Lecture 10

Operator Splitting

In many applications the combined effect of several physical (or chemical, etc.) phenomena is modelled. In these cases one has to solve a partial differential equation where the local time derivative of the modelled physical quantity equals the sum of several operators, describing how this quantity behaves in space. The idea behind operator splitting procedures is that, instead of the sum, we treat each spatial operator separately, i.e., we solve all the corresponding sub-problems. The solution of the original problem is then obtained from the solutions of the sub-problems. Since the sum usually contains operators of different nature, each corresponding to one physical phenomenon, the sub-problems may be easier to solve separately.

Consider the abstract Cauchy problem on the Banach space X of the form

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}u(t) = (A+B)u(t), \qquad t>0 \\ u(0) = u_0 \end{cases} \tag{10.1}$$

with densely defined, closed, and linear operators A and B. Throughout the lecture we suppose that $D := D(A) \cap D(B)$ is dense in X and $u_0 \in D$.

As an example, we explain how the simplest operator splitting procedure works. The main idea is to choose sub-problems which are easier to handle as the original problem. This can happen if there are particularly well-suited (fast, accurate, reliable, etc.) numerical methods to solve the sub-problems, or if the exact (analytical) solution of at least one of the sub-problems is known. First, one solves the sub-problem corresponding to the operator A on the time interval $[0,h]$ using the original initial value u_0. Then the second sub-problem, corresponding to the operator B, is solved on the same time interval but using the solution of the previous step as initial value. In the next step the sub-problems with A and B are solved on the next time interval $[h,2h]$, always taking the previous solution as initial value. We repeat this procedure recursively. The corresponding sub-problems can be formulated for $t \in ((k-1)h, kh]$ with $k \in \mathbb{N}$ and $u_{\mathrm{spl},h}(0) = u_0$ as follows:

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}u_A(t) = Au_A(t) \\ u_A((k-1)h) = u_{\mathrm{spl},h}((k-1)h) \end{cases} \quad \text{and} \quad \begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}u_B(t) = Bu_B(t) \\ u_B((k-1)h) = u_A(kh) \end{cases}$$

and we set $u_{\mathrm{spl},h}(kh) = u_B(kh)$.

Operator splittings can be mathematically handled in the same way as finite difference schemes, which were introduced in Definition 4.1, with the help of a strongly continuous function $F : [0,\infty) \to \mathscr{L}(X)$. By applying operator splitting, one computes the numerical solution at time $t > 0$ (more precisely, a sequence of numerical solutions) to problem (10.1) of the form

$$u_{\mathrm{spl},h}(t) = \left(F(\tfrac{t}{n})\right)^n u_0$$

with $h = \frac{t}{n}$ and $n \in \mathbb{N}$. Our aim is to establish splitting procedures being convergent in the sense

$$u(t) = \lim_{n\to\infty} u_{\mathrm{spl},h}(t) = \lim_{n\to\infty} \left(F(\tfrac{t}{n})\right)^n u_0$$

for all (or at least for many) $u_0 \in D$, for all $t \geq 0$. As usual, we set $nh = t$.

There are several splitting procedures in the literature. We collect here the most important ones which are often used in applications as well.

Definition 10.1. The **split solution** to problem (10.1) at time $t > 0$ is defined by

$$u_{\mathrm{spl},h}(t) = (F(h))^n \, u_0$$

for all $u_0 \in D$ and $n \in \mathbb{N}$ with $nh = t$. For the different operator splitting procedures, the strongly continuous function $F : [0, \infty) \to \mathscr{L}(X)$ is formally defined for all $h > 0$ as

Sequential splitting: $F_{\mathrm{seq}}(h) = \mathrm{e}^{hB}\mathrm{e}^{hA}$,

Marchuk–Strang splitting: $F_{\mathrm{MS}}(h) = \mathrm{e}^{\frac{h}{2}A}\mathrm{e}^{hB}\mathrm{e}^{\frac{h}{2}A}$,

Lie splitting: $F_{\mathrm{Lie}}(h) = \big(I - hB\big)^{-1}\big(I - hA\big)^{-1}$,

Peaceman–Rachford splitting: $F_{\mathrm{PR}}(h) = \big(I - \frac{h}{2}A\big)^{-1}\big(I + \frac{h}{2}B\big)\big(I - \frac{h}{2}B\big)^{-1}\big(I + \frac{h}{2}A\big)$.

Of course, due to the application of operator splitting, there appears a certain **splitting error** in the split solution.

In this chapter we show the convergence of the operator splitting procedures defined above, and we also derive some error bounds for their **local error**

$$\mathscr{E}_{u_0}\big(h, u(t)\big) = \mathscr{E}\big(h, u(t)\big) := \|F(h)u(t) - u(t+h)\|,$$

where the exact solution of problem (10.1) is $u(t) = \mathrm{e}^{t(A+B)}u_0$. Hence, the local error can be further rewritten as

$$\mathscr{E}\big(h, u(t)\big) = \big\|F(h)u(t) - \mathrm{e}^{(t+h)(A+B)}u_0\big\| = \big\|F(h)u(t) - \mathrm{e}^{h(A+B)}u(t)\big\|.$$

In order to obtain convergence and some error bounds, we have to investigate the difference $F(h) - \mathrm{e}^{h(A+B)}$. For the sequential splitting[1] this means $\mathrm{e}^{hB}\mathrm{e}^{hA} - \mathrm{e}^{h(A+B)}$ which in general differs from zero (unless $A, B \in \mathbb{C}$).

For simplicity we start with A and B being matrices.

