The exponential Rosenbrock-Euler method for nonsmooth initial data

Julia Schweitzer

Karlsruhe Institute of Technology
Institute for Applied and Numerical Mathematics
Kaiserstr. 89–93
D-76128 Karlsruhe
Germany
+49 721 608 42684
Julia.Schweitzer@kit.edu

Abstract

We consider the exponential Rosenbrock-Euler method for the solution of nonlinear parabolic abstract ordinary differential equations. For smooth solutions the convergence analysis is known, and the method is of order two. Here we investigate the convergence of the method in the case of nonsmooth initial conditions which result in derivatives of the solution with singularities at the origin. We give an error analysis that applies to the nonsmooth case and identify conditions on the problems for which we can still observe convergence order two. Furthermore we discuss examples with respect to these assumptions.

Keywords: Exponential integrators, Exponential Rosenbrock-Euler method, Semilinear parabolic equations, Nonsmooth initial data, Error bounds
2010 MSC: 65L20, 65L04, 65L05, 65L70, 65J08, 65J15

---

1. Introduction

High convergence order of a numerical time integration scheme requires temporal smoothness of the solution. For parabolic partial differential equations this follows form spatial smoothness as well as compatibility with the boundary conditions of the initial data. Moreover, the source term has to satisfy certain conditions. Consider for example the simplest parabolic equation, say $u'(t) = Au(t)$, $t > 0$, with an unbounded sectorial operator A on some Banach space. Then the implicit Euler approximation converges with full order one if the initial condition u_0 is in the domain of A^2.

In many applications, however, this rather strict assumption is not fulfilled. A simple example may be a diffusion-reaction equation which models the reaction of different chemicals being initially spatially separated. In that case, the functions describing the initial concentrations of the chemicals show jumps and thus are not even differentiable in space. Other such examples arise in option pricing models where the initial condition is usually a piecewise linear continuous function.

Nevertheless, these equations admit solutions with less regularity in time, the derivatives of the solution show singularities towards the origin. In order to analyse the convergence of time integration schemes for this class of problems independently of any spatial discretisation, they are usually considered in the framework of nonlinear parabolic abstract ordinary differential equations on Banach spaces.

There is a variety of papers that consider classical implicit methods for nonsmooth solutions. In [1], Crouzeix and Thomée studied classical implicit one-step methods for linear parabolic problems with nonsmooth initial conditions. In [5, 12, 13, 15, 16] the problems range from semilinear over quasilinear to fully nonlinear with different sources and measures of nonsmooth solutions. The methods under investigation are different forms of classical implicit or linearly implicit one-step methods.

If we turn our attention to exponential methods for the solution of parabolic problems with nonsmooth initial conditions, the list becomes remarkably short. In [4], the exponential Rosenbrock-Euler method was used to solve the Black-Scholes model for American option pricing, an example which fits into our framework. However, the convergence was only studied experimentally and no analysis was given. The method itself is not new. It was first proposed by Pope in 1963, [18], and was discussed in several works since then, e.g. [3, 8, 9, 19, 22]. In the case of sufficiently smooth solutions the method is known to have stiff convergence order two, see [9]. In the present paper we extend the error analysis given there to the case where the initial conditions are incompatible. We show that under certain additional conditions on the nonlinearity of the problem we can still obtain full convergence order two in most cases. Only for the worst case initial conditions an order reduction cannot be avoided. Moreover, in some cases the error bound characterises the sort of order reduction that can be expected if these additional conditions only hold for parameters that are not sufficient for full second order. The result is still valid for variable time step sizes as long as the sequence of time step sizes is quasi-uniform, see [20].

The paper is organised as follows. In Section 2 we state the natural conditions on the parabolic abstract ordinary differential equation and introduce intermediate spaces that characterise the compatibility of the initial condition. We also state the bounds on the exact solution and its derivatives that we use throughout the paper.

In Section 3 we briefly review the exponential Rosenbrock-Euler method and state the main result of the present paper.

In Section 4 we collect some preliminary work on the bounds of compositions of semigroups which are generated by operators $A + B_k$ where A is an unbounded, sectorial operator and the operators B_k are different, bounded perturbations. These results are used for the convergence proof, which itself is performed in Section 5.

To conclude the paper, we discuss two examples in Section 6 to illustrate the conditions which are required for the convergence.

2. Analytical framework

Let X be a Banach space equipped with a norm $\|\cdot\|_X$, and consider the abstract ordinary differential equation

$$u'(t) = F(u(t)) = Au(t) + f(u(t)) \ , \quad u(0) = u_0 \ , \tag{1}$$

on X. We assume $A : \mathcal{D}(A) \to X$ to be the generator of an analytic semigroup on X and $f : X \to X$ to be bounded, Lipschitz continuous, and twice Fréchet-differentiable with bounded derivatives in a strip along the exact solution.

Without loss of generality, let 0 be contained in the resolvent set of A. Thus, we can define fractional powers of $-A$. The domain $V_\alpha = \mathcal{D}((-A)^\alpha)$ of $(-A)^\alpha$ is a subspace of X, and we define the norm $\|\cdot\|_{V_\alpha} = \|(-A)^\alpha \cdot\|_X$ on V_α for $\alpha \geq 0$.

From standard semigroup theory we get the bound

$$\|e^{tA}\|_{X\leftarrow X} + \|(-tA)^\beta e^{tA}\|_{X\leftarrow X} \leq C \ , \quad t \in (0, T] \ , \tag{2}$$

for some constant $C \geq 0$ and $\beta \geq 0$, see e.g. [17, Theorem 2.6.13].

The mild solution of (1) is the solution of the variation of constants formula

$$u(t) = e^{tA}u_0 + \int_0^t e^{(t-\tau)A} f(u(\tau))\, d\tau \tag{3}$$

for some initial condition $u_0 \in X$. Note that for the given conditions the mild solution exists.

We now summarise bounds of the mild solution and its derivatives over a finite time interval $[0, T]$ for different regularity assumptions on the initial condition u_0. We would like to point out that all constants denoted by C may depend on α, T, bounds on f as well as higher derivatives thereof, and on bounds of the semigroup e^{tA}, but not on A directly.

Let u_0 be contained in V_α for $\alpha \geq 0$. The mild solution (3) of (1) satisfies the bounds

$$\|u(t)\|_X \leq C \tag{4a}$$

$$\|(-A)^{-\beta}u'(t)\|_X \leq Ct^{\gamma_1}\ , \quad \beta > -1 \tag{4b}$$

$$\|(-A)^{-\beta}u''(t)\|_X \leq Ct^{\gamma_2}\ , \quad \beta > 0 \tag{4c}$$

for $\gamma_1(\beta) = \min(0, \alpha + \beta - 1, \beta)$ and $\gamma_2(\beta) = \min(0, \alpha + \beta - 2, \beta - 1, \alpha - 1)$, on a finite time interval $(0, T]$. The first bound follows from Theorem 3.3.3 of [6]. The second bound for $\beta \leq 0$ is given in Theorem 3.5.2 of [6]. Note that the case of $\alpha \geq 1$ is an easy extension of the proof given there. For $\beta > 0$ the bound is obtained directly by estimating the differential equation multiplied by $(-A)^{-\beta}$ in a straight forward manner after inserting the variation of constants formula. The third bound is an easy consequence of the second. Note that the second bound for $\beta < 0$ is only required to prove the third. Throughout the remainder of the paper, it will only be used with $\beta \geq 0$ and thus γ_1 simplifies to $\min(0, \alpha + \beta - 1)$.

3. Convergence of the exponential Rosenbrock-Euler method with nonsmooth initial data

We now consider the exponential Rosenbrock-Euler method, which was first proposed by Pope in 1963, see [18]. In [9] it was shown that the method converges with stiff convergence order 2 for smooth solutions, i.e. u and its derivatives are all bounded.

In the present paper we derive error bounds for the exponential Rosenbrock-Euler method in the case of weaker regularity assumptions on the solution and its derivatives as discussed in the previous section. In this setting, several essential parts of the proof given in [9] do not work anymore. We also restrict ourselves to the second order Rosenbrock-Euler method since higher order methods would need stronger assumptions on the time regularity of the solution not given in our case.

For the sake of completeness and notation, we derive the method and review the φ-functions which are of common use in the context of exponential integrators.

