15th Internet Seminar on Evolution Equations
Solutions to the Exercises of Lecture 10
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Exercise 1. Compute the constant in the $\mathcal{O}(h^3)$ term in the formula (10.2).

We begin in the proof of Theorem 10.3 and compute

$$\begin{aligned}
\mathcal{E}_{seq}(t,h) &\leq \|(I + hB + \tfrac{h^2}{2}B^2 + \tfrac{h^3}{6}B^3 + \cdots)(I + hA + \tfrac{h^2}{2}A^2 + \tfrac{h^3}{6}A^3 + \cdots) \\
&\quad -(I + h(A+B) + \tfrac{h^2}{2}(A+B)^2 + \tfrac{h^3}{6}(A+B)^3) + \cdots \| \cdot \|u(t)\| \\
&= \|(I - I) + h(B+A) - h(A+B) + \tfrac{h^2}{2}(2BA + B^2 + A^2) \\
&\quad -\tfrac{h^2}{2}(A^2 + AB + BA + B^2) + \tfrac{h^3}{6}(B^3 + 3B^2A + 3BA^2 + A^3) \\
&\quad -\tfrac{h^3}{6}(A^3 + A^2B + ABA + BA^2 + B^2A + BAB + AB^2 + B^3) + \cdots \| \cdot \|u(t)\| \\
&\leq \|\tfrac{h^2}{2}(BA - AB) + \tfrac{h^3}{6}(2B^2A + 2BA^2 - A^2B - ABA - BAB - AB^2)\| \cdot \|u(t)\| \\
&\quad +\mathcal{O}(h^4) \cdot \|u(t)\|.
\end{aligned}$$

For the third order term we have

$$\begin{aligned}
&\tfrac{h^3}{6}(B^2A - BAB + B^2A - AB^2 + BA^2 - ABA + BA^2 - A^2B) \\
= \; &\tfrac{h^3}{6}(B[B,A] + [B^2,A] + [B,A]A + [B,A^2]).
\end{aligned}$$

So the constant in the $\mathcal{O}(h^3)$ term is

$$C = \tfrac{1}{6}\|B[B,A] + [B^2,A] + [B,A]A + [B,A^2]\|.$$

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

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

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

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

"(i)⇒(ii)" We have $[A,B] = AB - BA = 0$ and thus $AB = BA$ holds. Since A, $B \in \mathcal{L}(X)$ holds, the semigroups generated by A and B are given by

$$e^{tA} = \sum_{k=0}^{\infty} \frac{t^kA^k}{k!} \text{ and } e^{tB} = \sum_{k=0}^{\infty} \frac{t^kB^k}{k!}.$$

Thus, we can compute

$$\begin{aligned}
e^{tA}e^{tB} &= \sum_{k=0}^{\infty} \frac{t^kA^k}{k!} \sum_{k=0}^{\infty} \frac{t^kB^k}{k!} = \sum_{k=0}^{\infty} \sum_{j=0}^{k} \frac{A^{k-j}}{(k-j)!} \frac{B^j}{j!} \\
&= \sum_{k=0}^{\infty} \sum_{j=0}^{k} \frac{1}{k!}\binom{k}{j} A^{k-j}B^j = \sum_{k=0}^{\infty} \frac{t^k(A+B)^k}{k!} \\
&= e^{t(A+B)} = e^{tB}e^{tA}
\end{aligned}$$

where we used the Cauchy product formula and in the last step the binomial theorem (where the commutativity is used).

"(ii)⇒(i)" We have $[e^{tA}, e^{tB}] = e^{tA}e^{tB} - e^{tB}e^{tA} = 0$. With the formulas for e^{tA} and e^{tB} above, we get

$$\begin{aligned}
0 = e^{tA}e^{tB} - e^{tB}e^{tA} &= \sum_{k=0}^{\infty} \frac{t^k A^k}{k!} \sum_{k=0}^{\infty} \frac{t^k B^k}{k!} - \sum_{k=0}^{\infty} \frac{t^k B^k}{k!} \sum_{k=0}^{\infty} \frac{t^k A^k}{k!} \\
&= (I + tA + tB + \tfrac{t^2}{2}A^2 + \tfrac{t^2}{2}B^2 + t^2 AB + \tfrac{t^3}{6}A^3 + \cdots) \\
&\quad -(I + tB + tA + \tfrac{t^2}{2}B^2 + \tfrac{t^2}{2}A^2 + t^2 BA + \tfrac{t^3}{6}B^3 + \cdots) \\
&= t^2(AB - BA) + t^3(\cdots) + t^4(\cdots) + \cdots \\
&=: \sum_{k=2}^{\infty} c_k t^k.
\end{aligned}$$