10.1 Matrix case

Consider the problem (10.1) with operators $A, B \in \mathscr{L}(\mathbb{C}^d)$, which corresponds to a linear system of ordinary differential equations.
The exponential function of the matrices A, B can be formulated as power series, and the local error is then defined as

$$\mathscr{E}\big(h, u(t)\big) = \big\|\big(F(h) - \mathrm{e}^{h(A+B)}\big)u(t)\big\|.$$

We start with the investigation of the sequential splitting.

Proposition 10.2. *Consider the operators $A, B \in \mathscr{L}(\mathbb{C}^d)$. If they commute, i.e. $[A, B] := AB - BA = 0$, then the local error of the sequential splitting vanishes.*

[1] Sometimes is called as Lie–Trotter product formula, see Theorem 10.6.

The proof is left as Exercise 2.

In the next step we will prove the convergence of the sequential splitting for general, non-commuting operators.

Theorem 10.3. *The sequential splitting is first-order convergent for $A, B \in \mathscr{L}(\mathbb{C}^d)$.*

Proof. By the Lax equivalence theorem, Theorem 4.6, it is sufficient to show consistency and stability from Definition 4.1, for $t < t_0$. To prove the consistency, we first consider the local error

$$\begin{aligned}\mathscr{E}_{\mathrm{seq}}(t,h) &= \|F(h)u(h) - u(t+h)\| = \big\|\mathrm{e}^{hB}\mathrm{e}^{hA}u(t) - \mathrm{e}^{h(A+B)}u(t)\big\| \\ &\le \big\|\mathrm{e}^{hB}\mathrm{e}^{hA} - \mathrm{e}^{h(A+B)}\big\| \cdot \|u(t)\|.\end{aligned}$$

The local error can be expressed by the power series of the corresponding exponential functions (see also Exercise 1):

$$\begin{aligned}\mathscr{E}_{\mathrm{seq}}(t,h) &\le \|(I + hB + \tfrac{h^2}{2}B^2 + \dots)(I + hA + \tfrac{h^2}{2}A^2 + \dots) \\ &\quad - (I + h(A+B) + \tfrac{h^2}{2}(A+B)^2 + \dots)\| \cdot \|u(t)\| \\ &= \tfrac{h^2}{2}\|(AB - BA) + \dots\| \cdot \|u(t)\| \le \tfrac{h^2}{2}\|[A,B]\| \cdot \|u(t)\| + \mathcal{O}(h^3). \qquad (10.2)\end{aligned}$$

From this estimate consistency follows, since $\frac{1}{h}\mathscr{E}\big(h, u(t)\big) \to 0$ as $h \searrow 0$. We note that from the considerations above, we also conclude that the sequential splitting is of first order.

To show stability, we have to ensure the existence of a constant $M > 0$ such that $\big\|F_{\mathrm{seq}}(\frac{t}{n})^n\big\| \le M$ for all fixed $t < t_0$ and for all $n \in \mathbb{N}$. Since $t < t_0$, the boundedness of A and B implies that

$$\begin{aligned}\big\|F_{\mathrm{seq}}(\tfrac{t}{n})^n\big\| &\le \big\|F_{\mathrm{seq}}(\tfrac{t}{n})\big\|^n = \big\|\mathrm{e}^{\frac{t}{n}B}\mathrm{e}^{\frac{t}{n}A}\big\|^n \le \big\|\mathrm{e}^{\frac{t}{n}B}\big\|^n \cdot \big\|\mathrm{e}^{\frac{t}{n}A}\big\|^n \\ &\le \big(\mathrm{e}^{\frac{t}{n}\|B\|}\big)^n \cdot \big(\mathrm{e}^{\frac{t}{n}\|A\|}\big)^n = \mathrm{e}^{t\|B\|}\mathrm{e}^{t\|A\|} \le \mathrm{e}^{t_0\|B\|}\mathrm{e}^{t_0\|A\|} = \mathrm{e}^{t_0(\|A\|+\|B\|)} \le M.\end{aligned}$$ □

One can investigate the convergence of the Marchuk–Strang splitting analogously.

Proposition 10.4. *The Marchuk–Strang splitting is of second order for $A, B \in \mathscr{L}(\mathbb{C}^d)$.*

The proof is left as Exercise 3.

We see that in general the behaviour of the commutator of the operators A and B is of enormous importance for these results and also for the investigation of higher order splitting formulae. Here the Baker–Campbell–Hausdorff formula comes to help.[2]

Theorem 10.5 (Baker–Campbell–Hausdorff Formula)**.** *For $A, B \in \mathscr{L}(\mathbb{C}^d)$ and $h \in \mathbb{R}$ we have*

$$\mathrm{e}^{hB}\mathrm{e}^{hA} = \mathrm{e}^{h(A+B)+\Phi(A,B)}$$

with

$$\Phi(A,B) = \tfrac{h^2}{2}[A,B] + \tfrac{h^3}{12}[A-B,[A,B]] - \tfrac{h^4}{24}[B,[A,[A,B]]] + \dots$$

where $[A,B] = AB - BA$ denotes the commutator of A and B (appearing in all terms of the infinite sum above).

For a thorough investigation of operator splitting procedures in the context of matrices, we refer to the monograph by Faragó and Havasi,[3] or to the above cited monograph by Hairer, Lubich and Wanner.

Note that all the above considerations only make sense if $h\|A\|$ and $h\|B\|$ are small, otherwise the large constants will make the convergence very slow. This means that we need other approaches for unbounded operators, or even for matrices coming from discretisation of unbounded operators. One possible approach is presented in the following section.

[2] E. Hairer, Ch. Lubich, and G. Wanner, Geometric Numerical Integration, Springer-Verlag, 2008, Chapter III. 4.

