,\mathcal{K}_1(t)\,\mathcal{D}(t) + [\mathcal{K}_1(t), A + (B_C(t) - B)]\,\mathcal{S}(t)\,, \quad t \geq 0\,, \\ \mathcal{D}_1(0) = 0\,, \end{cases} \tag{49}$$

with $\mathcal{K}_1$ from (21).

Summarizing this analysis for $\mathcal{D} + \mathcal{T}$, we state the following result.

Lemma 5 (Representation of $\mathcal{D} + \mathcal{T}$, Lie–Trotter). *The error of $\mathcal{D}$ as an approximation for $-\mathcal{T}$ satisfies* (46)*,*

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\big(\mathcal{D} + \mathcal{T}\big)(t) = \big(A + B + C\big)\,\big(\mathcal{D} + \mathcal{T}\big)(t) + \mathcal{K}_1(t)\,\mathcal{L}(t) + \mathcal{D}_1(t)\,, \quad t \geq 0\,, \\ \big(\mathcal{D} + \mathcal{T}\big)(0) = 0\,. \end{cases}$$

Here, $\mathcal{D}_1$ from (45) *is the solution of* (49)*,*

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}_1(t) = \mathcal{D}_1(t)A + B_C(t)\,\mathcal{D}_1(t) + C\,\mathcal{D}_1(t) \\ \qquad\qquad + 2\,\mathcal{K}_1(t)\,\mathcal{D}(t) + [\mathcal{K}_1(t), A + (B_C(t) - B)]\,\mathcal{S}(t)\,, \quad t \geq 0\,, \\ \mathcal{D}_1(0) = 0\,, \end{cases}$$

where $\mathcal{D}$ and $\mathcal{K}_1$ are specified in Lemma 1. Due to $\mathcal{L}(0) = \mathcal{D}_1(0) = 0$ we also have $\big(\mathcal{D} + \mathcal{T}\big)'(0) = 0$.

Finally, we can formulate the following result.

Lemma 6 (Representation of $\widetilde{\mathcal{L}} - \mathcal{L}$, Lie–Trotter). *The deviation $\widetilde{\mathcal{L}} - \mathcal{L}$ satisfies* (44)*,*

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\big(\widetilde{\mathcal{L}} - \mathcal{L}\big)(t) = \big(\widetilde{\mathcal{L}} - \mathcal{L}\big)(t)A + B_C(t)\big(\widetilde{\mathcal{L}} - \mathcal{L}\big)(t) + C\big(\widetilde{\mathcal{L}} - \mathcal{L}\big)(t) \\ \qquad\qquad + \big(\mathcal{D} + \mathcal{T}\big)(t)\,, \quad t \geq 0\,, \\ \big(\widetilde{\mathcal{L}} - \mathcal{L}\big)(0) = 0\,, \end{cases}$$

where $\mathcal{D} + \mathcal{T}$ is specified in Lemma 5. Due to $\big(\mathcal{D} + \mathcal{T}\big)(0) = \big(\mathcal{D} + \mathcal{T}\big)'(0) = 0$ we also have $\big(\widetilde{\mathcal{L}} - \mathcal{L}\big)'(0) = \big(\widetilde{\mathcal{L}} - \mathcal{L}\big)''(0) = 0$. This yields the integral *representation*

$$\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)=\int_0^t \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\,\big(\mathcal{D}+\mathcal{T}\big)(\tau)\,\mathrm{e}^{(t-\tau)A}\,\mathrm{d}\tau$$

$$=\int_0^t \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\int_0^\tau \mathrm{e}^{(\tau-\tau_1)(A+B+C)}\big(\mathcal{K}_1(\tau_1)\,\mathcal{L}(\tau_1)+\mathcal{D}_1(\tau_1)\big)\mathrm{d}\tau_1\,\mathrm{e}^{(t-\tau)A}\,\mathrm{d}\tau.$$

Here,

$$\begin{aligned}
&\big(\mathcal{K}_1(\tau_1)\,\mathcal{L}(\tau_1)+\mathcal{D}_1(\tau_1)\big)=\mathcal{K}_1(\tau_1)\,\mathcal{L}(\tau_1)\\
&+\int_0^{\tau_1}\mathrm{e}^{\tau_1 C}\,\mathrm{e}^{(\tau_1-\tau_2)B}\,\mathrm{e}^{-\tau_2 C}\times\\
&\qquad\times\big(2\,\mathcal{K}_1(\tau_2)\,\mathcal{D}(\tau_2)+\big[\mathcal{K}_1(\tau_2),A+(B_C(\tau_2)-B)\big]\mathcal{S}(\tau_2)\big)\,\mathrm{e}^{(\tau_1-\tau_2)A}\,\mathrm{d}\tau_2\,,
\end{aligned}$$

where $\mathcal{D}$ and $\mathcal{K}_1$ are specified in Lemma 1.

In particular, for $C=0$ we have

$$[\mathcal{K}_1(t),A+(B_C(t)-B)]=\big[\big[B,A\big],A\big]\,. \tag{50}$$

Further expansion — Strang splitting method. For the Strang splitting method ($C=A$), $\mathcal{K}_1$ satisfies $\mathcal{K}_1(0)=0$, see (26). Furthermore, $\mathcal{D}_1$ from (45) satisfies the initial value problem (49) with $C=A$,

$$\begin{cases}
\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}_1(t)=\mathcal{D}_1(t)A+B_A(t)\,\mathcal{D}_1(t)+A\,\mathcal{D}_1(t)+2\,\mathcal{K}_1(t)\,\mathcal{D}(t)\\
\qquad\qquad+\underbrace{\big[\mathcal{K}_1(t),A+(B_A(t)-B)\big]}_{(*)}\,\mathcal{S}(t)\,,\quad t\geq 0\,,\\
\mathcal{D}_1(0)=0\,,
\end{cases} \tag{51}$$