If the power series $\sum_{k=2}^{\infty} c_k t^k$ is zero then all coefficients are zero, i.e. $c_k = 0$ for all $k \in \mathbb{N}$, and thus in particular $c_2 = AB - BA = 0$ that is $[A, B] = 0$ holds.

Exercise 3. Prove Proposition 10.4.

By the Lax equivalence theorem (more precisely Proposition 4.12), it is sufficient to show consistency, stability (Definition 4.1) and consistency of order 2 (Definition 4.11).
To prove the consistency, we first consider the local error

$$\begin{aligned}
\mathcal{E}_{\text{MS}}(h, u(t)) &= \|(F_{\text{MS}}(h) - e^{h(A+B)})u(t)\| = \|(e^{\frac{h}{2}A}e^{hB}e^{\frac{h}{2}A} - e^{h(A+B)})u(t)\| \\
&\le \|e^{\frac{h}{2}A}e^{hB}e^{\frac{h}{2}A} - e^{h(A+B)}\| \cdot \|u(t)\|.
\end{aligned}$$

By using the power series of the corresponding exponential functions we get

$$\begin{aligned}
\mathcal{E}_{\text{MS}}(h, u(t)) &\le \|(I + \tfrac{h}{2}A + \tfrac{h^2}{8}A^2 + \tfrac{h^3}{48}A^3 + \cdots)(I + hB + \tfrac{h^2}{2}B^2 + \tfrac{h^3}{6}B^3 + \cdots)(I + \tfrac{h}{2}A \\
&\quad + \tfrac{h^2}{8}A^2 + \tfrac{h^3}{48}A^3 + \cdots) - (I + h(A+B) + \tfrac{h^2}{2}(A+B)^2 + \tfrac{h^3}{6}(A+B)^3 \\
&\quad + \cdots)\| \cdot \|u(t)\| \\
&= \|(I + hB + \tfrac{h^2}{2}B^2 + \tfrac{h^3}{6}B^3 + \tfrac{h}{2}A + \tfrac{h^2}{2}AB + \tfrac{h^3}{4}AB^2 + \tfrac{h^2}{8}A^2 + \tfrac{h^3}{8}A^2B \\
&\quad + \tfrac{h^3}{48}A^3 + \cdots)(I + \tfrac{h}{2}A + \tfrac{h^2}{8}A^2 + \tfrac{h^3}{48}A^3 + \cdots) - (I + h(A+B) \\
&\quad + \tfrac{h^2}{2}(A+B)^2 + \tfrac{h^3}{6}(A+B)^3 + \cdots)\| \cdot \|u(t)\| \\
&= \|(I + h(A+B) + \tfrac{h^2}{2}(A+B)^2 + \tfrac{h^3}{6}A^3 + \tfrac{h^3}{6}B^3 + \tfrac{h^3}{8}BA^2 + \tfrac{h^3}{4}B^2A \\
&\quad + \tfrac{h^3}{4}ABA + \tfrac{h^3}{4}AB^2 + \tfrac{h^3}{8}A^2B + \cdots) - (I + h(A+B) + \tfrac{h^2}{2}(A+B)^2 \\
&\quad + \tfrac{h^3}{6}(A+B)^3 + \cdots)\| \cdot \|u(t)\| \\
&= h^3\|\alpha ABA + \beta A^2B + \gamma BA^2 + \delta AB^2 + \cdots\| \cdot \|u(t)\| \\
&\le C \cdot h^3 \cdot \|u(t)\| + \mathcal{O}(h^4) \cdot \|u(t)\|,
\end{aligned}$$

where $\alpha, \beta, \gamma, \delta, C \in \mathbb{R}_+$. The consistency follows from this estimate, since $\frac{1}{h}\mathcal{E}_{\text{MS}}(h, u(t)) \to 0$ (locally uniformly in t) as $h \searrow 0$. We note that from the considerations above, we also conclude that the MS splitting is of second order.