[3] I. Faragó, Á. Havasi, Operator Splittings and their Applications, Mathematics Research Developments, Nova Science Publishers, New York, 2009.

10.2 Exponential splittings

In this section we suppose that the operators A and B are the generators of strongly continuous semigroups on the Banach space X. For the sake of better understanding (since there will be more operators and the corresponding semigroups), we will use the notation $(\mathrm{e}^{tA})_{t\geq 0}$ for the semigroup generated by the operator A, and similarly for the other operators. Therefore, the splittings schemes have the same forms as in Definition 10.1. First we investigate the sequential and Marchuk–Strang splittings.

Under the condition that the operator $A+B$ with the domain $D := D(A)\cap D(B)$ is the generator of a strongly continuous semigroup, the convergence of the sequential splitting was already shown in Corollary 4.10. Since the proof is essentially the same if $A+B$ is not a generator, but its closure, we only state the theorem here. Note that the assertion follows from Chernoff's Theorem, Theorem **??**, applied to the operator F_{seq} defined above (see Exercise 4 as well).

Theorem 10.6 (Lie–Trotter Product Formula[4])**.** *Suppose that the operators A and B are the generators of strongly continuous semigroups. Suppose further that there exist constants $M \geq 1$ and $\omega \in \mathbb{R}$ such that*

$$\left\| \left(\mathrm{e}^{\frac{t}{n}B}\mathrm{e}^{\frac{t}{n}A} \right)^n \right\| \leq M\mathrm{e}^{\omega t} \tag{10.3}$$

holds for all $t \geq 0$ and $n \in \mathbb{N}$. Consider the sum $A + B$ on $D = D(A) \cap D(B)$, and assume that D and $\big(\lambda_0 - (A + B)\big)D$ are dense in X for some $\lambda_0 > \omega$. Then $C = \overline{A + B}$ generates a strongly continuous semigroup given by the sequential splitting, i.e.,

$$\mathrm{e}^{tC}u_0 = \lim_{n\to\infty} \left(\mathrm{e}^{\frac{t}{n}B}\mathrm{e}^{\frac{t}{n}A} \right)^n u_0$$

holds for all $u_0 \in X$ uniformly for t in compact intervals.

Although the theorem above ensures the convergence of the sequential splitting under rather weak conditions, it does not tell us anything about the convergence rate. To obtain certain error bounds, the sum $A+B$ with domain $D = D(A)\cap D(B)$ needs to be a generator as well. This leads to stronger conditions on the operators A and B.

We show the first-order convergence of the sequential splitting following the idea which was presented by Jahnke and Lubich for the Marchuk–Strang splitting.[5] To this end, we need some assumptions.

Assumption 10.7. Suppose that A generates a strongly continuous semigroup on the Banach space X, and let $B \in \mathscr{L}(X)$. Suppose further that there exist a subspace Y such that

$$D(A) \hookrightarrow Y \hookrightarrow X$$

with dense and continuous embeddings. We also assume that $D(A)$ is invariant under the operator B, and that Y is invariant under the semigroup $(\mathrm{e}^{tA})_{t\geq 0}$.

Note that this means in particular that there are constants K_1 and K_2 such that

$$\begin{aligned} \|f\|_Y &\leq K_1\|f\|_A \quad &&\text{holds for all } f \in D(A), \text{ and} \\ \|f\| &\leq K_2\|f\|_Y \quad &&\text{holds for all } f \in Y. \end{aligned}$$

[4]H. F. Trotter, "On the product of semi-groups of operators," Proc. Amer. Math. Soc. **10** (1959), 545–551.
[5]T. Jahnke and Ch. Lubich, "Error bounds for exponential operator splittings," BIT **40** (2000), 735–744.

We have already seen in the matrix case that the commutator of A and B plays an important role, when seeking an error bound. It motivates us to define it properly also for A, B being generators, and to bound it on an appropriate subspace. For $B \in \mathscr{L}(X)$ the commutator

$$[A, B]f = ABf - BAf$$

is only defined on $D(A)$. However, in some cases we may be able to extend this estimate for all $f \in Y$ for the subspace Y satisfying Assumption 10.7.

Assumption 10.8. Suppose that A generates a strongly continuous semigroup on the Banach space X, and that $B \in \mathscr{L}(X)$. Further suppose that there exists a constant $c_1 \geq 0$ such that

$$\|[A, B]f\| \leq c_1 \|f\|_Y \tag{10.4}$$

holds for all $f \in D(A)$ with Y being the appropriate subspace such as in Assumption 10.7.

Note that in this case the operator $[A, B]$ extends continuously to the entire space Y.

Example 10.9. Suppose that A generates a strongly continuous semigroup on the Banach space X, and let $B \in \mathscr{L}(X)$. Suppose further that there exist constants $\alpha \in (0, 1)$ and $c_1 \geq 0$ such that

$$\|[A, B]f\| \leq c_1 \|(-A)^\alpha f\|$$

holds for all $f \in D(A)$. Then the subspace $Y = D\big((-A)^\alpha\big)$ possesses all the properties listed in Assumption 10.7, see Lecture 7.

Now we are able to state the first-order convergence of the sequential splitting.

