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EXPONENT SPLITTING SCHEMES FOR EVOLUTION EQUATIONS WITH FRACTIONAL POWERS OF OPERATORS

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Abstract. We have considered the Cauchy problem for a first-order evolutionary equation with fractional powers of an operator. Such nonlocal mathematical models are used, for example, to describe anomalous diffusion processes. We want the transition to a new level in time to be solved usual problems. Computational algorithms are constructed based on some approximations of operator functions. Currently, when solving stationary problems with fractional powers of an operator, the most attention is paid to rational approximations. In the approximate solution of nonstationary problems, we come to equations with an additive representation of the problem operator. Additive-operator schemes are constructed by using different variants of splitting schemes. In the present work, the time approximations are based on approximations of the transition operator by the product of exponents. We use exponent splitting schemes of the first and second-order accuracy. The results of numerical experiments for a two-dimensional model problem with fractional powers of the elliptic operator are presented.

Key words. Evolutionary equation, fractional powers of an operator, rational approximation, exponent splitting scheme, stability of operator-difference schemes.

1. Introduction

Spatial effects in classical applied mathematical models (see, for example, [13, 31]) are described most often by elliptic operators of the second order. We relate dynamic processes to parabolic and hyperbolic equations by second-order equations [18, 39]. A characteristic feature of such models is locality in both time and space. The property of locality is manifested in the fact that we write all the terms of the constitutive equations, boundary and initial conditions at the same space-time points.

More and more attention is paid to the study of nonlocal mathematical models. In this regard, we can note the books [14, 17] and the bibliography is given in them. Nonlocality in time is due to the dependence of the system's state studied at a given point in time on the entire prehistory. Such mathematical descriptions of dynamic processes with memory are based on the use of integral and integrodifferential operators [21, 37]. Often (see, e.g., [6, 45]) these nonlocal-time models are associated with fractional derivatives.

Nonlocal models in space are constructed based on various generalizations of classical elliptic operators [7, 15]. In particular, much attention in the literature is paid to fractional Laplacian [16, 36]. Models using elliptic operator functions are involved to describe nonlocal stationary processes. In this case the fractional Laplacian is associated with the fractional degree of the Laplace operator. Local in time and nonlocal in space models are based on abstract parabolic equations with operator functions [57].

Different approaches are used in the approximate solution of stationary problems with operator functions. First of all, we can focus on the achievements of the theory and practice of methods for solving problems with matrix functions

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[20, 26]. For this purpose, the results of a nonlinear approximation of functions [10] are involved, providing an acceptable computational implementations. In [56] methods of rational approximations, approximations by sum and product of exponents with applications to problems with fractional powers of an operator have been distinguished.

We use the spectral definition of the fractional power of a self-adjoint operator in a finite-dimensional Hilbert space. In functional analysis [30] we have a representation based on the Dunford-Taylor integral [28] and the Balakrishnan formula [5]. We note the main approaches for approximate solutions with a fractional power of an operator (see, e.g., [8, 22, 32]) based on rational approximation. The first approach is based on an integral representation using specific quadrature formulas for the Balakrishnan formula [1, 9, 19, 53]. We easily obtain the necessary computational formulas for a rational approximation. The second approach involves using the results of the theory of a best uniform rational approximation of functions [23, 25, 27, 43]. In this case, we can obtain approximations of higher accuracy.

In the approximate solution of nonstationary problems with a fractional power of an operator, we can use standard unconditionally stable implicit time approximations [4, 40]. On the new time level we have a non-standard reaction and fractional diffusion type problems [2, 23, 52]. We can do things a little differently. First, we perform some approximation of a fractional power of an operator, and then we adapt the approximation in time to a peculiarities of the problem. With a rational approximation of a fractional power of an operator, we represent a problem operator as a sum of accessible operators. In this case, we can build time approximations based on the theory of additive operator-difference schemes [33, 48]. Various variants of such splitting schemes are constructed in [12, 51, 55, 54].

In the present paper, the splitting schemes are constructed based on an approximation of the transition operator to a new level in time [34, 48]. For evolution equations of the first order, the transition operator is represented as a product of exponents. For this reason, we call such time approximations exponent splitting schemes. When rational approximations of the fractional power of an operator are used, the operator terms are pairwise permutations. This property allows us to construct exponent splitting schemes most easily.

The paper is organized as follows. In Section 2, the Cauchy problem for the first and second-order evolution equations with a fractional power of a self-adjoint operator in a finite-dimensional Hilbert space is formulated. In Section 3, we discuss the problem of the rational approximations of the fractional power operator for nonstationary problems. The central part Section 4 is devoted to the construction and study of exponent splitting schemes. In Section 5, we address more general evolutionary equations. The results of the numerical solution of the two-dimensional model problem are presented in Section 6. The conclusions follow in Section 7.

2. Problem formulation

After finite-element or finite-volume approximations [29, 38] of elliptic operators, we have discrete analogs in corresponding finite-dimensional spaces. Let H be a finite-dimensional Hilbert space. The scalar product for $u, v \in H$ is (u, v), and the norm is $\|u\| = (u, u)^{1/2}$. For a self-adjoint and positive definite operator D, we define the Hilbert space H_D with scalar product and norm $(u, v)_D = (Du, v)$, $\|u\|_D = (u, v)_D^{1/2}$.

Let A be a self-adjoint positive definite operator ($A : H \to H$):

$$A = A^*, \quad \delta I \le A \le \Delta I, \quad \delta > 0, \tag{1}$$

where I is the identity operator in H.

We use the spectral definition of the fractional powers of the operator. We begin with the spectral problem

$$A\psi = \lambda \psi$$

for the operator A. For the eigenvalues, we have $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_K$, therefore in (1) $\delta = \lambda_1,\ \Delta = \lambda_K$. For each $u \in H$, we have the representation

$$u = \sum_{k=1}^{K} (u, \psi_k) \psi_k$$

via eigenfunctions $\psi_k,\ \|\psi_k\| = 1,\ k = 1, 2, \ldots, K$. For A^α, we have

$$A^\alpha u = \sum_{k=1}^{K} \lambda_k^\alpha (u, \psi_k) \psi_k, \quad 0 < \alpha < 1.$$

The object of our study is the Cauchy problem

$$\frac{du}{dt} + A^\alpha u = f(t), \quad 0 < t \leq T, \tag{2}$$

$$u(0) = u^0. \tag{3}$$

For the approximate solution of the problem (1)–(3), stability estimates for the initial data and the right-hand side are of crucial importance. For the exact solution of the problem (2), (3), we have the representation

$$u(t) = \exp\big(-tA^\alpha\big) u^0 + \int_0^t \exp\big(-(t-s)A^\alpha\big) f(s) ds, \quad 0 < t \leq T. \tag{4}$$

Taking into account (1), from (4), we obtain the a priori estimate

$$\|u(t)\| \leq \exp\big(-\delta^\alpha t\big) \|u^0\| + \int_0^t \exp\big(-\delta^\alpha (t-s)\big) \|f(s)\| ds, \quad 0 < t \leq T.$$

A rougher estimate (non-negative operator A) has the form

$$\|u(t)\| \leq \|u^0\| + \int_0^t \|f(s)\| ds, \quad 0 < t \leq T. \tag{5}$$

We will strive for similar stability estimates for the approximate solution.