To show stability, we have to ensure the existence of a constant $M > 0$ such that $\|F_{\text{MS}}(\frac{t}{n})^n\| \le M$ 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

$$\begin{aligned}
\|F_{\text{MS}}(\tfrac{t}{n})^n\| &\le \|F_{\text{MS}}(\tfrac{t}{n})\|^n = \|e^{\frac{t}{2n}A}e^{\frac{t}{n}B}e^{\frac{t}{2n}A}\|^n \le \|e^{\frac{t}{2n}A}\|^n \cdot \|e^{\frac{t}{n}B}\|^n \cdot \|e^{\frac{t}{2n}A}\|^n \\
&\le (e^{\frac{t}{2n}\|A\|})^n \cdot (e^{\frac{t}{n}\|B\|})^n \cdot (e^{\frac{t}{2n}\|A\|})^n \le e^{\frac{t_0}{2}\|A\|} \cdot e^{t_0\|B\|} \cdot e^{\frac{t_0}{2}\|A\|} \\
&= e^{t_0\|A\|} \cdot e^{t_0\|B\|} = e^{t_0(\|A\|+\|B\|)} =: M.
\end{aligned}$$

Exercise 4. Prove Theorem 10.6.

Proof: We consider the function $F : [0, \infty) \to \mathcal{L}(X)$ defined by

$$F(t) = e^{tB}e^{tA}.$$

Clearly, $F(0) = I$ and by (10.3) we obtain

$$\|F(t)^n\| \leq Me^{\omega nt}$$

for all $n \in \mathbb{N}$ and $t \geq 0$. For $f \in D = D(A) \cap D(B)$ we calculate

$$\begin{aligned} \lim_{h \searrow 0} \left\| \tfrac{F(h)f-f}{h} - Af - Bf \right\| &\leq \lim_{h \searrow 0} \|e^{hB}\| \left\| \tfrac{e^{hA}f-f}{h} - Af \right\| + \lim_{h \searrow 0} \|e^{hB}Af - Af\| \\ &\quad + \lim_{h \searrow 0} \left\| \tfrac{e^{hB}f-f}{h} - Bf \right\| \\ &= 0 \end{aligned}$$

as A and B are the generators of e^{tA} and e^{tB}, respectively, $\sup_{h\in[0,1]} \|e^{hB}\| < \infty$, and the semigroup (e^{tB}) is strongly continuous. Thus

$$(A + B)f = \lim_{h \searrow 0} \tfrac{F(h)f-f}{h}$$

exists for all $f \in D$. Moreover, $(\lambda_0 - (A + B))D$ is dense in X. Consequently, the statement of Theorem 10.6 follows from Chernoff's Product Formula (Theorem 5.12).

Exercise 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

$$\left\| \left(e^{\frac{t}{n}B}e^{\frac{t}{n}A}\right)^n \right\| \leq Me^{\omega t}$$

holds for all $t \geq 0$ and $n \in \mathbb{N}$, then there exist constants M_1, $M_2 \geq 1$ and ω_1, $\omega_2 \in \mathbb{R}$ such that

$$\left\| \left(e^{\frac{t}{n}A}e^{\frac{t}{n}B}\right)^n \right\| \leq M_1e^{\omega_1 t}$$

and

$$\left\| \left(e^{\frac{t}{2n}A}e^{\frac{t}{n}B}e^{\frac{t}{2n}A}\right)^n \right\| \leq M_2e^{\omega_2 t}$$