The exponential Rosenbrock-Euler method is based on a continuous linearisation of (1) along the numerical solution. For some point u_n in the state space, this linearisation is given by

$$u'(t) = J_n u(t) + g_n(u(t)) \ , \tag{5}$$

where J_n denotes the Fréchet derivative of F evaluated at u_n,

$$J_n = \mathrm{D}F(u_n) = A + \mathrm{D}f(u_n) \ ,$$

and g_n is the nonlinear remainder,

$$g_n(u(t)) = F(u(t)) - J_n u(t) \ .$$

The exponential Rosenbrock-Euler method is given by applying the variation of constants formula (3) to the linearised equation (5), freezing the nonlinearity at the numerical solution u_n and integrating exactly,

$$u_{n+1} = e^{hJ_n} u_n + h\varphi_1(hJ_n) g_n(u_n) = u_n + h\varphi_1(hJ_n) F(u_n) \ . \tag{6}$$

The function φ_1 is one of the well known φ-functions, which are entire functions given by

$$\varphi_k(z) = \int_0^1 e^{(1-\tau)z} \frac{\tau^{k-1}}{(k-1)!} \, d\tau \ , \quad k \geq 1 \ , \quad z \in \mathbb{C} \ .$$

To improve the convergence rate of this method for problems with nonsmooth initial data, we require the following additional assumption on the nonlinearity of the problem.

Assumption 1. *There exists some* $\beta \in [0, 2)$ *such that the nonlinearity of the abstract initial value problem* (1) *satisfies the condition*

$$\|(-A)^{-\beta} \mathrm{D}f(v) (-A)^{\beta}\|_{X \leftarrow X} \leq C \tag{7}$$

for v in a strip along the exact solution. Moreover, the bound

$$\|(-A)^{-\beta}\mathrm{D}^2 f(u(t))(u'(t),u'(t))\|_X \le Ct^{\alpha+\beta-2}\ , \quad t>0\ , \tag{8}$$

holds for the exact solution with $u_0 \in V_\alpha$. In the case of $\beta \ge 1$, we additionally require the bound (7) *to hold for some $\eta \in (\beta-1,1)$ in the role of β.*

The main part of the paper consists of the proof of the following theorem on the convergence of the exponential Rosenbrock-Euler method under weak regularity assumptions. The proof will be given within the next two sections.

Theorem 1. *Consider an abstract initial value problem* (1) *with initial condition $u_0 \in V_\alpha$ for $\alpha \in [0,2)$ such that the solution satisfies the bounds* (4) *for $t \in (0,T]$ and that fulfils Assumption 1 for some β such that $\alpha+\beta>0$. For the numerical solution consider the exponential Rosenbrock-Euler method* (6) *applied with constant time step size $h>0$. Then, the error of the numerical solution at time $t_{n+1}=(n+1)h \le T$ is bounded by*

$$\begin{aligned}\|u_{n+1}-u(t_{n+1})\|_X \le{}& Ch^{1+\alpha+\beta}\Big(t_{n+1}^{-\beta}+\int_h^T \tau^{-\beta}\ d\tau\Big)\\ &+Ch^2\Big(t_{n+1}^{\alpha-1}+\int_h^T \tau^{\alpha-1}\ d\tau\Big)\\ &+Ch^2\Big(t_{n+1}^{-\beta}+\int_h^T \tau^{-\beta}\ d\tau\Big)\int_h^T \tau^{\gamma_2(\beta)}\ d\tau\\ &+Ch^2\Big(t_{n+1}^{\gamma_2(\beta)}+\int_h^T \tau^{\gamma_2(\beta)}\ d\tau\Big)\int_h^T \tau^{-\beta}\ d\tau\ .\end{aligned}$$

The constants depend on the bounds of the solution as well as the nonlinearity, α, β and T, but not on n or h.

Remark 1. The result easily extends to variable time step sizes with a quasi-uniform sequence of time step sizes $(h_k)_k$ such that $h_k \le Ch_{\min}$. The details can be found in [20].

Remark 2. This error bound is of order 2 if all time step sizes appear with powers greater or equal than 2. Obviously, the first term yields the condition $\alpha+\beta \ge 1$. But also the lower limits of the integrals may possibly lead to order reduction. We obtain a logarithmic perturbation of the second order error estimate if any of the powers of the integrands is equal to -1, and order reduction if any of the powers of the integrands is less than -1.

Thus, to keep all powers of the time step sizes greater or equal to 2 for a given α, we require Assumption 1 to hold with some β such that $1 > \beta > 1-\alpha$ and such that $\gamma_2(\beta) > -1$.

For $\alpha \in [1, 2)$ the first condition is satisfied for all $\beta \in [0, 1)$. But from $\gamma_2(\beta) = \min(0, \alpha + \beta - 2, \beta - 1, \alpha - 1) = \min(0, \beta - 1) > -1$ we see, that Assumption 1 is required for some $\beta \in (0, 1)$ to obtain full convergence order 2. If Assumption 1 only holds in the trivial case of $\beta = 0$ we expect a logarithmic perturbation of second order.

Consider the case of $\alpha \in (0, 1)$. If Assumption 1 holds for some $1 > \beta > 1 - \alpha$ we have $\gamma_2(\beta) = \alpha + \beta - 2 > -1$ and thus also obtain full convergence order 2.

In the worst case, namely $\alpha = 0$, the condition $1 > \beta > 1 - \alpha$ is a contradiction, and therefore we cannot obtain full order 2 for $\alpha = 0$.

In the case that the nonlinearity of the problem does not yield the appropriate conditions (7) and (8) for full order 2, the error bound also shows that an order reduction should be expected. In some cases, where specific values for α and β can be obtained, the order reduction can be quantified.

4. Operator bounds for compositions of semigroups

In the next section we will see that the error of the exponential Rosenbrock-Euler method involves stability bounds on the operators

$$S_{n,0} = e^{hJ_n} \cdots e^{hJ_0} \ , \quad S_{-1,0} = I \ , \tag{9}$$

which are compositions of analytical semigroups with perturbed generators. We will call them perturbed semigroups. The operator bounds of such compositions are essential for the error analysis of the method. Hence, it is important to bound them independently of the number of time steps. Indeed, it is desirable for the composition of perturbed semigroups each on a short time step to behave like one single semigroup on the sum over all time steps. Therefore, the goal of this section is to derive stability bounds for the composition of perturbed semigroups which reflect the original bound (2).

Recall that A is the generator of an analytic semigroup. Then for bounded operators B and B_k, $k = 0, \ldots, n$, the operators $J = A + B$ and $J_k = A + B_k$ also generate analytic semigroups.

In the sequel we require some condition on the interchangeability of the bounded operators with fractional powers of $-A$. Therefore, we introduce the notation $B^{(\beta)} = (-A)^{-\beta} B (-A)^{\beta}$ and assume that $B^{(\beta)} : X \to X$ is bounded with $M^{(\beta)} = \|(-A)^{-\beta} B (-A)^{\beta}\|_{X \leftarrow X}$ denoting the norm of the operator. A similar notation $B_k^{(\beta)}$ and $M_k^{(\beta)}$ is used for the operators B_k. The assumption of $B^{(\beta)}$ being bounded will be discussed in Section 6.

For the ease of presentation we only consider the operator norms $M_k^{(\beta)}$ to be uniformly bounded. Note however that it is possible to track and analyze the exact dependence of the results of this section on the operator norms for more general cases.

To start with we collect two preliminary results.

Lemma 2. *Under the given assumptions, the bound*

$$\|(-tA)^{-\mu} e^{tJ} (-tA)^{\nu}\|_{X \leftarrow X} \leq C \ , \quad t \in (0, T]$$

holds for $\nu - \mu < 1$ with a constant C that depends on T and $M^{(\mu)}$. Additionally, the bound holds for $\mu = -1$ and $\nu = 0$ as well as $\mu = 0$ and $\nu = 1$ with with a constant C that depends on T and $M^{(0)}$.

Proof. For the proof, we first consider the function $u_\lambda(t) = (-tA)^{\lambda} e^{tA} x$ for an arbitrary $x \in X$. For $t \in (0, T]$ let Δt be such that $t + \Delta t > 0$. Then we have

$$\begin{aligned}
\|u_\lambda(t + \Delta t) - u_\lambda(t)\|_X &= \Big\| \int_t^{t+\Delta t} u_\lambda'(\tau) \ d\tau \Big\|_X \\
&= \Big\| \int_t^{t+\Delta t} \big(\lambda \tau^{\lambda - 1} (-A)^{\lambda} e^{\tau A} x + (-\tau A)^{\lambda} A e^{\tau A} x \big) \ d\tau \Big\|_X \\
&\leq \Big| \int_t^{t+\Delta t} \tau^{-1} \ d\tau \Big| \ C \|x\|_X \\
&= C \big| \log(t + \Delta t) - \log(t) \big| \ \|x\|_X \ .
\end{aligned}$$

For any $t \in (0, T]$ this tends to zero for $\Delta t \to 0$ and arbitrary $x \in X$. Therefore, u_λ is continuous for all $t \in (0, T]$.

