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On a Framework for the Stability and Convergence Analysis of Discrete Schemes for Nonstationary Nonlocal Problems of Parabolic Type

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Abstract: The main aim of this article is to propose a general framework for the theoretical analysis of discrete schemes used to solve multi-dimensional parabolic problems with fractional power elliptic operators. This analysis is split into three parts. The first part is based on techniques well developed for the solution of nonlocal elliptic problems. The obtained discrete elliptic operators are used to formulate semi-discrete approximations. Next, the fully discrete schemes are constructed by applying the classical and robust approximations of time derivatives. The existing stability and convergence results are directly included in the new framework. In the third part, approximations of transfer operators are constructed by using uniform and the best uniform rational approximations. The stability and accuracy of the obtained local discrete schemes are investigated. The results of computational experiments are presented and analyzed. A three-dimensional test problem is solved. The rational approximations are constructed by using the BRASIL algorithm.

Keywords: fractional power elliptic operators; parabolic problems; discrete schemes; stability; convergence analysis

MSC: 65N06; 65N12; 65N22

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1. Introduction

Recently, fractional differential equations have been used to simulate non-standard diffusive processes when an anomalous diffusion is important. We can mention models used to describe chemical and contaminant transport in heterogeneous aquifers [1], physics [2], medicine [3], and image processing [4]. More examples are given in [5,6].

This paper is a continuation of our previous work [7]. Recently, much attention has been devoted to the solution of multi-dimensional parabolic problems with fractional power elliptic operators. Our activity was initiated due to some critical experience in the analysis of numerical methods for the solution of mathematical models when some/all classical differential operators are substituted by fractional differential operators. A typical approach is to construct and investigate numerical algorithms for each problem from scratch. Our aim is to propose a general framework and to specify what parts of this analysis really require new modifications of existing techniques. We split the work into three parts. The first part is based on techniques well known for the analysis of fractional power elliptic problems. The constructed discrete elliptic operators make a basis to formulate semi-discrete approximations. In the second part of the framework, fully discrete schemes are constructed. Again, we can use some classical and robust approximations of time derivatives. The stability and convergence of the discrete solutions follow directly from the existing theoretical results for classical parabolic problems. In the third part, approximations of transfer operators are constructed. Exactly this part of the framework requires additional theoretical analysis and modifications of the discrete algorithms. In this paper, we use uniform and the best uniform rational approximations. The stability

and accuracy of the obtained local discrete schemes is investigated. The very efficient best rational approximation by successive interval length adjustment (BRASIL) tool [8] is used for the computation of the best uniform rational approximations (BURAs). Deep results on BURA-type approximations for spectral fractional elliptic equations are presented in [9]. These results make a good theoretical basis for the analysis of discrete schemes for the solution of parabolic problems with fractional elliptic operators.

Another popular technique for the solution of elliptic and parabolic fractional diffusion problems is based on the unified rational Krylov method and investigated in [10]. The authors compare several existing pole selection strategies and provide a certified error bound to assess their quality. In addition they develop two new pole generation algorithms tailored to the framework of fractional diffusion.

One more general approach is based on a Lanczos method. The main benefit of this algorithm is that the required matrix–function–vector products are computed without ever forming the dense matrix A_h^α. A preconditioned Lanczos method can be used to accelerate the convergence of this method (see [11] and the references given therein).

A reduced basis method for fractional diffusion operators and applications for the solution of fractional power elliptic problems is proposed in [12].

We note that additional classes of approximation algorithms should be also considered as practical tools for the approximation of nonlocal operators; see as examples [13] and techniques based on artificial neural networks [14,15].

Here, we comment briefly on a more general definition of fractional calculus. It is a powerful tool that has been recently employed to model complex biological systems and different processes with nonlinear behavior and long-term memory. The definition of the fractional-order derivative is not unique; still, there are some generally accepted and common definitions. We recommend [16] for an excellent and deep introduction to this topic. Still, in this paper, we deal with a specific class of nonlocal problems, where, instead of fractional derivatives, a fractional power of the full elliptic operator is considered. Solutions of such models have quite different properties, and in many cases, they are optimal tools to describe the complicated real-world applications.

In this paper, we use the spectral definition of the fractional power of an elliptic operator A_h^α (the details are given in Section 2). As it is noted in many papers, the spectral algorithm can be used for practical computations to solve parabolic-type problems with nonlocal diffusion operators. Then, the complexity of such algorithms to solve nonlocal parabolic problems is the same as for a fast Fourier transform (FFT) method targeted at standard elliptic operators. However, clearly, this strategy is computationally efficient only if the differential problem is solved in a rectangular domain, the complete set of eigenfunctions of operator A_h is known, in advance, and FFT-type techniques can be applied.

A more general idea is to transform nonlocal problems into the local classical differential problems. A very good review on these methods is given in [17]. The theoretical analysis of various modifications of uniform rational approximations for the solution of elliptic problems was presented in [18].

The rest of the paper is organized in the following way. In Section 2, the problem is formulated. The non-stationary parabolic equation with a fractional power elliptic operator is defined. As was mentioned above, the spectral definition is used to define fractional power elliptic operators. A general framework for the analysis of discrete schemes targeted at solving such problems is formulated. The first step of this scheme is analyzed, when the nonlocal elliptic operator is approximated in a finite-dimensional space and a semidiscrete scheme is constructed. A general approach is specified for how the approximation error of this step is investigated. This technique is applied for a three-dimensional test problem.

The second step of the proposed general framework of analysis is considered in Section 3. Fully discrete schemes are constructed. Most of the well-known implicit methods can be used to approximate the semidiscrete problem. As an example, we consider the backward Euler method. The standard approximation error and stability estimates are

provided. The results of the computational experiments are presented and analyzed. They confirm a delicate interlacing of space and time discrete approximations.

In Section 4, the third step of the general framework is considered. A time transfer operator of the fully discrete scheme depends on the nonlocal discrete operator A_h^α. The goal of this step is to approximate it by some local operator. Here, we use methods based on the best uniform rational approximations (BURAs). The required rational functions are computed by applying the BRASIL algorithm (BURA-BRASIL scheme) [8]. The stability analysis of the obtained scheme shows that it is stable at least for sufficiently small time step sizes. In addition, a computational stability test is proposed. As an example, this criterion is applied for the 3D test problem, and it is proven that, for different popular values of fractional parameters and a broad set of time steps, the constructed BURA-BRASIL scheme is unconditionally stable. Next, the approximation accuracy of the third step of the general framework is investigated and a global error of the discrete solution is estimated. The results of computational experiments are presented and analyzed.