We approximate in time using a uniform grid with a step τ. We use the notation $y^n = y(t^n),\ t^n = n\tau,\ n = 0, \ldots, N,\ N\tau = T$. From (4), we obtain

$$u^{n+1} = \exp\big(-\tau A^\alpha\big) u^n + \int_{t^n}^{t^{n+1}} \exp\big(-(t^{n+1}-s)A^\alpha\big) f(s) ds, \quad n = 0, \ldots, N-1. \tag{6}$$

With (5) we associate the estimate on the time level

$$\|u^{n+1}\| \leq \|u^n\| + \int_{t^n}^{t^{n+1}} \|f(s)\| ds, \quad n = 0, \ldots, N-1. \tag{7}$$

An approximate solution of the problem (2), (3) based on the representation (6) is provided, first of all, by choosing some approximation of the transition operator $\exp\big(-\tau A^\alpha\big)$. For the integral term in the right-hand side of (6) some quadrature formula of appropriate accuracy is used. Thus, for the approximate solution we have

$$y^{n+1} = S(A^\alpha) y^n + F^n(A^\alpha, f), \quad n = 0, \ldots, N-1, \tag{8}$$

$$y^0 = u^0, \tag{9}$$

where

$$S(A^\alpha) \approx \exp\big(-\tau A^\alpha,\big), \quad F^n(A^\alpha, f) \approx \int_{t^n}^{t^{n+1}} \exp\big(-(t^{n+1}-s)A^\alpha\big) f(s) ds.$$

In this approach, the problems that A^α generates are solved after approximation by time.

For example, using the Euler explicit discretization, we have $S(A^\alpha) = I - \tau A^\alpha$. In this case, we correlate the equation (2) to equation

$$\frac{y^{n+1}-y^n}{\tau} + A^\alpha y^n = \varphi^n, \quad n = 0, \dots, N-1, \tag{10}$$

with

$$\varphi^n = f^n, \quad F^n(A^\alpha, f) = \tau f^n.$$

The stability conditions of the scheme (1), (9), (10) are well known [40, 41] and have the form $\tau \le 2\|A^\alpha\|^{-1}$. Under these conditions, we have the a priori estimate

$$\|y^{n+1}\| \le \|u^0\| + \tau\|\varphi^n\|, \quad n = 0, \dots, N-1.$$

The computational realization of the scheme (9), (10) is provided by calculating $A^\alpha y^n$. For this purpose, we can use approximations of A^α. We have implemented a similar technique for solving non-stationary problems with fractional powers of an operator in the papers [46, 49].

Using the Euler implicit discretization, we have

$$\frac{y^{n+1}-y^n}{\tau} + A^\alpha y^{n+1} = \varphi^n, \quad n = 0, \dots, N-1, \tag{11}$$

where, for example,

$$\varphi^n = f^{n+1}, \quad F^n(A^\alpha, f) = \tau(I + \tau A^\alpha)^{-1} f^{n+1}.$$

The difference scheme (1), (9), (11) belongs to the class of unconditionally stable schemes. The transition operator is approximated as $S(A^\alpha) = (I + \tau A^\alpha)^{-1}$. The computational difficulties are generated by the need to compute $S(A^\alpha)y^n$ at each time level. We cannot directly use any approximations of the fractional power of the operator. Some rational approximations of $(I + \tau A^\alpha)^{-1}$ are considered in [2, 23, 52].

We consider an approach to an approximate solution of the problem (1)–(3) with a prior approximation of A^α by some operator D. In this case, we approximate (6) by the relation

$$y^{n+1} = S(D)y^n + F^n(D, f), \quad n = 0, \dots, N-1, \tag{12}$$

where

$$D \approx A^\alpha, \quad S(D) \approx \exp\big(-\tau D\big).$$

After choosing the operator D, we construct some approximations $S(D)$ in (12).

3. Rational approximations of the fractional power of an operator

When approximating operator functions, rational approximations, approximations by sum or product of exponents are used (see, e.g., [56]). When solving non-stationary problems with the fractional power of an operator, we focus most attention on the rational approximation.

We use a rational approximation of A^α in the form

$$D = D(A) \approx A^\alpha, \quad D(A) = AR(A), \quad R(A) = a_0 I + \sum_{i=1}^{m} a_i (b_i I + A)^{-1} \tag{13}$$

with the coefficients

$$a_0 \geq 0, \quad a_i > 0, \quad b_i > 0, \quad i = 0, 1, \dots, m. \tag{14}$$

Under these constraints, we have

$$D = D^* > 0, \quad DA = AD. \tag{15}$$

For the fractional power of a positively determined self-adjoint operator there is an integral representation (the Balakrishnan formula) [5])

$$A^{-\beta} = \frac{\sin(\beta\pi)}{\pi} \int_0^\infty \theta^{-\beta} (\theta I + A)^{-1} d\theta, \quad 0 < \beta < 1. \tag{16}$$

For $A^\alpha,\ 0 < \alpha < 1$, we put [54, 55]

$$A^\alpha = A A^{-\beta}, \quad \beta = 1 - \alpha. \tag{17}$$

The most straightforward approach to constructing a rational approximation of the operator $A^{-\beta}$ involves applying some quadrature formula for the integral on the right-hand side (16). In this case,

$$A^{-\beta} \approx \frac{\sin(\beta\pi)}{\pi} \sum_{i=1}^{m} w_i \theta_i^{-\beta} (\theta_i I + A)^{-1}, \tag{18}$$

where w_i are the weights of the quadrature formula, and $\theta_i,\ i = 1, \dots, m$, are the nodes of the quadrature formula. Taking into account (17), (18) for the coefficients of rational approximation (13), we get

$$a_0 = 0, \quad a_i = \frac{\sin(\beta\pi)}{\pi} w_i \theta_i^{-\beta}, \quad b_i = \theta_i, \quad i = 1, \dots, m.$$

The integrand has a singularity at $\theta \to 0$ and the unboundedness of the integration interval. Therefore, direct use of the Balakrishnan formula is not very convenient for constructing quadrature formulas. Many works are concerned with constructing quadrature formulas using new integration variables.