Next we want to analyse the function $v_{\mu,\nu}(t) = (-tA)^{-\mu} e^{tJ} (-tA)^{\nu} x$. To transfer the properties of $u_{\nu-\mu}$ to $v_{\mu,\nu}$, we generalise the proof of Proposition 3.1.2 in [17]. To this end we consider the integral equation

$$e^{tJ} = e^{tA} + \int_0^t e^{(t-\tau)A} B e^{\tau J} \ d\tau \ , \tag{10}$$

multiply it from both sides with the appropriate powers of $(-tA)$, apply it to some $x \in X$ and obtain

$$v_{\mu,\nu}(t) = u_{\nu-\mu}(t) + t^{\nu-\mu} \int_0^t \tau^{\mu-\nu} e^{(t-\tau)A} B^{(\mu)} v_{\mu,\nu}(\tau)\ d\tau\ . \tag{11}$$

Up to now it is not clear whether a solution to this equation exists. But if a unique solution exists, it coincides with the function $v_{\mu,\nu}$. In the following we will construct a solution to (11) and show its uniqueness. For this purpose we recursively define the sequence of functions

$$\begin{aligned} v_0(t) &= u_{\nu-\mu}(t)\ , \\ v_k(t) &= t^{\nu-\mu} \int_0^t \tau^{\mu-\nu} e^{(t-\tau)A} B^{(\mu)} v_{k-1}(\tau)\ d\tau\ , \quad k \geq 1\ . \end{aligned}$$

We conclude by induction that the functions v_k are continuous for $t \in (0, T]$, and

$$\begin{aligned} \|v_k(t)\|_X &\leq C \frac{CM^{(\mu)}t}{\mu-\nu+1}\ \frac{C^{k-1}{M^{(\mu)}}^{k-1}t^{k-1}}{(\mu-\nu+2)\cdots(\mu-\nu+k)} \|x\|_X \\ &\leq C \frac{CM^{(\mu)}t}{\mu-\nu+1}\ \frac{C^{k-1}{M^{(\mu)}}^{k-1}t^{k-1}}{(k-1)!} \|x\|_X \end{aligned}$$

for $k \geq 1$ and $\nu - \mu < 1$. We now set

$$v(t) = \sum_{k\geq 0} v_k(t)\ .$$

If we consider

$$\begin{aligned} \sum_{k\geq 0} \|v_k(t)\|_X &\leq C\Big(1 + \frac{CM^{(\mu)}t}{\mu-\nu+1} \sum_{k\geq 0} \frac{C^n {M^{(\mu)}}^k t^k}{k!}\Big)\|x\|_X \\ &\leq C e^{CM^{(\mu)}t} \|x\|_X\ , \end{aligned}$$

we observe that the series converges uniformly. Therefore v is continuous for $t \in (0, T]$ and every $x \in X$. It is straightforward to check that v is a solution to the integral equation (11). The uniqueness of the solution is shown by a contradiction argument and using a continuous Gronwall inequality, see Lemma A.1. Hence $v(t) = v_{\mu,\nu}(t)$. The last inequality then induces the desired bound.

Now we consider the case $\mu = 0$ and $\nu = 1$ and obtain

$$\begin{aligned}\|e^{tJ}tA\|_{X\leftarrow X} &\leq \|e^{tJ}tJ\|_{X\leftarrow X} + \|e^{tJ}tB\|_{X\leftarrow X} \\ &= \|tJe^{tJ}\|_{X\leftarrow X} + \|e^{tJ}tB\|_{X\leftarrow X} \leq C(1+tM^{(0)}) \ .\end{aligned}$$

The last case $\mu = -1$ and $\nu = 0$ follows analogously. □

Lemma 3. *Under the same assumptions as before, the bound*

$$\|(-tA)^{-\mu}\left(e^{tJ} - e^{tA}\right)(-tA)^{\nu}\|_{X\leftarrow X} \leq Ct \ , \quad t \in (0,T] \ ,$$

holds for a pair of μ and ν, such that there is a λ with $\lambda - \mu, \nu - \lambda < 1$ and with a constant C that depends on T and $M^{(\lambda)}$.

Proof. Similar to the previous proof, we incorporate the integral representation (10) for the difference of the two semigroups. Let $x \in X$ be arbitrary. Then we obtain

$$\begin{aligned}&(-tA)^{-\mu}(e^{tJ} - e^{tA})(-tA)^{\nu}x \\ &= t^{\nu-\mu}\int_0^t (-A)^{-\mu}e^{(t-\tau)A}Be^{\tau J}(-A)^{\nu}x \ d\tau \\ &= t^{\nu-\mu}\int_0^t (-A)^{\lambda-\mu}e^{(t-\tau)A}B^{(\lambda)}(-A)^{-\lambda}e^{\tau J}(-A)^{\nu}x \ d\tau \ .\end{aligned}$$

We apply the previous lemma to $(-\tau A)^{-\lambda}e^{\tau J}(-\tau A)^{\nu}$ and make use of the standard bound on analytic semigroups (2) for the term $(-(t-\tau)A)^{\lambda-\mu}e^{(t-\tau)A}$ to obtain

$$\|(-tA)^{-\mu}(e^{tJ} - e^{tA})(-tA)^{\nu}x\|_X \leq CM^{(\lambda)}t^{\nu-\mu}\int_0^t (t-\tau)^{\mu-\lambda}\tau^{\lambda-\nu} \ d\tau\|x\|_X \ .$$

Thus, we can conclude the assertion. □

Now we are ready to state the main results of this section. The proofs use similar techniques to e.g. [16].

Lemma 4. *Let A be the generator of an analytic semigroup, $J_k = A + B_k$ with uniformly bounded perturbations B_k and $t_{n+1} = (n+1)h$ with $h > 0$. Then for $\beta \in [0,1)$, the composition of perturbed analytic semigroups satisfies the bound*

$$\|e^{hJ_n}\cdots e^{hJ_0}(-t_{n+1}A)^{\beta}\|_{X\leftarrow X} \leq C$$

with a constant C that depends on $M_k^{(0)}$ and T, but not on h or n.

Proof. To begin with, we expand the composition of the perturbed semigroups into a telescopic sum where the first two terms are treated explicitly,

$$
\begin{aligned}
S_{n,0}(-t_{n+1}A)^\beta = e^{t_{n+1}A}(-t_{n+1}A)^\beta &+ t_{n+1}^\beta e^{(t_{n+1}-t_1)A}\left(e^{hJ_0}-e^{hA}\right)(-A)^\beta \\
&+ t_{n+1}^\beta \sum_{k=1}^{n} e^{(t_{n+1}-t_{k+1})A}\left(e^{hJ_k}-e^{hA}\right) S_{k-1,0}(-A)^\beta \ .
\end{aligned}
$$

The first of the three parts is readily bounded by the standard bound on analytic semigroups (2). For the second term the fractional power of $-A$ appears together with the difference of the perturbed semigroups. Thus we use Lemma 3 with $0 < \nu = \beta < 1$ and $\mu = \lambda = 0$. The remaining sum yields a sum which can be treated by a Gronwall lemma using Lemma 3 with $\mu = \nu = 0$,

$$
\begin{aligned}
\|S_{n,0}(-t_{n+1}A)^\beta\|_{X\leftarrow X} \le C &+ t_{n+1}^\beta C h^{1-\beta} M_0^{(0)} \\
&+ t_{n+1}^\beta C \sum_{k=1}^{n} h M_k^{(0)} t_k^{-\beta} \|S_{k-1,0}(-t_k A)^\beta\|_{X\leftarrow X} \ .
\end{aligned}
$$

Since we consider the problem on a bounded time domain $[0,T]$, we obtain

$$
\|S_{n,0}(-t_{n+1}A)^\beta\|_{X\leftarrow X} \le C + C\sum_{k=1}^{n} h t_k^{-\beta} \|S_{k-1,0}(-t_k A)^\beta\|_{X\leftarrow X} \ .
$$

To this estimate we apply the simple version of the discrete Gronwall Lemma A.2, and obtain the desired result with a constant depending on the sum

$$
\sum_{k=1}^{n} h t_k^{-\beta} \le C t_{n+1}^{1-\beta} \le C T^{1-\beta} \ ,
$$

which was bounded using Lemma B.1. Thus we obtain the desired result. □

Lemma 5. *Let A be the generator of an analytic semigroup, $J_k = A + B_k$ with uniformly bounded perturbations B_k, and $t_{n+1} = (n+1)h$ with $h > 0$. Then for $\beta \in [1,2)$, the composition of perturbed analytic semigroups satisfies the bound*

$$
\|e^{hJ_n}\cdots e^{hJ_0}(-t_{n+1}A)^\beta\|_{X\leftarrow X} \le C
$$

with a constant C that depends on T, $M_k^{(0)}$ as well as $M_0^{(\eta)}$ for some $\eta \in (\beta-1,1)$, but not on h or n.