thus we also have $\mathcal{D}_1'(0)=0$. For the derivative of the term $(*)$ in the inhomogeneity of (51) we obtain (see (9),(27))

$$\begin{aligned}
&\tfrac{\mathrm{d}}{\mathrm{d}t}\big[\mathcal{K}_1(t),A+(B_A(t)-B)\big]\\
&\quad=\big[\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{K}_1(t),A+(B_A(t)-B)\big]+\big[\mathcal{K}_1(t),\tfrac{\mathrm{d}}{\mathrm{d}t}B_A(t)\big]\\
&\quad=\big[\mathrm{e}^{tA}\big[A,B\big]\,\mathrm{e}^{-tA},A+B\big],A+(B_A(t)-B)\big]\\
&\qquad+\big[\big[A+B_A(t),A+B\big],\mathrm{e}^{tA}\big[A,B\big]\,\mathrm{e}^{-tA}\big]\,.
\end{aligned}$$

This yields the following version of Lemma 5 for the case of the Strang splitting method.

Lemma 7 (Representation of $\mathcal{D}+\mathcal{T}$, Strang). *The error of $\mathcal{D}$ as an approximation for $\mathcal{T}$ satisfies* (46) *with $C = A$,*

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\big(\mathcal{D}+\mathcal{T}\big)(t) = \big(A+B+A\big)\,\big(\mathcal{D}+\mathcal{T}\big)(t) + \mathcal{K}_1(t)\,\mathcal{L}(t) + \mathcal{D}_1(t)\,, \quad t \geq 0\,, \\ \big(\mathcal{D}+\mathcal{T}\big)(0) = 0\,. \end{cases}$$

Here, $\mathcal{D}_1$ from (45) *is the solution of* (51),

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}_1(t) = \mathcal{D}_1(t)A + B_A(t)\,\mathcal{D}_1(t) + A\,\mathcal{D}_1(t) \\ \qquad\qquad + \underbrace{2\,\mathcal{K}_1(t)\,\mathcal{D}(t) + \big[\mathcal{K}_1(t), A + (B_A(t)-B)\big]\,\mathcal{S}(t)}_{(\,*\,)}\,, \quad t \geq 0\,, \\ \mathcal{D}_1(0) = 0\,, \end{cases}$$

and it also satisfies $\mathcal{D}_1'(0) = 0$. The factor $(\,*\,)$ in the inhomogeneity can be written as

$$2\,\mathcal{K}_1(t)\,\mathcal{D}(t) + \int_0^t \Big(\big[\big[\mathrm{e}^{\tau A}\,[A,B]\,\mathrm{e}^{-\tau A}, A+B\big], A + (B_A(\tau)-B)\big] \\ + \big[\big[A+B_A(\tau), A+B\big], \mathrm{e}^{\tau A}\big[A,B\big]\mathrm{e}^{-\tau A}\big]\Big)\,\mathrm{d}\tau\;\mathcal{S}(t)\,, \tag{52}$$

where $\mathcal{D}$ and $\mathcal{K}_1$ are specified in Lemma 2. Due to $\mathcal{L}(0) = \mathcal{D}_1(0) = 0$ we also have $\big(\mathcal{D}+\mathcal{T}\big)'(0) = 0$. Moreover, due to $\mathcal{D}_1'(0) = \mathcal{K}_1(0) = 0$, we also have $\big(\mathcal{D}+\mathcal{T}\big)''(0) = 0$.

Finally, we can formulate the following result.

Lemma 8 (Representation of $\widetilde{\mathcal{L}}-\mathcal{L}$, Strang). *The deviation $\widetilde{\mathcal{L}}-\mathcal{L}$ satisfies* (44) *with $C = A$,*

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t) = \big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t)A + B_A(t)\,\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t) \\ \qquad\qquad + A\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(t) + \;\big(\mathcal{D}+\mathcal{T}\big)(t)\,, \quad t \geq 0\,, \\ \big(\widetilde{\mathcal{L}}-\mathcal{L}\big)(0) = 0\,. \end{cases}$$

Here, $\mathcal{D}+\mathcal{T}$ is specified in Lemma 7. Due to $\big(\mathcal{D}+\mathcal{T}\big)(0) = \big(\mathcal{D}+\mathcal{T}\big)'(0) = \big(\mathcal{D}+\mathcal{T}\big)''(0) = 0$ we also have $\big(\widetilde{\mathcal{L}}-\mathcal{L}\big)'(0) = \big(\widetilde{\mathcal{L}}-\mathcal{L}\big)''(0) = \big(\widetilde{\mathcal{L}}-\mathcal{L}\big)'''(0) = 0$.

This yields the integral representation

$$\begin{aligned}\big(\widetilde{\mathcal{L}} - \mathcal{L}\big)(t) &= \int_0^t \mathrm{e}^{tA}\, \mathrm{e}^{(t-\tau)B}\, \mathrm{e}^{-\tau A}\, \big(\mathcal{D} + \mathcal{T}\big)(\tau)\, \mathrm{e}^{(t-\tau)A}\, \mathrm{d}\tau \\ &= \int_0^t \mathrm{e}^{tA}\, \mathrm{e}^{(t-\tau)B}\, \mathrm{e}^{-\tau A} \int_0^\tau \mathrm{e}^{(\tau-\tau_1)(A+B+A)}\, \big(\mathcal{K}_1(\tau_1)\, \mathcal{L}(\tau_1) \\ &\qquad + \mathcal{D}_1(\tau_1)\big)\, \mathrm{d}\tau_1\, \mathrm{e}^{(t-\tau)A}\, \mathrm{d}\tau\,.\end{aligned} \tag{53}$$