For example, in [9] to remove the singularity at $\theta \to 0$ uses new variable θ: $\theta = \exp(\theta)$. From (16), we have

$$A^{-\beta} = \frac{\sin(\beta\pi)}{\pi} \int_{-\infty}^\infty \exp\big((1-\beta)\eta\big) \big(\exp(\eta) I + A\big)^{-1} d\eta.$$

We have an integral on a finite interval (see, e.g., [1, 19] at $\theta = \mu(1-\eta)(1+\eta)^{-1},\ \mu > 0$. In this case, from (16), we get

$$A^{-\beta} = \frac{2\mu^{1-\beta} \sin(\pi\beta)}{\pi} \int_{-1}^1 (1-\eta)^{-\beta} (1+\eta)^{\beta-1} \big(\mu(1-\eta) I + (1+\eta) A\big)^{-1} d\eta.$$

Using (see [53]) $\theta = \eta^{1/(1-\beta)} (1-\eta)^{-\mu/\beta}$, the formula (16) takes the form

$$A^{-\beta} = \frac{\sin(\pi\beta)}{(1-\beta)\pi} \int_0^1 (1-\eta)^{\mu-1} \Big(1 + \Big(\mu \frac{1-\beta}{\beta} - 1\Big)\eta\Big) \Big(\eta^{\frac{1}{1-\beta}} I + (1-\eta)^{\frac{\mu}{\beta}} A\Big)^{-1} d\eta \tag{19}$$

with the parameter $\mu > 1$. We can restrict ourselves to standard quadrature formulas since we integrate on a finite interval and avoid the integrand's singularity. The paper [3] applies a single-exponential and a double-exponential transform of the integrand function for the integral representation with $\theta = \eta^2$.

In rational approximation (13), it is necessary to focus on achieving a given accuracy at a minimum m. For this purpose, additional information about the bounds of the operators A and $\widetilde{A}$ is involved. Given (17) we match (13) with a rational approximation of the function $\lambda^{-\beta},\ \beta = 1-\alpha$: $\lambda^{-\beta} \approx R(\lambda;\beta),\ \lambda_1 \le \lambda \le \lambda_K$. We estimate the error of this approximation as ε:

$$|\lambda^{-\beta} - R(\lambda;\beta)| \le \varepsilon, \quad \lambda_1 \le \lambda \le \lambda_K. \tag{20}$$

In the case of (13), the inequality (20) gives

$$\|(A^\alpha - D(A))A^{-1}\| \le \varepsilon. \tag{21}$$

Based on these accuracy estimates of the rational approximation of the fractional powers of the operator, we can obtain corresponding accuracy estimates for the approximate solution of the Cauchy problem (1)–(3).

Denote by $v(t)$ the approximate solution of the problem (1)–(3) when approximating the operator A^α by the operator $D(A)$. For $v(t)$ we have the Cauchy problem

$$\frac{dv}{dt} + D(A)v = f(t), \quad 0 < t \le T, \tag{22}$$

$$v(0) = u^0. \tag{23}$$

Theorem 1. *Let $u(t)$ be the solution of (1)-(3) and $v(t)$ be the solution of (22), (23) with the self-adjoint non-negative operator $D(A)$, $AD(A) = D(A)A$. Then for $u - v$ if the inequality (21) is satisfied, the estimation*

$$\|u(t) - v(t)\| \le \varepsilon t\|Au_0\| + \varepsilon \int_0^t \int_0^s \|Af(\zeta)\| d\zeta\, ds \tag{24}$$

holds.

Proof. For $w = u - v$ from (2) and (22) it follows

$$\frac{dw}{dt} + A^\alpha u - D(A)v = 0.$$

Adding and subtracting $A^\alpha v$, we get

$$\frac{dw}{dt} + A^\alpha w + (A^\alpha - D(A))v = 0.$$

By multiplying scalarly by w, we have

$$\|w(t)\| \frac{d\|w(t)\|}{dt} \le \big((D(A) - A^\alpha)v, w\big).$$

By this we come to the inequality

$$\frac{d\|w(t)\|}{dt} \le \|(A^\alpha - D(A))v\|. \tag{25}$$

If the inequality (21) is satisfied, then for the right-hand side of (25), we have

$$\|(A^\alpha - D(A))v\| = \|(A^\alpha - D(A))A^{-1}Av\| \le \varepsilon\|Av\|.$$

This gives the inequality

$$\|w(t)\| \le \varepsilon \int_0^t \|Av(s)\| ds. \tag{26}$$

Considering the permutability of the operators A and $D(A)$ to solve equation (22), we get an estimate

$$\frac{d\|Av(t)\|}{dt} \le \|Af(t)\|.$$

To do this, let's multiply equation (22) scalarly by $A^2 v$. From this estimate follows that

$$\int_0^t \|Av(s)\| ds \leq \|Au_0\| t + \int_0^t \int_0^s \|Af(\zeta)\| d\zeta \, ds.$$

Under these conditions, from (26), we have the provable estimate (24). □

Comparison of the estimate (24) for the error with the estimate (5) for the solution of (2), (3) shows that the estimate (24) is not optimal with respect to the smoothness of the dates u_0 and f. We can partially reduce the constraints on the smoothness of the initial data and the right-hand side of the problem (2), (3) by increasing the accuracy requirements for rational approximation. From this point of view, it is more acceptable (see [56]) to estimate not the absolute, but the relative error of the function approximation.

4. Approximations of the transition operator

The time approximation is provided by choosing S in (12). With a rational approximation (13) for the operator D, we have an additive representation

$$D = \sum_{i=0}^{m} D_i, \quad D_0 = a_0 A, \quad D_i = a_i A (b_i I + A)^{-1}, \quad i = 1, 2, \dots, m. \tag{27}$$

For the operator terms in (27), we have

$$D_i = D_i^* \geq 0, \quad D_i D_j = D_j D_i, \quad i, j = 0, 1, \dots, m, \tag{28}$$

under the assumptions (14).

Under the conditions (27), (28), we get

$$\exp\big(-\tau D\big) = \exp\Big(-\tau \sum_{i=0}^{m} D_i\Big) = \prod_{i=0}^{m} \exp\big(-\tau D_i\big). \tag{29}$$

Thereby the time transition operator from one level to another (the operator exponent $\exp\big(-\tau D\big)$) is split into the product of the operator exponents $\exp\big(-\tau D_i\big)$, $i = 0, 1, \dots, m$. Given (29), we can construct exponent splitting schemes when

$$S(D) = \prod_{i=0}^{m} S(D_i). \tag{30}$$

For the transition operator, we use the representation

$$\exp\big(-\tau D\big) = S(D) + \tau^{\gamma} Q(D) + \mathcal{O}(\tau^{\gamma+1}). \tag{31}$$

Using (12), the error of the approximate solution of the evolution equation (2) is $\mathcal{O}(\tau^{\gamma-1})$. In modern computational practice, the schemes of the first ($\gamma = 2$) and second ($\gamma = 3$) order of accuracy receive the most attention. When choosing a method for approximate solution of the Cauchy problem for a first-order evolution equation with a self-adjoint operator, instead of the standard unconditional stability condition, one can focus on the more stringent SM-stability (Spectral Mimetic stability) conditions [47]. In this case, the scheme has ϱ-stability, and spectral monotonicity, which is asymptotically stable.