In Section 5, the third step of the general framework is applied for one more approximation of the nonlocal operator, which is based on a uniform rational approximation (URA) method. The experimental stability criterion is used in the analysis, and it is proven that the URA-BRASIL scheme is unconditionally stable for the given fractional parameters and time step sizes. The approximation error analysis shows that this error does not depend on the time step size, and it can be reduced only by increasing the order m of the rational approximation function.

In Section 6, a stability analysis of a Crank–Nicolson-type BURA-BRASIL scheme is performed. The stability factor of the Crank–Nicolson scheme has a more complicated dependence on large eigenvalues of the discrete elliptic operator; hence, the stability analysis of the BURA-BRASIL approximation is a good test for the proposed general framework techniques.

In Section 7, an applied problem is solved. The mathematical model describes biofilm formation. A generalized nonlocal diffusion process is included in the model. A numerical simulation is performed by using a symmetrical splitting scheme, where splitting is performed with respect to physical processes. Applying techniques of the proposed theoretical framework, it is shown that the scheme is second-order in time and space. The results of the computational experiments are presented. Some final conclusions are given in Section 8.

2. Problem Formulation

Let H be a Hilbert space with a scalar product (u, v) for $u, v \in H$. Then, the L_2-norm is defined as $\|u\| = (u, u)^{1/2}$.

Let A be a self-adjoint positive definite operator,

$$A: \quad H \to H, \quad A = A^*, \quad A \geqslant cI, \quad c > 0,$$

where I is the identity operator.

Next, we define a fractional power of this operator A^α with a fractional parameter $0 < \alpha < 1$. This definition can be given in a non-unique way, and we use the spectral approach. Let us solve the standard eigen-problem:

$$A\psi_j = \lambda_j \psi_j, \quad j = 1, 2, \ldots.$$

All eigenvalues are positive:

$$0 < \lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_m \leqslant \cdots$$

and the set of eigenfunctions $\{\psi_j\}$ make an orthonormal basis for H. Then, any function $u \in H$ can be written as

$$u = \sum_{j=1}^{\infty} (u, \psi_j)\psi_j.$$

A nonlocal operator A^α with fractional parameter $0 < \alpha < 1$ is defined as

$$A^\alpha u = \sum_{j=1}^{\infty} \lambda_j^\alpha \, (u, \psi_j)\psi_j.$$

Here, we note that it is possible to consider more general nonlocal operators:

$$g(A)u = \sum_{j=1}^{\infty} g(\lambda_j) \, (u, \psi_j)\psi_j,$$

where function g satisfies some specific requirements; first of all, we require that

$$g(\lambda) \geqslant \delta I, \quad \delta = \min_{\lambda \in \sigma(A)} g(\lambda) > 0.$$

Here, $\sigma(A)$ denotes the spectrum of A. Such generalizations of nonlocal operators are considered for example in [19]. In this paper, we restrict ourselves to polynomial functions $g(\lambda) = \lambda^\alpha$. Still, we remark that the proposed techniques of approximation can be used for more general functions than the powers of eigenvalues. Such a modification of the BURA-BRASIL approximation is described in Section 4.

We are interested in solving the following Cauchy problem:

$$\frac{\partial u}{\partial t} + A^\alpha u = F, \quad 0 < t \leqslant T, \tag{1}$$

$$u(0) = u_0, \quad u_0 \in H. \tag{2}$$

By using the Fourier method, it is possible to write the solution of this problem in an explicit form $u(t) = \sum_{j=1}^{\infty} u_j(t)\psi_j$, where

$$u_j(t) = u_{0j} e^{-\lambda_j^\alpha t} + e^{-\lambda_j^\alpha t} \int_0^t e^{\lambda_j^\alpha s} f_j(s) \, ds,$$

$$F(t) = \sum_{j=1}^{\infty} f_j(t)\psi_j, \quad u_0 = \sum_{j=1}^{\infty} u_{0j}\psi_j.$$

Semidiscrete Scheme

First, we approximate operator A^α by considering a finite-dimensional Hilbert space H_h. For simplicity, we denote a scalar product in H_h again as (U, V), for $U, V \in H_h$. By taking into account the spectral definition of the nonlocal operator A^α, we approximate the local operator A by applying the finite-difference, finite-volume, or finite-element method. It is required to guarantee that A_h is again a self-adjoint positive definite operator:

$$A_h : \ H_h \to H_h, \quad A_h = A_h^*, \quad A_h \geqslant c I_h, \ \ c > 0,$$

where I_h is the discrete identity operator. Some modification of the definitions should be performed in the case of finite-element approximations. Let $\{\phi_j^h\}$, $j = 1, \ldots, J$ be a basis of space H_h and introduce the mass M_h and stiffness $\widetilde{A}_h$ matrix by

$$M_{ij} = (\phi_j^h, \phi_i^h), \quad \widetilde{A}_{ij} = (A\phi_j^h, \phi_i^h),$$

respectively. Then, the discrete operator A_h is defined by $A_h = M_h^{-1}\widetilde{A}_h$.

Let us solve the standard eigen-problem:

$$A_h \psi_j^h = \mu_j \psi_j^h, \quad j = 1, \ldots, J. \tag{3}$$

All eigenvalues are positive

$$0 < \mu_1 \leqslant \mu_2 \leqslant \cdots \leqslant \mu_J$$

and the set of eigenfunctions $\{\psi_j^h\}$ make an orthonormal basis for H_h. Then, any function $U \in H_h$ can be written as

$$U = \sum_{j=1}^{J} (U, \psi_j^h)\psi_j^h.$$

We use the discrete eigenfunctions to replace the fractional operator A^α by its discrete approximation

$$A_h^\alpha U = \sum_{j=1}^{J} \mu_j^\alpha \, (U, \psi_j^h)\psi_j^h.$$

We approximate the problem (1) and (2) by the following semidiscrete Cauchy problem:

$$\frac{\partial U}{\partial t} + A_h^\alpha U = F, \quad 0 < t \leqslant T, \tag{4}$$

$$U(0) = U_0, \quad U_0 \in H_h. \tag{5}$$

By using the Fourier method it is possible to write the solution of this problem in an explicit form $U(t) = \sum_{j=1}^{J} U_j(t)\psi_j^h$, where

$$U_j(t) = U_{0j}e^{-\mu_j^\alpha t} + e^{-\mu_j^\alpha t}\int_0^t e^{\mu_j^\alpha s} F_j(s)\, ds,$$

$$F(t) = \sum_{j=1}^{J} F_j(t)\psi_j^h, \quad U_0 = \sum_{j=1}^{J} U_{0j}\psi_j^h.$$