Here,

$$\begin{aligned}&\big(\mathcal{K}_1(\tau_1)\, \mathcal{L}(\tau_1) + \mathcal{D}_1(\tau_1)\big) = \mathcal{K}_1(\tau_1)\, \mathcal{L}(\tau_1) \\ &+ \int_0^{\tau_1} \mathrm{e}^{\tau_1 C}\, \mathrm{e}^{(\tau_1-\tau_2)B}\, \mathrm{e}^{-\tau_2 C} \\ &\times \underbrace{\big(2\, \mathcal{K}_1(\tau_2)\, \mathcal{D}(\tau_2) + \big[\mathcal{K}_1(\tau_2), A + (B_C(\tau_2) - B)\big] \mathcal{S}(\tau_2)\big)}_{(\,*\,)}\, \mathrm{e}^{(\tau_1-\tau_2)A}\, \mathrm{d}\tau_2\,,\end{aligned} \tag{54}$$

where $\mathcal{D}$ and $\mathcal{K}_1$ are specified in Lemma 2, and the factor $(\,*\,)$ is represented in terms of (52)*.*

4.2.2. Analysis of the quadrature error $\mathcal{P} - \widetilde{\mathcal{L}}$

The estimator $\mathcal{P}$ has been defined as a quadrature approximation to the integral representation for $\widetilde{\mathcal{L}}$ (see (38)),

$$\widetilde{\mathcal{L}}(t) = \int_0^t \underbrace{\mathrm{e}^{tC}\, \mathrm{e}^{(t-\tau)B}\, \mathrm{e}^{-\tau C}\, \mathcal{D}(\tau)\, \mathrm{e}^{(t-\tau)A}}_{=\mathcal{F}(\tau;t)}\, \mathrm{d}\tau\,, \quad t \geq 0\,,$$

Our aim is to show that

$$\big(\mathcal{P} - \widetilde{\mathcal{L}}\big)(t) = \mathcal{O}\big(t^{p+2}\big)\,, \quad t \geq 0\,,$$

with $p = 1$ for the Lie–Trotter splitting method and $p = 2$ for the Strang splitting method ($C = A$), respectively. To this end we employ standard local error representations.

- For the second order trapezoidal quadrature (Lie–Trotter splitting method), see (38) and (39), the error admits the representation

$$\mathcal{P}(t) - \widetilde{\mathcal{L}}(t) = \int_0^t \tfrac{1}{2}\, \tau(t-\tau)\, \partial_\tau^2 \mathcal{F}(\tau;t)\, \mathrm{d}\tau\,.$$

- For the third order Hermite quadrature (Strang splitting method), see (41), the error admits the representation

$$\mathcal{P}(t) - \widetilde{\mathcal{L}}(t) = \int_0^t \tfrac{1}{6}\,\tau(t-\tau)^2\,\partial_\tau^3 \mathcal{F}(\tau;t)\,\mathrm{d}\tau\,.$$

By definition of the defect operator $\mathcal{D}$ (see (15)) and the splitting operator $\mathcal{S}$ (see (4)) we have

$$\begin{aligned}
\mathcal{F}(\tau;t) &= \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\,\big[\mathcal{S}(\tau),A\big]\,\mathrm{e}^{(t-\tau)A} \\
&\qquad + \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}\,\big(B_C(\tau)-B\big)\,\mathcal{S}(\tau)\,\mathrm{e}^{(t-\tau)A} \\
&= \mathrm{e}^{tC}\,\mathrm{e}^{tB} A\,\mathrm{e}^{tA} + \mathrm{e}^{tC} B\,\mathrm{e}^{tB}\,\mathrm{e}^{tA} \\
&\qquad - \mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\,\mathrm{e}^{-\tau C}(A+B)\,\mathrm{e}^{\tau C}\,\mathrm{e}^{\tau B}\,\mathrm{e}^{tA} \\
&= \mathrm{e}^{tC}\mathrm{e}^{tB}\Big((A+B) - \mathrm{e}^{-\tau B}\mathrm{e}^{-\tau C}\,(A+B)\,\mathrm{e}^{\tau C}\mathrm{e}^{\tau B}\Big)\,\mathrm{e}^{tA}
\end{aligned}$$

for $0 \le \tau \le t$. The respective derivatives can be determined by a routine calculation, with the help of the following lemma.

Lemma 9. *Consider* $\mathcal{U}(\tau) = \mathrm{e}^{-\tau B}\mathrm{e}^{-\tau C}\,X\,\mathrm{e}^{\tau C}\mathrm{e}^{\tau B}$ *with some constant operator* X. *Then,*

$$\mathcal{U}'(\tau) = \mathrm{e}^{-\tau B}\mathrm{e}^{-\tau C}\,[X,C]\,\mathrm{e}^{\tau C}\mathrm{e}^{\tau B} + [\mathcal{U}(\tau),B]. \tag{55}$$

Proof. We let $\mathcal{H}(\tau) = \mathrm{e}^{\tau C}\mathrm{e}^{\tau B}$ and $\hat{\mathcal{H}}(\tau) = \mathrm{e}^{-\tau B}\mathrm{e}^{-\tau C}$. We compute