For the implicit SM-stable scheme (Euler's backward method), we have

$$S(D) = (I + \tau D)^{-1} \tag{32}$$

when

$$F^n(D, f) = \tau f^{n+1}, \quad Q(D) = -\frac{1}{2} D^2, \quad \gamma = 2.$$

The possibility of solving the stationary problem based on the scheme (12), (32) is provided by setting $F^n(D, f) = (I + \tau D)^{-1} f^{n+1}$ (see equation (11)).

Among the second-order accuracy schemes, we note the symmetric scheme (the Crank-Nicholson scheme) when

$$S(D) = \Big(I - \frac{\tau}{2} D\Big)\Big(I + \frac{\tau}{2} D\Big)^{-1} \tag{33}$$

when

$$F^n(D, f) = \tau\Big(I + \frac{\tau}{2} D\Big)^{-1} f^{n+1/2}, \quad Q(D) = \frac{1}{12} D^3, \quad \gamma = 3.$$

The main drawback of the scheme (12), (33) is that this scheme is not a SM-stable scheme.

The simplest SM-stable scheme of the second order of accuracy corresponds to choosing

$$S(D) = \Big(I + \tau D + \frac{\tau}{2} D^2\Big)^{-1} \tag{34}$$

when

$$F^n(D, f) = \tau\Big(I + \frac{\tau}{2} D\Big)^{-1} f^{n+1/2}, \quad Q(D) = -\frac{1}{6} D^3, \quad \gamma = 3.$$

This scheme is not very convenient for computational implementation since you need to work with D^2.

We proposed [50] a factorized scheme of the second order of accuracy when a transition operator is approximated by the operator

$$S(D) = \Big(I + 2\sigma\tau D + \Big(\sigma^2 - \frac{1}{2}\Big)\tau^2 D^2\Big)(I + \tau D)^{-1}(I + \sigma\tau D)^{-2}, \tag{35}$$

In this case, we have

$$F^n(D, f) = \tau\Big(I + \frac{\tau}{2} D\Big)^{-1} f^{n+1/2}, \quad Q(D) = \Big(\frac{1}{3} - \sigma\Big) D^3, \quad \gamma = 3.$$

The scheme (12), (35) at parameter values $\sigma \geq \sigma_0 = 1/\sqrt{2}$ is a SM-stable scheme. The basic error term is minimal at $\sigma = \sigma_0$.

Here is a small comment on the computational complexity of the transition from one level in time to another when using different approximations in time. We restrict ourselves to the case of problems with a homogeneous right-hand side ($f(t) = 0$ in (2)). When using the Euler scheme (32) it is necessary to solve the problem $Gy = \varphi$ when $G = I + \tau D$. We solve a similar problem using the Crank-Nocolson scheme (33) ($G = I + 0.5\tau D$). We must solve a significantly more complicated problem for SM-stable scheme (34) when $G = I + \tau D + 0.5\tau D^2$. For this reason, such approximations are practically not used in computational practice for approximate solutions of parabolic IVP. The computational cost for the scheme (35) is three times higher than for the Euler scheme (33): we solve one problem with $G = I + \tau D$ and two — with $G = I + \sigma\tau D$.

Theorem 2. *Let D be a self-adjoint non-negative operator. Then the first-order accuracy scheme (9), (12), (32) is unconditionally stable and an a priori estimate for the approximate solution is*

$$\|y^{n+1}\| \leq \|u^0\| + \sum_{k=0}^{n} \tau \|f^{k+1}\|, \quad n = 0, \dots, N-1. \tag{36}$$

For unconditionally stable schemes of second-order accuracy (9), (12) when $S(D)$ is given by the relations (33)–(35), the stability estimate on the initial data and right-hand side is

$$\|y^{n+1}\| \leq \|u^0\| + \sum_{k=0}^{n} \tau \|f^{k+1/2}\|, \quad n = 0, \dots, N-1. \tag{37}$$

Proof. If $S(D)$ is defined according to (32)–(35), then $\|S(D)\| \leq 1$. For the first-order accuracy scheme, we have $\|F^n(D,f)\| \leq \tau \|f^{n+1}\|$. Under these conditions, from (12), we obtain a time estimate on a single time level

$$\|y^{n+1}\| \leq \|y^n\| + \tau \|f^{n+1}\|.$$

From this inequality follows the inequality (37). Similarly, for second-order accuracy schemes, we get a similar inequality (37). □

Similarly, exponent splitting schemes are constructed when we used splitting (27), (28). For individual operator terms like (31), we have

$$\exp\big(-\tau D_i\big) = S(D_i) + \tau^\gamma Q(D_i) + \mathcal{O}(\tau^{\gamma+1}), \quad i = 0, 1, \dots, m. \tag{38}$$

Given the pairwise permutability of the operators $D_i,\ i = 0, 1, \dots, m$, we get

$$\exp\big(-\tau D\big) = \prod_{i=0}^{m} \exp\big(-\tau D_i\big) = \prod_{i=0}^{m} \big(S(D_i) + \tau^\gamma Q(D_i)\big) + \mathcal{O}(\tau^{\gamma+1}).$$

Given that $S(D_i) = I + \mathcal{O}(\tau)$, we have

$$\exp\big(-\tau D\big) = \prod_{i=0}^{m} S(D_i) + \tau^\gamma \sum_{i=0}^{m} Q(D_i) + \mathcal{O}(\tau^{\gamma+1}).$$

Thus in (31) the representation (30) for $S(D)$ takes place and

$$Q(D) = \sum_{i=0}^{m} Q(D_i). \tag{39}$$

For the scheme (9), (12), (30), (39) of the first order, we have

$$S(D_i) = (I + \tau D_i)^{-1}, \quad i = 0, 1, \dots, m, \tag{40}$$

and

$$F^n(D,f) = \tau f^{n+1}, \quad Q(D_i) = -\frac{1}{2} D_i^2, \quad \gamma = 2, \quad i = 0, 1, \dots, m.$$

With (9), (12), (30), we associate the exponent splitting scheme with

$$S(D_i) = \Big(I - \frac{\tau}{2} D_i\Big)\Big(I + \frac{\tau}{2} D_i\Big)^{-1}, \quad i = 0, 1, \dots, m, \tag{41}$$

and

$$F^n(D,f) = \tau \prod_{i=0}^{m} \Big(I + \frac{\tau}{2} D_i\Big)^{-1} f^{n+1/2}, \quad Q(D_i) = \frac{1}{12} D_i^3, \quad \gamma = 3, \quad i = 0, 1, \dots, m.$$

In this case, we have

$$F^n(D,f) = \tau \Big(I + \frac{\tau}{2} D\Big)^{-1} f^{n+1/2} + \mathcal{O}(\tau^2).$$

Similarly (34), we can set

$$S(D_i) = \Big(I + \tau D_i + \frac{\tau}{2} D_i^2\Big)^{-1}, \quad i = 0, 1, \dots, m, \tag{42}$$

and

$$F^n(D,f) = \tau \prod_{i=0}^{m} \Big(I + \frac{\tau}{2} D_i\Big)^{-1} f^{n+1/2},\ Q(D_i) = -\frac{1}{6} D_i^3,\ \gamma = 3,\ i = 0,1,\dots,m.$$

The exponent splitting scheme (9), (12), (30), (42) is a SM-stable scheme.