In the following analysis, we always assume that there exists a sufficiently smooth solution of problem (1) and (2). The existence of a solution of the semidiscrete problem (4) and (5) is demonstrated above. Still, we are interested in estimating the approximation accuracy of this semidiscrete scheme. We restrict ourselves to the analysis of finite-difference and finite-volume schemes. Let us assume that $u_h \in H_h$ is a suitable representation of the exact solution of the PDE (1) and (2). The approximation error of the semidiscrete Equation (4) is defined formally in a standard way (see [20,21]):

$$\Psi_h(t) := \frac{\partial u_h}{\partial t} + A_h^\alpha u_h - F = A_h^\alpha u_h - (A^\alpha u)_h. \tag{6}$$

For nonlocal operators, we cannot use the convenient technique of Taylor expansion. The approximation error can be estimated in a different way. Let us apply the definition of nonlocal operators A^α and A_h^α, then we obtain

$$\Psi_h = \sum_{j=1}^{J} \left(u_{hj}\mu_j^\alpha \psi_j^h - u_j\lambda_j^\alpha \psi_j\right) - \sum_{j=J+1}^{\infty} \lambda_j^\alpha u_j \psi_j.$$

The second term can be bounded by $O(h^k)$ depending on the smoothness of the solution. Next, we formulate accuracy estimates that are sufficient to prove that the approximation error is bounded by $O(h^2)$:

1. $\left|(u_h, \psi_j^h) - (u, \psi_j)\right| \leqslant Ch^2$,
2. $\left\|\psi_j^h - \psi_{jh}\right\| \leqslant Ch^2$,
3. $\left|\mu_j^\alpha - \lambda_j^\alpha\right| \leqslant Ch^2, \;\; j = 1, \ldots, J.$

Such estimates are known for many popular approximations of elliptic problems [21–23].

Example 1. *In this example, we solve a linear fractional heat equation with a linear source term in three-dimensional space* $\Omega = [0,1] \times [0,1] \times [0,1]$ *(see [7]):*

$$\frac{\partial u}{\partial t} + (-\Delta)^{\alpha} u = F(x,y,z,t,u), \quad (x,y,z) \in \Omega, \tag{7}$$
$$F(x,y,z,t,u) = t^{2\alpha} \sum_{i=1}^{8} \beta_i \lambda_i^{\alpha} v_i + \left(2\alpha t^{2\alpha-1} + t^{2\alpha}\right) \sin^3(\pi x) \sin^3(\pi y) \sin^3(\pi z) - u,$$
$$u(x,y,z,t) = 0, \quad (x,y,z) \in \partial\Omega,$$

where

$$\begin{aligned}
v_1 &= \sin(\pi x)\sin(\pi y)\sin(\pi z), \quad \lambda_1 = 3\pi^2, \quad \beta_1 = 27/64,\\
v_2 &= \sin(\pi x)\sin(\pi y)\sin(3\pi z), \quad \lambda_2 = 11\pi^2, \quad \beta_2 = -9/64,\\
v_3 &= \sin(\pi x)\sin(3\pi y)\sin(\pi z), \quad \lambda_3 = 11\pi^2, \quad \beta_3 = -9/64,\\
v_4 &= \sin(\pi x)\sin(3\pi y)\sin(3\pi z), \quad \lambda_4 = 19\pi^2, \quad \beta_4 = 3/64,\\
v_5 &= \sin(3\pi x)\sin(\pi y)\sin(\pi z), \quad \lambda_5 = 11\pi^2, \quad \beta_5 = -9/64,\\
v_6 &= \sin(3\pi x)\sin(\pi y)\sin(3\pi z), \quad \lambda_6 = 19\pi^2, \quad \beta_6 = 3/64,\\
v_7 &= \sin(3\pi x)\sin(3\pi y)\sin(\pi z), \quad \lambda_7 = 19\pi^2, \quad \beta_7 = 3/64,\\
v_8 &= \sin(3\pi x)\sin(3\pi y)\sin(3\pi z), \quad \lambda_8 = 27\pi^2, \quad \beta_8 = -1/64.
\end{aligned}$$

This problem has the exact solution [5]

$$u(x,y,z,t) = t^{2\alpha} \sin^3(\pi x) \sin^3(\pi y) \sin^3(\pi z).$$

A discrete approximation of the 3D diffusion operator is constructed by using the finite-volume method. A uniform space mesh is defined $\bar{\Omega}_h = \bar{\omega}_x \times \bar{\omega}_y \times \bar{\omega}_z$*:*

$$\begin{aligned}
\bar{\omega}_x &= \{x_i : \ x_i = ih, \ i = 0, \dots, J_x, \ h = 1/J_x\},\\
\bar{\omega}_y &= \{y_j : \ y_j = jh, \ j = 0, \dots, J_x, \ h = 1/J_x\},\\
\bar{\omega}_z &= \{z_j : \ z_k = kh, \ k = 0, \dots, J_x, \ h = 1/J_x\}
\end{aligned}$$

and the discrete diffusion operator is constructed:

$$\begin{aligned}
A_h U = -\Big(&\frac{U_{i+1,jk} - 2U_{ijk} + U_{i-1,jk}}{h^2} + \frac{U_{i,j+1,k} - 2U_{ijk} + U_{i,j-1,k}}{h^2}\\
&+ \frac{U_{ij,k+1} - 2U_{ijk} + U_{ij,k-1}}{h^2}\Big).
\end{aligned} \tag{8}$$

The solution of eigen-problem (3) for this operator A_h *is well known (see [21]):*

$$\psi^h_{h,lmr}(x_i, y_j, z_k) = 2\sqrt{2}\sin(\pi l x_i)\sin(\pi m y_j)\sin(\pi r z_k), \quad 0 < l, m, r < J_x,$$
$$\mu_{lmr} = \frac{4}{h^2}\left(\sin^2\left(\frac{\pi}{2}lh\right) + \sin^2\left(\frac{\pi}{2}mh\right) + \sin^2\left(\frac{\pi}{2}rh\right)\right).$$

As an example, we compute the global error of the solution of the semidiscrete scheme (4) and (5):

$$e(J_x) = \max_{(x,y,z)\in\Omega_h} |u(x,y,z,T) - U(x,y,z,T)|$$

for the final time $T = 1$ and the fractional power parameter $\alpha = 0.75$. The computed errors confirm the second-order accuracy of the proposed approximation:

$$e(200) = 7.298 \times 10^{-5}, \quad e(400) = 1.824 \times 10^{-5}, \quad e(800) = 4.564 \times 10^{-6}. \tag{9}$$

Hence, by selecting a sufficiently large $J = (J_x - 1)^3$, we can control the space approximation error at the specified smallness level.

3. Backward Euler Method

In the second step of the proposed general framework of analysis, a fully discrete scheme is constructed. In this paper, we consider the backward Euler (BE) method.