$$\begin{aligned}
\mathcal{U}'(\tau) &= \tfrac{\mathrm{d}}{\mathrm{d}\tau}\,\hat{\mathcal{H}}(\tau)\,X\,\mathcal{H}(\tau) \\
&= \hat{\mathcal{H}}'(\tau)\,X\,\mathcal{H}(\tau) + \hat{\mathcal{H}}(\tau)\,X\,E'(\tau) \\
&= \hat{\mathcal{H}}(\tau)\mathcal{H}(\tau)\hat{\mathcal{H}}'(\tau)\,X\,\mathcal{H}(\tau) + \hat{\mathcal{H}}(\tau)\,X\,E'(\tau)\hat{\mathcal{H}}(\tau)\mathcal{H}(\tau) \\
&= \hat{\mathcal{H}}(\tau)\,\big(\mathcal{H}(\tau)(\mathcal{H}(\tau)\hat{\mathcal{H}}'(\tau)\,X + X\,E'(\tau)\hat{\mathcal{H}}(\tau)\big)\,\mathcal{H}(\tau) \\
&= \hat{\mathcal{H}}(\tau)\,\big(X\,E'(\tau)\hat{\mathcal{H}}(\tau) - E'(\tau)\hat{\mathcal{H}}(\tau)\,X\big)\,\mathcal{H}(\tau) \\
&= \hat{\mathcal{H}}(\tau)\,\big[X, E'(\tau)\hat{\mathcal{H}}(\tau)\big]\,\mathcal{H}(\tau). \qquad \square
\end{aligned}$$

We can thus determine the partial derivatives of $\mathcal{F}$:

Quadrature error — Lie–Trotter splitting method. The desired result for the Lie–Trotter splitting method, $\big(\mathcal{P}-\widetilde{\mathcal{L}}\big)(t)=\mathcal{O}(t^3)$, holds true provided that $\partial_\tau^2\mathcal{F}(\tau;t)$ is bounded. We have

$$\begin{aligned}&\partial_\tau\mathcal{F}(\tau;t)=\\&=\mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\Big(\big[B,\mathrm{e}^{-\tau C}(A+B)\,\mathrm{e}^{\tau C}\big]+\mathrm{e}^{-\tau C}\big[C,A+B\big]\,\mathrm{e}^{\tau C}\Big)\,\mathrm{e}^{\tau B}\,\mathrm{e}^{tA}\end{aligned}\tag{56}$$

for $0\le\tau\le t$, and

$$\begin{aligned}\partial_\tau^2\mathcal{F}(\tau;t)=-\mathrm{e}^{tC}\,\mathrm{e}^{(t-\tau)B}\Big(&\big[B,\big[B,\mathrm{e}^{-\tau C}(A+B)\,\mathrm{e}^{\tau C}\big]\big]\\&+2\,\big[B,\mathrm{e}^{-\tau C}[C,A+B]\,\mathrm{e}^{\tau C}\big]+\mathrm{e}^{-\tau C}\,\big[C,[C,A+B]\big]\,\mathrm{e}^{\tau C}\Big)\,\mathrm{e}^{\tau B}\,\mathrm{e}^{tA}\end{aligned}\tag{57}$$

for $0\le\tau\le t$. In particular, for $C=0$ we obtain

$$\partial_\tau^2\mathcal{F}(\tau;t)=\mathrm{e}^{(t-\tau)B}\,\big[B,\big[B,A\big]\big]\,\mathrm{e}^{\tau B}\,\mathrm{e}^{tA}\,,\quad 0\le\tau\le t\,.\tag{58}$$

Quadrature error — further expansion for the Strang splitting method. The desired result for the Strang splitting method, $\big(\mathcal{P}-\widetilde{\mathcal{L}}\big)(t)=\mathcal{O}(t^4)$, holds true provided that $\partial_\tau^3\mathcal{F}(\tau;t)$ is bounded.

First, for $C=A$, (57) simplifies to

$$\begin{aligned}\partial_\tau^2\mathcal{F}(\tau;t)=-\mathrm{e}^{tA}\,\mathrm{e}^{(t-\tau)B}\Big(&\big[B,\big[B,A+\mathrm{e}^{-\tau A}B\,\mathrm{e}^{\tau A}\big]\big]\\&+2\,\big[B,\mathrm{e}^{-\tau A}[A,B]\,\mathrm{e}^{\tau A}\big]+\mathrm{e}^{-\tau A}\big[A,[A,B]\big]\,\mathrm{e}^{\tau A}\Big)\,\mathrm{e}^{\tau B}\,\mathrm{e}^{tA}\,.\end{aligned}$$

Thus,

$$\begin{aligned}\partial_\tau^3\mathcal{F}(\tau;t)=\mathrm{e}^{tA}\,\mathrm{e}^{(t-\tau)B}\Big(&\big[B,\big[B,\big[B,A+\mathrm{e}^{-\tau A}B\,\mathrm{e}^{\tau A}\big]\big]\big]\\&+3\,\big[B,\big[B,\mathrm{e}^{-\tau A}[A,B]\,\mathrm{e}^{\tau A}\big]\big]+3\,\big[B,\mathrm{e}^{-\tau A}\big[A,[A,B]\big]\,\mathrm{e}^{\tau A}\big]\\&+\mathrm{e}^{-\tau A}\big[A,\big[A,[A,B]\big]\big]\,\mathrm{e}^{\tau A}\Big)\,\mathrm{e}^{\tau B}\,\mathrm{e}^{tA}\,,\quad 0\le\tau\le t\,.\end{aligned}\tag{59}$$

Lemma 10. *The quadrature error $\mathcal{P}-\widetilde{\mathcal{L}}$ satisfies*

$$(\mathcal{P}-\widetilde{\mathcal{L}})(t)=\mathcal{O}\big(t^{p+2}\big)$$

with $p=1$ for the Lie–Trotter splitting method and $p=2$ for the Strang splitting method, respectively, provided the derivatives $\partial_\tau^2\mathcal{F}(\tau;t)$ (see (57)) or $\partial_\tau^3\mathcal{F}(\tau;t)$ (see (59)), respectively, remain bounded.

4.2.3. Synopsis: Asymptotical correctness of local error estimator $\mathcal{P}$

Proposition 1. *The a posteriori local error estimator defined in* (38)–(43) *is asymptotically correct, i.e.,*

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

with $p = 1$ for the Lie–Trotter splitting method and $p = 2$ for the Strang splitting method, respectively, provided the data quantities (commutator expressions) influencing the deviation $\widetilde{\mathcal{L}} - \mathcal{L}$ (see Lemma 6, Lemma 8) and the quadrature error $\mathcal{P} - \widetilde{\mathcal{L}}$ (see Lemma 10) remain bounded.

