Numerical solution of nonstationary problems for a space-fractional diffusion equation

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Applied problems

Many applied mathematical models involve both sub-diffusion (fractional in time) and super-diffusion (fractional in space) operators (see, e.g., Podlubny [1998], Uchaikin [2013]). Super-diffusion problems are treated as evolutionary problems with a fractional power of an elliptic operator. For example, suppose that in a bounded domain Ω on the set of functions $u(\boldsymbol{x}) = 0,\ \boldsymbol{x} \in \partial\Omega$, there is defined the operator $\mathcal{A}$: $\mathcal{A}u = -\triangle u,\ \boldsymbol{x} \in \Omega$. We seek the solution of the Cauchy problem for the equation with the fractional power elliptic operator:

$$\frac{du}{dt} + \mathcal{A}^\alpha u = f(t), \quad 0 < \alpha < 1, \quad 0 < t \leq T,$$

$$u(0) = u_0,$$

for a given $f(\boldsymbol{x}, t)$, $u_0(\boldsymbol{x})$, $\boldsymbol{x} \in \Omega$ using the notation $f(t) = f(\cdot, t)$.

Approximation in space

For approximation in space, we can apply finite volume or finite element methods oriented to using arbitrary domains and irregular computational grids (Knabner and Angermann [2003], Quarteroni and Valli [1994]).
After this, we formulate the corresponding Cauchy problem with a fractional power of a self-adjoint positive definite discrete elliptic operator (see Bonito and Pasciak [2015], Szekeres and Izsák [2016]) — a fractional power of a symmetric positive definite matrix (Higham [2008]).

Time-dependent problems

In the study of difference schemes for time-dependent problems of BVP for PDE, the general theory of stability (well-posedness) for operator-difference schemes (Samarskii [2001], Samarskii et al. [2002]) is in common use.

At the present time, the exact (matching necessary and sufficient) conditions for stability are obtained for a wide class of two- and three-level difference schemes considered in finite-dimensional Hilbert spaces.

We emphasize a constructive nature of the general theory of stability for operator–difference schemes, where stability criteria are formulated in the form of operator inequalities, which are easy to verify. In particular, the backward Euler scheme and Crank–Nicolson scheme are unconditionally stable for a non-negative operator.

Problems with fractional powers of operators

Problems in numerical solving unsteady problems with fractional powers of operators appear in using the simplest explicit approximations in time. A practical implementation of such approach requires the matrix function-vector multiplication. For such problems, different approaches (see Higham [2008]) are available.

Algorithms for solving systems of linear equations associated with fractional elliptic equations that are based on Krylov subspace methods with the Lanczos approximation are discussed, e.g., in Ilić et al. [2008].

The simplest variant is associated with the explicit construction of the solution using the eigenvalues and eigenfunctions of the elliptic operator with diagonalization of the corresponding matrix (Bueno-Orovio et al. [2014], Ilic et al. [2006]). Unfortunately, all these approaches demonstrate very high computational complexity for multidimensional problems.

Approximation of the original operator

There does exist a general approach to solve approximately equations involving a fractional power of operators based on an approximation of the original operator and then taking fractional power of its discrete variant. Using the Dunford-Cauchy formula the elliptic operator is represented as a contour integral in the complex plane.

In Bonito and Pasciak [2015], there was presented a more promising variant of using quadrature formulas with nodes on the real axis, which are constructed on the basis of the corresponding integral representation for the power operator (see Krasnoselskii et al. [1976], Carracedo et al. [2001]).

In this case, the inverse operator of the problem has an additive representation, where each term is an inverse of the original elliptic operator. A similar rational approximation to the fractional Laplacian operator is studied in Aceto and Novati [2017].

Our approach

We have proposed (Vabishchevich [2015]) a numerical algorithm to solve an equation for fractional power elliptic operators that is based on a transition to a pseudo–parabolic equation.
For an auxiliary Cauchy problem, the standard two-level schemes are applied. The computational algorithm is simple for practical use, robust, and applicable to solving a wide class of problems. A small number of time steps is required to find a solution.
This computational algorithm for solving equations with fractional power operators is promising for transient problems.

1D problems

As for one-dimensional problems for the space-fractional diffusion equation, an analysis of stability and convergence for this equation was conducted in Jin et al. [2014] using finite element approximation in space.

A similar study for the Crank–Nicolson scheme was conducted earlier in Tadjeran et al. [2006] using finite difference approximations in space.

We highlight separately the works Huang et al. [2008], Sousa [2012], Meerschaert and Tadjeran [2004], where numerical methods for solving one–dimensional transient problems of convection and space–fractional diffusion equation are considered.

Multidimensional problems

In Vabishchevich [2016], an unsteady problem is considered for a space–fractional diffusion equation in a bounded domain. To construct approximation in time, regularized two-level schemes are used (see Vabishchevich [2014]).

The numerical implementation is based on solving the equation with the fractional power of the elliptic operator using an auxiliary Cauchy problem for a pseudo–parabolic equation (Vabishchevich [2015]).

Some more general unsteady problems are considered in Vabishchevich [2016].

This work

In the present work, standard two-level schemes are applied to solve numerically a Cauchy problem for an evolutionary equation of first order with a fractional power of the operator.

The numerical implementation is based on the rational approximation of the operator at a new time-level.

When implementing the explicit scheme, the fractional power of the operator is approximated on the basis of Gauss-Jacobi quadrature formulas for the corresponding integral representation. In this case, we have (see Frommer et al. [2014]) a Pade–type approximation of the power function with a fractional exponent. A similar approach is used when considering implicit schemes.

