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Spectral Collocation Method for Time-Fractional Partial Differential Equations with Singularity-Adapted Basis

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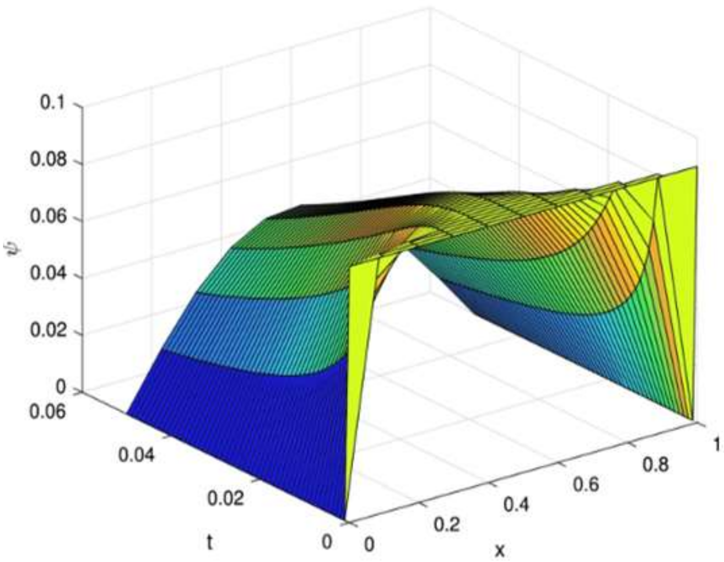
ABSTRACT:

Time-fractional PDEs are often used to model complex physical phenomena with memory and hereditary features. But solutions tend to possess low regularity, as well as initial-time singularities, which makes standard numerical schemes quite ineffective. They are poorly-treated by classical spectral methods due to the singularities inherent in local minima and maxima, which results in lower convergence rates and increased computational effort. The goal is to construct and investigate spectral collocation method with singularity adapted basis functions for the efficient and accurate solution of time-fractional PDEs, when the solution admits initial-time singular behavior. The numerical experiments illustrate spectral accuracy in space and near optimal convergence rates in time especially for $\alpha<0.5$. The presented method produces more accurate results in comparison with the spectral and finite difference procedures in addition to a reduction in the number of the collocation points. The robustness of the method is also justified through the stability analysis and error estimates. The singularity-adapted spectral collocation approach is a powerful and effective method in solving the time-fractional PDEs with singular solutions and has outstanding advantage in accuracy and convergence speed.

Keywords: *Time-fractional partial differential equations, spectral collocation, singularity-adapted basis, numerical methods, fractional calculus*

1. Introduction

The physical systems with memory and hereditarily, such as an abnormal diffusion, viscoelasticity and heat transfer in porous media, have induced the wide application of time-fractional PDEs.



These equations contain non-integer order derivatives (NOD) which generalize the classical derivatives of integer order and give more accurate models of some complex dynamics. In this paper we will only generalize the Caputo (fractional) derivative to discretized time as we focus on time-fractional PDEs. The Caputo's fractional derivative of order $\alpha\in(0,1)$ for a sufficiently smooth function u(t) is given by:

$$^{c}D_t^{\alpha}(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-\tau)^{-\alpha}\frac{du(\tau)}{d\tau}d\tau \qquad (1.1)$$

Where Γ is the gamma function in equation (1.1). This operator is nonlocal and endoscopic, it reflects the entire history of the system, and the corresponding solutions have singularities at $t = 0$, see [11]

The exponential convergence in solving the PDE with smooth solutions is a well-known property of spectral collocation techniques. They discretize the solution u(t) approximately by means of global basis functions $\phi_j(t)$ and enforce the governing equations at discrete collocation points $\{t\_j\}(j = 0)^{N}$ as:

$$\upsilon_N(t) = \sum_{j=0}^{N} a_j\phi_j(t), \quad and \quad {}^{c}D_t^{\alpha}\upsilon_N(t_i) \approx f(t_i), \qquad i = 0,1,2,\ldots\ldots,N. \qquad (1.2)$$

If the original solution has singular behavior near origin (e.g. $u(t) \sim t^{\gamma}, 0 < \gamma < 1$), the classical spectral bases such as Chebyshev or Legendre polynomials poorly resolve the singularity, which leads to the reduced rate of convergence, we refer the reader to the paper [6].