In concrete applications, rigorous bounds for the deviation $\mathcal{P}-\mathcal{L}$ are obtained by analyzing the respective influence quantities.

5. Application to linear Schrödinger equations

5.1. Theoretical bounds

In this section, we establish the regularity assumptions on the exact solution necessary for our a priori and a posteriori error estimates to be well-defined such that our asymptotical results hold true for a linear Schrödinger equation (1) with sufficiently regular potential. For the Lie–Trotter splitting method, we only consider the case $C = 0$, and for the Strang splitting method we set $C = A$.

We generally restrict ourselves to the leading terms and evaluate the commutators appearing in the error representation. The fact that the commutators can be bounded in terms of the listed commutators of the data operators applied to suitable arguments is indicated by the asymptotic equivalence sign $\sim$; more precisely, for operators $\mathcal{C}, L$ the relation $\mathcal{C} \sim L$ signifies that there is a constant $C > 0$ such that $\|\mathcal{C}v\| \leq C\,\|Lv\|$. We thus investigate the following commutators:

- A priori, Lie–Trotter ($C = 0$) (see (25),(35)):

$$\mathcal{C}_1 \sim [A, B]\,. \tag{60}$$

- A priori, Strang ($C = A$) (see (29),(36)):

$$\mathcal{C}_2 \sim \left[\mathrm{e}^{tA}\,[A, B]\,\mathrm{e}^{-tA}, A + B\right]. \tag{61}$$

- A posteriori, Lie–Trotter ($C = 0$), leading term (see Lemma 6 and (50)):

$$\mathcal{C}_3 \sim \big[A, \big[A, B\big]\big] \,. \tag{62}$$

- A posteriori, Strang ($C = A$), leading term (see Lemma 8 and (52)):

$$\begin{aligned} \mathcal{C}_4 \sim \big[\big[\mathrm{e}^{tA}[A,B]\mathrm{e}^{-tA}, A+B\big], A + (B_A - B)\big] \\ + \big[\big[A + B_A, A+B\big], \mathrm{e}^{tA}\,[A,B]\,\mathrm{e}^{-tA}\big] \,. \end{aligned} \tag{63}$$

- A posteriori, Lie–Trotter ($C = 0$) , quadrature (see (58)):

$$\mathcal{C}_5 \sim \big[[A,B], B\big] \,. \tag{64}$$

- A posteriori, Strang ($C = A$) , quadrature (see (59)):

$$\begin{aligned} \mathcal{C}_6 \sim \big[B, \big[B, \big[B, A + \mathrm{e}^{-tA}\,B\,\mathrm{e}^{tA}\big]\big]\big] + 3\,\big[B, \big[B, \mathrm{e}^{-tA}\,[A,B]\,\mathrm{e}^{tA}\big]\big] \\ + 3\,\big[B, \mathrm{e}^{-tA}\big[A,[A,B]\big]\mathrm{e}^{tA}\big] + \mathrm{e}^{-tA}\big[A, \big[A,[A,B]\big]\big]\mathrm{e}^{tA} \,. \end{aligned} \tag{65}$$

In the following estimates, we restrict ourselves to the linear Schrödinger equation, where

$$A = \mathrm{i}\Delta \,, \qquad B = \mathrm{i}V,$$

with a smooth and bounded multiplication operator V on the underlying Banach space $\mathcal{B} = L^2(\mathbb{R}^d)$. We are omitting factors $\frac{1}{2}$ and -1, respectively, which do not affect the following considerations.

First we show that in the estimation of the commutators listed above, it is admissible to ignore the contributions from the flows $\mathrm{e}^{\pm tA}$, for $A = \mathrm{i}\Delta$. As usual, H^k denotes the Sobolev space of k times weakly differentiable functions and $\mathcal{C}^k$ the space of functions with k continuous derivatives.

Lemma 11. *Let $j, k \in \mathbb{N}$, and $\alpha, \beta, \psi : \mathbb{R}^d \to \mathbb{C}$ be sufficiently smooth. Then,*

$$\begin{cases} \big\|\big[\mathrm{e}^{tA}\alpha\,\mathrm{e}^{-tA}, \beta\big]\psi\big\|_{L^2} \le C\big(\|\alpha\|_{\mathcal{C}^0}, \|\beta\|_{\mathcal{C}^0}, \|\psi\|_{L^2}\big) \,, \\ \big\|\big[\mathrm{e}^{tA}\alpha\,\partial_x^j \mathrm{e}^{-tA}, \beta\,\partial_x^k\big]\psi\big\|_{L^2} \le C\big(\|\alpha\|_{\mathcal{C}^k}, \|\beta\|_{\mathcal{C}^j}, \|\psi\|_{H^{k+j-1}}\big), \quad k+j \ge 1 \,. \end{cases}$$

Proof. The proposition follows by direct computation using the product rule for differentiation and $\partial_x^j\,\mathrm{e}^{tA}\psi = \mathrm{e}^{tA}\partial_x^j\psi,\ j \ge 0$, for $A = \mathrm{i}\Delta,\ \psi \in H^j$. The latter relation is immediate from the solution representation of the free Schrödinger equation using the Fourier transform [10]. □

We now derive estimates for the relevant commutators in (60)–(65) in the present setting. The inequality we employ is $\|\phi\,\psi\|_{L^2} \leq \|\phi\|_{L^\infty}\|\psi\|_{L^2}$ [11]. We first list the estimates for the commutators with generic argument ϕ.