Theorem 10.10. *Consider operators A, B and a subspace Y satisfying Assumption 10.7. Under Assumption 10.8 the sequential splitting is first-order convergent.*

Proof. Let $h \in (0, t_0]$. By applying Proposition 4.12, it is sufficient to show the stability and the first-order consistency. Since A is a generator and B is bounded, by Exercise 5.5 the sum $A + B$ with domain $D(A)$ generates a semigroup. After applying the renorming procedure (see Exercise C.4) and shifting the generators in the appropriate way, we may assume that A, B, and $A + B$ generate contraction semigroups, that is, for all $t \geq 0$ we have

$$\big\|\mathrm{e}^{tA}\big\| \leq 1, \quad \big\|\mathrm{e}^{tB}\big\| \leq 1, \quad \text{and} \quad \big\|\mathrm{e}^{t(A+B)}\big\| \leq 1. \tag{10.5}$$

In particular, for $t < t_0$ this proves the stability of F_{seq}. Note that although the rescaling does not effect the order of convergence, it may modify the constants appearing in the estimates and it may have effect how small the time step h has to be chosen.

To show the first-order consistency (see Definition 4.11), we have to ensure the existence of a constant M, depending on c_1 and $\|B\|$, such that for all $f \in D(A) \subset Y$ we have

$$\mathscr{E}_{\mathrm{seq}}(h, f) = \big\|F_{\mathrm{seq}}(h)f - \mathrm{e}^{h(A+B)}f\big\| \leq Mh^2 \|f\|_Y. \tag{10.6}$$

Taylor's Formula from Exercise C.2 implies

$$\mathrm{e}^{hB}g = g + hBg + \int_0^h (h - s)B^2 \mathrm{e}^{sB} g \,\mathrm{d}s$$

for all $g \in X$. In particular, for $g = \mathrm{e}^{hA} f$ we have

$$\mathrm{e}^{hB}\mathrm{e}^{hA} f = \mathrm{e}^{hA} f + hB\mathrm{e}^{hA} f + \int_0^h (h-s) B^2 \mathrm{e}^{sB}\mathrm{e}^{hA} f \,\mathrm{d}s. \tag{10.7}$$

On the other hand, note that the solution of the initial value problem $\frac{\mathrm{d}}{\mathrm{d}t} v(t) = (A+B)v(t)$, $v(0) = v_0$, can be expressed by the variation-of-constants formula as

$$v(h) = \mathrm{e}^{hA} v_0 + \int_0^h \mathrm{e}^{(h-s)A} B v(s) \,\mathrm{d}s,$$

which implies

$$\mathrm{e}^{h(A+B)} f = \mathrm{e}^{hA} f + \int_0^h \mathrm{e}^{(h-s)A} B \mathrm{e}^{s(A+B)} f \,\mathrm{d}s.$$

Using the variation-of-constants formula for the term $v(s) = B\mathrm{e}^{s(A+B)} f$ once again, we obtain

$$\mathrm{e}^{h(A+B)} f = \mathrm{e}^{hA} f + \int_0^h \mathrm{e}^{(h-s)A} B \mathrm{e}^{sA} f \,\mathrm{d}s + \int_0^h \mathrm{e}^{(h-s)A} B \Big(\int_0^s \mathrm{e}^{(s-r)A} B \mathrm{e}^{r(A+B)} f \,\mathrm{d}r \Big) \mathrm{d}s. \tag{10.8}$$

Subtracting (10.7) from (10.8), the local error can be written as

$$\begin{aligned} \mathscr{E}_{\mathrm{seq}}(h, f) &= \big\| \mathrm{e}^{hB}\mathrm{e}^{hA} f - \mathrm{e}^{h(A+B)} f \big\| \\ &\le \Big\| hB\mathrm{e}^{hA} f - \int_0^h \mathrm{e}^{(h-s)A} B \mathrm{e}^{sA} f \,\mathrm{d}s \Big\| + \|(R_1 - R_2) f\| \end{aligned} \tag{10.9}$$

with
$$R_1 f = \int_0^h (h-s) B^2 \mathrm{e}^{sB}\mathrm{e}^{hA} f \,\mathrm{d}s$$

and
$$R_2 f = \int_0^h \mathrm{e}^{(h-s)A} B \Big(\int_0^s \mathrm{e}^{(s-r)A} B \mathrm{e}^{r(A+B)} f \,\mathrm{d}r \Big) \mathrm{d}s.$$

For a continuously differentiable function $\eta : \mathbb{R} \to X$, the fundamental theorem of calculus implies that

$$\eta(s) = \eta(h) + \int_h^s \eta'(r) \,\mathrm{d}r,$$

and therefore

$$h\eta(h) - \int_0^h \eta(s) \,\mathrm{d}s = h\eta(h) - \int_0^h \eta(h) \,\mathrm{d}s - \int_0^h \Big(\int_h^s \eta'(r) \,\mathrm{d}r \Big) \mathrm{d}s = \int_0^h \Big(\int_s^h \eta'(r) \,\mathrm{d}r \Big) \mathrm{d}s. \tag{10.10}$$

We note that this corresponds to the error of the a first-order quadrature rule (the right rectangular rule). In particular, for

$$\eta(s) = \mathrm{e}^{(h-s)A} B \mathrm{e}^{sA} f,$$

being continuously differentiable because $D(A)$ is invariant under B, we have

$$h\eta(h) - \int_0^h \eta(s)\mathrm{d}s = hB\mathrm{e}^{hA}f - \int_0^h \mathrm{e}^{(h-s)A}B\mathrm{e}^{sA}f\mathrm{d}s$$

being exactly the first term in (10.9) to be estimated. For this special choice of η we obtain

$$\begin{aligned}\eta'(s) &= \mathrm{e}^{(h-s)A}(-A)B\mathrm{e}^{sA}f + \mathrm{e}^{(h-s)A}BA\mathrm{e}^{sA}f\\ &= -\mathrm{e}^{(h-s)A}(AB-BA)\mathrm{e}^{sA}f = -\mathrm{e}^{(h-s)A}[A,B]\mathrm{e}^{sA}f,\end{aligned}$$