A more computationally convenient SM-stable scheme ($\sigma \geq \sigma_0 = 1/\sqrt{2}$) of the second order of accuracy (see 35)) is related to choosing

(43)

$$S(D_i) = \Big(I + 2\sigma\tau D_i + \Big(\sigma^2 - \frac{1}{2}\Big)\tau^2 D_i^2\Big)(I + \tau D_i)^{-1}(I + \sigma\tau D_i)^{-2},\ i = 0,1,\dots,m,$$

and

$$F^n(D,f) = \tau \prod_{i=0}^{m} \Big(I + \frac{\tau}{2} D_i\Big)^{-1} f^{n+1/2},\ Q(D_i) = \Big(\frac{1}{3} - \sigma\Big) D_i^3,\ \gamma = 3,\ i = 0,1,\dots,m.$$

Further consideration follows the proof of the theorem 2. The result is the following statement.

Theorem 3. *Let the conditions (27), (28) for the operator D be satisfied in the scheme (9), (12). Then the first-order accuracy exponent splitting scheme (9), (12), (30), (39), (40) is unconditionally stable and an a priori estimate for the approximate solution (36) is valid. For unconditionally stable exponent splitting schemes of second-order accuracy (9), (12), (30), (39) when $S(D_i)$ $i = 0,1,\dots,m$, is given by the relations (41)–(43), the stability estimate (36) on the initial data and right-hand side holds.*

Let us briefly discuss the organization of calculations when applying exponent splitting schemes. To find an approximate solution on a new time level, we can start by calculating the last term in (12). For the first-order scheme (see (40)), there is no problem. For the second order scheme (see (41)–(43)) we can use

$$\varphi^0 = f^{n+1/2}, \quad \Big(I + \frac{\tau}{2} D_i\Big)\varphi^{i+1} = \varphi^i, \quad i = 0,1,\dots,m, \quad F^n(D,f) = \tau\varphi^{m+1}.$$

Given the representation (30), we find an approximate solution on a new time level as follows

$$v^0 = y^n, \quad \varphi^{i+1} = S(D_i)\varphi^i, \quad i = 0,1,\dots,m, \quad y^{n+1} = v^{m+1} + F^n(D,f).$$

For the first-order scheme, from (40), we get

$$(I + \tau D_i)\varphi^{i+1} = \varphi^i, \quad i = 0,1,\dots,m.$$

Under rational approximation (27), we have

$$(I + \tau a_0 A)\varphi^1 = \varphi^0, \quad \big(b_i I + (1 + \tau a_i)A\big)\varphi^{i+1} = (b_i I + A)\varphi^i, \quad i = 1,2,\dots,m.$$

We have similar computational formulas for other exponent splitting schemes of second-order accuracy (33)–(35). Thus, the transition to a new level in time is provided by solving $m+1$ of standard problems with operators of type $cI + dA,\ c,d =$ const.

5. Other problems

The considered technique of approximate solution of nonstationary problems with fractional powers of the operator based on rational approximation can be used for some other problems. We note, first of all, the problems with the operator function. We will assume that the function $g(\lambda)$ does not have poles and $g(\lambda) \geq 0$ an $[\delta, +\infty)$. Let instead of equation (2), the desired function $u(t)$ satisfy equation

$$\frac{du}{dt} + g(A)u = f(t), \quad 0 < t \leq T, \quad g(A) \geq 0. \tag{44}$$

In this case,

$$g(A)u = \sum_{k=1}^{K} g(\lambda_k)(u, \psi_k)\psi_k, \quad 0 < \alpha < 1.$$

The most straightforward situation for the Cauchy problem for the equation (44) is related to the use of a rational approximation of the operator function $g(A)$ itself:

$$g(A) \approx a_0 I + \sum_{i=1}^{m} a_i (b_i I + A)^{-1}.$$

The approximation (13) corresponds to choosing

$$g(A) \approx a_0 A + \sum_{i=1}^{m} a_i A (b_i I + A)^{-1}.$$

We can construct rational approximations for the operator function of A^{-1} (see, e.g., [22, 25]). At $g(A) = \widetilde{g}(\widetilde{A})$, $\widetilde{A} = A^{-1}$, we use

$$\widetilde{g}(\widetilde{A}) = a_0 I + \sum_{i=1}^{m} a_i (b_i I + \widetilde{A})^{-1}.$$

For the operator function $g(A)$, this gives a rational approximation

$$g(A) = a_0 I + \sum_{i=1}^{m} a_i A (I + b_i A)^{-1}.$$

Let us also note some more general nonstationary problems with fractional powers of the operator. Consider, for example, an evolution equation of the first-order with the operator at the time derivative

$$B\frac{du}{dt} + A^{\alpha} u = f(t), \quad 0 < t \leq T, \tag{45}$$

when B is a self-adjoint positively definite operator.

It is convenient to transform equation (45) by formally introducing a new unknown quantity $\widetilde{u} = B^{1/2} u$. In this case, we have

$$\frac{d\widetilde{u}}{dt} + B^{-1/2} A^{\alpha} B^{-1/2} \widetilde{u} = B^{-1/2} f(t), \quad 0 < t \leq T. \tag{46}$$

With the rational approximation of A^{α}, we have

$$D \approx A^{\alpha}, \quad D = \sum_{i=0}^{m} D_i.$$

To equation (46) we assign

$$\frac{dv}{dt} + \widetilde{D} v = B^{-1/2} f(t), \quad 0 < t \leq T, \tag{47}$$

where

$$\widetilde{D} = \sum_{i=0}^{m} \widetilde{D}_i, \quad \widetilde{D}_i = B^{-1/2} D_i B^{-1/2}, \quad i = 0, 1, \ldots, m.$$

When constructing time approximations for equation (47), we distinguish two cases. In the first case, the consequence is the pairwise permutation of the operators $\widetilde{D}_i,\ i = 0,1,\dots,m$ and the following equality

$$\exp\big(-\tau\widetilde{D}\big) = \prod_{i=0}^{m} \exp\big(-\tau\widetilde{D}_i\big). \tag{48}$$

We can use the exponent splitting schemes discussed above.