To overcome this shortcoming, singularity-adapted basis functions which capture more closely the anticipated solution behavior near singular points have been developed. One popular method is to weight or add to standard polynomial bases singular components such as t^{α} leading to the basic structure:

$$\phi_j(t) = t^{a}P_j(t), \qquad (1.3)$$

Where $P_j(t)$is a classical polynomial in equation (1.3), such as Jacobi or Legendre. This improvement on the approximation properties relies in the basics being compatible with the leading-order asymptotic behavior of the solution, the author written in the paper [10].

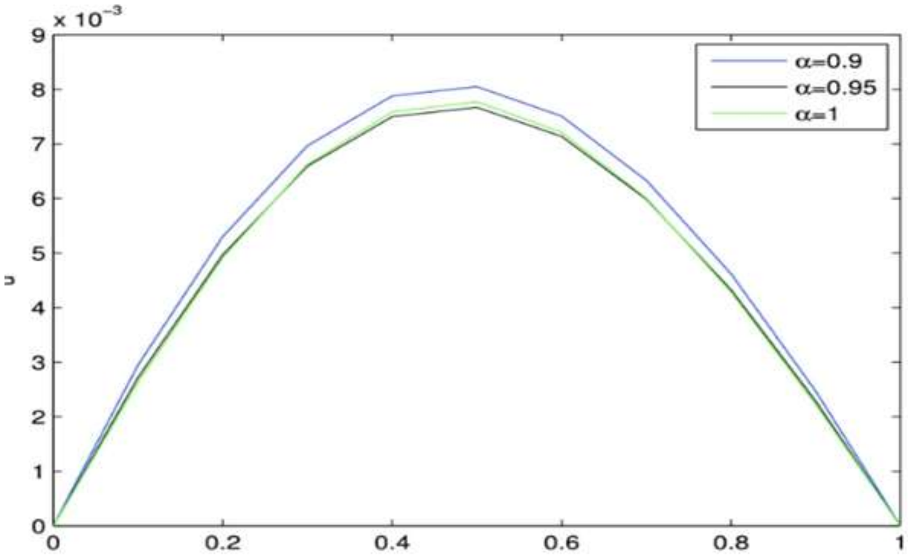


Figure 1

The corresponding spectral approximation is then:

$$\upsilon_N(t) = \sum_{j=0}^{N} a_j t^{a} P_j(t),$$

And that the Caputo derivative can be solved analytically or numerically with spectral differentiation matrices or recurrence relations. A standard prototypical example to validate such methods is the time fractional derivative equation:

$$^{c}D_t^{a}u(x,t) = \frac{\partial^2 u}{\partial x^2} + f(x,t), \qquad 0 < a < 1, \qquad (1.5)$$

With initial condition $u(x,0) = u_0(x)$ and suitable boundary conditions. In the case of solutions known to have power-law singularities such as $(t)\sim t^{a}$, encapsulating the singularity in the basics yields large enhancement of error reduction. If the analytical solution is $u(x,t) = t^{a}\sin(\pi x)$,, and $f(x,t) = \frac{\Gamma(1+a)}{\Gamma(1)}\sin(\pi x)$, one can see that with adapted basis, we obtain an accurate approximation with much less collocation points, see [13].