Elliptic operator

In a bounded polygonal domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$ with the Lipschitz continuous boundary $\partial\Omega$, we search the solution for the problem with a fractional power of an elliptic operator. Define the elliptic operator as

$$\mathcal{A}u = -\mathrm{div} k(\boldsymbol{x}) \mathrm{grad}\, u + c(\boldsymbol{x})u$$

with coefficients $0 < \underline{k} \leq k(\boldsymbol{x}) \leq \overline{k}$, $c(\boldsymbol{x}) \geq 0$. The operator $\mathcal{A}$ is defined on the set of functions $u(\boldsymbol{x})$ that satisfy on the boundary $\partial\Omega$ the following conditions:

$$k(\boldsymbol{x}) \frac{\partial u}{\partial n} + g(\boldsymbol{x})u = 0, \quad \boldsymbol{x} \in \partial\Omega,$$

where $g(\boldsymbol{x}) \geq 0$, $\boldsymbol{x} \in \partial\Omega$.

Spectral problem

In the Hilbert space $H = L_2(\Omega)$, we define the scalar product and norm in the standard way:

$$(u, v) = \int_\Omega u(\boldsymbol{x}) v(\boldsymbol{x}) d\boldsymbol{x}, \quad \|u\| = (u, u)^{1/2}.$$

For the spectral problem

$$\mathcal{A}\varphi_k = \lambda_k \varphi_k, \quad \boldsymbol{x} \in \Omega,$$

$$k(\boldsymbol{x}) \frac{\partial \varphi_k}{\partial n} + g(\boldsymbol{x}) \varphi_k = 0, \quad \boldsymbol{x} \in \partial\Omega,$$

we have

$$\lambda_1 \leq \lambda_2 \leq ...,$$

and the eigenfunctions φ_k, $\|\varphi_k\| = 1$, $k = 1, 2, ...$ form a basis in $L_2(\Omega)$. Therefore,

$$u = \sum_{k=1}^{\infty} (u, \varphi_k) \varphi_k.$$

Fractional power of the operator

Let the operator $\mathcal{A}$ be defined in the following domain:

$$D(\mathcal{A}) = \{u \mid u(\boldsymbol{x}) \in L_2(\Omega),\ \sum_{k=0}^{\infty} |(u, \varphi_k)|^2 \lambda_k < \infty\}.$$

The operator $\mathcal{A}$ is self-adjoint and positive definite:

$$\mathcal{A} = \mathcal{A}^* \geq \delta I, \quad \delta > 0,$$

where I is the identity operator in H. For δ, we have $\delta = \lambda_1$. In applications, the value of λ_1 is unknown (the spectral problem must be solved). Therefore, we assume that $\delta \leq \lambda_1$. Let us assume for the fractional power of the operator $\mathcal{A}$:

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

Mathematically complete definition of fractional powers of elliptic operators is given in Carracedo et al. [2001], Yagi [2009].

Nonstationary problems

We seek the solution of a Cauchy problem for the evolutionary first-order equation with the fractional power of the operator $\mathcal{A}$. The solution $u(\boldsymbol{x}, t)$ satisfies the equation

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

and the initial condition

$$u(0) = u_0.$$

The key issue in the study of computational algorithms for solving the Cauchy problem is to establish the stability of the approximate solution with respect to small perturbations of the initial data and the right-hand side in various norms.

Discrete elliptic operator

To solve numerically the problem, we employ finite element approximations in space (see, e.g., Brenner and Scott [2008], Thomée [2006]). We define the bilinear form

$$a(u, v) = \int_\Omega (k \operatorname{grad} u \operatorname{grad} v + c\, uv)\, d\boldsymbol{x} + \int_{\partial\Omega} g\, uv d\boldsymbol{x}.$$

We have

$$a(u, u) \geq \delta \|u\|^2.$$

Define the subspace of finite elements $V^h \subset H^1(\Omega)$ and the discrete elliptic operator A as

$$(Ay, v) = a(y, v), \quad \forall\ y, v \in V^h.$$

Fractional power of the operator

For the spectral problem $A\widetilde{\varphi}_k = \widetilde{\lambda}_k$ we have

$$\widetilde{\lambda}_1 \leq \widetilde{\lambda}_2 \leq ... \leq \widetilde{\lambda}_{M_h}, \quad \|\widetilde{\varphi}_k\| = 1, \quad k = 1, 2, ..., M_h.$$

The domain of definition for the operator A is

$$D(A) = \{y \mid y \in V^h, \ \sum_{k=0}^{M_h} |(y, \widetilde{\varphi}_k)|^2 \widetilde{\lambda}_k < \infty\}.$$

The operator A acts on the finite dimensional space V^h and

$$A = A^* \geq \underline{\delta}_h I, \quad \underline{\delta}_h > 0,$$

where $\underline{\delta}_h \leq \lambda_1 \leq \widetilde{\lambda}_1$. For the fractional power of the operator A:

$$A^\alpha y = \sum_{k=1}^{M_h} (y, \widetilde{\varphi}_k) \widetilde{\lambda}_k^\alpha \widetilde{\varphi}_k.$$

In detail: Acosta and Borthagaray [2017], Szekeres and Izsák [2016].

Time-dependent problems

We put into the correspondence the operator equation for $w(t) \in V^h$:

$$\frac{dw}{dt} + A^\alpha w = \psi(t), \quad 0 < t \le T,$$

$$w(0) = w_0,$$

where $\psi(t) = Pf(t)$, $w_0 = Pu_0$ with P denoting L_2-projection onto V^h.

Now we obtain an elementary a priori estimate for the solution assuming that the solution of the problem, coefficients of the elliptic operator, the right-hand side and initial conditions are sufficiently smooth.