In the second case, the operators B and A are not permutations, and equality (48) is not valid. The construction of schemes of the first order of accuracy is based on the approximation

$$\exp\big(-\tau\widetilde{D}\big) = \prod_{i=0}^{m} \exp\big(-\tau\widetilde{D}_i\big) + \mathcal{O}(\tau^2).$$

For second-order schemes, the symmetrization [34, 48]

$$\exp\big(-\tau\widetilde{D}\big) = \prod_{i=0}^{m} \exp\Big(-\frac{\tau}{2}\widetilde{D}_i\Big) \prod_{j=0}^{m} \exp\Big(-\frac{\tau}{2}\widetilde{D}_{m-j}\Big) + \mathcal{O}(\tau^3)$$

is involved.

Let us also note the main possibilities of constructing exponent splitting schemes for the equation

$$\frac{du}{dt} + A^\alpha u + Bu = f(t), \quad 0 < t \le T, \quad B \ge 0. \tag{49}$$

For the solution of the Cauchy problem (1), (3), (19)we have the representation

$$u(t) = \exp\big(-t(A^\alpha + B)\big)u^0 + \int_0^t \exp\big(-(t-s)(A^\alpha + B)\big) f(s)ds, \quad 0 < t \le T.$$

In the particular case $DA = AB$, we can construct exponent splitting schemes as before. In the general case $DA \neq AB$, time approximations are based on operator exponent approximations

$$\exp\big(-\tau(D+B)\big) = \exp(-\tau D)\exp(-\tau B) + \mathcal{O}(\tau^2),$$

for first-order accuracy schemes. Similarly, we use

$$\exp\big(-\tau(D+B)\big) = \exp\Big(-\frac{\tau}{2}D\Big)\exp\Big(-\frac{\tau}{2}B\Big)\exp\Big(-\frac{\tau}{2}B\Big)\exp\Big(-\frac{\tau}{2}D\Big) + \mathcal{O}(\tau^3),$$

for schemes of the second-order of accuracy.

6. Numerical experiments

The problems of rational approximation and computational implementation of exponent splitting schemes are discussed in the example of the boundary value problem for equations with fractional powers of a two-dimensional operator in a rectangle.

6.1. Rational approximations. To unify the problem of calculating the coefficients of rational approximation of the fractional power of an operator, we will pass from the operator A to the operator $\bar{A} = \delta^{-1}A$. The problem of finding the minimal eigenvalue of a positively defined finite-dimensional operator is standard in numerical analysis. It is solved using (see, for example, [11, 44]) the inverse iteration method for eigenvalues. For the spectrum of the operator $\bar{A}$ we have

$$\bar{A} = \delta^{-1}A, \quad \sigma(\bar{A}) \in [1,q], \quad q = \frac{\lambda_K}{\lambda_1}.$$

For a rational approximation of the function $\lambda^{-\beta}$ we use

$$\lambda^{-\beta} \approx R(\lambda;\beta), \quad \lambda \in [1,q], \quad 0<\beta<1. \tag{50}$$

The rational approximation of the fractional power of the operator (13) corresponds to

$$\lambda^{\alpha} = \lambda\lambda^{1-\alpha} \approx \lambda R(\lambda; 1-\alpha), \quad \lambda \in [1,q], \quad 0<\alpha<1.$$

We estimate the error by the values $\varepsilon_r(\lambda) = \lambda^{\alpha} - \lambda R(\lambda;1-\alpha)$, $\lambda \in [1,q]$.

The construction of rational approximations $R(\lambda; 1-\alpha)$ is an independent problem of computational mathematics [10]. The best uniform rational approximations based on the Remez algorithm are used in [24]. The AAA algorithm [35] uses the representation of the rational approximant in barycentric form. From recent works in this direction, we note the article [27], which considers the best uniform rational approximations to real scalar functions in the setting of zero defect. In our numerical experiments we used the open-source Python package baryrat by Clemens Hofreither (https://github.com/c-f-h/baryrat).

Evaluate the accuracy of the approximation of the rational approximation $R(\lambda; 1-\alpha)$ by the value $\bar{\varepsilon}_r(\lambda) = \lambda^{\alpha-1} - R(\lambda; 1-\alpha)$, $\lambda \in [1,q]$, $0<\alpha<1$, so $\varepsilon_r(\lambda) = \lambda\bar{\varepsilon}_r(\lambda)$. The effect of the parameter $q = 10^{\nu}$ (the width of the approximation interval) is shown in Fig. 1. The calculations were performed at $m = 10$ for various values of α. At sufficiently large ν, the influence of q does not appear. In this case, the approximating function

$$R(\lambda; 1-\alpha) = a_0 + \sum_{i=1}^{m} \frac{a_i}{b_i + \lambda},$$

has constant $a_0 \approx 0$, and it can be neglected.

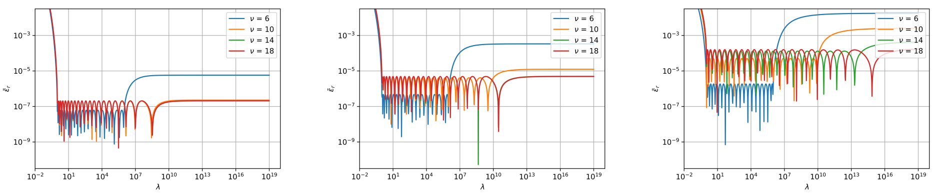

FIGURE 1. Approximation error $\bar{\varepsilon}_r(\lambda)$ at $\alpha = 0.25$ (left), $\alpha = 0.5$ (center), and $\alpha = 0.75$ (right) for different values of $q = 10^{\nu}$ ($m = 10$).

Increasing the accuracy is achieved by increasing m (see Fig. 2). The calculations were performed for $\alpha = 0, 0.5, 0.75$ and different values of m. The approximation error over the interval $[1, 10^{\nu}]$, $\nu = 18$ will be estimated by the value $\max|\bar{\varepsilon}_r(\lambda)|$. The accuracy of the rational approximation of the function $\lambda^{\alpha-1}$ for $0.01 \le \alpha \le 0.99$ is shown in Fig. 3. We observe a decrease in accuracy as the parameter α increases.

6.2. The test problem. We perform numerical experiments for a nonstationary problem containing a fractional power of the Laplace operator. We find the solution $w(\boldsymbol{x}, t)$ of the equation

$$\frac{\partial w}{\partial t} + (-\triangle)^{\alpha} w = 0, \quad \boldsymbol{x} \in \Omega, \quad 0 < t \le T,$$

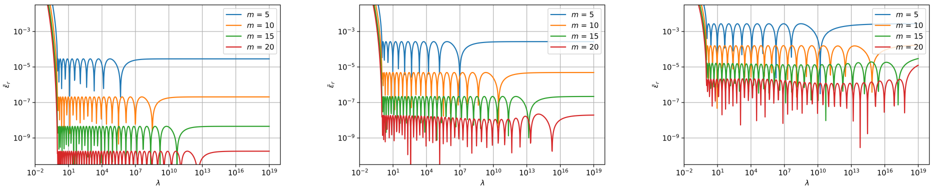

FIGURE 2. Approximation error $\bar{\varepsilon}_r(\lambda)$ at $\alpha = 0.25$ (left), $\alpha = 0.5$ (center), and $\alpha = 0.75$ (right) for different values of m ($\nu = 18$).