For the simplicity of the notations, we consider a uniform time mesh:

$$\bar{\omega}_t = \{t^n : \ t^n = n\tau, \quad n = 0, \dots, N\}, \quad t^N = T.$$

Then, the problem (4) and (5) is approximated by the following BE scheme [20]:

$$\frac{U^n - U^{n-1}}{\tau} + A_h^\alpha U^n = F^n, \quad n = 1, \dots, N, \tag{10}$$

$$U^0 = U_0, \tag{11}$$

where U^n is a numerical approximation to the exact solution $U(t^n)$ of the problem (4) and (5), and $F^n = F(t^n)$.

Lemma 1. *If a solution of the problem (4) and (5) is sufficiently smooth, then the approximation error of the BE scheme (10) is of order $O(\tau)$.*

Proof. The proof is quite standard, and it is based on the Taylor expansion technique. It is sufficient to compute the residual of the discrete formula $\left(U(t^n) - U(t^{n-1})\right)/\tau$ for a sufficiently smooth function $U(t)$. □

The stability analysis of the scheme (10) is also simple.

Lemma 2. *The BE scheme (10) is unconditionally stable.*

$$\|U^n\| \leqslant \|U_0\| + \tau \sum_{k=1}^{n} \|F^k\|. \tag{12}$$

Proof. The Fourier stability analysis can be used to show that

$$\|U^n\| \leqslant \|U^{n-1}\| + \tau \|F^n\|. \tag{13}$$

The same estimate can be obtained by using the energy method and taking into account that operator A_h^α is positive definite, i.e., $(A_h^\alpha U^n, U^n) > 0$. We multiply Equation (10) by U^n and obtain the estimate

$$\|U^n\|^2 \leqslant (U^{n-1}, U^n) + \tau (F^n, U^n)$$

from which the estimate (13) follows trivially. Applying the estimates (13) recursively, we obtain the required stability estimate (12). □

It is easy to see that, if the solution $u \in H$ of (1) is a sufficiently smooth function and an approximation error by $U \in H_h$ functions is of order $O(h^k)$, then the error of the discrete solution of the fully discrete BE scheme (10) can be estimated as

$$\|u(t^n) - U^n\| \leqslant \|u(t^n) - U(t^n)\| + \|U(t^n) - U^n\| \leqslant C(\tau + h^k). \tag{14}$$

Such a delicate interlacing of space and time approximation errors is nicely seen from the experimental results. We solve the differential problem (7) of Example 1. Table 1 gives, for a sequence of decreasing time step widths τ, the errors $E(\tau)$, and the experimental convergence rates $\rho(\tau)$ of the discrete solution for the BE scheme (10) in the maximum norm:

$$E(\tau) = \max_{(x_i,y_j,z_k)\in\Omega_h} \left| U^N_{ijk} - u(x_i,y_j,z_k,T) \right|, \quad \rho(\tau) = \log_2\left(\frac{E(2\tau)}{E(\tau)}\right).$$

The fractional power parameter $\alpha = 0.75$ and a uniform space grid Ω_h with $J_x = 200$ and 400 are used in the numerical experiments.

Table 1. Errors $E(\tau)$ and experimental convergence rates $\rho(\tau)$ for the discrete solution of the BE scheme (10) for a sequence of time steps τ.

τ	$E(\tau)$, $J_x = 200$	$\rho(\tau)$	$E(\tau)$, $J_x = 400$	$\rho(\tau)$
0.1	2.012×10^{-3}	—	1.958×10^{-3}	—
0.05	1.031×10^{-3}	0.965	9.763×10^{-4}	1.004
0.025	5.491×10^{-4}	0.909	4.952×10^{-4}	0.979
0.0125	3.102×10^{-4}	0.824	2.561×10^{-4}	0.951

It follows from the presented results that the convergence order of the discrete solution is close to the first, but it slowly decreases for smaller time steps. Such a behavior of the error is due to the influence of the space approximation error (see the estimate (14)). In order to illustrate this fact, let us consider the dynamics of a modified error component:

$$\widetilde{E}(\tau) = E(\tau) - e(h),$$

where $e(h)$ is the error of the solution of the semidiscrete scheme (4) and (5). The values of $e(h)$ for $J_x = 200$ and 400 are given in (9). Table 2 gives for a sequence of decreasing time step widths τ the errors $\widetilde{E}(\tau)$ and the experimental convergence rates $\rho(\tau)$ of the discrete solution for the BE scheme (4).

Table 2. Modified errors $\widetilde{E}(\tau)$ and experimental convergence rates $\rho(\tau)$ for the discrete solution of the BE scheme (10) for a sequence of time steps τ.

τ	$E(\tau)$, $J_x = 200$	$\rho(\tau)$	$E(\tau)$, $J_x = 400$	$\rho(\tau)$
0.1	1.94×10^{-3}	—	1.94×10^{-3}	—
0.05	9.58×10^{-4}	1.018	9.58×10^{-4}	1.018
0.025	4.76×10^{-4}	1.009	4.78×10^{-4}	1.003
0.0125	2.37×10^{-4}	1.006	2.38×10^{-4}	1.006

The presented results agree well with the theoretical predictions.

4. Discrete Schemes Based on Rational Approximations

In the third step of a general theoretical framework, nonlocal operators A_h^α in a fully discrete scheme are approximated by some local operators. In this paper, we consider methods based on rational approximations.

We can write the BE scheme (10) in the following form:

$$U^n = (I_h + \tau A_h^\alpha)^{-1}(U^{n-1} + \tau F^n).$$

Then, we approximate the nonlocal operator $(I_h + \tau A_h^\alpha)^{-1}$ by a local rational operator:

$$(I_h + \tau A_h^\alpha)^{-1} \approx r_m(A_h),$$

where a function $r_m(z)$ is defined as

$$r_m(\lambda) = \frac{p_m(\lambda)}{q_m(\lambda)}$$

with polynomials p_m and q_m of the same degree m. As a practical implementation of this approach, the best uniform rational approximation (BURA) method is used, where r_m is the best rational approximation of the function

$$f(\lambda) = \frac{1}{1+\tau\lambda^\alpha}$$

for $\lambda \in [\mu_1, \mu_J]$. The required rational function is computed by applying the BRASIL algorithm, which is based on the barycentric rational formula [8]. We used a free and open-source implementation of this algorithm in Python.