- For $\mathcal{C}_1$ we obtain

$$\begin{aligned}\|\mathcal{C}_1\phi\|_{L^2} &\sim \big\|[B,A]\phi\big\|_{L^2}\\ &= \big\|[\,\mathrm{i}V,\mathrm{i}\Delta]\phi\big\|_{L^2}\\ &\leq \|(\Delta V)\phi\|_{L^2} + 2\|(\nabla V)\cdot(\nabla\phi)\|_{L^2} \leq C\,(\|V\|_{C^2},\|\phi\|_{H^1})\,.\end{aligned}$$

- The leading term of $\mathcal{C}_3$ reduces to

$$\begin{aligned}\|\mathcal{C}_3\,\phi\|_{L^2} &\sim \big\|\big[[B,A],A\big]\phi\big\|_{L^2}\\ &= \|2\,\mathrm{i}\,(\Delta V)(\Delta\phi) - \mathrm{i}\,(\Delta^2\,V)\phi - 6\,\mathrm{i}\,(\Delta V)(\Delta\phi)\\ &\qquad -\ 4\,\mathrm{i}\,(\nabla^3 V)\cdot(\nabla\phi)\|_{L^2}\\ &\leq C\,(\|V\|_{C^4},\|\phi\|_{H^2})\,.\end{aligned}$$

- The leading term of $\mathcal{C}_5$ is given by

$$\begin{aligned}\|\mathcal{C}_5\,\phi\|_{L^2} &\sim \big\|\big[B,[B,A]\big]\phi\big\|_{L^2}\\ &= \|-2\,\mathrm{i}\,(\nabla V)\cdot(\nabla V)\,\phi\|_{L^2}\\ &\leq C\,(\|V\|_{\mathcal{C}^1},\|\phi\|_{L^2})\,.\end{aligned}$$

- As a further illustration of the procedure, we also include the estimate for $\mathcal{C}_2$. This also follows by the above considerations and Lemma 11.

$$\begin{aligned}\|\mathcal{C}_2\,\phi\|_{L^2} \sim\ &\big\| -4\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\Delta V)\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\Delta\phi)\\ &\quad -\ 4\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\nabla^3 V)\cdot(\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}\nabla\phi)\\ &\quad +\ 2\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\nabla V)\cdot\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}V(\nabla\phi)\\ &\quad -\ 2\,V\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\nabla V)\cdot\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\nabla\phi)\\ &\quad -\ \mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\Delta^2\,V)\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}\phi\\ &\quad +\ 2\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\Delta V)\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}V\phi\\ &\quad +\ 2\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\nabla V)\cdot(\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}\,\nabla V)\phi\\ &\quad -\ V\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}(\Delta V)\,\mathrm{e}^{\mathrm{i}t\Delta}\mathrm{e}^{\mathrm{i}tV}\phi\big\|_{L^2}\\ \leq\ &C(\|V\|_{C^4},\|\phi\|_{H^2})\,.\end{aligned}$$

- It is straightforward to extend the above arguments to the remaining terms $\mathcal{C}_4$ and $\mathcal{C}_6$. Note that the dominant term with highest appearing derivatives is in both cases

$$\big\| \big[[[B,A],A],A\big]\phi \big\|_{L^2} \leq C\left(\|V\|_{C^6}, \|\phi\|_{H^3}\right).$$

  As a consequence, we obtain

$$\begin{aligned} \|\mathcal{C}_4\,\phi\|_{L^2} &\leq C(\|V\|_{C^6}, \|\phi\|_{H^3})\,, \\ \|\mathcal{C}_6\,\phi\|_{L^2} &\leq C(\|V\|_{C^6}, \|\phi\|_{H^3})\,. \end{aligned}$$

These commutators act on terms which are composed of the flows of the evolution equation and the subproblems arising in the splitting scheme. We therefore need the following regularity results.

Lemma 12. *Let $m \geq 0$ and $t \in \mathbb{R}$.*

(i) *If $\phi \in H^m(\mathbb{R}^3)$ then $\mathrm{e}^{\mathrm{i}t\Delta}\phi \in H^m(\mathbb{R}^3)$.*
(ii) *If $\phi \in H^m(\mathbb{R}^3)$ and $V \in \mathcal{C}^m$ then $\mathrm{e}^{\mathrm{i}tV}\phi \in H^m(\mathbb{R}^3)$.*
(iii) *If $\phi \in H^m(\mathbb{R}^3)$ and $V \in \mathcal{C}^m$ then $\mathrm{e}^{\mathrm{i}t(\Delta-V)}\phi \in H^m(\mathbb{R}^3)$.*

Proof. The first statement is a direct consequence of the representation of $\mathrm{e}^{\mathrm{i}t\Delta}\phi$ by means of the Fourier transform [10]. The second one follows from the product rule of differentiation. For the third statement, we consider the original Schrödinger equation (1) with $d = 1$, recast as

$$\begin{cases} \partial_t \psi(x,t) = (A + B(x))\,\psi(x,t)\,, \\ \psi(x,0) = \phi(x)\,, \end{cases} \qquad x \in \mathbb{R}\,, \quad t \geq 0\,.$$

The space derivative of its solution satisfies

$$\begin{cases} \partial_t\,\partial_x \psi(x,t) = (A + B(x))\,\partial_x\psi(x,t) + \partial_x B(x)\,\psi(x,t)\,, \\ \partial_x\psi(x,0) = \partial_x\phi(x)\,, \end{cases} \qquad x \in \mathbb{R}\,, \quad t \geq 0\,.$$

Estimation of $\partial_x\psi(x,t)$ is straightforward by means of the variation-of-constants formula

$$\partial_x\psi(x,t) = \mathrm{e}^{t(A+B(x))}\partial_x\phi(x) + \int_0^t \mathrm{e}^{(t-\tau)(A+B(x))}\partial_x B(x)\,\psi(x,\tau)\mathrm{d}\tau\,.$$

These arguments directly extend to the case of arbitrary dimension $d > 1$ and higher-order space derivatives. $\square$

We are now ready to state the main results of the present work.