Stability of the solution

Let us multiply equation by w and integrate it over the domain Ω:

$$\left(\frac{dw}{dt}, w\right) + (A^\alpha w, w) = (\psi, w).$$

In view of the self-adjointness and positive definiteness of the operator A^α, we have

$$\left(\frac{dw}{dt}, w\right) \leq (\psi, w).$$

The latter inequality leads us to the desired a priori estimate:

$$\|w(t)\| \leq \|w_0\| + \int_0^t \|\psi(\theta)\| d\theta.$$

We will focus on this estimate for the stability of the solution with respect to the initial data and the right-hand side in constructing discrete analogs.

Simplest scheme

We use simplest explicit and implicit two–level schemes. Let τ be a step of a uniform grid in time such that $w^n = w(t^n), \ t^n = n\tau$, $n = 0, 1, ..., N, \ N\tau = T$. It seems reasonable to begin with

$$\frac{w^{n+1} - w^n}{\tau} + A^\alpha w^n = \psi^n, \quad n = 0, 1, ..., N-1,$$

$$w^0 = w_0.$$

Advantages and disadvantages of explicit schemes for the standard parabolic problem ($\alpha = 1$) are well-known, i.e., these are a simple computational implementation and a time step restriction.
In our case ($\alpha \neq 1$), the main drawback (conditional stability) remains, whereas the advantage in terms of implementation simplicity does not exist.

Numerical implementation

The approximate solution at a new time-level is determined as

$$w^{n+1} = w^n - \tau A^\alpha w^n + \tau \psi^n.$$

Thus, we must calculate $A^\alpha w^n$.
The numerical implementation is based on the following representation:

$$w^{n+1} = -\tau A r^n + w^n + \tau \psi^n, \quad r^n = A^{\alpha-1} w^n.$$

We construct a numerical algorithm that employ the rational approximation of the operator

$$A^{-\beta}, \quad \beta = 1 - \alpha, \quad 0 < \beta < 1.$$

In this case, we solve standard problems that are related to the operator A.

Integral representation

We use an approximation for $A^{-\beta}$ based on integral representation of a self-adjoint and positive definite operator A (see, e.g., Krasnoselskii et al. [1976], Carracedo et al. [2001]):

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

The approximation of $A^{-\beta}$ is based on the use of one or another quadrature formulas for the right-hand side.
Various possibilities in this direction are discussed in Bonito and Pasciak [2015].
One possibility is special Gauss–Jacobi quadrature formulas considered in Frommer et al. [2014], Aceto and Novati [2017].
Just this approximation of the operator $A^{-\beta}$ is used in the present work.

Gauss quadrature formulas

To achieve higher accuracy in approximating the the right-hand side, it is natural to focus on the use of Gauss quadrature formulas. Some possibilities of constructing quadratures directly for half-infinite intervals are investigated, for example, in the work Gautschi [1991].
The classical Gauss quadrature formulas can be used via introducing a new variable of integration (see Frommer et al. [2014]):

$$\theta = \mu \frac{1-\eta}{1+\eta}, \quad \mu > 0.$$

Gauss–Jacobi quadrature formula

We have

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

To approximate the right-hand side, we apply the Gauss–Jacobi quadrature formula with the weight $(1-\eta)^{\tilde{\alpha}}(1+\eta)^{\tilde{\beta}})$ (see Ralston and Rabinowitz [2001]):

$$\int_{-1}^{1} f(t)(1-\eta)^{\tilde{\alpha}}(1+\eta)^{\tilde{\beta}}d\eta \approx \sum_{m=1}^{M}\omega_m f(\eta_m), \quad \alpha,\beta > -1.$$

Here $\eta_1,\eta_2,...,\eta_M$ are the roots of the Jacobi polynomial $J_M(\eta;\tilde{\alpha},\tilde{\beta})$ of degree M. The weights $\omega_1,\omega_2,...,\omega_M$ are given by the formula

$$\omega_m = -\frac{2M+\tilde{\alpha}+\tilde{\beta}+2}{M+\tilde{\alpha}+\tilde{\beta}+1}\frac{\Gamma(M+\tilde{\alpha}+1)\Gamma(M+\tilde{\beta}+1)}{\Gamma(M+\tilde{\alpha}+\tilde{\beta}+1)(M+1)!}\frac{2^{\tilde{\alpha}+\tilde{\beta}}}{J'_M(\eta_m;\tilde{\alpha},\tilde{\beta})J_{M+1}(\eta_m;\tilde{\alpha},\tilde{\beta})},$$

where Γ denotes the gamma function.

Computational scheme

For the fractional power of the operator A, we get

$$A^{-\beta} \approx R_M(A), \quad R_M(A) = \sum_{m=1}^{M} d_m (c_m I + A)^{-1},$$

where

$$\tilde{\alpha} = -\beta, \quad \tilde{\beta} = \beta - 1, \quad d_m = \frac{2\mu^{1-\beta}\sin(\pi\beta)}{\pi} \frac{\omega_m}{1+\eta_m}, \quad c_m = \mu \frac{1-\eta_m}{1+\eta_m}.$$

The approximate solution of the problem $r^n = A^{\alpha-1} w^n$ is associated with solving M standard problems
$r_m^n = (c_m I + A)^{-1} w^n, \ m = 1, 2, ..., M.$
We employ the scheme

$$w^{n+1} = -\tau A R_M(A) w^n + w^n + \tau \psi^n, \quad n = 0, 1, ..., N-1.$$

Stability conditions

For a finite-dimensional self-adjoint operator A, in addition to the lower bound, the following upper bound holds:

$$A \leq \overline{\delta}_h I,$$

where $\overline{\delta}_h = \mathcal{O}(h^{-2})$. Thus

$$\underline{\delta}_h^\alpha I \leq A^\alpha \leq \overline{\delta}_h^\alpha I, \quad 0 < \alpha < 1.$$

Similar estimates we have also for $AR_M(A)$:

$$\underline{\gamma}_h I \leq AR_M(A) \leq \overline{\gamma}_h I, \quad 0 < \alpha < 1,$$

with some $\underline{\gamma}_h, \overline{\gamma}_h > 0$.