Proof. Following the same lines as the previous proof yields too pessimistic bounds. Thus we slightly alter the proof. To begin with, we split the composition of the perturbed semigroups into

$$S_{n,0}(-t_{n+1}A)^{\beta} = e^{t_{n+1}A}(-t_{n+1}A)^{\beta} + \left(S_{n,0} - e^{t_{n+1}A}\right)(-t_{n+1}A)^{\beta} \ .$$

The first term is directly bounded by a constant using (2). The main part of the proof is to bound the second term, which we denote by $t_{n+1}^{\beta}\Delta_n$ and expand into a telescopic sum,

$$\begin{aligned}
\Delta_n &= \left(S_{n,0} - e^{t_{n+1}A}\right)(-A)^{\beta} \\
&= \sum_{k=0}^{n} e^{(t_{n+1}-t_{k+1})A}(e^{hJ_k} - e^{hA})S_{k-1,0}(-A)^{\beta} \\
&= \sum_{k=0}^{n} e^{(t_{n+1}-t_{k+1})A}(e^{hJ_k} - e^{hA})\left(\Delta_{k-1} + e^{t_kA}(-A)^{\beta}\right) \ ,
\end{aligned}$$

using the convention $\Delta_{-1} = 0$. The operator norm of the part of the sum that contains the Δ_{k-1} yields a sum which can be treated by a Gronwall lemma using the standard bound for analytic semigroups (2) and Lemma 3 for $\mu = \nu = 0$,

$$\left\| \sum_{k=1}^{n} e^{(t_{n+1}-t_{k+1})A}(e^{hJ_k} - e^{hA})\Delta_{k-1} \right\|_{X\leftarrow X} \le C \sum_{k=1}^{n} h\|\Delta_{k-1}\|_{X\leftarrow X} \ .$$

For the remaining terms we insert identity operators $(-A)^{\eta}(-A)^{-\eta}$ for some $\eta \in (\beta - 1, 1)$ and obtain

$$\begin{aligned}
(\star) :&= \sum_{k=0}^{n} e^{(t_{n+1}-t_{k+1})A}(e^{hJ_k} - e^{hA})e^{t_kA}(-A)^{\beta} \\
&= \sum_{k=1}^{n-1} e^{(t_{n+1}-t_{k+1})A}(-A)^{\eta}(-A)^{-\eta}(e^{hJ_k} - e^{hA})(-A)^{\eta}e^{t_kA}(-A)^{\beta-\eta} \\
&\quad + e^{(t_{n+1}-t_1)A}(-A)^{\eta}(-A)^{-\eta}\left(e^{hJ_0} - e^{hA}\right)(-A)^{\beta} \\
&\quad + \left(e^{hJ_n} - e^{hA}\right)(-A)^{\eta}e^{t_nA}(-A)^{\beta-\eta} \ .
\end{aligned}$$

In order to estimate the operator norm of $(\star)$ the standard bound on analytic semigroups (2) is applied several times. Moreover, we employ Lemma 3 with

$0 < \mu = \nu = \eta < 1$ and $\lambda = 0$ for the first term, for the second term we choose $\mu = \lambda = \eta$ and $\nu = \beta$. Note that this introduces the dependence of the constant C on $M_0^{(\eta)}$. For the last term Lemma 3 is applicable with $\mu = \lambda = 0$ and $\nu = \eta$. This yields

$$\begin{aligned}\|(\star)\|_{X\leftarrow X} \le C \sum_{k=1}^{n-1} h(t_{n+1} - t_{k+1})^{-\eta} t_k^{\eta-\beta} \\ + C(t_{n+1} - t_1)^{-\eta} h^{1-\beta+\eta} + Ch^{1-\eta} t_n^{\eta-\beta} \le Ct_{n+1}^{1-\beta} \; .\end{aligned}$$

For the last inequality, we used Lemma B.2. Putting the estimates together, the operator norm of Δ_n can be bounded by

$$\|\Delta_n\|_{X\leftarrow X} \le Ct_{n+1}^{1-\beta} + C \sum_{k=1}^{n} h \|\Delta_{k-1}\|_{X\leftarrow X} \; .$$

We now employ the general case of the discrete Gronwall Lemma A.2 and Lemma B.1 which yields

$$\|\Delta_n\|_{X\leftarrow X} \le Ct_{n+1}^{1-\beta} + C \sum_{k=1}^{n} h t_k^{1-\beta} \le Ct_{n+1}^{1-\beta} + Ct_{n+1}^{2-\beta} \; .$$

Recall that in the operator bound of the first equation of this proof $\|\Delta_n\|_{X\leftarrow X}$ is multiplied by t_{n+1}^{β}. Thus the powers of t_{n+1} are always positive and can therefore be estimated on bounded time intervals by T. Combining all bounds concludes the proof. □

5. Convergence proof

In this section we employ the results on the composition of perturbed semigroups from Section 4 and conclude the proof of Theorem 1.

Proof of Theorem 1. Following the standard procedure in the error analysis of exponential time stepping methods, we derive a defect representation of the error. To this end we employ the abbreviation $G_n(t) = g_n(u(t))$ where $u(t)$ is the exact solution and consider

$$u(t_{n+1}) = e^{hJ_n} u(t_n) + h\varphi_1(hJ_n) G_n(t_n) + \delta_{n+1}$$

which is equivalent to

$$\delta_{n+1} = h\int_0^1 e^{(1-\tau)hJ_n} G_n(t_n + h\tau)\, d\tau - h\varphi_1(hJ_n)G_n(t_n) \tag{12}$$

using the variation of constants formula (3) applied to the linearised equation (5). Thus, the error of the exponential Rosenbrock-Euler method is given by the recursion relation

$$\begin{aligned} e_{n+1} &= u_{n+1} - u(t_{n+1}) = e^{hJ_n} e_n + h\varphi_1(hJ_n)\big(g_n(u_n) - G_n(t_n)\big) - \delta_{n+1}\ , \\ e_0 &= 0\ , \end{aligned}$$

assuming that we start with the exact initial value. The solution of the recursion is given by

$$e_{n+1} = \sum_{k=0}^{n} S_{n,k+1}\Big(h\varphi_1(hJ_k)\big(g_k(u_k) - G_k(t_k)\big) - \delta_{k+1}\Big)\ . \tag{13}$$

Here we used the notation for the composition of the semigroups with generators J_k given in equation (9). Note that we set $S_{n,n+1} = I$.

We thus remain with the task of bounding the term (13). For its first part we obtain

$$\Big\|\sum_{k=1}^{n} S_{n,k+1} h\varphi_1(hJ_k)\big(g_k(u_k) - G_k(t_k)\big)\Big\|_X \le CL\sum_{k=1}^{n} h\|S_{n,k+1}\|_{X\leftarrow X}\|e_k\|_X$$

by using the Lipschitz continuity of g_k. With the bound for compositions of perturbed semigroups (see Lemma 4) we obtain $\|S_{n,k+1}\|_{X\leftarrow X} \le C$.