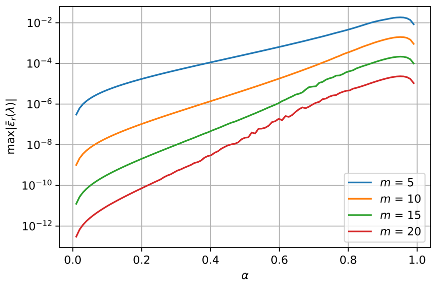

FIGURE 3. Approximation error $\bar{\varepsilon}_r(\lambda)$ for different values of m ($\nu = 18$).

when $\Omega = \{\boldsymbol{x} \mid \boldsymbol{x} = (x_1, x_2),\ 0 < x_k < 1,\ k = 1, 2\}$. The boundary and initial conditions are

$$w(\boldsymbol{x}, t) = 0, \quad \boldsymbol{x} \in \Omega, \quad 0 < t \le T, \quad w(\boldsymbol{x}, 0) = u^0(\boldsymbol{x}), \quad \boldsymbol{x} \in \Omega.$$

The most straightforward approach to an approximate solution to this Cauchy problem is based on difference approximation over space (see, for example, [40, 42]). We use a uniform grid

$$\overline{\omega} = \{\boldsymbol{x} \mid \boldsymbol{x} = (x_1, x_2), \quad x_k = i_k h_k, \quad i_k = 0, 1, ..., N_k, \quad N_k h_k = 1,\ k = 1, 2\},$$

where $\overline{\omega} = \omega \cup \partial\omega$ and ω is the set of interior nodes, whereas $\partial\omega$ is the set of boundary nodes of the grid. In the Hilbert space $H = L_2(\omega)$ for grid functions $u(\boldsymbol{x})$ such that $u(\boldsymbol{x}) = 0,\ \boldsymbol{x} \notin \omega$ the scalar product and the norm are defined as follows:

$$(u, w) = \sum_{\boldsymbol{x} \in \omega} u(\boldsymbol{x})\, w(\boldsymbol{x})\, h_1 h_2, \quad \|u\| = (u, u)^{1/2}.$$

After approximation in space, we have a discrete problem (1)–(3) with $u^0(\boldsymbol{x}) = w^0(\boldsymbol{x}),\ \boldsymbol{x} \in \omega$. For $u(\boldsymbol{x}) = 0,\ \boldsymbol{x} \notin \omega$, the Laplace grid operator A can be written as

$$\begin{aligned} Au = & -\frac{1}{h_1^2}(u(x_1 + h_1, h_2) - 2u(\boldsymbol{x}) - u(x_1 - h_1, h_2)) \\ & -\frac{1}{h_2^2}(u(x_1, x_2 + h_2) - 2u(\boldsymbol{x}) - u(x_1, x_2 - h_2)), \quad \boldsymbol{x} \in \omega. \end{aligned}$$

The grid operator A approximates the differential operator $\triangle$ on smooth functions with accuracy $\mathcal{O}\left(|h|^2\right)$, $|h|^2 = h_1^2 + h_2^2$. In the computational implementation, we use direct methods for solving the grid equations based on the fast Fourier transform [40, 42]. In our case, we have

$$\lambda_1 = \delta = \sum_{k=1}^{2} \frac{4}{h_k^2} \sin^2 \frac{\pi}{2N_k}, \quad \lambda_K = \Delta = \sum_{k=1}^{2} \frac{4}{h_k^2} \cos^2 \frac{\pi}{2N_k}$$

in a two-sided inequality (1).

6.3. Accuracy of exponent splitting schemes. Many factors affect the accuracy of approximate solutions to nonstationary problems with the fractional power of the elliptic operator. For our test problem, we will distinguish the main ones: (i) the parameter α (a crucial characteristic of the mathematical model), (ii) the exponent splitting scheme (the time approximation), and (iii) the time step (the convergence of the approximate solution to the exact solution). We take the initial condition as

$$u^0(\boldsymbol{x}) = 16x_1(1-x_1)x_2(1-x_2), \quad \max_{\boldsymbol{x}\in\Omega} u^0(\boldsymbol{x}) = u^0(\boldsymbol{x}_0) = 1, \quad \boldsymbol{x}_0 = (0.5, 0.5).$$

We will put $T = 0.1$ and use a fairly detailed computational grid over the space with $N_1 = N_2 = 256$. The exact solution of the test problem in the center of the computational domain with a value of $\alpha = 0.25, 0.5, 0.75$ is shown in Fig. 4.

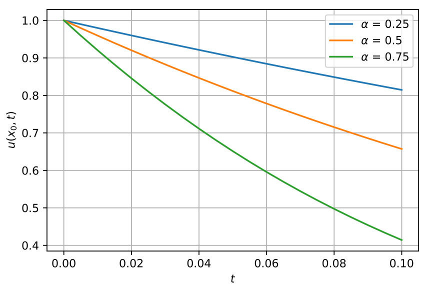

FIGURE 4. The exact solution at the point $\boldsymbol{x}_0 = (0.5, 0.5)$ at various values of α.

The influence of the rational approximation error is estimated by $\varepsilon_1(t) = \|v(\boldsymbol{x}, t) - u(\boldsymbol{x}, t)\|$, where $v(\boldsymbol{x}, t)$ is the solution of the homogeneous ($f(t) = 0$) problem (22), (23). The computational data for different values of m are shown in Fig. 5. We find good accuracy at sufficiently small m. The error of the approximate solution increases as α increases. This behavior is consistent with the data on the error of rational approximation (see Fig. 3).

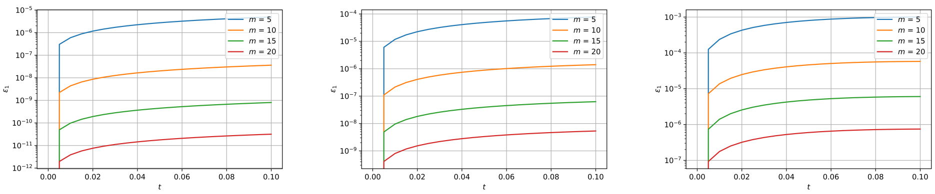

FIGURE 5. The error of the solution of the unsteady problem $\varepsilon_1(t)$ at $\alpha = 0.25$ (left), $\alpha = 0.5$ (center), and $\alpha = 0.75$ (right) for different values of m ($\nu = 18$).