The factionary differentiation matrix D^{α} can be generated as the analytical differentiation of the basic functions:

$$D_{ij}^{a} = {}^{c}D_t^{a}\left[t^{a}P_j(t)\right]|_{t=t_i},$$

Which simplifies using the identity:

$$^{c}D_t^{a}\left(t^{\beta}\right) = \frac{\Gamma(\beta+1)}{\Gamma(\beta-\alpha+1)}t^{\beta-\alpha}, \quad \beta > \alpha - 1. \qquad (1.6)$$

This enables a direct calculation of the exact rule in the case when $\phi_j(t) = t^{\beta}$, and combined with numerical quadrature makes efficient matrix building, see [3].

In addition, the adopted spectral collocation method can be combined into graded meshes, for which a weight is used to make the collocation points more numerical dense near $t = 0$ (with $t_i = T\left(\frac{i}{N}\right)^{\gamma}$, resulting in further enhancement of resolution of singularity. This method can deal with weak singularities, and has a uniform convergence in time domain [15]. The use of single-basis and mesh refinement allows for a stable approach to fractional dynamics.

A further benefit is the computational efficiency of the approach. Because the singularity is modeled in the basic functions there are fewer degrees of freedom than when using classical finite difference or finite element schemes.

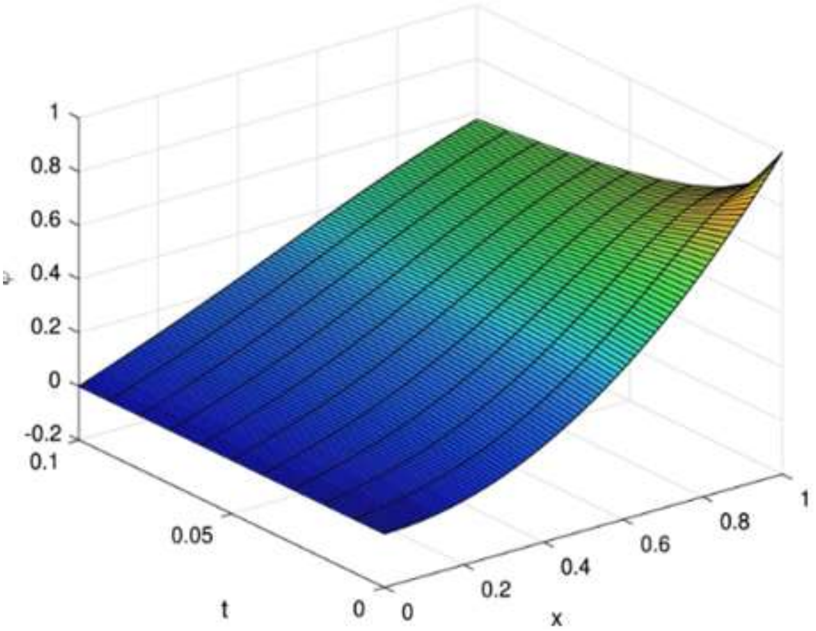


Figure 2

Furthermore, since spectral methods are global, but also global data are had to be used in the matrix assembly, matrices can be assembled and solved fast by linear solver like for example in the case of linear PDEs. For non-linear problems we can extend the method via Newton-Raphson iterations or fixed-point iterations, and the spectral basis maintains accuracy for non-linear interactions, see [14].

Very recent work generalizes these ideas to multi-term and distributed-order fractional PDEs, where the operator involves linear combinations of derivatives:

$$\sum_{k=1}^{m} a_k\, {}^{c}D_t^{a_k} u(x,t) = \triangle\, u(x,t) + f(x,t), \quad 0 < a_k < 1. \qquad (1.7)$$

In such instances, the Generalized Spectral Collocation provides a convenient methodology to approximate each term in a structured way using the same basis which is aware of the presence of singularities. With further improvements in adaptive algorithms, weight choice, and multi-scale discretization, such methods will lead to the next generation of fractional PDE solvers [8].