Next we consider the second term of (13), namely the sum over the defects

$$\sum_{k=0}^{n} S_{n,k+1}\delta_{k+1} = S_{n,1}\delta_1 + \delta_{n+1} + \sum_{k=1}^{n-1} S_{n,k+1}\delta_{k+1}\ .$$

In order to estimate this, we expand $G_k(t_k+h\tau)$ from (12) into a Taylor series. For $k = 0$ and $k = n$ we expand up to order one and for the remaining part of the sum up to order two,

$$\begin{aligned} \delta_{k+1} &= h^2\int_0^1 e^{(1-\tau)hJ_k}\int_0^\tau G_k'(t_k + h\sigma)\, d\sigma\, d\tau \\ &= h^2\varphi_2(hJ_k)G_k'(t_k) + h^3\int_0^1 e^{(1-\tau)hJ_k}\int_0^\tau (\tau - \sigma)G_k''(t_k + h\sigma)\, d\sigma\, d\tau\ . \end{aligned}$$

Denoting the integrals of the h^3-term by $\delta_{k+1}^{(3)}$, this yields

$$\begin{aligned}\sum_{k=1}^{n-1} S_{n,k+1}\delta_{k+1} &= \sum_{k=1}^{n-1} S_{n,k+1}h^2\varphi_2(hJ_k)G_k'(t_k) + \sum_{k=1}^{n-1} S_{n,k+1}h^3\delta_{k+1}^{(3)} \\ &=: \Sigma_n^{(2)} + \Sigma_n^{(3)}\end{aligned}$$

for the inner terms. We first consider $\Sigma_n^{(2)}$ which can be bounded by

$$\begin{aligned}\|\Sigma_n^{(2)}\|_X &\leq \sum_{k=1}^{n-1} h^2 \|S_{n,k+1}\|_{X\leftarrow X}\|\varphi_2(hJ_k)\|_{X\leftarrow X}\|G_k'(t_k)\|_X \\ &\leq C\sum_{k=1}^{n-1} h^2\|G_k'(t_k)\|_X \ .\end{aligned}$$

Here we take advantage of the definition of g_k and therefore of the linearisation. Thus, we obtain

$$\|G_k'(t_k)\|_X = \big\|\big(\mathrm{D}f(u(t_k)) - \mathrm{D}f(u_k)\big)u'(t_k)\big\|_X \leq C\|e_k\|_X t_k^{\alpha-1} \ .$$

The error of the method is then given by

$$\|e_{n+1}\|_X \leq C\sum_{k=1}^{n} h\|e_k\|_X + a_{n+1} \leq a_{n+1} + C\sum_{k=1}^{n} ha_k$$

with $a_1 = \|\delta_1\|_X$, $a_2 = \|\delta_2\|_X + \|S_{1,1}\delta_1\|_X$ and $a_{n+1} = \|\delta_{n+1}\|_X + \|S_{n,1}\delta_1\|_X + \|\Sigma_n^{(3)}\|_X$ for $n > 1$ using the discrete Gronwall Lemma A.2.

We first consider the defects δ_{n+1} without the composition of the perturbed semigroups. In the case of $n > 0$ this can be bounded directly by

$$\|\delta_{n+1}\|_X \leq Ch^2\int_0^1\int_0^\tau \|G_n'(t_n + h\sigma)\|_X \ d\sigma \ d\tau \leq Ch^2 t_n^{\alpha-1}$$

where we used $\|G_n'(t_n+h\sigma)\|_X = \|\mathrm{D}g_n(u(t_n+h\sigma))u'(t_n+h\sigma)\|_X$ as well as the bound on the derivative of the solution given in (4). In the case $n = 0$ we insert a fractional power of $(-A)^{-\nu}(-A)^{\nu}$ for either $\nu = \beta$ or $\nu = \eta$ or $\nu = 0$ such that $\alpha + \nu > 0$ and $0 \leq \nu < 1$. This yields

$$\|\delta_1\|_X \leq h^2\int_0^1 \|e^{(1-\tau)hJ_0}(-A)^{\nu}\|_{X\leftarrow X}\int_0^\tau \|(-A)^{-\nu}G_0'(h\sigma)\|_X \ d\sigma \ d\tau \ .$$

From the bound of the derivative of the solution given in (4) we can deduce

$$\begin{aligned}\|(-A)^{-\nu}G_0'(t)\|_X &\le \|(-A)^{-\nu}\mathrm{D}g_0(u(t))(-A)^{\nu}\|_{X\leftarrow X}\|(-A)^{-\nu}u'(t)\|_X \\ &\le Ct^{\alpha+\nu-1}\end{aligned}$$

which requires condition (7) for $\nu=\beta$ or $\nu=\eta$ for $\alpha=0$. For the first defect we thus obtain

$$\|\delta_1\|_X \le Ch^2\int_0^1 \big((1-\tau)h\big)^{-\nu}\int_0^\tau \big(h\sigma\big)^{\alpha+\nu-1}\,d\sigma\,d\tau \le Ch^{1+\alpha}$$

using Lemma 2 with $\mu=0$. Note that the integrals exist for our choice of ν.

Next, we consider the defect of the first time step multiplied by a composition of perturbed semigroups. We again insert identity operators in form of fractional powers of $-A$ and obtain

$$\begin{aligned}&\|S_{n,1}\delta_1\|_X \\ &= h^2\Big\|S_{n,1}(-A)^{\beta}\int_0^1 (-A)^{-\beta}e^{(1-\tau)hJ_0}(-A)^{\beta}\int_0^\tau (-A)^{-\beta}G_0'(h\sigma)\,d\sigma\,d\tau\Big\|_X \\ &\le h^2\|S_{n,1}(-A)^{\beta}\|_{X\leftarrow X}\int_0^1 \|(-A)^{-\beta}e^{(1-\tau)hJ_0}(-A)^{\beta}\|_{X\leftarrow X} \\ &\qquad\qquad \int_0^\tau \|(-A)^{-\beta}G_0'(h\sigma)\|_X\,d\sigma\,d\tau\ .\end{aligned}$$

Similarly as above and at the cost of condition (7) for β we can estimate $\|(-A)^{-\beta}G_0'(h\sigma)\|_X$ and apply Lemma 2 with $\mu=\nu=\beta$. Since $\alpha+\beta>0$, the integral remains bounded and we obtain

$$\|S_{n,1}\delta_1\|_X \le Ch^{1+\alpha+\beta}\|S_{n,1}(-A)^{\beta}\|_{X\leftarrow X} \le Ch^{1+\alpha+\beta}(t_{n+1}-t_1)^{-\beta}\ .$$

The last inequality follows from the analytical versions of the bounds for compositions of perturbed semigroups from Lemma 4 or Lemma 5 for $0\le\beta<1$ or $1\le\beta<2$, respectively.

It remains to bound the last part $\Sigma_n^{(3)}$ of the sum over the defects. We first consider a single addend and insert fractional powers of $-A$ again. This yields

$$\begin{aligned}P_k := S_{n,k+1}(-A)^{\beta}&\int_0^1 (-A)^{-\beta}e^{(1-\tau)hJ_k}(-A)^{\beta} \\ &\qquad\int_0^\tau (\tau-\sigma)(-A)^{-\beta}G_k''(t_k+h\sigma)\,d\sigma\,d\tau\ .\end{aligned}$$

For the second derivative $(-A)^{-\beta}G_k''(t)$ we compute the estimate

$$\begin{aligned}\|(-A)^{-\beta}G_k''(t)\|_X &\le \|(-A)^{-\beta}\mathrm{D}g_k(u(t))(-A)^{\beta}\|_{X\leftarrow X}\|(-A)^{-\beta}u''(t)\|_X \\ &\qquad + \|(-A)^{-\beta}\mathrm{D}^2 f(u(t))(u'(t),u'(t))\|_X \\ &\le Ct^{\gamma_2(\beta)}\end{aligned}$$

using both conditions (7) and (8) as well as the bounds on the derivatives of the exact solution (4). Thus, we obtain

$$\begin{aligned}\|P_k\|_X &\le \|S_{n,k+1}(-A)^{\beta}\|_{X\leftarrow X}\int_0^1 \|(-A)^{-\beta}e^{(1-\tau)hJ_k}(-A)^{\beta}\|_{X\leftarrow X} \\ &\qquad \int_0^\tau (\tau-\sigma)\|(-A)^{-\beta}G_k''(t_k+h\sigma)\|_X \; d\sigma \; d\tau \\ &\le C(t_{n+1}-t_{k+1})^{-\beta}\int_0^1\int_0^\tau (\tau-\sigma)(t_k+h\sigma)^{\gamma_2(\beta)} \; d\sigma \; d\tau \\ &\le C(t_{n+1}-t_{k+1})^{-\beta}t_k^{\gamma_2(\beta)}\end{aligned}$$

employing the bounds for the composition of perturbed semigroups from the previous section for β as well as Lemma 2 with condition (7) and taking into account that the integrals are bounded. Hence, we obtain

$$\begin{aligned}\|\Sigma_n^{(3)}\|_X &\le \sum_{k=1}^{n-1} h^3\|P_k\|_X \le C\sum_{k=1}^{n-1} h^3(t_{n+1}-t_{k+1})^{-\beta}t_k^{\gamma_2(\beta)} \\ &\le Ch^2\Big(t_{n+1}^{-\beta}\int_h^T \tau^{\gamma_2(\beta)} \; d\tau + t_{n+1}^{\gamma_2(\beta)}\int_h^T \tau^{-\beta} \; d\tau\Big)\end{aligned}$$

by applying Lemma B.2.