and

$$\|\eta'(s)\| \le \big\|\mathrm{e}^{(h-s)A}\big\| \cdot \big\|[A,B]\mathrm{e}^{sA}f\big\| \le c_1\|\mathrm{e}^{sA}f\|_Y = c\big\|\mathrm{e}^{sA}\big\|_Y\big\|f\big\|_Y,$$

where we used condition (10.4) for $\mathrm{e}^{sA}f \in Y$. Formula (10.10) implies the estimate for the first term in (10.9):

$$\begin{aligned}\Big\|hB\mathrm{e}^{hA}f - \int_0^h \mathrm{e}^{(h-s)A}B\mathrm{e}^{sA}f\mathrm{d}s\Big\| &\le \int_0^h \Big(\int_s^h \big\|\eta'(r)\big\|\,\mathrm{d}r\Big)\mathrm{d}s \qquad (10.11)\\ &\le \int_0^h \Big(\int_s^h c\big\|\mathrm{e}^{sA}\big\|_Y\|f\|_Y\mathrm{d}r\Big)\mathrm{d}s \le K\cdot h^2\mathrm{e}^{\omega h}\|f\|_Y \le K'\cdot h^2\|f\|_Y,\end{aligned}$$

for some constant $K' \ge 0$, where we used $h \le t_0$ in the last step. For the second term in (10.9) we have the rough estimate $\|(R_1-R_2)f\| \le \|R_1f\| + \|R_2f\|$ with

$$\begin{aligned}\|R_1f\| &= \Big\|\int_0^h (h-s)B^2\mathrm{e}^{sB}\mathrm{e}^{hA}f\mathrm{d}s\Big\| \le \int_0^h (h-s)\|B^2\|\cdot\big\|\mathrm{e}^{sB}\big\|\cdot\big\|\mathrm{e}^{hA}\big\|\cdot\|f\|\mathrm{d}s\\ &\le \frac{h^2}{2}\|B\|^2\cdot\|f\| \qquad (10.12)\end{aligned}$$

and

$$\begin{aligned}\|R_2f\| &= \Big\|\int_0^h \mathrm{e}^{(h-s)A}B\Big(\int_0^s \mathrm{e}^{(s-r)A}B\mathrm{e}^{r(A+B)}f\mathrm{d}r\Big)\mathrm{d}s\Big\|\\ &\le \int_0^h \big\|\mathrm{e}^{(h-s)A}\big\|\cdot\|B\|\Big(\int_0^s \big\|\mathrm{e}^{(s-r)A}\big\|\cdot\|B\|\cdot\big\|\mathrm{e}^{r(A+B)}\big\|\cdot\|f\|\mathrm{d}r\Big)\mathrm{d}s\\ &\le \frac{h^2}{2}\|B\|^2\cdot\|f\|. \qquad (10.13)\end{aligned}$$

Estimates (10.11), (10.12), and (10.13) imply the desired error bound for (10.9) with an appropriate constant M depending on c_1 and $\|B\|$. □

If operator A generates an analytic semigroup of type $(0,\omega)$ with $\omega < 0$, even stronger estimates hold, requiring bounds only on the norm of the initial value u_0. Recall that in this case there is a constant $M > 0$ so that the estimates

$$\big\|A\mathrm{e}^{tA}\big\| \le \frac{M}{t}, \quad \big\|(A+B)\mathrm{e}^{t(A+B)}\big\| \le \frac{M}{t}, \quad \text{and hence } \big\|A\mathrm{e}^{t(A+B)}\big\| \le \frac{M}{t} \qquad (10.14)$$

hold for all $t > 0$, see Corollary 9.22.

Theorem 10.11. *Suppose that A generates an analytic semigroup of type $(1,\omega)$ with $\omega < 0$ on the Banach space X, and $B \in \mathscr{L}(X)$. Suppose further that Assumptions 10.7 and 10.8 hold with $Y = D\big((-A)^\alpha\big)$ for some $\alpha \in (0,1)$, i.e.,*

$$\|[A,B]f\| \le c\|(-A)^\alpha f\| \quad \text{holds for all } f \in D(A).$$

Then the global error of the sequential splitting is bounded by

$$\|u_{\mathrm{seq},h}(nh) - u(nh)\| \le hM_0 \log(n)\|u_0\|,$$

for all $u_0 \in X$ and $n > 1$, $n \in \mathbb{N}$, $h \ge 0$, $nh \in [0,t_0]$. In particular, the sequential splitting converges in the operator norm like $\frac{\log n}{n}$.

Proof. As before, we assume that all occurring semigroups are contraction semigroups. Applying the telescopic identity, the global error can be written with the help of the local error as

$$\begin{aligned}
\|u_{\mathrm{seq},h}(nh) - u(nh)\| &= \big\|F_{\mathrm{seq}}(h)^n u_0 - \mathrm{e}^{nh(A+B)}u_0\big\| \\
&= \Big\|\sum_{j=0}^{n-1} F_{\mathrm{seq}}(h)^{n-j-1}\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)\mathrm{e}^{jh(A+B)}u_0\Big\| \\
&\le \sum_{j=0}^{n-1} \|F_{\mathrm{seq}}(h)\|^{n-j-1} \cdot \big\|\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)\mathrm{e}^{jh(A+B)}u_0\big\| \\
&\le \quad \|F_{\mathrm{seq}}(h)\|^{n-1}\big\|\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)u_0\big\| \\
&\quad + \sum_{j=1}^{n-1} \|F_{\mathrm{seq}}(h)\|^{n-j-1}\big\|\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)A^{-1}\big\| \cdot \big\|A\mathrm{e}^{jh(A+B)}u_0\big\|
\end{aligned}$$

for all $u_0 \in D(A)$. Since $\|F_{\mathrm{seq}}(h)\| \le 1$, we obtain

$$\begin{aligned}
\|u_{\mathrm{seq},h}(nh) - u(nh)\| \le{}& \big\|\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)u_0\big\| \\
&+ \sum_{j=1}^{n-1} \big\|\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)A^{-1}\big\| \cdot \big\|A\mathrm{e}^{jh(A+B)}u_0\big\|. \qquad (10.15)
\end{aligned}$$