Basic Statement

Theorem 1. *If*

$$\tau \leq \tau_0 = \frac{2}{\overline{\gamma}_h},$$

then the scheme is stable in H and the solution satisfies the following estimate:

$$\|w^{n+1}\| \leq \|w^0\| + \tau \sum_{j=0}^{n} \|\psi^j\|, \quad n = 0, 1, ..., N-1.$$

The function $zR_M(z)$ for $z \geq z_0 > 0$ is a positive and monotonically increasing function. In view of this, we have

$$\overline{\gamma}_h < \lim_{z \to \infty} zR_M(z) = \overline{\gamma}(M, \alpha), \quad \alpha = 1 - \beta,$$

where

$$\overline{\gamma}(M, \alpha) = \sum_{m=1}^{M} d_m.$$

Remark

Special attention (see Frommer et al. [2014], Aceto and Novati [2017]) should be given to the problem of choosing the parameter μ. Taking into account the definition of the operator A, we are interested in the best approximation of $A^{-\beta}$ for the smallest (principal) eigenvalue $\widetilde{\lambda}_1$.

In Frommer et al. [2014], there is established a remarkable fact that $R_M(z)$ corresponds to a Pade–type approximation for the function $z^{-\beta}$ with expansion point μ.

Thus, the optimal choice corresponds to the selection $\mu = \underline{\delta}_h$. In this case, we have $\underline{\gamma} = \underline{\delta}_h^\alpha$.

The computational complexity of finding $\underline{\delta}_h = \widetilde{\lambda}_1$ (the principal eigenvalue of a discrete self-adjoint elliptic operator of second order) is not high. To this end, it is possible to use standard algorithms (see, e.g., Saad [2011]) and the corresponding software (see Hernandez et al. [2005]).

Two-level schemes with weights

Unconditionally stable schemes are constructed on the basis of implicit approximations in time. Here we consider standard two-level schemes with weights. For a constant weight parameter σ $(0 < \sigma \leq 1)$, we define

$$w^{n+\sigma} = \sigma w^{n+1} + (1-\sigma) w^n.$$

Let us consider the implicit scheme

$$\frac{w^{n+1} - w^n}{\tau} + A^\alpha w^{n+\sigma} = \psi^{n+\sigma}, \quad n = 0, 1, ..., N-1.$$

For $\sigma = 1/2$, the difference scheme is the symmetric scheme (the Crank–Nicolson scheme). It approximates the differential problem with the second order by τ, whereas for other values of σ, we have only the first order.

Computational implementation

Rewrite the scheme in the form

$$\frac{w^{n+\sigma} - w^n}{\sigma \tau} + A^\alpha w^{n+\sigma} = \psi^{n+\sigma}, \quad n = 0, 1, ..., N-1.$$

In view of this, the transition to a new time-level involves the solution of the problem

$$(\nu I + A^\alpha) w^{n+\sigma} = \chi^n, \quad \nu = \frac{1}{\sigma \tau}.$$

For this problem, we construct the rational approximation of the operator

$$(\nu I + A^\alpha)^{-1}, \quad 0 < \alpha < 1.$$

Integral representation

The necessary approximation is based on the following integral representation:

$$(\nu I + A^\alpha)^{-1} = \frac{\sin(\pi\alpha)}{\pi} \int_0^\infty \frac{\theta^\alpha}{\theta^{2\alpha} + 2\theta^\alpha \nu \cos(\pi\alpha) + \nu^2} (A + \theta I)^{-1} d\theta,$$

taken from the work Carracedo et al. [2001].
Using the new variable θ, we arrive at the representation

$$(\nu I + A^\alpha)^{-1} = \frac{2\mu^{1-\alpha}\sin(\pi\alpha)}{\pi} \int_{-1}^1 (1-\eta)^{-\alpha}(1+\eta)^{\alpha-1} g(\eta;\nu,\alpha) \big(\mu(1-\eta)I + (1+\eta)A\big)^{-1} d\eta,$$

where

$$g^{-1}(\eta;\nu,\alpha) = 1 + 2\nu\cos(\pi\alpha)\mu^{-\alpha}\left(\frac{1+\eta}{1-\eta}\right)^\alpha + \nu^2\mu^{-2\alpha}\left(\frac{1+\eta}{1-\eta}\right)^{2\alpha}.$$

Operator approximation

The Gauss quadrature formula is used (see Gautschi [2004]) with the weight function

$$(1-\eta)^{-\alpha}(1+\eta)^{\alpha-1} g(\eta_m;\nu,\alpha).$$

We get

$$(\nu I + A^\alpha)^{-1} \approx R_M(A;\nu), \quad R_M(A;\nu) = \sum_{m=1}^{M} d_m^\nu (c_m I + A)^{-1}.$$

Thereby $R_M(A;0) = R_M(A)$.
For $\sigma > 0$, an approximate solution is obtained from

$$\begin{aligned} R_M^{-1}(A;\nu) w^{n+\sigma} &= \nu w^n + \psi^{n+\sigma}, \\ w^{n+1} &= \frac{1}{\sigma}(w^{n+\sigma} - (1-\sigma) w^n), \quad n = 0,1,...,N-1. \end{aligned}$$