Now that we have bounds for all individual terms appearing in the error we can estimate the sum $\sum_{k=1}^n ha_k$ from the Gronwall lemma. We split it into three parts and use Lemma B.1 several times for all of them. Firstly we have

$$\sum_{k=1}^n h\|\delta_k\|_X \le Ch^{2+\alpha} + C\sum_{k=2}^n h^3 t_{k-1}^{\alpha-1} \le Ch^2\int_h^T \tau^{\alpha-1} \; d\tau \; .$$

Next consider

$$\sum_{k=2}^{n} h\|S_{k-2,1}\delta_1\|_X \le C\sum_{k=2}^{n} h^{2+\alpha+\beta}(t_k-t_1)^{-\beta}$$
$$\le Ch^{1+\alpha+\beta}\int_{t_2}^{t_{n+1}}(\tau-t_1)^{-\beta}\,d\tau \le Ch^{1+\alpha+\beta}\int_h^T \tau^{-\beta}\,d\tau\ .$$

Finally we estimate

$$\sum_{k=3}^{n} h\|\Sigma_{k-1}^{(3)}\|_X$$
$$\le Ch^2\Big(\int_h^T \tau^{\gamma_2(\beta)}\,d\tau\ \sum_{k=3}^{n} ht_k^{-\beta} + \int_h^T \tau^{-\beta}\,d\tau\ \sum_{k=3}^{n} ht_k^{\gamma_2(\beta)}\Big)$$
$$\le Ch^2\int_h^T \tau^{\gamma_2(\beta)}\,d\tau\ \int_h^T \tau^{-\beta}\,d\tau\ .$$

Combining all bounds yields the desired bound.

In the course of the proof we used the bounds on the composition of perturbed semigroups from Lemma 4 and in the case of $1\le\beta<2$ also from Lemma 5. This requires the operators $B_k^{(0)}$, and in the case of Lemma 5 also $B_k^{(\eta)}$ for $\eta\in(1-\beta,1)$, to be uniformly bounded. This is indeed the case since

$$B_k^{(0)} = J_k - A = \mathrm{D}f(u_k)\ ,$$

and the Fréchet derivative of f is bounded in a strip along the exact solution. In the case of $1\le\beta<2$, we also need to consider

$$B_k^{(\eta)} = (-A)^{-\eta}(J_k-A)(-A)^{\eta} = (-A)^{-\eta}\mathrm{D}f(u_k)(-A)^{\eta}$$

for some $\eta\in(\beta-1,1)$ which results in the additional condition (7) for η. This completes the proof. □

6. Discussion of the assumptions and examples

The assumptions (7) and (8) on the nonlinearity of the initial value problem (1) need some discussion. We only give the details for (7) since the discussion for (8) follows the same lines by fixing one argument of the bilinear form. Inequality (7) holds of course true if A and $B = \mathrm{D}f(v)$ commute for all v in a strip along the exact solution. Since commutativity is a rather strict assumption, which we would like to avoid, it is interesting to discuss whether the product of the operators can be bounded otherwise. A direct estimate of the three operators one by one is not feasible since we want to apply the product to elements of X for which $(-A)^\beta$ is unbounded for positive β. In general the product of these operators can be estimated by extending the space X to spaces $V_{-\beta}$ such that $(-A)^\beta : X \to V_{-\beta}$ as well as $(-A)^{-\beta} : V_{-\beta} \to X$ are bounded. This leads to the question, whether $V_{-\beta}$ is invariant under the operation of B. But these spaces are rather unhandy for actual computation. Therefore, for reflexive spaces X we choose the characterisation via the dual problem. Thus, for $x \in V_\beta$ consider

$$\begin{aligned} \|(-A)^{-\beta} B (-A)^\beta x\|_X &= \sup_{\substack{y \in X^\star \\ \|y\|_{X^\star} \le 1}} |\langle y, (-A)^{-\beta} B (-A)^\beta x \rangle| \\ &= \sup_{\substack{y \in X^\star \\ \|y\|_{X^\star} \le 1}} |\langle (-A^\star)^\beta B^\star (-A^\star)^{-\beta} y, x \rangle| \ . \end{aligned}$$

This expression is bounded if $\|(-A^\star)^\beta B^\star (-A^\star)^{-\beta}\|_{X^\star \leftarrow X^\star}$ is bounded. The dual operator is easier to handle than the original operator since here we first apply the bounded operator. This composition of operators is bounded if $\mathcal{D}((-A^\star)^\beta)$ is invariant under the operation of $B^\star$. In that case the second expression is bounded for all $x \in X$ and we can interpret $(-A)^{-\beta} B (-A)^\beta$ as the adjoint operator of the bounded operator $(-A^\star)^\beta B^\star (-A^\star)^{-\beta} : X^\star \to X^\star$, which is defined and bounded on all of X.

Let us restrict ourselves even further and consider the Sobolev setting, where the dual space of $V_{-\beta}$ coincides with V_β. We consider $\Omega = \mathbb{R}^d$, the d-dimensional torus $\Omega = \mathbb{T}^d$ with periodic boundary conditions or an open subset $\Omega \subset \mathbb{R}^d$ with homogeneous Dirichlet boundary conditions and set $X = L_2(\Omega)$.

For a generator of an analytic semigroup A, we know form [14, Proposition 2.2.15] that the domains $V_\alpha = \mathcal{D}((-A)^\alpha)$ of fractional powers of A are interpolation spaces of V_1 and X. Thus for a nonnegative selfadjoint strongly elliptic second order differential operator A such that $V_1 = H^2(\Omega)$ for $\Omega = \mathbb{R}^d$ or $\Omega = \mathbb{T}^d$ we can identify V_α with $H^{2\alpha}(\Omega)$ since $V_1 = \mathcal{D}(A)$ and $H^2(\Omega)$ yield the same interpolation spaces with respect to complex interpolation with X.

In the case of Ω being an open subset of $\mathbb{R}^d$ the case is slightly more complicated. We have $H_0^2(\Omega) \subset V_1 = H^2(\Omega) \cap H_0^1(\Omega) \subset H^2(\Omega)$ and consider the interpolation spaces for each of these spaces with $X = L_2(\Omega)$. The fractional Sobolev spaces $H^{2\alpha}(\Omega)$ can be defined by interpolation of $H^2(\Omega)$ with X. The same holds for $H_0^2(\Omega)$ except for 2α being an integer plus $1/2$, see [11, Theorem 11.6]. By construction of the interpolation methods the inclusion $V_1 \subset H^2(\Omega)$ yields $V_\alpha \subseteq H^{2\alpha}(\Omega)$ for all α and $H_0^{2\alpha}(\Omega) \subseteq V_\alpha$ for most α since we interpolate with the same space X. Thus in all cases it is sufficient to check the assumptions in $H^{2\alpha}(\Omega)$.

A wide range of applications yields a multiplier for $\mathrm{D}f(v)$, namely a function g which defines a bounded linear operator on X by pointwise multiplication. An extensive characterisation of multipliers for which fractional Sobolev spaces stay invariant can be found in the paper of Strichartz [21].

As a first example let us consider the class of equations with analytic functions (possibly with the constant term equal to zero depending on whether the constant functions are part of the space in question) of the solution as nonlinearities. This includes e.g. reaction-diffusion equations modelling problems from chemical reactions over combustion theory to population spreading. Prominent examples of equations are the Allen-Cahn equation with $f(u) = u^2 - u^3$, Fisher's equation with $f(u) = u - u^2$ and the Zeldovich equation with $f(u) = u(1-u)(u-a)$ for $0 < a < 1$.

We know from [21] that $H^{2\beta}(\Omega)$ for $\Omega \subset \mathbb{R}^d$ one of the above is invariant under pointwise multiplication with its own functions if $2\beta > d/2$. This yields the inequalities (7) and (8) for any $\beta > 1/4$ in the one-dimensional case, i.e. for $d = 1$. Note that this calculation directly extends to analytic functions of the solution as multipliers.