Theorem 1. *The Lie–Trotter splitting method applied to the linear Schrödinger equation* (1) *satisfies the following local error estimates.*

(i) *A priori: If* $V \in \mathcal{C}^2$ *and* $\|\psi_0\|_{H^1} \leq M$*, then*

$$\|\mathcal{L}(t)\psi_0\|_{L^2} \leq C\,t^2,$$

with a constant $C > 0$ *depending in particular on* M*.*

(ii) *A posteriori: If* $V \in \mathcal{C}^4$ *and* $\|\psi_0\|_{H^2} \leq M$*, then* $\mathcal{P}(t)\psi_0$ *is well-defined in* $L^2(\mathbb{R}^3)$ *and there holds*

$$\|(\mathcal{P} - \mathcal{L})(t)\psi_0\|_{L^2} \leq C\,t^3.$$

Theorem 2. *The Strang splitting method applied to linear Schrödinger equation* (1) *satisfies the following local error estimates.*

(i) *A priori: If* $V \in \mathcal{C}^4$ *and* $\|\psi_0\|_{H^2} \leq M$*, then*

$$\|\mathcal{L}(t)\psi_0\|_{L^2} \leq C\,t^3,$$

with a constant $C > 0$ *depending in particular on* M*.*

(ii) *A posteriori: If* $V \in \mathcal{C}^6$ *and* $\|\psi_0\|_{H^3} \leq M$*, then* $\mathcal{P}(t)\psi_0$ *is well-defined in* $L^2(\mathbb{R}^3)$ *and there holds*

$$\|(\mathcal{P} - \mathcal{L})(t)\psi_0\|_{L^2} \leq C\,t^4.$$

Remark 1. From the above results it is straightforward to deduce the respective global bounds: The stability of the splitting schemes in the linear case is a direct consequence of the fact that the operators A, B, C, and H have been assumed to generate unitary semigroups, and the global orders relate to the local orders in the usual way by the standard Lady Windermere's fan argument [12].

5.2. Numerical illustrations

In the following, we illustrate the theoretical results of Theorems 1 and 2 by numerical examples for the harmonic oscillator in three space dimensions and a linear Schrödinger equation involving a periodic potential in two space dimensions. In particular, we confirm the asymptotical correctness of our a posteriori local error estimators for the Lie–Trotter and Strang splitting methods.

k	Δt	$\|\mathcal{L}(\Delta t)\,\psi_0\|_{L^2}$	$\kappa_{\mathcal{L}}$	$\kappa_{\mathcal{P}-\mathcal{L}}$
0	$1.0000 \cdot 10^{0}$	$5.8059 \cdot 10^{-1}$	1.88	3.39
1	$5.0000 \cdot 10^{-1}$	$1.5765 \cdot 10^{-1}$	2.00	2.96
2	$1.2500 \cdot 10^{-1}$	$9.7704 \cdot 10^{-3}$	2.00	2.99
3	$1.5625 \cdot 10^{-2}$	$1.5247 \cdot 10^{-4}$	2.00	2.99
4	$9.7656 \cdot 10^{-4}$	$5.9558 \cdot 10^{-7}$	2.00	2.99
5	$3.0517 \cdot 10^{-5}$	$5.8162 \cdot 10^{-10}$	—	—

Table 1: Local errors and associated orders for the Lie–Trotter splitting method applied to the harmonic oscillator in 3D.

Harmonic oscillator. We first consider the time-dependent linear Schrödinger equation (1) in three space dimensions subject to the scaled harmonic potential

$$V(x) = V(x_1, x_2, x_3) = \sum_{j=1}^{3} \omega_j\, x_j^2\,, \qquad \omega = (\omega_1, \omega_2, \omega_3) = (0.9, 1, 1.1)\,.$$

We choose the initial state such that the exact solution is given by

$$\psi(x,t) = \mathrm{e}^{-\mathrm{i}\,\mu\,t}\, H_0^{\omega}(x)\,, \qquad \mu = \tfrac{1}{2} \sum_{j=1}^{3} \omega_j\,, \quad H_0^{\omega}(x) = \prod_{j=1}^{3} \sqrt[4]{\tfrac{\omega_j}{\pi}}\, \mathrm{e}^{-\frac{1}{2}\,\omega_j^2\, x_j^2}\,,$$

serving as a reliable reference solution. For the space discretization, we utilize fast Fourier transform (FFT) techniques, truncating the unbounded domain to the bounded domain $\Omega = [-8,8] \times [-8,8] \times [-8,8]$; due to the fact that

k	Δt	$\|\mathcal{L}(\Delta t)\,\psi_0\|_{L^2}$	$\kappa_{\mathcal{L}}$	$\kappa_{\mathcal{P}-\mathcal{L}}$
0	$1.0000 \cdot 10^{0}$	$1.7775 \cdot 10^{-1}$	3.02	3.77
1	$5.0000 \cdot 10^{-1}$	$2.1826 \cdot 10^{-2}$	3.00	3.94
2	$1.2500 \cdot 10^{-1}$	$3.3777 \cdot 10^{-4}$	3.00	3.99
3	$1.5625 \cdot 10^{-2}$	$6.5928 \cdot 10^{-7}$	3.00	3.99
4	$9.7656 \cdot 10^{-4}$	$1.6095 \cdot 10^{-10}$	—	—

Table 2: Local errors and associated orders for the Strang splitting method applied to the harmonic oscillator in 3D.