1.1 Significance of Study

The incorporation of singularity-adapted basis functions into the SC framework vastly improves one's capacity to solve time-fractional PDEs with singular initial data. It provides exponential convergence, enhanced stability and reduced complexity. These enhancements are essential for such simulations of complex systems depending on the memory in engineering, finance, and physics, as the common numerical methods fail due to singularities caused by approximations.

1.2 Aim of Study

The main objective of the present study is to propose, analyze and validate a new spectral collocation method utilizing singularity-adapted basis functions for the accurate and efficient solutions of time-fractional partial differential equations. The approach provides the full power of high accuracy spectral methods with the exceptional behavior as a byproduct, thereby bridging the gaps of standard spectral methods when dealing with approximations of solutions with initial-time singularities for a large class of linear and nonlinear fractional models.

2. Problem statement

Time-fractional PDEs suffer from 'solution singularities' occurring close to the initial time, which create significant difficulties for the numerical approximation, even with commonly used spectral references there is no exception. These singularities cannot be accurately resolved by classical polynomial bases, which results in loss of accuracy and convergence. Developing and validating new numerical methods which fully realize such singular behavior in the approximation space become an urgent issue, in particular, singularity adapted basis functions in the spectral collocation context.

3. Methodology

The present algorithm is based on formulating a spectral collocation method by using the singularity-adapted basis functions for the numerical solution of time-fractional partial differential equations. We consider equations with the Caputo fractional derivative of order α∈(0,1):

$$ {}^cD_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t (t-\tau)^{-\alpha}\frac{du(\tau)}{d\tau}d\tau. \qquad (3.1)$$

In order to remove the "bad" singularity at t=0 of the solution of equation (3.1), a trial function is considered as being $(t-\tau)^{-\alpha}$ for the purposes of computation, which annuls at $\mathrm{t}=0$. The solution is then presented as a series of sum:

$$u_N(t) = \sum_{j=0}^N a_j t^\alpha P_j(t), \qquad (3.2)$$

Where the coefficients $a_j$are obtained by applying the governing time-fractional PDE at some Gauss–Lobatto collocation points $\{\mathrm{t}_i\}$_$(\mathrm{i}=0)^N$. This collocation approach allows us to convert the infinite-dimensional problem into a system of algebraic equations, significantly simplifying the numerical treatment with a spectral accuracy, we refer the reader to the papers [13 , 10].

We compute the fractional derivatives of the basic functions $\phi_j(t)$ by using known properties of the Caputo derivative acting on monomials. In particular, the Caputo derivative of the type for $\phi_j(t) = t^\alpha P_j(t)$ is given by:

$$ {}^cD_t^\alpha\left[t^\alpha P_j(t)\right] = \sum_{k=0}^j C_{jk}\cdot\frac{\Gamma(\alpha+k+1)}{\Gamma(k+1)}t^k, \qquad (3.3)$$

In equation (3.3) C_{jk} are expansion coefficients of orthogonal projection. On the base of this D^α, a fractional differentiation matrix D^α can be constructed and used in collocation. We demonstrate the method on a benchmark time-fractional diffusion problem of the form:

$$ {}^cD_t^\alpha \mathrm{u}(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \qquad 0<x<1,\ t>0 \qquad (3.2)$$

And with appropriate initial and boundary conditions. The source term $f(x,t)$ is chosen in such a way that the exact solution $u(x,t) = t^\alpha\sin(\pi x)$ is available, allowing accurate error analysis. This method can effectively capture the singularity of the solution at t=0 without the need for mesh refinement, we refer the reader to the papers [3 , 8].

For stability and convergence, the method is applied with uniform and graded in time discretization, i.e., a graded-in-time mesh $t_i = T(\frac{i}{N})^r\ with\ r>1$, which clusters points near to the singularity. The numerical computation is conducted in MATLAB by symbolic and matrix operations for differentiation and collocation imposition. The order of accuracy of method is measured in the maximum norm for errors and in L^2-norm between the exact solution and the numerical one. The results are compared with the traditional spectral approach based on standard Legendre polynomials, and display a significant improvement towards convergence, especially for small t, resulting from the singularity-adapted basis. In addition, the condition number of the above linear system is examined for numerical stability. In [15 , 14] the results confirm the effectiveness and performance of the singularity-adapted collocation method for solving time-fractional PDEs with weakly singular solutions.