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

Let (M_A, ω_A) and (M_B, ω_B) be the types of the semigroups generated by A and B. Then we get

$$\begin{aligned} \|(e^{\frac{t}{n}A}e^{\frac{t}{n}B})^n\| &= \|e^{\frac{t}{n}A}(e^{\frac{t}{n}B}e^{\frac{t}{n}A})^{n-1}e^{\frac{t}{n}B}\| \\ &\leq \|e^{\frac{t}{n}A}\| \, \|e^{\frac{t}{n}B}\| \, \|(e^{\frac{(n-1)t}{(n-1)n}B}e^{\frac{(n-1)t}{(n-1)n}A})^{n-1}\| \\ &\leq M_Ae^{\frac{t}{n}\omega_A}M_Be^{\frac{t}{n}\omega_B}Me^{\frac{(n-1)t}{n}\omega} \\ &= (M_AM_BM)e^{t\cdot(\frac{\omega_A}{n}+\frac{\omega_B}{n}+\frac{\omega(n-1)}{n})} \\ &\leq (M_AM_BM)e^{t\cdot(|\omega_A|+|\omega_B|+|\omega|)} \\ &=: M_1e^{t\omega_1} \end{aligned}$$

and

$$
\begin{aligned}
\|(e^{\frac{t}{2n}A}e^{\frac{t}{n}B}e^{\frac{t}{2n}A})^n\| &= \|e^{\frac{t}{2n}A}(e^{\frac{t}{n}B}e^{\frac{t}{2n}A}e^{\frac{t}{2n}A})^{n-1}e^{\frac{t}{n}B}e^{\frac{t}{2n}A}\| \\
&\leq M_A e^{\frac{t}{2n}\omega_A} M_B e^{\frac{t}{n}\omega_B} M_A e^{\frac{t}{2n}\omega_A} \|(e^{\frac{t}{n}B}e^{\frac{t}{2n}A}e^{\frac{t}{2n}A})^{n-1}\| \\
&= (M_A^2 M_B) e^{\frac{t}{n}\omega_A} e^{\frac{t}{n}\omega_B} \|(e^{\frac{t}{n}B}e^{\frac{t}{n}A})^{n-1}\| \\
&\leq (M_A^2 M_B) e^{\frac{t}{n}\omega_A} e^{\frac{t}{n}\omega_B} M e^{\frac{(n-1)t}{n}\omega} \\
&= (M_A^2 M_B M) e^{t\cdot(\frac{\omega_A}{n}+\frac{\omega_B}{n}+\frac{\omega(n-1)}{n})} \\
&\leq (M_A^2 M_B M) e^{t\cdot(|\omega_A|+|\omega_B|+|\omega|)} \\
&=: M_2 e^{t\omega_2}.
\end{aligned}
$$

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

Under Assumption 10.7. we have a generator A of a strongly continuous semigroup on X and $B \in \mathcal{L}(X)$. Using only shifting of the generators and the renorming procedure we want to acquire generators A' and B', each generating a contraction semigroup, with the additional property that the sum $A' + B'$ generates a contraction semigroup as well.

We start by noting the type (M, ω) of the semigroup generated by A.

In the next step we shift the semigroup by subtracting ω from the generator, hence the new generator is $A - \omega$. This leaves us with a semigroup of the type $(M, 0)$, allowing us to use the renorming procedure from excercise C.4.

By switching from the current norm $\|\cdot\|$ on X to the equivalent norm $|||\cdot|||$ from exercise C.4 our semigroup gains the desired type $(1, 0)$.

Since the norms are equivalent, B is still a bounded operator on X, which means that the generated semigroup e^{tB} is of the type $(1, |||B|||)$. By shifting the generator to $B' := B - |||B|||$, which is obviously still a bounded operator on X, the generated semigroup gains his final type $(1, 0)$.

The last step, motivated by the theorem we will use afterwards, is another shifting of our first generator. The final version of the first generator is $A' := A - \omega - |||B||| = A - (\omega + |||B|||)$, whose generated semigroup bears the type $(1, -|||B|||)$.

Both A' and B' now generate contraction semigroups. Furthermore the conditions of theorem 6.13 are now satisfied and therefore $(A' + B')$ with $D(A' + B') = D(A')$ generates a semigroup of the type $(1, -|||B||| + |||B|||) = (1, 0)$, which means that $A' + B'$ generates a contraction semigroup as well. The three equations in (10.5) follow immediately.

Exercise 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.