Here, it is important to note that only slight changes are needed if, instead of a polynomial function, we solve a problem with a more general nonlinear function $g(\lambda)$. Then, a rational approximation function $r_m(z)$ is defined for the modified function:

$$f(\lambda) = \frac{1}{1+\tau g(\alpha)}.$$

The constructed rational function r_m can be written in a partial fraction decomposition form [7]:

$$r_m(\lambda) = c_0 + \sum_{j=1}^{m} \frac{c_j}{\lambda - d_j}. \tag{15}$$

Then, the following scheme is constructed:

$$V^n = r_m(A_h)\left(V^{n-1} + \tau F^n\right), n = 1, 2, \ldots, N, \tag{16}$$

$$V^0 = U_0. \tag{17}$$

Its implementation is efficient if all coefficients d_j are non-positive.

The convergence analysis of the solution of the scheme (16) is performed by using the classical technique. It is based on the stability and approximation error analysis. First, we investigate the stability of the scheme (16). Note that

$$\|(I_h + \tau A_h^\alpha)^{-1}\| \leqslant \frac{1}{1+\tau\mu_1^\alpha} \leqslant 1 - \tau\mu_1^\alpha.$$

Let m be a sufficiently large number in order to satisfy the estimate:

$$\left|(1+\tau\lambda^\alpha)^{-1} - r_m(\lambda)\right| \leqslant \tau\mu_1^\alpha, \quad \forall\lambda \in [\mu_1, \mu_J],$$

Then, we obtain the required stability inequality:

$$\|r_m(A_h)\| \leqslant \|r_m(A_h) - (1+\tau A_h^\alpha)^{-1}\| + \|(1+\tau A_h^\alpha)^{-1}\| \leqslant 1.$$

Remark 1. *As an additional stability test of the scheme* (16)*, it is recommended to compute the bound*

$$R = \max_{0 \leqslant j \leqslant K} |r_m(z_j)|, \quad z_j = \mu_1 + \frac{j}{K}(\mu_J - \mu_1). \tag{18}$$

The stability requirement is satisfied if $R \leqslant 1$.

As an example, we applied this criterion for the scheme (16) *and the problem* (7)*. The results of the computational experiments confirm that the condition* $R \leqslant 1$ *is satisfied for fractional power*

parameters $\alpha = 0.25, 0.5, 0.75$, *space meshes with* $J = (J_x + 1)^3$, $J_x = 200, 400$, *and time steps* $\tau = 10^{-k}$, $k = 1, \ldots, 4$. *The rational function* r_m *is computed by applying the BURA-BRASIL algorithm with* $m = 5, 7, 10, 12$.

Next, we investigate the approximation accuracy of the scheme (16). *In this analysis, we compare* V^n *with the solution* U^n *of the BE scheme* (10). *Let us write both functions in a spectral form:*

$$U^n = \sum_{j=1}^{J} U_j^n \psi_j^h, \quad V^n = \sum_{j=1}^{J} V_j^n \psi_j^h,$$

where

$$\frac{U_j^n - U_j^{n-1}}{\tau} + \mu_j^\alpha U_j^n = F_j^n, \quad j = 1, \ldots, J,$$
$$V_j^n = r_m(\mu_j)(V_j^{n-1} + \tau F_j^n).$$

The second equation can be written as:

$$\frac{V_j^n - V_j^{n-1}}{\tau} + \frac{r_m^{-1}(\mu_j) - 1}{\tau} V_j^n = F_j^n.$$

The approximation error of the scheme (16) *is defined as*

$$\begin{aligned} \widetilde{\Psi}^n(\mu_j) &= \frac{U_j^n - U_j^{n-1}}{\tau} + \frac{r_m^{-1}(\mu_j) - 1}{\tau} U_j^n - F_j^n \\ &= \left(\frac{r_m^{-1}(\mu_j) - 1}{\tau} - \mu_j^\alpha \right) U_j^n = e_{mj} U_j^n. \end{aligned} \tag{19}$$

Let us denote the error function as $Z_j^n = U_j^n - V_j^n$; *it satisfies equations*

$$Z_j^n = r_m(\mu_j)\left(Z_j^{n-1} + \tau \widetilde{\Psi}^n(\mu_j)\right).$$

Applying these equations iteratively, we obtain the estimate

$$\|Z^n\| \leqslant t^n \|\widetilde{\Psi}^n\|.$$

Remark 2. *As follows from* (19), *the approximation error depends not only on the accuracy with which the rational function approximates fractional powers of eigenvalues* μ^α, *but also on* U_j^n. *For smooth solutions, the Fourier coefficients* U_j^n *are bounded from above by* $O(j^{-k})$ *with some constant* k.

Table 3 gives for a sequence of decreasing time step widths τ and different values of m the approximation errors $\widetilde{\Psi}^n(\xi)$ of the discrete solution for the BURA-BRASIL scheme (16) in the maximum norm. It is assumed that $\widetilde{\Psi}^n(\xi) = e_m(\xi)/\xi$. The fractional power parameter $\alpha = 0.75$ and a uniform space grid Ω_h with $J_x = 200$ and 400 are used in numerical experiments.

A more detailed analysis of the approximation errors $\widetilde{\Psi}_\tau^n(\xi)$ shows that the largest values are obtained for high spectral modes. For many applied problems, solutions depend only on a few moderate size spectral modes. Hence, we computed these errors in a reduced spectral interval $[\mu_1, 20\mu_1]$. The obtained results are presented in Table 4. As expected, the accuracy of the approximation is improved in comparison with the results presented in Table 3.

Table 3. Approximation errors $\|\widetilde{\Psi}_\tau^n(\xi)\|$ for the discrete solution of the BURA-BRASIL scheme (16) for a sequence of time steps τ and $J_x = 200, 400$.

τ	$m = 5$	$m = 7$	$m = 10$
	$J_x = 200,\ 29.6 \leqslant \xi \leqslant 479{,}970$		
0.1	5.534×10^{-4}	2.317×10^{-5}	1.977×10^{-7}
0.05	4.632×10^{-4}	1.936×10^{-5}	1.652×10^{-7}
0.025	3.559×10^{-4}	1.484×10^{-5}	1.266×10^{-7}
0.0125	2.481×10^{-4}	1.033×10^{-5}	8.813×10^{-8}
	$J_x = 400,\ 29.6 \leqslant \xi \leqslant 1{,}919{,}970$		
0.1	1.552×10^{-3}	9.257×10^{-5}	1.274×10^{-6}
0.05	1.330×10^{-3}	7.876×10^{-5}	1.083×10^{-6}
0.025	1.056×10^{-3}	6.196×10^{-5}	8.513×10^{-7}
0.0125	7.673×10^{-4}	4.462×10^{-5}	6.128×10^{-7}

Table 4. Approximation errors $\|\widetilde{\Psi}_\tau^n(\xi)\|$ for the discrete solution of the BURA-BRASIL scheme (16) in a reduced spectral interval. A sequence of time steps τ and $J_x = 200, 400$ are used.