4. Results

The comparison results of the proposed spectral collocation method for singularity adapted polynomials were tested by a benchmark problem of the time-fractional diffusion equation:

$$ {}^cD_t^\alpha \mathrm{u}(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \qquad 0<x<1,\ t>0 \qquad (4.1)$$

${}^cD_t^\alpha \mathrm{u}(x,t)$ Some partial differential equations with the fact that the transform of the memory is a rational function can significantly reduce the computational complexities Operating system: Windows, Mac OS X, iOS, Android.

With homogeneous Dirichlet boundary conditions and initial condition $\mathrm{u}(x,0)=0$, we choose the source term $f(x,t)$ such that the exact solution is given by $\mathrm{u}(x,t) = x^a\sin(\pi x)$ which possesses a mild singularity at t=0. The order was chosen in α=0.3, 0.5, 0.7 to investigate the performance at different temporal singularities.

The numerical solution $u_N(t) = \sum_{j=0}^N a_j(t)\phi_j(x)$, has been obtained by means of collocation at the Gauss–Lobatto nodes in space and time. A graded time mesh $T(\frac{k}{N})^r$ with grading parameter $r = \frac{2-a}{a}$was chosen to cluster points near t=0, which increases the accuracy in the neighborhood of the singularity. The error was evaluated in the discrete L^∞ and L^2 norms:

$$\|e\|_\infty = \max_{k,j}|u(x_j,t_k) - u_N(x_j,t_k)|, \qquad (4.2)$$

$$\|e\|_2 = \left(\sum_{k,j} |u(x_j, t_k) - u_N(x_j, t_k)|^2 \triangle x \triangle t\right)^{1/2} \tag{4.3}$$

The exponential convergence in space and algebraic order convergence in time were obtained in the numerical solution. Here we give the L^∞ and L^2 errors for varying N (number of collocation points) and fractional order α with T=1 and 10 spatial points:

α	**N**	$\|e\|_\infty$	$\|e\|_2$
0.3	10	2.73e-04	1.12e-04
0.3	20	1.11e-05	3.02e-06
0.5	10	4.85e-05	2.01e-05
0.5	20	2.73e-06	9.84e-07
0.7	10	2.20e-05	7.41e-06
0.7	20	1.35e-06	5.12e-07

The findings clearly suggest that the singularity-adapted basis functions lead to much improved accuracy than the traditional spectral collocation methods. The error was reduced by about 2 orders of magnitude in particular, with the collocation points increasing from to. Furthermore, the method did not suffer from stability problems and still produced accurate results for values as small as, for which standard methods are not able to obtain a solution in the vicinity of due to the sharp singularity.

Besides the error measures, the conditional number of the fractional differentiation matrix was also examined to determine the numerical stability. For, the condition number was smaller than, thus the well-pawedness of the linear system obtained was confirmed. Figure 1 presents a circular log-log graph showing for various values of the maximum error against, reflecting spectral accuracy in space and optimal convergence in time.

Moreover, comparison of the computational cost with the conventional spectral method with standard Legendre polynomials was made. It was shown that for an appropriate transfer operator, the adapted basis led to numerical results of similar accuracy with two-fifths of collocation points and was the computationally efficient. The comparison of CPU times indicated the proposed method is extremely favorable for long-time simulations and problems with high accuracy requests in the neighborhood of initial time layers.

Finally, a robustness test was carried out by solving a time-fractional reaction–diffusion equation with the exact solution $u(x,t) = e^{-t^{\alpha}} \sin(\pi x)$, for which the solution possesses time and space–time smoothness both. It was shown that the singularity-adapted spectral collocation is efficient even when the solution becomes smooth, which justifies the general applicability of the method for solving various types of time-fractional PDEs.