Since $A + B$ generates an analytic semigroup, we have

$$\big\|A\mathrm{e}^{jh(A+B)}\big\| \le \frac{M}{jh}$$

for all $j = 1, \ldots, n$. For $g \in X$ we have $A^{-1}g \in D(A) \hookrightarrow D((-A)^\alpha)$, and hence

$$\big\|\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)A^{-1}g\big\| \le h^2 C\|A^{-1}g\|_{(-A)^\alpha} \le h^2 C'\|g\|.$$

Hence, for the second term in (10.15) we obtain

$$\sum_{j=1}^{n-1} \big\|\big(F_{\mathrm{seq}}(h) - \mathrm{e}^{h(A+B)}\big)A^{-1}\big\| \cdot \big\|A\mathrm{e}^{jh(A+B)}u_0\big\| \le \sum_{j=1}^{n-1} h^2 C'\frac{M}{jh} \le hC'' \log(n).$$

Consider now the case $j = 0$, that is, the first term in (10.15). To this end, we have to estimate the operator norm of the local error. By (10.9), we have

$$\mathscr{E}_{\mathrm{seq}}(h, f) \le \Big\| hB\mathrm{e}^{hA}u_0 - \int_0^h \mathrm{e}^{(h-s)A}B\mathrm{e}^{sA}u_0\mathrm{d}s \Big\| + \|(R_1 - R_2)u_0\| .$$

Note that by (10.12) and (10.13) the inequality

$$\|(R_1 - R_2)\| \le \|R_1\| + \|R_2\| \le h^2\|B\|^2.$$

holds. We conclude by means of (10.11) that

$$\begin{aligned}
\Big\| hB\mathrm{e}^{hA}u_0 - \int_0^h \mathrm{e}^{(h-s)A}B\mathrm{e}^{sA}u_0\mathrm{d}s \Big\| &\le \int_0^h \Big(\int_s^h \Big\| \mathrm{e}^{(h-r)A}[A,B]\mathrm{e}^{rA}u_0 \Big\| \,\mathrm{d}r \Big) \mathrm{d}s \\
&\le \int_0^h \Big(\int_s^h \Big\| \mathrm{e}^{(h-r)A}[A,B](-A)^{-\alpha}(-A)^{\alpha}\mathrm{e}^{rA}u_0 \Big\| \,\mathrm{d}r \Big) \mathrm{d}s \\
&\le \int_0^h \Big(\int_s^h \Big\| \mathrm{e}^{(h-r)A}[A,B](-A)^{-\alpha} \Big\| \cdot \|(-A)^{\alpha}\mathrm{e}^{rA}u_0\| \,\mathrm{d}r \Big) \mathrm{d}s,
\end{aligned}$$

where by Assumption 10.8 we have $[A, B](-A)^{-\alpha} \in \mathscr{L}(X)$. By using Corollary 9.22, we obtain that

$$\begin{aligned}
\Big\| hB\mathrm{e}^{hA}u_0 - \int_0^h \mathrm{e}^{(h-s)A}B\mathrm{e}^{sA}u_0\mathrm{d}s \Big\| &\le \|[A,B](-A)^{-\alpha}\| \int_0^h \int_s^h \big\|(-A)^{\alpha}\mathrm{e}^{rA}u_0\big\| \,\mathrm{d}r\mathrm{d}s \\
&\le K \int_0^h \int_s^h \frac{1}{r^{\alpha}} \mathrm{d}r\mathrm{d}s\|u_0\| \le K' h^{2-\alpha}\|u_0\|.
\end{aligned}$$

Putting the pieces together we arrive at

$$\|u_{\mathrm{seq},h}(nh) - u(nh)\| \le K'h^{2-\alpha}\|u_0\| + hC'' \log(n)\|u_0\| \le M_0 h \log(n)\|u_0\|. \qquad \square$$

The following two results of Jahnke and Lubich about the Marchuk–Strang splitting can be proved by a slightly more detailed analysis, we postpone the proofs to the project phase.

Theorem 10.12. *Suppose that A generates a semigroup of type $(1, \omega)$ with $\omega < 0$ on the Banach space X, and $B \in \mathscr{L}(X)$. Suppose further that Assumptions 10.7 and 10.8 hold with $Y = D((-A)^{\alpha})$ for some $\alpha \in (0, 1)$, i.e.,*

$$\|[A, B]f\| \le c\|(-A)^{\alpha}f\| \quad \text{holds for all } f \in D(A). \tag{10.16}$$

Then the Marchuk–Strang splitting is first-order convergent on $D((-A)^{\alpha})$. If in addition there exist constants $c_2 \ge 0$ and $1 \le \beta \le 2$ such that

$$\|[A, [A, B]]g\| \le c_2\big\|(-A)^{\beta}g\big\| \tag{10.17}$$

holds for all $g \in D(A^2)$, then the Marchuk–Strang splitting is convergent of second order on $D((-A)^{\beta})$.