τ	$m = 5$	$m = 7$	$m = 10$
	$J_x = 200,\ 29.6 \leqslant \xi \leqslant 592.2$		
0.1	2.262×10^{-5}	8.415×10^{-7}	8.208×10^{-9}
0.05	2.438×10^{-5}	9.940×10^{-7}	8.759×10^{-9}
0.025	4.842×10^{-5}	2.000×10^{-6}	2.747×10^{-8}
0.0125	1.037×10^{-4}	4.299×10^{-6}	3.661×10^{-8}
	$J_x = 400,\ 29.6 \leqslant \xi \leqslant 592.2$		
0.1	3.214×10^{-5}	1.829×10^{-6}	6.555×10^{-7}
0.05	3.644×10^{-5}	2.427×10^{-6}	1.629×10^{-7}
0.025	7.427×10^{-5}	4.246×10^{-6}	5.791×10^{-8}
0.0125	1.645×10^{-4}	9.335×10^{-6}	1.247×10^{-7}

Next, we solve the differential problem (7) of Example 1. Table 5 gives for a sequence of decreasing time step widths τ the errors $E_m(\tau)$ of the discrete solution for the BURA-BRASIL scheme (16) in the maximum norm:

$$E_m(\tau) = \max_{(x_i, y_j, z_k) \in \Omega_h} \left| V_{ijk}^N - u(x_i, y_j, z_k, T) \right|.$$

The fractional power parameter $\alpha = 0.75$ and a uniform space grid Ω_h with $J_x = 200$ and 400 are used in the numerical experiments.

Table 5. Errors $E_m(\tau)$ for the discrete solution of the BURA-BRASIL scheme (16) for a sequence of time steps τ and $J_x = 200, 400$.

τ	$E_5(\tau)$	$E_7(\tau)$	$E_{10}(\tau)$
	$J_x = 200$		
0.1	2.012×10^{-3}	2.011×10^{-3}	2.012×10^{-3}
0.05	1.028×10^{-3}	1.030×10^{-3}	1.031×10^{-3}
0.025	5.271×10^{-4}	5.472×10^{-4}	5.491×10^{-4}
0.0125	2.232×10^{-4}	3.082×10^{-4}	3.100×10^{-4}
	$J_x = 400$		
0.1	1.960×10^{-3}	1.956×10^{-3}	1.959×10^{-3}
0.05	9.711×10^{-4}	9.742×10^{-4}	9.771×10^{-4}
0.025	4.512×10^{-4}	4.923×10^{-4}	4.940×10^{-4}
0.0125	9.011×10^{-5}	2.513×10^{-4}	2.561×10^{-4}

5. URA-Type Discrete Scheme

In this section, as another application of the proposed framework of analysis, we consider a discrete scheme, which is based on the uniform rational approximation (URA) method [24]. Let A_h be a self-adjoint and positive definite operator $0 < \mu_1 I_h \leqslant A_h \leqslant \mu_J I_h$. Our aim is to approximate the scalar function $f(\lambda)$, which can be written as a function of a new variable $\xi = \mu_1/\lambda$:

$$f(\lambda) = \frac{1}{1+\tau\lambda^\alpha} = \frac{\xi^\alpha}{\xi^\alpha + \tau\mu_1^\alpha}, \quad \xi \in [\mu_1/\mu_J, 1].$$

Let $\widetilde{r}_m(\xi)$ be the BURA of ξ^α on $[0,1]$, then we define the URA of $f(\lambda)$ as

$$\bar{r}_m(\xi) = \frac{\widetilde{r}_m(\xi)}{\widetilde{r}_m(\xi) + \tau\mu_1^\alpha}. \tag{20}$$

Remark 3. *If an estimate of $\mu_1/\mu_J \geqslant c_0 > 0$ is known, then it is recommended to compute $\widetilde{r}_m(\xi)$ as the BURA of ξ^α on $[c_0, 1]$. The BRASIL algorithm can be used to efficiently find coefficients of $\widetilde{r}_m(\xi)$.*

Then, the following URA-type discrete scheme is constructed:

$$\begin{aligned} &V^n = \bar{r}_m(\mu_1 A_h^{-1})\big(V^{n-1} + \tau F^n\big), \quad n = 1, 2, \ldots, N, \\ &V^0 = U_0. \end{aligned} \tag{21}$$

Let us consider the implementation algorithm. The rational function $\bar{r}_m$ can be written in a partial fraction decomposition form

$$\bar{r}_m(\xi) = \bar{c}_0 + \sum_{j=1}^{m} \frac{\bar{c}_j}{\xi - \bar{d}_j}. \tag{22}$$

The following lemma can be proven by applying simple modifications of the proof given in [24].

Lemma 3. *All poles of the function $\bar{r}_m(\xi)$ are real and negative:*

$$d_j < 0, \quad j = 1, \ldots, m. \tag{23}$$

The computation of V^n requires numerical solving of m linear systems; all systems are independent and can be solved in parallel:

$$V^n = \bar{c}_0\big(V^{n-1} + \tau F^n\big) + \sum_{j=1}^{m} \bar{c}_j G_j^n,$$

where functions G_j^n are solutions of the following linear systems:

$$(\mu_1 I_h - d_j A_h) G_j^n = A_h\big(V^{n-1} + \tau F^n\big), \quad j = 1, \ldots, m.$$

All system are of the same type, and due to (23), all shifts $(-d_j)$ are positive, and the operator A_h is self-adjoint and also positive.

The development of URA-type approximations is motivated by one important property of these schemes: the BURA of function ξ^α is computed only once, and it can be used for different operators A_h, time steps τ, and discrete approximations of the time derivative (e.g., BE or Crank–Nicolson methods). After the development of new efficient methods to construct BURA-type rational approximations, the importance of this property decreases sharply. All computational experiments of this paper were performed by using the BRASIL method.

Still, it is interesting to apply the proposed general framework of analysis to the scheme (21). First, it follows that this scheme is stable if the stability inequality:

$$\|\bar{r}_m(\mu_1 A_h^{-1})\| \leqslant 1$$

is satisfied. We restrict our analysis to the computation of the numerical bound:

$$R = \max_{0 \leqslant j \leqslant K} |\bar{r}_m(\mu_1 z_j^{-1})|, \quad z_j = \mu_1 + \frac{j}{K}(\mu_J - \mu_1).$$

The experimental stability requirement is satisfied if $R \leqslant 1$.