Main result

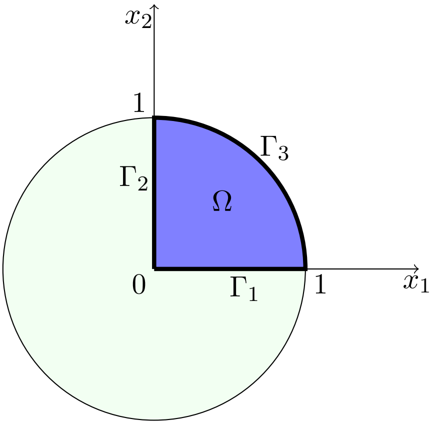
Theorem 2. *The difference scheme for $\sigma \geq 0.5$ and*

$$R_M^{-1}(A;\nu) \geq \nu I$$

is unconditionally stable in H and its solution satisfies the a priori estimate

$$\|w^{n+1}\| \leq \|w^0\| + \tau \sum_{j=0}^{n} \|\psi^{j+\sigma}\|, \quad n = 0, 1, ..., N-1.$$

Computational domain



Test problem

Consider the equation

$$\mathcal{A}u = -\Delta u, \quad \boldsymbol{x} \in \Omega,$$

with the boundary conditions

$$\frac{\partial u}{\partial n} = 0, \quad \boldsymbol{x} \in \Gamma_1, \quad \boldsymbol{x} \in \Gamma_2,$$

$$\frac{\partial u}{\partial n} + gu = 0, \quad \boldsymbol{x} \in \Gamma_3, \quad g = \text{const}.$$

We study the case, where the solution depends only on r, and $r = (x_1^2 + x_2^2)^{1/2}$. By virtue of this

$$\mathcal{A}u = -\frac{1}{r}\frac{d}{dr}\left(r\frac{du}{dr}\right), \quad 0 < r < 1,$$

$$\frac{du}{dr} + gu = 0, \quad r = 1.$$

Exact solution

The solution of the spectral problem

$$-\frac{1}{r}\frac{d}{dr}\left(r\frac{d\varphi_k}{dr}\right) = \lambda_k\varphi_k, \quad 0 < r < 1,$$

$$\frac{d\varphi_k}{dr} + g\varphi_k = 0, \quad r = 1,$$

is well-known. Eigenfunctions are represented as zero-order Bessel functions:

$$\varphi_k(r) = J_0(\sqrt{\lambda_k}r),$$

whereas eigenvalues $\lambda_k = \nu_k^2$, where $\nu_k,\ k = 1, 2, ...$ are roots of the equation

$$\nu J_0^{'}(\nu) + \mu J_0(\nu) = 0.$$

The general solution of the homogeneous Cauchy:

$$u(r,t) = \sum_{k=1}^{\infty} a_k \exp(-\nu_k^{2\alpha}t) J_0(\nu_k r).$$

Test solution

To study the accuracy of the approximate solution of the time-dependent equation with the fractional power of an elliptic operator, we use the exact solution

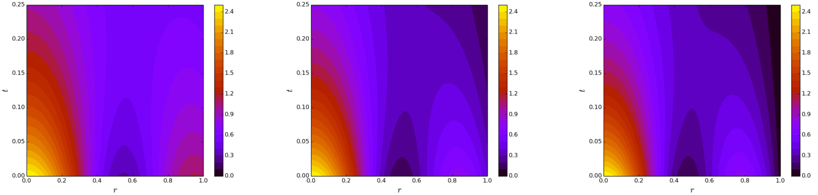
$$u(r,t) = \exp(-\nu_1^{2\alpha} t) J_0(\nu_1 r) + 1.5 \exp(-\nu_3^{2\alpha} t) J_3(\nu_3 r), \quad r = (x_1^2 + x_2^2)^{1/2}.$$

The values of the roots $\nu_1, \ \nu_3$ for different values of the boundary condition μ are given in Table.

Table: The roots of equation

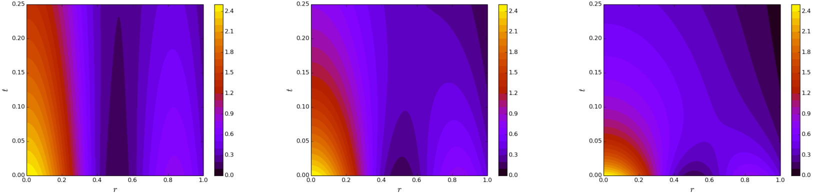
k	$g=1$	$g=10$	$g=100$
1	1.25578371	2.17949660	2.38090166
3	7.15579917	7.95688342	8.56783165

The exact solution for $T = 0.25$ at different values of g



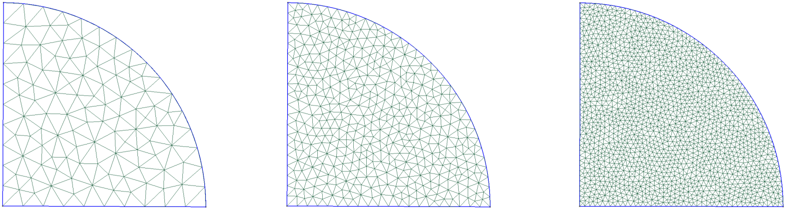
The solution for different g ($\alpha = 0.5$):
left: $g = 1$; center: $g = 10$; right: $g = 100$.

The exact solution for $T = 0.25$ at different values of α



The solution for different α $(g = 10)$:
left: $\alpha = 0.25$; center: $\alpha = 0.5$; right: $\alpha = 0.75$.

Calculation FEM grid



Left: 1 — 123 vertices and 208 cells;
center: 2 — 461 vertices and 848 cells;
right: 3 — 1731 vertices and 3317 cells.

Computational implementation

The finite element approximation in space is based on the use of continuous P_1 Lagrange element, namely, piecewise-linear elements. The calculations were performed using the computing platform FEniCS for solving partial differential equations (website http://fenicsproject.org, Logg et al. [2012], Alnæs et al. [2015]). To solve spectral problems with symmetrical matrices, we use the SLEPc library (Scalable Library for Eigenvalue Problem Computations, http://slepc.upv.es, Hernandez et al. [2005]). We apply the Krylov-Schur algorithm, a variation of the Arnoldi method, proposed by Stewart [2001].