The results from Theorem 1 can now be applied to the one-dimensional case for initial data $u_0 \in V_\alpha \subseteq H^{2\alpha}(\Omega)$ for any $\alpha > 1/4$. Due to the smoothing property of the parabolic problem as well as the fact that $f(u(t)) \in V_\alpha \subset X$ for all t the solution stays in V_α for all times. In this case the condition $1 > \beta > 3/4 > 1 - \alpha$ can always be fulfilled.

Therefore, for a large class of applications we obtain full convergence order 2 for initial data only in $H^{2\alpha}(\mathbb{R})$ for $\alpha > 1/4$. For initial conditions which are less smooth the operator $(-A)^{-\beta}B(-A)^{\beta}$ looses smoothness. Moreover, the nonlinearity f does not necessarily map X onto itself anymore. Therefore the assumptions from Theorem 1 are no longer satisfied.

We demonstrate this experimentally for the example of an exponential

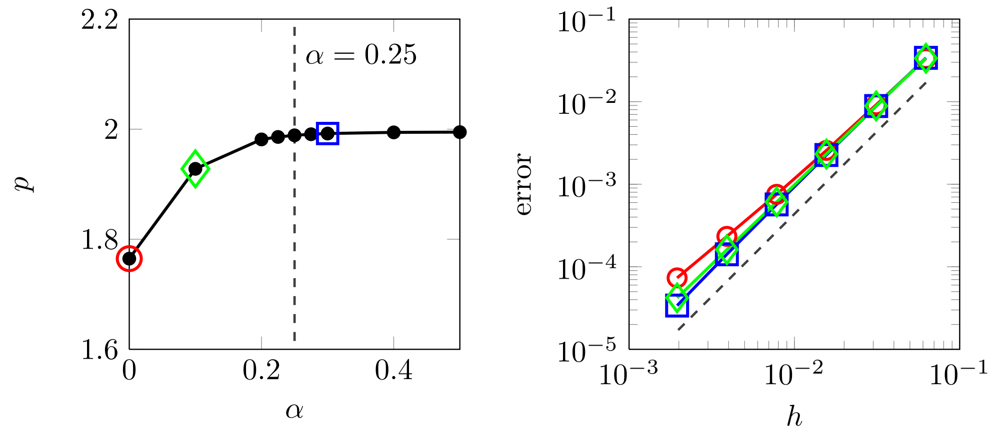

Figure 1: **Left:** The numerically computed order is plotted versus the smoothness parameter α of the initial condition. **Right:** The error is plotted versus the time step size in a double logarithmic plot for a few chosen values of α. The dashed line indicates order 2 as reference.

reaction model

$$u'(t,z) = \partial_z^2 u(t,z) + e^{u(t,z)} \ , \quad (t,z) \in [0,1] \times [0,1] \ ,$$

with periodic boundary conditions. Here we have $X = L_2([0,1])$ and $V_1 = H^2_{\text{per}}([0,1])$. To construct initial values which are contained in V_α for a given α we consider a function v_0 represented as a Fourier expansion

$$v_0(z) = \sum_{k\in\mathbb{Z}} \hat{v}_k^{(0)} e^{i2\pi k}$$

which is in $L_2([0,1])$ if the coefficients satisfy

$$\sum_{k\in\mathbb{Z}} |\hat{v}_k^{(0)}|^2 < \infty \ .$$

We choose $\hat{v}_k^{(0)} = (1+(2\pi k)^2)^{-1/4-\varepsilon}$ for arbitrary small $\varepsilon > 0$ and obtain $v_0 \in L_2([0,1])$. From this we compute $v_\alpha = (I-\partial_z^2)^{-\alpha} v_0 \in V_\alpha$ by setting $\hat{v}_k^{(\alpha)} = (1+(2\pi k)^2)^{-\alpha} \hat{v}_k^{(0)}$ and take $u_\alpha \in V_\alpha$ to be the normalised real part of v_α. For the computation we consider $N = 512$ Fourier modes. Since the cutoff of the Fourier modes already is a smoothing factor for the data, we choose $\varepsilon = 0$ in order to avoid further smoothing. The order is then numerically estimated in the common way for different values of $\alpha \in [0, 0.5]$. In the left part of Figure 1 we plot the numerically computed order versus the smoothness parameter α of the initial condition. In the right part the error is plotted versus the time step size in a double logarithmic plot for a few chosen values of α indicated by similar markers in the left picture. This clearly shows that for $\alpha > 1/4$ we do obtain the predicted order 2. For $\alpha < 1/4$, order reduction can be observed. This gives numerical evidence that the assumptions claimed in Theorem 1 are hard assumptions. Note that for the computation of the φ_1-function of the matrices times a vector we use diagonalisation to avoid any additional errors which might be introduced by computationally more advantageous but approximative iterative methods.

As a second example we discuss the Black-Scholes model for American option pricing. A derivation is given for example in [2], and a numerical convergence study of the exponential Rosenbrock-Euler method applied to this problem is presented in [4], where convergence of order two was observed in numerical experiments. Now let us discuss whether this example fulfils the assumptions for convergence. To that end we restate the particular equations. We consider the value $v(t, z)$ of an American put option. It depends on $t = T - \tau \in \mathbb{R}_0^+$ which denotes the time to expiry for a time horizon T at a given time τ, and the asset price $z \in \mathbb{R}^+$. Further, we consider the payoff function $v^\star(z) = \max(Z - z, 0)$, where Z is the strike price. The shifted value of the option $u(t, z) = v(t, z) - \varphi(z)$, where φ is a smooth L_2-function that satisfies $\varphi(0) = Z$ and $\lim_{z\to\infty} \varphi(z) = 0$, fulfils homogeneous Dirichlet boundary conditions at $z = 0$. Then the Black-Scholes model yields the set of equations

$$
\begin{aligned}
u'(t, z) - Au(t, z) - A\varphi(z) + \rho \min\bigl(u(t, z) + \varphi(z) - v^\star(z), 0\bigr) &= 0 \\
u(0, z) &= v^\star(z) - \varphi(z) \\
u(t, 0) = \lim_{z\to\infty} u(t, z) &= 0
\end{aligned}
$$

with the Black-Scholes operator given as

$$
A = \frac{\sigma^2}{2} z^2 \partial_z^2 + rz\partial_z - rI \ .
$$

The parameters are given by the volatility σ, and the risk-free interest rate r, while ρ is a penalisation parameter.

For this equation we have $\mathcal{D}(A) = H_0^1(\mathbb{R}^+) \cap H^2(\mathbb{R}^+) = V_1$. Furthermore, we know that the optimal exercise price which is the moving boundary of the problem and consists of all z, where $u + \varphi - v^\star = 0$, is a set of measure 0. Therefore, we can calculate the Fréchet derivatives of the nonlinearity. The first Fréchet derivative is a characteristic function as a multiplier and the second Fréchet derivative is zero. Thus the second condition (8) of Assumption 1 is obsolete. In [21] it is shown that for characteristic functions of intervals as multipliers $H^{2\beta}(\mathbb{R}^+) = V_\beta$ stays invariant for $\beta < 1/4$. From the same result we can deduce that the initial condition, which is a continuous, piecewise smooth function, is contained in $H^{2\alpha}(\mathbb{R}^+) = V_\alpha$ for $\alpha < 3/4$. Therefore this problem is just outside the range of the full convergence order 2 of the method since $\beta < 1/4$ contradicts $\beta > 1 - \alpha > 1/4$. Nevertheless, the condition holds for $\beta = 1/4 - \varepsilon_1$ and $\alpha = 3/4 - \varepsilon_2$ which yields convergence order $1 + \alpha + \beta = 2 - \varepsilon_1 - \varepsilon_2$ with arbitrary small $\varepsilon_i > 0$. However, in numerical experiments this would not be distinguishable from full order 2.

As we can see from these two examples, the conditions (7) and (8) are hard assumptions on the problem that we want to solve. Nevertheless, there are classes of examples that satisfy these assumptions even in the case where the operators do not commute.

Acknowledgements

The author would like to thank Alexander Ostermann for the careful reading of the manuscript and a lot of helpful comments, Volker Grimm for many inspiring discussions and Roland Schnaubelt for valuable hints especially to the paper of Strichartz.

This work was supported by the Deutsche Forschungsgemeinschaft via GRK 1294.