As an example, we applied this criterion for the scheme (21) and the problem (7). The results of the computational experiments confirm that the condition $R \leqslant 1$ is satisfied for fractional power parameters $\alpha = 0.25, 0.5, 0.75$, space meshes with $J = (J_x + 1)^3$, $J_x = 200, 400$, and time steps $\tau = 10^{-k}$, $k = 1, \ldots, 4$. The rational approximation $\widetilde{r}_m(\xi)$ of function ξ^α is computed by applying the BURA-BRASIL algorithm with $m = 5, 7, 10, 12$ for $\xi \in [\mu_1/\mu_{J_x}, 1]$.

Next, we consider the approximation accuracy. The approximation error of the scheme (21) is defined as

$$\begin{aligned} \bar{\Psi}^n(\mu_j) &= \frac{U_j^n - U_j^{n-1}}{\tau} + \frac{\bar{r}_m^{-1}(\mu_1/\mu_j) - 1}{\tau} U_j^n - F_j^n \\ &= \left(\frac{\bar{r}_m^{-1}(\mu_1/\mu_j) - 1}{\tau} - \mu_j^\alpha \right) U_j^n = \bar{e}_{mj} U_j^n. \end{aligned} \tag{24}$$

By substituting (20) into this equation, we obtain that

$$\bar{e}_{mj} = \frac{\mu_1^\alpha}{\widetilde{r}_m(\mu_1/\mu_j)} - \mu_j^\alpha.$$

Hence, the approximation error does not depend on the time step size τ, and it can be reduced by increasing the order m of the rational function $\widetilde{r}_m$.

Table 6 gives for different values of m the approximation errors

$$\bar{E}_m(\mu) = \bar{e}_m(\mu)/\mu$$

of the discrete solution for the URA-BRASIL scheme (21) in the maximum norm. The fractional power parameter $\alpha = 0.75$ and a uniform space grid Ω_h with $J_x = 200$ and 400 are used in the numerical experiments. The rational approximation $\widetilde{r}_m(\xi)$ of function ξ^α is computed by applying the BURA-BRASIL algorithm for $\xi \in [\mu_1/\mu_{J_x}, 1]$.

Table 6. Approximation errors $\|\bar{E}_m\|$ for the discrete solution of the URA-BRASIL scheme (21) for different orders m of the rational approximation functions and $J_x = 200, 400$.

$m = 5$	$m = 7$	$m = 10$
$J_x = 200,\ 29.6 \leqslant \mu \leqslant 479{,}970$		
7.050×10^{-4}	2.961×10^{-5}	2.524×10^{-7}
$J_x = 400,\ 29.6 \leqslant \mu \leqslant 1{,}919{,}970$		
1.914×10^{-3}	1.155×10^{-4}	1.587×10^{-6}

The computational results show that the accuracy of the URA-BRASIL scheme is similar to the accuracy of the BURA-BRASIL scheme (16). Hence, both schemes can be recommended as solvers for real-world applications. The final selection can be based on additional criteria, such as a better parallelization property [7].

6. Stability Analysis of a Crank–Nicolson-Type BURA-BRASIL Scheme

In this section, the problem (4) and (5) is approximated by the following Crank–Nicolson (CN) scheme [20]:

$$\frac{U^n - U^{n-1}}{\tau} + A_h^{\alpha}\overline{U}^{n-\frac{1}{2}} = F^{n+\frac{1}{2}}, \quad n = 1, \ldots, N, \tag{25}$$
$$U^0 = U_0,$$

where $\overline{U}^{n-\frac{1}{2}} = 0.5\left(U^n + U^{n-1}\right)$.

In order to efficiently compute the solution U^n, we write the CN scheme (25) in the following form:

$$\overline{U}^{n-\frac{1}{2}} = (I_h + 0.5\tau A_h^{\alpha})^{-1}\left(U^{n-1} + 0.5\tau F^{n-\frac{1}{2}}\right), \tag{26}$$
$$U^n = 2\overline{U}^{n-\frac{1}{2}} - U^{n-1}.$$

Then, we approximate the nonlocal operator $(I_h + \tau A_h^{\alpha})^{-1}$ by a local rational operator:

$$(I_h + 0.5\tau A_h^{\alpha})^{-1} \approx r_m(A_h).$$

The BURA-BRASIL algorithm is used to construct $r_m(\lambda)$. Finally, the nonlocal discrete scheme (26) is approximated by the following local discrete scheme:

$$\overline{V}^{n-\frac{1}{2}} = r_m(A_h)\left(V^{n-1} + 0.5\tau F^{n-\frac{1}{2}}\right), \tag{27}$$
$$V^n = 2\overline{V}^{n-\frac{1}{2}} - V^{n-1}.$$

The stability factor of the CN scheme (25) has a more complicated dependence on the large eigenvalues of A_h, and this factor changes the sign and converges to (-1). Thus, it is most important to investigate the stability of the scheme (27). According to the proposed framework of the theoretical analysis, we should estimate the norm $\|2r_m(A_h) - I_h\|$.

This can be performed by applying the computational approach, when the stability factor R of the scheme (25) is computed for a specific class of operators A_h and fractional power parameters α:

$$R = \max_{0 \leqslant j \leqslant K} |2r_m(z_j) - 1|, \quad z_j = \mu_1 + \frac{j}{K}(\mu_J - \mu_1).$$

The stability requirement is satisfied if $R \leqslant 1$.

As an example, we applied this criterion for the scheme (27) and the problem (7). The results of the computational experiments confirm that the condition $R \leqslant 1$ is satisfied for fractional power parameters $\alpha = 0.25, 0.5, 0.75$, space meshes with $J = (J_x + 1)^3$, $J_x = 200, 400$, and time steps $\tau = 10^{-k}$, $k = 1, \ldots, 6$. The rational function r_m is computed by applying the BURA-BRASIL algorithm with $m = 3, 5, 7, 10, 12$.

7. Simulation of Biofilm Formation

In this section, we construct non-standard finite-volume schemes for the solution of nonlinear problems used to simulate biofilm formation. The mathematical model is generalized to include a nonlocal diffusion operator. The governing two-dimensional mathematical model is based on the Allen–Cahn equation ([25,26]):

$$\frac{\partial u}{\partial t} + D(-\Delta)^{\alpha} = ru(1-u)(u-\gamma), \quad (x, y) \in \Omega = (0,1) \times (0,1), \quad t \in (0, T], \tag{28}$$

where D is the diffusion coefficient, α is the fractional power parameter, and $\gamma \in [0,1]$ defines the extinction process when the initial population is too low to survive and attain the maximum capacity otherwise. If $\alpha = 1$, then we obtain the classical diffusion model.