We choose the space discretization for the Schrödinger equation

$$i\frac{\partial u}{dt} = -\Delta u + Vu.$$

Code (MATLAB) :

```
function [u,U] = solver(T,N,V,U0,tau,split)
```

```
% ============================================================
% Semi-discretization method for Schrödinger equation with splittings
% ============================================================
 % input parameters:
 % N                    defines number of line
 % T                    final time
 % V                    potential (2π-periodic)
 % u0                   vector with initial values
 % tau                  step size of splitting method
 % spilt                splitting method
 %                      split = 1: Sequential splitting
 %                      split = 2: Marchuk-Strang splitting
 % output parameters:
 % U                    approximations in the grid points (ODE)
 % u                    approximations in the grid points (PDE)
% ============================================================
% arrange grid
l = -N : N-1;
x = l*pi/N;
% arrange initial value vector
U = zeros(2*N,T);
U(:,1) = U0;
% choose splitting method and compute solution for ODE
if split == 1
  for k = 1 : T
      U(:,k+1) = expm(i*tau*diag((i*l).^2))*fft(eye(2*N))*diag(exp(-i/2*tau*V))*ifft(eye(2*N))*U(:,k);
  end
end
if split == 2
  for k = 1 : T
      U(:,k+1) = fft(eye(2*N))*diag(exp(-i/2*tau*V))*ifft(eye(2*N))*expm(i*tau*diag((i*l).^2))
      *fft(eye(2*N))*diag(exp(-i/2*tau*V))*ifft(eye(2*N))* U(:,k);
  end
end
% compute solution for PDE
u = zeros(2*N,T);
for l = 1 : T
  for k = 1 : 2*N
      u(:,l) = u(:,l) + (exp(i*k*x)*U(k,l))';
  end
end
end
```

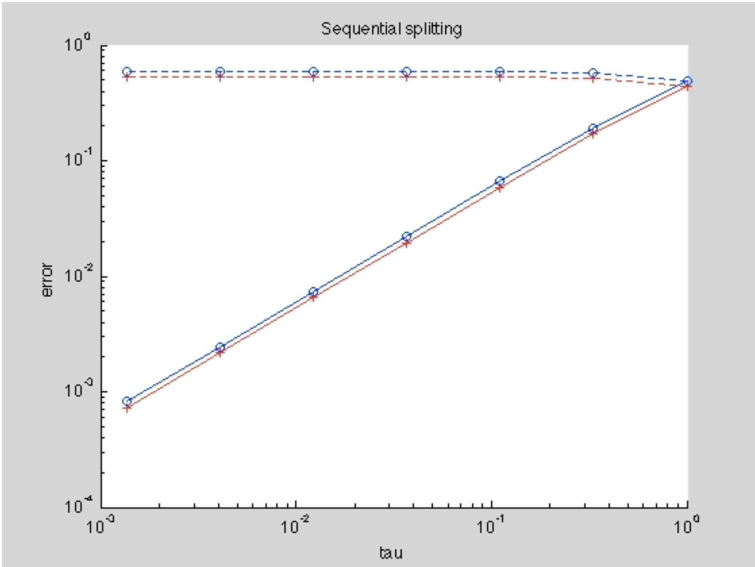

Figure 1: Error versus step size; smooth potential ($V(x) = 1 - \cos x$). The red curve corresponds to the initial value $\hat{U}^0_{(1)}$, and the blue one to the initial value $\hat{U}^0_{(2)}$.The dashed lines indicate the error divided by τ.