The value

$$\varepsilon_2(t^n) = \|y^n(\boldsymbol{x}) - u(\boldsymbol{x}, t^n)\|, \quad n = 0, 1, \ldots, N,$$

is evaluate the accuracy of the difference schemes. The effect of the time step for the Euler exponent splitting scheme when the transition operator is approximated according to (30), (40) is illustrated by the data in Fig. 6. The rational approximation of the fractional powers of the operator is obtained when $m = 20$. A theoretical first-order convergence on τ and a decrease in accuracy as the parameter α increases is observed.

The calculated data for the second-order scheme (30), (41) are given in Fig. 7. The influence of the approximation error of the fractional degree of the operator appears at small time steps ($N = 80$) for $\alpha = 0.75$. Similar data for the second-order SM-stable scheme (30), (42) are given in Fig. 8. On our test problem, the properties of the SM-stable scheme practically do not appear the disadvantages of the Crank-Nicolson scheme over the implicit Euler scheme in solving many parabolic problems.

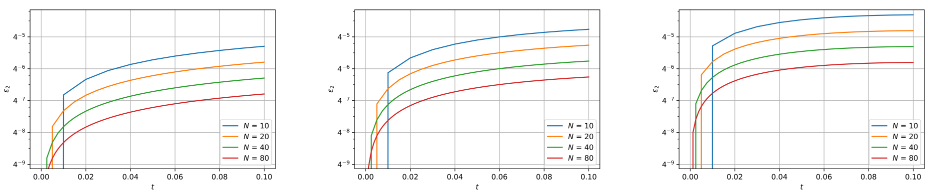

FIGURE 6. Euler exponent splitting scheme (40) at $\alpha = 0.25$ (left), $\alpha = 0.5$ (center), and $\alpha = 0.75$ (right) for different values of N ($m = 20,\ \nu = 18$).

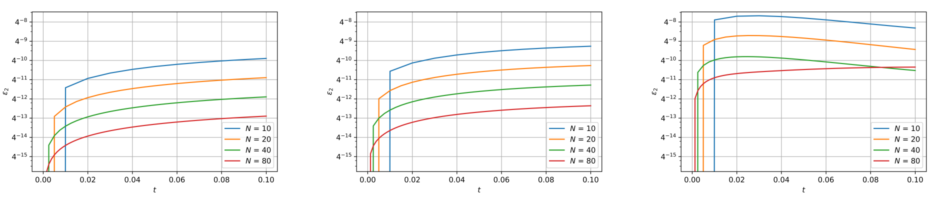

FIGURE 7. Crank-Nicolson exponent splitting scheme (41) at $\alpha = 0.25$ (left), $\alpha = 0.5$ (center), and $\alpha = 0.75$ (right) for different values of N ($m = 20,\ \nu = 18$).

The SM-stable scheme (30), (43) is related to the solution of usual problems on a new time level. We have the computational data for this scheme in Fig. 9. Again we observe the convergence of the approximate solution to the exact solution with the second-order of τ. The accuracy of this scheme is lower than that of the SM-stale exponent splitting scheme (30), (42) and Crank-Nicolson exponent splitting scheme (30), (41). This fact is consistent with the corresponding expressions for the main part of the approximation error of the transition operator (39).

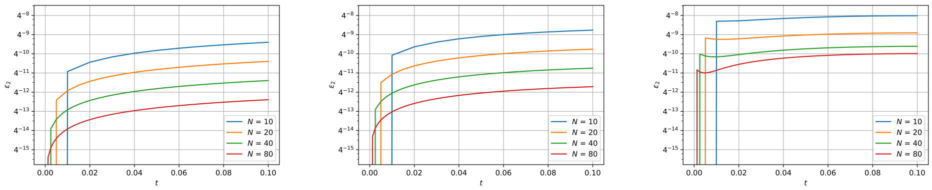

FIGURE 8. SM-stale exponent splitting scheme (42) at $\alpha = 0.25$ (left), $\alpha = 0.5$ (center), and $\alpha = 0.75$ (right) for different values of N $(m = 20,\ \nu = 18)$.

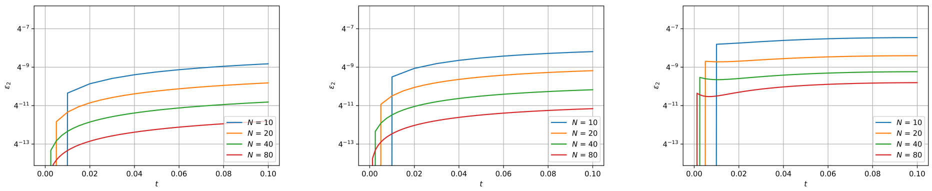

FIGURE 9. Exponent splitting scheme (43) with $\sigma = \sigma_0$ at $\alpha = 0.25$ (left), $\alpha = 0.5$ (center), and $\alpha = 0.75$ (right) for different values of N $(m = 20,\ \nu = 18)$.

7. Conclusions

We can summarize the results of our study as follows.

(1) The Cauchy problem for a first-order evolution equation with a fractional power of a self-adjoint positive definite operator A is considered in a finite-dimensional Hilbert space. Standard two-level approximations are not computationally practical; problems are generated by the need to solve a non-standard grid equation with $A^\alpha,\ 0 < \alpha < 1$ to find an approximate solution in a new time level.

(2) The computational algorithm is based on a rational approximation of the fractional powers of the operator. In this case, we have an evolution equation with operator $D(A)$, which appears as a sum of the positive definite operators $D_i(A),\ i = 0, 1, \dots, m$. We can provide the transition to a new level in time by solving usual grid problems using additive-operator schemes (splitting schemes) technology. We obtain estimates of the closeness of the approximate and exact solutions to the evolution problem with fractional powers of the operator.

(3) We construct unconditionally stable exponent splitting schemes using various approximations of the transition operator with the account of pairwise permutation of operators $D_i(A),\ i = 0, 1, \dots, m$. An implicit scheme of the first order of accuracy (analog of the implicit Euler scheme) and the symmetric scheme of the second order of accuracy (analog of the Crank-Nicholson scheme) are distinguished. SM-stable schemes to which the implicit Euler scheme belongs, but the Crank-Nicholson scheme does not belong, are particularly important for computational practice. We have investigated two types of such exponent splitting schemes of second-order accuracy.

(4) We have noted some more general non-classical non-stationary problems for which the constructed exponent splitting schemes can be used. In particular, rational approximations can be applied to the numerical solution of the Cauchy problem with operator functions. More general evolution equations may include some operator B at time derivative, be an additional term to A^{α}.

(5) The accuracy of the constructed exponent splitting schemes is illustrated by examples of calculations for a two-dimensional test problem with a fractional power of the Laplace operator using finite-difference approximations on a uniform grid over space. The best rational approximation was performed using the open-source Python package `baryrat`. We investigated the influence of the power (α parameter) and the time step when using different exponent splitting schemes.

Acknowledgments

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