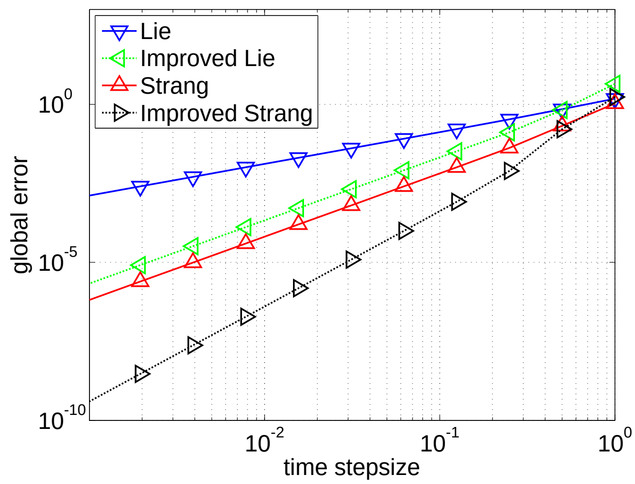

Figure 1: Global errors versus time stepsizes for the Lie–Trotter and Strang splitting methods and the improved approximations.

the exact solution remains localized, the effect from the artificial periodic boundary conditions is negligible. We use $M = 100$ equidistant grid points per spatial direction to suppress the influence of the spatial error. In Tables 1 and 2 we display the following quantities for the Lie–Trotter and Strang splitting methods.

- The local errors $\|\mathcal{L}(\Delta t)\,\psi_0\|_{L^2}$ for decreasing time stepsizes $\Delta t = 2^{-k}$, $k \geq 0$.

- The local orders $\kappa_{\mathcal{L}} \approx p + 1$, computed from the local errors associated with two successive time stepsizes, confirm the theoretical result $\mathcal{L}(\Delta t)\,\psi_0 = \mathcal{O}(\Delta t^{p+1})$ with $p = 1$ for the Lie–Trotter splitting method and with $p = 2$ for the Strang splitting method, see Theorems 1 and 2.

- The orders $\kappa_{\mathcal{P}-\mathcal{L}} \approx p+2$ associated with $\|(\mathcal{P}-\mathcal{L})(\Delta t)\,\psi_0\|_{L^2}$, confirming the theoretical result $(\mathcal{P} - \mathcal{L})(\Delta t)\,\psi_0 = \mathcal{O}(t^{p+2})$.

Periodic potential. As a further illustration, we include the global errors of the Lie–Trotter and Strang splitting methods when applied to the linear

Schrödinger equation (1) in two space dimensions subject to the periodic potential

$$V(x) = V(x_1, x_2) = 5 \left(\sin^2(\tfrac{\pi}{4} x_1) + \sin^2(\tfrac{\pi}{4} x_2) \right),$$

and the WKB-type initial condition

$$\psi_0(x) = \rho_0(x) \, \mathrm{e}^{\mathrm{i}\, \sigma_0(x)} \, , \quad \rho_0(x) = \mathrm{e}^{-(x_1^2 + x_2^2)} \, , \quad \sigma_0(x) = \ln \left(\mathrm{e}^{x_1 + x_2} + \mathrm{e}^{-(x_1 + x_2)} \right) .$$

As before, we use FFT techniques and perform the computation on the bounded domain $\Omega = [-8, 8] \times [-8, 8]$ with $M = 100$ equidistant grid points per spatial direction. The errors are computed with respect to a reference solution which was obtained by a fourth-order splitting scheme proposed in [13], applied with constant time stepsize $\Delta t = 2^{-11}$. It should be noted that any a posteriori local error estimator can also be used to improve the asymptotic quality of the numerical approximation by adding it to the basic solution. In our case, this results in approximations of convergence orders two and three for the Lie–Trotter and Strang splitting methods, respectively. For our numerical example, the global errors at the final time $T = 1$ are displayed in Figure 1, showing order one for the Lie–Trotter splitting method, order two for both the improved Lie–Trotter approximation and the Strang splitting method, and order three for the improved Strang approximation.

6. Conclusions

In this paper we have introduced a posteriori local error estimators based on the defect correction principle for time-splitting methods and analyzed applications to linear evolution equations of Schrödinger type. We have proven that our a posteriori local error estimators for the Lie–Trotter and Strang splitting methods are asymptotically correct, that is, the error of the error estimator as compared to the exact local error asymptotically tends to zero faster than the error itself. The respective bounds depend on certain iterated commutators of the involved operators, which translates to regularity assumptions on the exact solution of the Schrödinger equation. Besides, we recover the expected a priori local and global error bounds for the Lie–Trotter and Strang splitting methods. We have confirmed our theoretical results by numerical illustrations for time-dependent linear Schrödinger equations. Further numerical experiments given in [14] demonstrate that our local error estimators can indeed serve as the basis for efficient adaptive time-stepping.

We have focussed on the linear case in this paper, as the construction and analysis of the error estimators is technically even more involved in the nonlinear case and requires to resort to the technique of Lie derivatives. Thus, in the nonlinear case, the construction of the defect and neighboring problem is not a straightforward extension of the linear case. This will be addressed in future work on nonlinear Schrödinger-type equations such as Gross–Pitaevskii systems or systems resulting from model reductions of the linear multi-particle Schrödinger equation like the multi-configuration Hartree-Fock method or time–dependent density functional theory.

Extension to higher-order splitting schemes was not considered in this paper to keep the presentation focussed on the main ideas. Higher-order splitting methods for an evolution equation involving the two operators A, B are based on compositions of subflows $\mathrm{e}^{tb_j B}, \mathrm{e}^{ta_j A}$ with suitably chosen coefficients a_j, b_j. The extension of the present approach can be carried out by systematically combining defect terms associated with these subflows to represent the defect of the overall splitting operator. Moreover, appropriate higher-order quadrature will find employment in the construction of the associated error estimators.

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