Appendix A. Gronwall inequalities

In this section we state the Gronwall lemmata used throughout the paper. Lemma A.1 is a special case of Lemma 4 from [10] whereas Lemma A.2 is a straightforward extension of Lemmata 2 and 3 as well as the comments following Lemma 2 form [10].

Lemma A.1. *Assume that a, b and h are real-valued continuous functions on an interval $[0, T]$, and let b and h be nonnegative. If the continuous function e satisfies*

$$e(t) \leq a(t) + b(t) \int_0^t h(\tau) e(\tau) \; d\tau$$

for all $t \in [0,T]$*, then*

$$e(t) \le a(t) + b(t)\int_0^t h(\tau)a(\tau)e^{\int_\tau^t h(\sigma)b(\sigma)\ d\sigma}\ d\tau$$

holds for all $t \in [0,T]$*.*

Lemma A.2. *Assume that* $(e_n)_n$*,* $(a_n)_n$ *and* $(h)_n$ *be real-valued sequences and let* $(h)_n$ *be nonnegative. If the sequence* $(e_n)_n$ *satisfies*

$$e_n \le a_n + \sum_{k=0}^{n-1} he_k$$

for $n = 0,\ldots,N$*, then*

$$e_n \le a_n + \sum_{k=0}^{n-1} ha_k e^{\sum_{l=k+1}^{n-1} h}$$

is valid for $n = 0,\ldots,N$*. If in addition* $a_n \le C$ *for* $n = 0,\ldots,N$*, then the estimate*

$$e_n \le Ce^{\sum_{k=0}^{n-1} h}$$

holds for $n = 0,\ldots,N$ *with the same constant* C*.*

Appendix B. Two technical sums

Lemma B.1. *For* $h, \alpha > 0$ *and* $t_k = kh$ *the bound*

$$\sum_{k=1}^{n} ht_k^{-\alpha} \le 2^\alpha \int_{t_1}^{t_{n+1}} \tau^{-\alpha}\ d\tau$$

holds.

Proof. This proof is a variant of Lemma 4.10 from [7]. For $\alpha > 0$ we obtain

$$t_{k+1}^{-\alpha} = (t_k + h)^{-\alpha} \ge (2t_k)^{-\alpha} = 2^{-\alpha}t_k^{-\alpha}\ .$$

This yields

$$\sum_{k=1}^{n} ht_k^{-\alpha} \le 2^\alpha \sum_{k=1}^{n} ht_{k+1}^{-\alpha}\ .$$

The latter sum, as opposed to the first sum, is a lower Riemann sum for the integral $\int_{t_1}^{t_{n+1}} \tau^{-\alpha}\ d\tau$ and can thus be bounded by its value. □

Lemma B.2. *For $h, \alpha, \beta > 0$ and $t_k = kh$ the bound*

$$\sum_{k=1}^{n-1} h t_k^{-\alpha} (t_{n+1} - t_{k+1})^{-\beta} \le C\Big(t_{n+1}^{-\beta} \int_h^{t_{n+1}} \tau^{-\alpha} \, d\tau + t_{n+1}^{-\alpha} \int_h^{t_{n+1}} \tau^{-\beta} \, d\tau \Big)$$

holds with a constant C that depends on α and β, but is independent of h and n.

Proof. We choose the index $n_\star = \lceil \frac{n+1}{2} \rceil$ and divide the sum into two parts. In each sum, the decaying part is bounded by the value at $\frac{t_{n+1}}{2}$,

$$\begin{aligned}
&\sum_{k=1}^{n_\star} h t_k^{-\alpha} (t_{n+1} - t_{k+1})^{-\beta} + \sum_{k=n_\star+1}^{n-1} h t_k^{-\alpha} (t_{n+1} - t_{k+1})^{-\beta} \\
&\le \Big(\frac{t_{n+1}}{2}\Big)^{-\beta} \sum_{k=1}^{n_\star} h t_k^{-\alpha} + \Big(\frac{t_{n+1}}{2}\Big)^{-\alpha} \sum_{k=n_\star+1}^{n-1} h (t_{n+1} - t_{k+1})^{-\beta} \\
&\le C t_{n+1}^{-\beta} \sum_{k=1}^{n} h t_k^{-\alpha} + C t_{n+1}^{-\alpha} \sum_{k=0}^{n-1} h (t_{n+1} - t_{k+1})^{-\beta} \ .
\end{aligned}$$

To both remaining sums, in the latter case with the transformation $\tilde{t} = t_{n+1} - t$, we apply the previous Lemma and obtain the desired result. □

References

[1] M. Crouzeix and V. Thomée. On the discretization in time of semilinear parabolic equations with nonsmooth initial data. *Math. Comp.*, 49(180):359–377, 1987.

[2] J. de Frutos. Implicit-explicit Runge-Kutta methods for financial derivatives pricing models. *European J. Oper. Res.*, 171(3):991–1004, 2006.

[3] H. De la Cruz, R.J. Biscay, F. Carbonell, T. Ozaki, and J.C. Jimenez. A higher order local linearization method for solving ordinary differential equations. *Appl. Math. Comput.*, 185(1):197–212, 2007.

[4] M.A. Gondal. Exponential Rosenbrock integrators for option pricing. *J. Comput. Appl. Math.*, 234(4):1153–1160, 2010.

[5] C. González, A. Ostermann, C. Palencia, and M. Thalhammer. Backward Euler discretization of fully nonlinear parabolic problems. *Math. Comp.*, 71(237):125–145 (electronic), 2002.

[6] D. Henry. *Geometric theory of semilinear parabolic equations*, volume 840 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin-New York, 1981.

[7] M. Hochbruck, M. Hönig, and A. Ostermann. A convergence analysis of the exponential Euler iteration for nonlinear ill-posed problems. *Inverse Problems*, 25(7):075009, 18, 2009.

[8] M. Hochbruck and A. Ostermann. Explicit integrators of Rosenbrock-type. *Oberwolfach Reports*, 3(2):1107–1110, 2006.

[9] M. Hochbruck, A. Ostermann, and J. Schweitzer. Exponential Rosenbrock-type methods. *SIAM J. Numer. Anal.*, 47(1):786–803, 2008/09.

[10] G.S. Jones. Fundamental inequalities for discrete and discontinuous functional equations. *J. Soc. Indust. Appl. Math.*, 12:43–57, 1964.

[11] J.-L. Lions and E. Magenes. *Non-homogeneous boundary value problems and applications. Vol. I.* Springer-Verlag, New York-Heidelberg, 1972. Translated from the French by P. Kenneth, Die Grundlehren der mathematischen Wissenschaften, Band 181.

[12] C. Lubich and A. Ostermann. Linearly implicit time discretization of non-linear parabolic equations. *IMA J. Numer. Anal.*, 15(4):555–583, 1995.

[13] C. Lubich and A. Ostermann. Runge-Kutta time discretization of reaction-diffusion and Navier-Stokes equations: nonsmooth-data error estimates and applications to long-time behaviour. *Appl. Numer. Math.*, 22(1-3):279–292, 1996.

[14] A. Lunardi. *Analytic semigroups and optimal regularity in parabolic problems*. Progress in Nonlinear Differential Equations and their Applications, 16. Birkhäuser Verlag, Basel, 1995.

[15] A. Ostermann and M. Thalhammer. Non-smooth data error estimates for linearly implicit Runge-Kutta methods. *IMA J. Numer. Anal.*, 20(2):167–184, 2000.

[16] A. Ostermann and M. Thalhammer. Convergence of Runge-Kutta methods for nonlinear parabolic equations. *Appl. Numer. Math.*, 42(1-3):367–380, 2002.

[17] A. Pazy. *Semigroups of linear operators and applications to partial differential equations*, volume 44 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 1983.

[18] D.A. Pope. An exponential method of numerical integration of ordinary differential equations. *Comm. ACM*, 6:491–493, 1963.

[19] J.I. Ramos and C.M. García-López. Piecewise-linearized methods for initial-value problems. *Appl. Math. Comput.*, 82(2-3):273–302, 1997.

[20] J. Schweitzer. The exponential Rosenbrock-Euler method with variable time step sizes for nonsmooth initial data. Technical report, Karlsruhe Institute of Technology, 2014.

[21] R.S. Strichartz. Multipliers on fractional Sobolev spaces. *J. Math. Mech.*, 16:1031–1060, 1967.

[22] M. Tokman. Efficient integration of large stiff systems of ODEs with exponential propagation iterative (EPI) methods. *J. Comput. Phys.*, 213(2):748–776, 2006.