Discrete operator A

Table presents the lower and upper bounds of the operator spectrum on various grids for different values of the parameter g in the boundary condition.

Table: The spectrum bounds of the operator A

g	$\delta = \lambda_1$	grid	$\underline{\delta}_h$	$\overline{\delta}_h$
1	1.57699272630	1	1.57959231369	4225.51507674
		2	1.57763558651	17104.1780271
		3	1.57715815735	74989.7519112
10	4.75020542941	1	4.76409956820	4252.23867499
		2	4.75363764524	17143.1279728
		3	4.75108440807	74989.7519112
100	5.66869271459	1	5.68846224707	7310.80621520
		2	5.67358161306	22017.7463507
		3	5.66994292109	74989.7519112

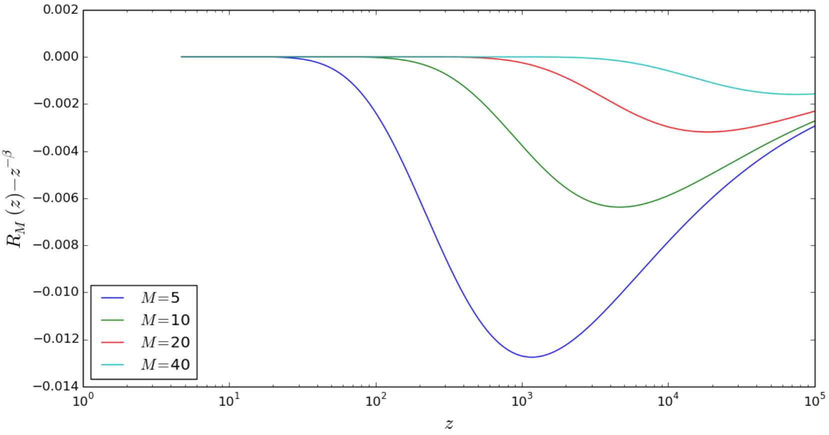
Approximation error

The numerical solution is compared with the exact one at the final time moment $u(\boldsymbol{x}, T)$. Error estimation is performed in $L_2(\Omega)$ and $L_\infty(\Omega)$:

$$\varepsilon_2 = \|w^N(\boldsymbol{x}) - u(\boldsymbol{x}, T)\|, \quad \varepsilon_\infty = \max_{\boldsymbol{x} \in \Omega} |w^N(\boldsymbol{x}) - u(\boldsymbol{x}, T)|.$$

Figure shows the absolute error arising from the approximation of $z^{-\beta}$ by the function $R_M(z)$ for $\beta = 0.5$ and $g = 10$. In this case, $\mu = \delta$ and $R_M(z_0) = z_0^{-\beta}$.
We see higher accuracy near the left boundary $z = z_0$, whereas for large z, the approximation accuracy decreases. The effect of increasing accuracy with increasing number of nodes of the quadrature formula is clearly observed.

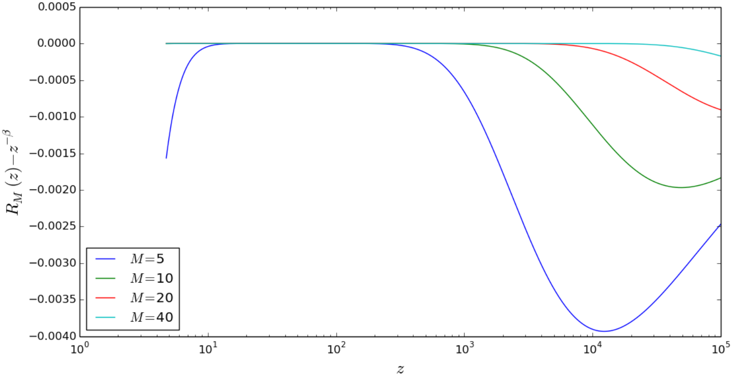
Approximation error for $\beta = 0.5$



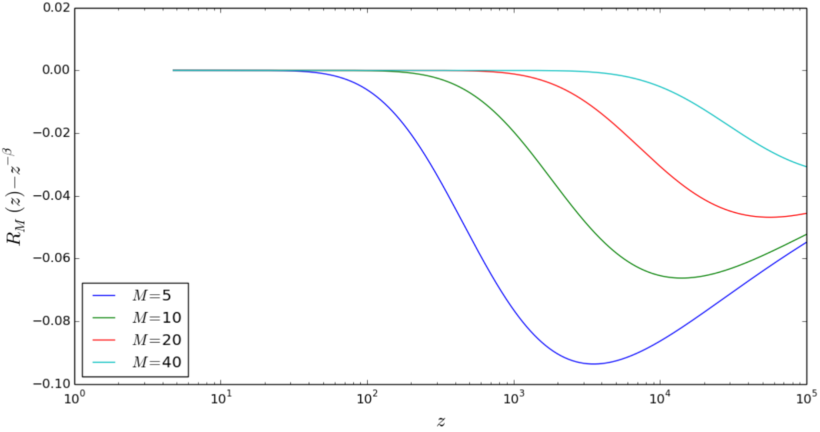
$\mu = \delta,\ z_0^{-\beta} = 0.458821546223$

Approximation error for $\beta = 0.5$ ($\mu = 50$)

Decreasing the approximation accuracy at $z \approx z_0$, we can increase the accuracy for other values of z. Figure demonstrates the approximation accuracy for $\mu = 50$. In this case $R_M(\mu) = \mu^{-\beta}$.