Theorem 10.13. *Suppose that A generates an analytic semigroup on the Banach space X, and $B \in \mathscr{L}(X)$. Suppose further that B leaves $D(A)$ invariant and that conditions* (10.17) *and* (10.16) *hold for all $f, g \in D(A^2)$ with $c_1, c_2 \geq 0$, $\alpha \leq 1$, and $\beta = 1$. Then the global error of the Marchuk–Strang splitting is bounded by*

$$\|u_{\mathrm{MS},h}(nh) - u(nh)\| \leq h^2 M_0 \log(n) \|u_0\|$$

for all $u_0 \in X$.

10.3 Example

Consider the m-dimensional Schrödinger equation on $\Omega = (-\pi, \pi)^m$:

$$\begin{cases} \partial_t w(t,x) = \mathrm{i}\Delta w(t,x) - \mathrm{i}V(x)w(t,x), & x \in \Omega,\ t > 0 \\ w(0,x) = w_0(x), & x \in \Omega \end{cases} \tag{10.18}$$

with periodic boundary conditions, some given initial function w_0, and a C^4 potential $V : \mathbb{R}^m \to \mathbb{C}$ being 2π-periodic in every coordinate direction, and transform the equation to an abstract Cauchy problem in $\mathrm{L}^2(\Omega)$.

Let

$$\mathrm{C}^\infty_{\mathrm{per}}(\Omega) := \bigl\{ f \in \mathrm{C}^\infty(\mathbb{R}^m) : f \text{ is } 2\pi\text{-periodic in each coordinate direction} \bigr\},$$

and for $f \in \mathrm{C}^\infty_{\mathrm{per}}(\Omega)$ we define

$$\|f\|^2_{\mathrm{H}^1(\Omega)} := \|f\|^2_{\mathrm{L}^2(\Omega)} + \|\partial_1 f\|^2_{\mathrm{L}^2(\Omega)} + \cdots + \|\partial_m f\|^2_{\mathrm{L}^2(\Omega)}$$

$$\|f\|^2_{\mathrm{H}^2(\Omega)} := \|f\|^2_{\mathrm{L}^2(\Omega)} + \|\partial_1 f\|^2_{\mathrm{L}^2(\Omega)} + \cdots + \|\partial_m f\|^2_{\mathrm{L}^2(\Omega)} + \sum_{i,j=1}^m \|\partial_i \partial_j f\|^2_{\mathrm{L}^2(\Omega)}.$$

The completion of

$$\bigl\{ f|_\Omega : f \in \mathrm{C}^\infty_{\mathrm{per}}(\Omega) \bigr\}$$

with respect to the norms $\|\cdot\|_{\mathrm{H}^1(\Omega)}$ and $\|\cdot\|_{\mathrm{H}^2(\Omega)}$ is denoted by $\mathrm{H}^1_{\mathrm{per}}(\Omega)$ and $\mathrm{H}^2_{\mathrm{per}}(\Omega)$, respectively. Both are Banach spaces for the respective norms.

Now we split the operator C according to the different physical phenomena:

$$A = \mathrm{i}\Delta \qquad \text{and} \quad B = -M_{\mathrm{i}V}$$

with the corresponding domains

$$D(A) = \mathrm{H}^2_{\mathrm{per}}(\Omega)$$

and

$$D(B) = \mathrm{L}^2(\Omega).$$

Of course, since V is a bounded function, the multiplication operator $M_{\mathrm{i}V}$ is bounded on L^2. By using the Lumer–Phillips theorem, Theorem 6.3, one can show that $\mathrm{i}\Delta$ generates a contraction semigroup T on $\mathrm{L}^2(\Omega)$ (and, since $-\mathrm{i}\Delta$ does this, too, the semigroup operators are invertible, in fact they are unitary). By assumption B leaves $D(A)$ invariant.

In order to prove the first-order convergence of sequential splitting and the second-order convergence of Marchuk–Strang splitting, we have to verify the assumptions of Theorems 10.10 and 10.12, respectively. It remains to bound the norm of the commutators $[A, B]$ and $[A, [A, B]]$ on appropriate subspaces. To get an idea how to choose the subspaces, we *formally* compute the commutators:

$$[A, B]f = ABf - BAf = \Delta(Vf) - V(\Delta f) = (\Delta V)f + 2(\nabla V)^\top \cdot (\nabla f)$$

and

$$[A, [A, B]]g = A\big([A, B]g\big) - [A, B]\big(Ag\big) = \mathrm{i}\big(\Delta(\Delta V)\big)g + 4\mathrm{i}\big(\nabla(\Delta V)\big)^\top \cdot (\nabla g) + 4\mathrm{i}(\Delta V)(\Delta g).$$

They contain first- and second-order derivatives of the functions f and g, and their norms can be estimated as follows:

$$\|[A, B]f\|_2 \le \|\Delta V\|_\infty \cdot \|f\|_2 + \|2(\nabla V)\|_\infty \cdot \|\nabla f\|_2 \le K(\|f\|_2 + \|\nabla f\|_2) \le K\|f\|_{\mathrm{H}^1}$$

and $$\|[A, [A, B]]g\|_2 \le \|\mathrm{i}\big(\Delta(\Delta V)\big)\|_\infty \cdot \|g\|_2 + \|4\mathrm{i}\big(\nabla(\Delta V)\big)\|_\infty \cdot \|\nabla g\|_2 + \|4\mathrm{i}(\Delta V)\|_\infty \cdot \|\Delta g\|_2 \le K'(\|g\|_2 + \|\nabla g\|_2 + \|\Delta g\|_2) \le K'\|g\|_{\mathrm{H}^2}$$

for some constants $K, K' \ge 0$. By using again multiplicators as in Section 1.1 one can compute the fractional powers of $-\mathrm{i}\Delta$ (see also Exercise 7.2), and obtain that with the choice $Y = \mathrm{H}^1_{\mathrm{per}}(\Omega)$ and $\alpha = \frac{1}{2}$ and $\beta = 1$, the assumptions in Theorems 10.10 and 10.12 are fulfilled. Thus we conclude that the sequential splitting is of first order, and the Marchuk–Strang splitting is of second order for this problem.