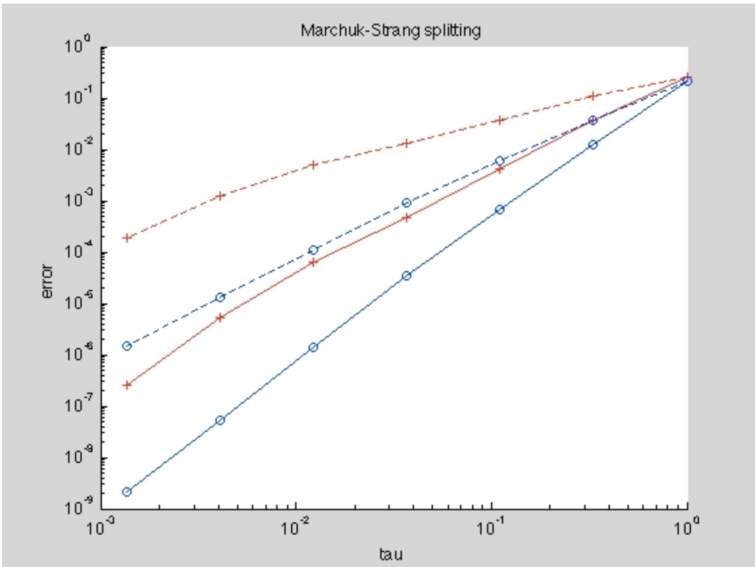

Figure 2: Error versus step size; smooth potential (V(x)=1-cosx). The red curve corresponds to the initial value $\hat{U}^0_{(1)}$, and the blue one to the initial value $\hat{U}^0_{(2)}$. The dashed lines indicate the error divided by τ.

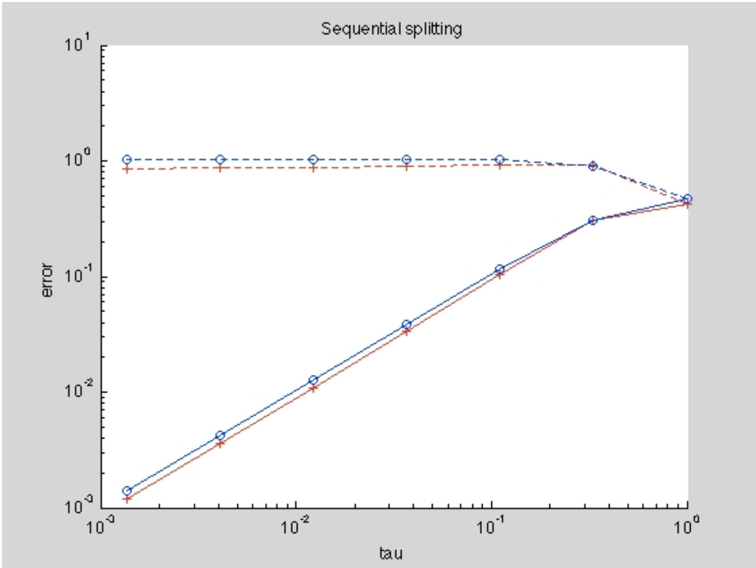

Figure 3: Error versus step size; nonsmooth potential ($V(x) = x + \pi$). The red curve corresponds to the initial value $\hat{U}^0_{(1)}$, and the blue one to the initial value $\hat{U}^0_{(2)}$.The dashed lines indicate the error divided by τ.

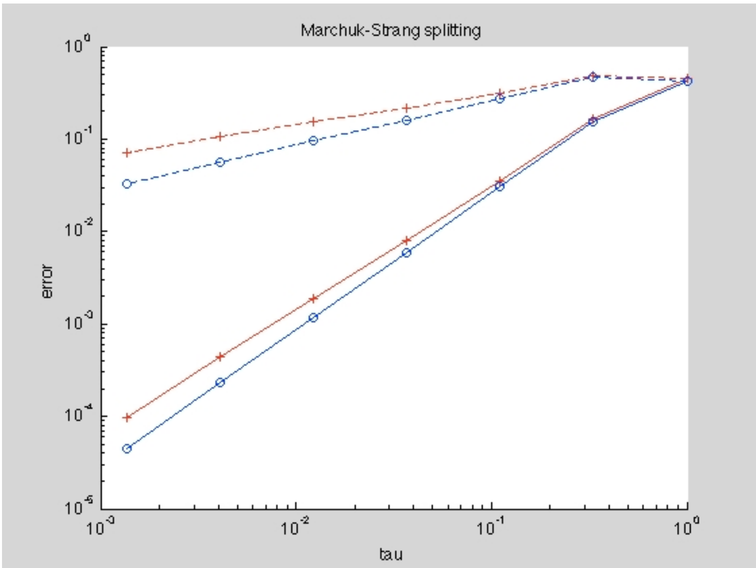

Figure 4: Error versus step size; nonsmooth potential ($V(x) = x + \pi$). The red curve corresponds to the initial value $\hat{U}^0_{(1)}$, and the blue one to the initial value $\hat{U}^0_{(2)}$. The dashed lines indicate the error divided by τ.