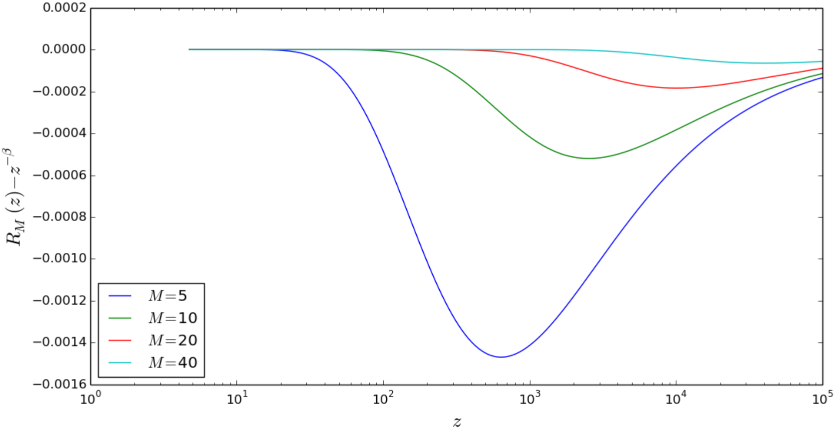


Approximation error for $\beta = 0.25$



$$\mu = \delta, \; z_0^{-\beta} = 0.677363673534$$

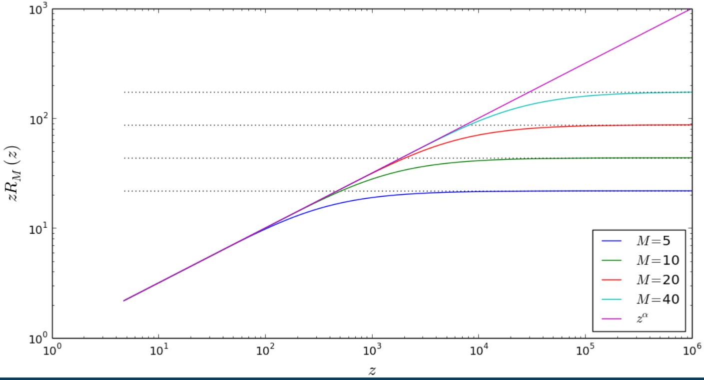
Approximation error for $\beta = 0.75$



$$\mu = \delta,\ z_0^{-\beta} = 0.310789048046$$

Approximation of A^α ($\alpha = 0.5$) for various M

The numerical implementation of the explicit scheme involves the approximation of the operator A^α by the expression $AR_M(A)(\beta = 1 - \alpha)$. Peculiarities of this approximation at $\alpha = 0.5$, $g = 10$ are shown in Figure.



Operator of explicit scheme

The upper bounds of the operator $AR_M(A)$ are given in Table for $g = 10$.

Increasing $\overline{\gamma}(M, \alpha)$ with increasing the number of quadrature formula nodes M results from increasing the accuracy of approximation of the unbounded operator A^α.

As α decreases, the value of $\overline{\gamma}(M, \alpha)$ decreases drastically.

Table: The upper bounds of the operator $AR_M(A)$

M	$\overline{\gamma}(M, 0.25)$	$\overline{\gamma}(M, 0.5)$	$\overline{\gamma}(M, 0.75)$
5	4.4602175	21.794966	142.00220
10	6.3106349	43.589932	401.45610
20	8.9256294	87.179864	1135.3565
40	12.623116	174.35973	3211.1792

Explicit scheme

Now we present numerical results obtained using the explicit scheme.
We confine ourselves to the case $\alpha = 0.5$ with the value of the boundary condition parameter $g = 10$.
It is interesting to identify the dependence of accuracy on grids in space and time.
In our case, we should also study the influence of the number of quadrature formula nodes M. Tables demonstrates the numerical solution convergence for decreasing the time step and increasing the accuracy of approximation of the fractional power operator.

Error of the solution for the explicit scheme

Table: Grid 2 ($\mu = 10, \alpha = 0.5$)

M	N	25	50	100	200
5	ε_2	0.00436648	0.00207328	0.00094905	0.00041937
	ε_∞	0.01896717	0.00927482	0.00447550	0.00216564
10	ε_2	0.00507635	0.00277981	0.00164515	0.00108352
	ε_∞	0.02186657	0.01217982	0.00738292	0.00499609
20	ε_2	0.00507902	0.00278251	0.00164787	0.00108627
	ε_∞	0.02187724	0.01219044	0.00739354	0.00500671
40	ε_2	0.00507902	0.00278251	0.00164787	0.00108627
	ε_∞	0.02187723	0.01219043	0.00739352	0.00500669

Spatial grid refinement

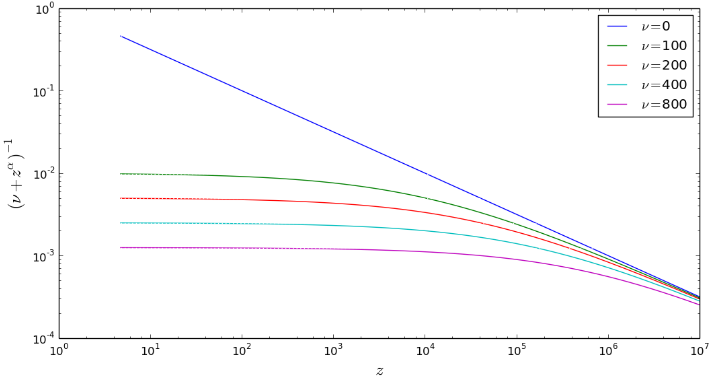
Table: Error of the solution for various spatial grids
($\mu = 10, \alpha = 0.5, M = 20$)

grid	N	25	50	100	200
1	ε_2	0.00641387	0.00419465	0.00310833	0.00257568
	ε_∞	0.02505950	0.01634587	0.01202969	0.00988175
2	ε_2	0.00507902	0.00278251	0.00164787	0.00108627
	ε_∞	0.02187724	0.01219044	0.00739354	0.00500671
3	ε_2	0.00472777	0.00241442	0.00126921	0.00069981
	ε_∞	0.02077071	0.01081355	0.00588308	0.00342987