One can show even more (see Exercise 7): Theorems 10.10 and 10.12 apply also to the semi-discretisation of the problem. By applying a certain operator splitting procedure, the numerical solution of problem (10.18) needs the approximation of the semigroups generated by the operators A and B. The multiplication is a pointwise calculation at every grid point. The semigroup generated by operator $A = \mathrm{i}\Delta$ can be approximated by applying some spectral method, see Appendix A. Using the approximation results presented in Lecture 3, we can imagine how such a combined method works. For more details, we refer to the project phase.

Now we illustrate the results above by presenting some figures showing the behaviour of the global error of the Marchuk–Strang splitting as a function of the time step h. We suppose $m = 1$. In the first case the smooth potential $V(x) = 1 - \cos x$ was used with random initial data in $\mathrm{H}^1_{\mathrm{per}}(-\pi, \pi)$, indicated by red circles, and with random initial data in $\mathrm{H}^2_{\mathrm{per}}(-\pi, \pi)$, indicated by blue stars. In the second case we used the non-smooth potential $V(x) = x + \pi$. One can see that in the case of the smooth potential the convergence is of higher order for the initial data being in $\mathrm{H}^2_{\mathrm{per}}(-\pi, \pi)$ than lying only in $\mathrm{H}^1_{\mathrm{per}}(-\pi, \pi)$. Thus, the numerical experiments are in line with the theoretical results. We note that the numerical experiments suggest that the non-smoothness of the potential does not allow a higher order convergence in general.

Remark 10.14. The commutator conditions stay the same for the corresponding parabolic problem

$$\partial_t w(t, x) = \Delta w(t, x) - V(x)w(t, x),$$

such as the heat equation with special source term, the linearised reaction-diffucion equation, or the imaginary-time Schrödinger equation. Thus, the considerations above apply to them as well.

Exercises

1. Compute the constant in the $\mathcal{O}(h^3)$ term in the formula (10.2).

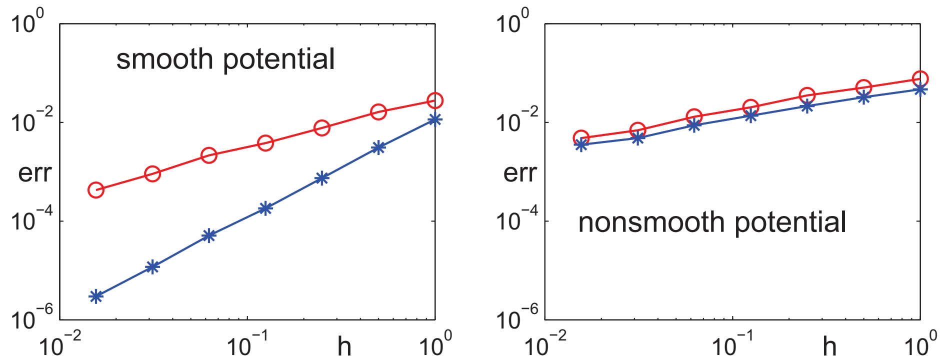

Figure 10.1: Global error of Marchuk–Strang splitting as a function of the time step h.

2. Let X be a Banach space and let $A, B \in \mathscr{L}(X)$. Prove that the following assertions are equivalent:

(i) $[A, B] = 0$.

(ii) For all $t \geq 0$ we have $[\mathrm{e}^{tA}, \mathrm{e}^{tB}] = 0$.

Show that under these equivalent conditions one has $\mathrm{e}^{tA}\mathrm{e}^{tB} = \mathrm{e}^{t(A+B)}$.

3. Prove Proposition 10.4.

4. Prove Theorem 10.6.

5. Let A and B be the generators of strongly continuous semigroups. Show that if there exist constants $M \geq 1$ and $\omega \in \mathbb{R}$ such that

$$\left\| \left(\mathrm{e}^{\frac{t}{n}B} \mathrm{e}^{\frac{t}{n}A} \right)^n \right\| \leq M\mathrm{e}^{\omega t} \tag{10.19}$$

holds for all $t \geq 0$ and $n \in \mathbb{N}$, then there exist constants $M_1, M_2 \geq 1$ and $\omega_1, \omega_2 \in \mathbb{R}$ such that

$$\left\| \left(\mathrm{e}^{\frac{t}{n}A} \mathrm{e}^{\frac{t}{n}B} \right)^n \right\| \leq M_1\mathrm{e}^{\omega_1 t}$$

and

$$\left\| \left(\mathrm{e}^{\frac{t}{2n}A} \mathrm{e}^{\frac{t}{n}B} \mathrm{e}^{\frac{t}{2n}A} \right)^n \right\| \leq M_2\mathrm{e}^{\omega_2 t}$$

holds as well for all $t \geq 0$ and $n \in \mathbb{N}$.

6. Work out the details of the conditions appearing in (10.5).

7. Study the space discretisation of the Schrödinger equation (10.18) which you can find as an example in the paper of Jahnke and Lubich. Implement the method together with the sequential and Marchuk–Strang splittings, and solve the equation numerically.