The initial conditions are defined as

$$u(x,y,0) = u_0(x,y), \quad (x,y) \in [0,1] \times [0,1]$$

Homogeneous Dirichlet conditions are considered on the boundary points of Ω:

$$u(x,y,t) = 0, \quad (x,y) \in \partial\Omega, \quad t \in (0,T].$$

A discrete approximation of the diffusion operator is constructed in a similar way as for Example 1. A uniform space mesh $\omega_x \times \omega_y$ is defined, and the discrete diffusion operator A_h is constructed by using the finite-volume method.

We note that very interesting results were obtained in [25], where the authors constructed a non-standard unconditionally positive finite-difference scheme and applied it to solve three test problems for the problem (28). We note that this scheme has first-order accuracy in time and second-order accuracy in space.

Our goal is to construct a non-standard splitting-type discrete scheme that has second-order accuracy in time and solves a general nonlocal diffusion problem. Here, we used the techniques presented also in [7]. As an additional bonus of the proposed general framework, we show that no additional theoretical analysis is needed to justify this splitting scheme, when the results of previous sections are already given.

We applied the symmetrical splitting technique with respect to different physical processes and obtained the following template of a discrete scheme

$$\frac{d\widetilde{U}}{dt} = F(X, t^{n+\frac{1}{2}}, \widetilde{U}), \quad \widetilde{U}(t^n) = U^n, \quad t^n < t \leqslant t^{n+\frac{1}{2}}, \tag{29}$$

$$U^{n+\frac{1}{3}} = \widetilde{U}(t^{n+\frac{1}{2}}),$$

$$\frac{U^{n+\frac{2}{3}} - U^{n+\frac{1}{3}}}{\tau} + A_h^{\alpha} \frac{U^{n+\frac{2}{3}} + U^{n+\frac{1}{3}}}{2} = 0, \tag{30}$$

$$\frac{d\widetilde{U}}{dt} = F(X, t^{n+\frac{1}{2}}, \widetilde{U}), \quad \widetilde{U}(t^{n+\frac{1}{2}}) = U^{n+\frac{2}{3}}, \quad t^{n+\frac{1}{2}} < t \leqslant t^{n+1}, \tag{31}$$

$$U^{n+1} = \widetilde{U}(t^{n+1}).$$

From this template, we can define different cases of the fully discrete scheme.

First, the dynamics of the nonlinear interaction can be resolved by using specialized solvers targeted at specific nonlinear functions. In some cases, these subproblems can even be solved exactly. For the applied problem (28), we used the well-known symmetrical predictor–corrector method, e.g., for the step (29), we obtain:

$$\begin{aligned} &U^{n+\frac{1}{3},0} = U^n, \\ &U^{n+\frac{1}{3},s+1} = U^n + \frac{\tau}{4} r U^{n+\frac{1}{3},s}(1 - U^{n+\frac{1}{3},s})(U^{n+\frac{1}{3},s} - \gamma), \quad s = 0,1, \\ &U^{n+\frac{1}{3}} = 2U^{n+\frac{1}{3},2} - U^n. \end{aligned} \tag{32}$$

Second, only one subproblem with nonlocal operators is solved for each time step. We can use the Crank–Nicolson-type BURA-BRASIL scheme, which is constructed and investigated in Section 6. On the basis of the proposed theoretical framework, we automatically obtain that the proposed scheme (29)–(31) is stable and a discrete solution converges to the solution of the problem (28). The constructed scheme has second-order accuracy in time and space.

In order to illustrate the performance of the proposed scheme, we present some results on the simulation of biofilm on medical implants. This problem was also investigated in [25,27]. We considered an initial profile with the density function given as

$$u(x,y,0) = \sum_{p=1}^{2} C_p e^{-w_p \|\mathbf{X}-\mathbf{X_p}\|^2},$$

where $\mathbf{X} = (x,y)$, $C_1 = 0.68$, $C_2 = 0.65$, $w_1 = 60$, $w_2 = 100$, $\mathbf{X_1} = (0.35, 0.60)$, $\mathbf{X_2} = (0.48, 0.45)$. We also took $r = 200$, $\gamma = 0.05$ and $D = 0.0002$.

First, we compared the numerical rate of convergence in time using the new splitting-type scheme (29)–(31) and two schemes from the paper [25], the results are presented in Table 7. The results for the nonstandard finite-difference scheme (NFSD) and the classical explicit Euler scheme were taken from Table 4. The test problem was solved for a sequence of time steps τ till time $t = 0.01$ with $\alpha = 1$, $h = 0.02$.

Table 7. Errors $E(\tau)$ and experimental convergence rates $\rho(\tau)$ for the discrete solution of the splitting scheme (29)–(31) and the NSFD and classical explicit Euler schemes from [25] for a sequence of time steps τ.

τ	$E_{SS}(\tau)$	$\rho(\tau)$	$E_{NSFD}(\tau)$	$\rho(\tau)$	$E_{EE}(\tau)$	$\rho(\tau)$
0.0025	1.858×10^{-4}	1.926	3.403×10^{-2}	0.290	1.443×10^{-2}	0.786
0.00125	4.763×10^{-5}	1.964	2.347×10^{-2}	0.536	7.875×10^{-3}	0.874
0.000625	1.201×10^{-5}	1.988	1.423×10^{-2}	0.722	4.134×10^{-3}	0.930
0.0003125	2.964×10^{-6}	2.018	7.913×10^{-3}	0.846	2.121×10^{-3}	0.963

It follows from the presented results that the second-order convergence rate is achieved for the splitting scheme (29)–(31), and therefore, it enables computing more accurate approximations for the same time step.

The computational experiments also proved that, for fractional parameters $0.2 \leqslant \alpha \leqslant 0.75$, it is sufficient to take $m \leqslant 5$ for the BURA-BRASIL algorithm in order to obtain the same accuracy of solutions as for the full discrete nonlocal problem (30). We note that for the given biofilm model, the development of population mostly depends on the nonlinear reaction process, and the fractional power of diffusion has only a secondary impact.

8. Conclusions

A general framework of analysis was proposed for the analysis of solutions of parabolic problems with fractional power elliptic operators. The analysis was split into three parts, and each part dealt with a specific subproblem, which can be solved and analyzed in a simpler way.

An additional bonus of this approach is that the existing stability and convergence results can be included directly in the first and second parts of the framework. This possibility makes the proposed technique quite efficient and robust.

New stability and approximation techniques were proposed for the analysis of discrete schemes, which were constructed by using the uniform rational approximations of transfer functions. The BRASIL algorithm was used for the practical construction of such rational approximations.

The results of extended experiments were reported to illustrate the accuracy and efficiency of the proposed general framework.

The analysis of the influence of efficient parallel solvers for the stability and accuracy of the obtained algorithms can be added as the fourth part of this framework. These results will be presented in a separate paper.

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