Function $(\nu + z^\alpha)^{-1}$ for $\alpha = 0.5, z \geq z_0 = \delta$ at various ν

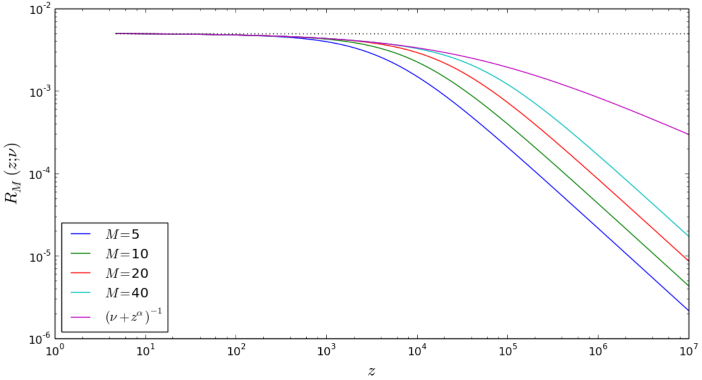
The numerical implementation of implicit schemes is associated with the function $(\nu + z^\alpha)^{-1}$.

The function $(\nu + z^\alpha)^{-1}$, which corresponds to our test problem for $\alpha = 0.5$, is shown in Figure.

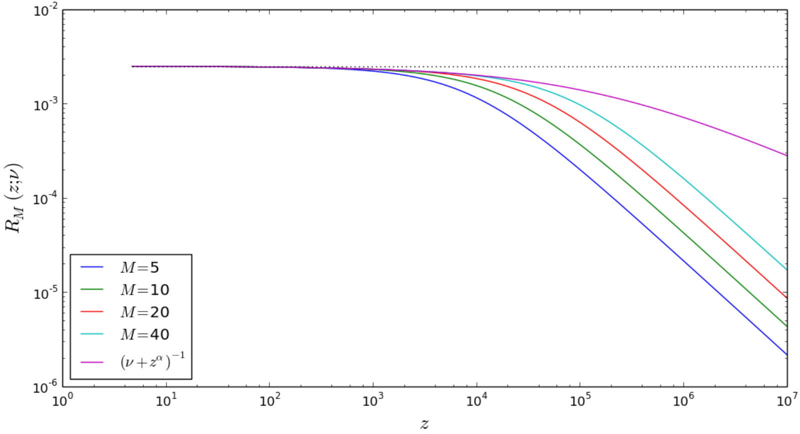


Function $R_M(z;\nu)$ for $\alpha = 0.5, \nu = 200$ at various M

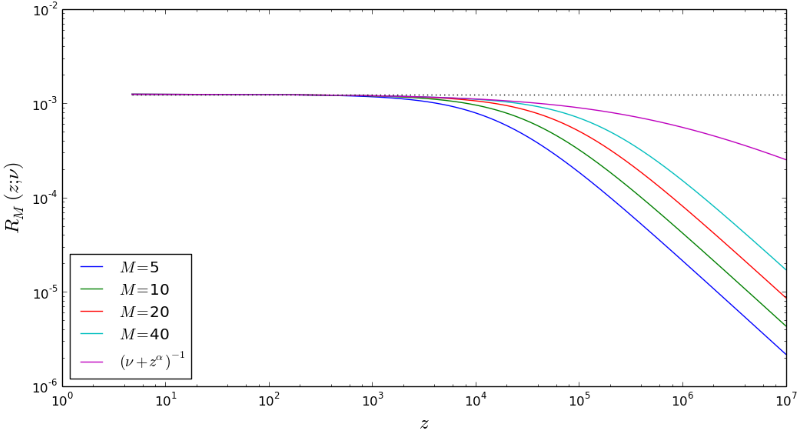
Figure shows the approximating function $R_M(z;\nu)$ for $\nu = 200$ with $\mu = \delta$. Operator approximations were designed using the package ORTHPOL (see Gautschi [1994]).



Function $R_M(z;\nu)$ for $\alpha = 0.5, \nu = 400$ at various M



Function $R_M(z;\nu)$ for $\alpha = 0.5, \nu = 800$ at various M



Implicit scheme

The accuracy of the approximate solution of the test problem was investigated for $\alpha = 0.5, \mu = 10$, and $g = 10$.
able demonstrates the dependence of the solution accuracy on the grid in time for various numbers M.

Table: Error of the solution for the implicit scheme on grid 2

M	N	25	50	100	200
5	ε_2	0.00326281	0.00111138	0.00044581	0.00078676
	ε_∞	0.01672817	0.00699940	0.00208775	0.00313725
10	ε_2	0.00394436	0.00173870	0.00063823	0.00018398
	ε_∞	0.01975034	0.01002383	0.00511271	0.00264674
10	ε_2	0.00394696	0.00174126	0.00064056	0.00018400
	ε_∞	0.01976054	0.01003442	0.00512346	0.00265756
10	ε_2	0.00394696	0.00174126	0.00064056	0.00018399
	ε_∞	0.01976037	0.01003433	0.00512339	0.00265750

Conclusion

1. There is considered a nonclassical problem with the initial data, which is described by an evolutionary equation of first order with a fractional power of an elliptic operator. The multidimensional problem is approximated in space using standard finite element piecewise-linear approximations.
2. The explicit scheme is implemented using a Pade-type approximation for the fractional power elliptic operator. Sufficient conditions for the stability of the explicit scheme are formulated. They do not depend on spatial grid steps.
3. Rational approximation is employed to implement implicit schemes. It is based on a computational generation of Gauss quadrature formulas for an integral representation of the operator of transition to a new time-level.
4. Possibilities of the proposed algorithms were demonstrated through numerical solving a test two-dimensional problem.

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