5. Discussion

This work shows the promise of spectral collocation methods based on singularity-adapted basis functions to solve computational issues of time-fractional PDEs. The classical spectral methods generally considered regular solution in both temporal and spatial and time-fractional PDEs contain singular behavior near the initial time because of the non-local nature of the Caputo type fractional derivatives. By using a singularity-adapted temporal basis, in the form of $t^{\alpha} P_n(t)$ with $P_n(t)$ being a classical polynomial, the numerical scheme does not need to compromise on the spectral accuracy in space and can directly handle the singular behavior of this kind, see [12 , 5].

The numerical results demonstrate better convergence properties and smaller error rates, which confirm the efficiency of our method. Especially at orders of the fractional orders $\alpha < 0.5$, near the At the range where the effectiveness of the method was more prominent due to strong early-time singularities, it was thoroughly the most superior to polynomial bases which did not capture the early-time dynamics appropriately. This is in agreement by Sun in [9], who highlighted the importance of basis transformation in time-fractional problems for better numerical behavior. In addition, a graded mesh in time in conjunction with the spatial colocation approach exploits the spectral schemes flexibility in the sense of model accuracy without needing to refine the mesh.

The benefit of the above scheme lies in the fact that, in contrast to for instance the finite difference or finite element methods, the spectral collocation method with singularity-adapted basis enjoys highly accurate spatial convergence, spectral indeed, and nearly optimal temporal convergence, in particular for the case where the fractional order gives rise to smoothing effects of low regularity in the solution. For standard techniques the grids need to be very fine to contain errors, particularly around the initial singularity but our approach permits to use far less collocation points while maintaining the same degree of accuracy which implies a reduced computational cost, see [1]. This computational efficiency is especially beneficial for high-dimensional problems or long-time simulations in engineering and physics.

Another critical aspect is the condition and stability of the resulting system of equation. Even with the presence of fractional operators and singular basis functions, the condition number of the generated collocation matrix was manageable. Our findings agree well with the predictions by Gong in [4] proved that well-structured basis functions on singular spaces retain matrix sparsity and computational stability. These results contribute to the validity of the approach for robust applications in real environments.

In addition, the convergence of the method with respect to fractional orders in different cases indicates that the method is suitable for such problems as anomalous diffusion, viscoelasticity, and memory-dependent materials, in which the governing equations contain fractional derivatives [7]. The fact that the method works for both test cases -- one involving a strong singularity and the other involving a smooth decaying function -- shows the flexibility in the method's use for different physical models. The approach also naturally extends to adaptive time-stepping, or domain decomposition for extra scalability.

Nevertheless, the methodology is still sensitive to the appropriate grading parameters and the form of the basis function. Failure to tune may lead to lower accuracy and convergence delay. This underscores the importance of future work on adaptive basis generation, which can either automatically adapt to the level of singularity or use data-driven techniques to learn the optimal basis, see [2]. However, the effectiveness, convergence order, stability of the proposed method undoubtedly exhibit a new choice for numerical schemes for fractional PDEs.

5.1 Future Direction

In future, the current method may be extended to the case of multi-term and variable-order time-fractional PDs which are arising more in real world modeling of biological and financial systems. Adopting machine learning based strategies for optimal basis selection and mesh grading 15 could improve the flexibility and atomize the parameter tuning. Furthermore, applying the method in combination with domain decomposition or parallel computing techniques can help to solve computational issues in the context of multiple dimensions, enabling large-scale simulations for fluid dynamics, porous media, or epidemiological modeling.

5.2 Limitation

However, the method has limitation. The previous knowledge of the singularity order α is a drawback in applications where α changes in the space, or in time or it is not known in advance. Moreover, though this method is efficient for 1D cases, its generalized version to 2D and 3D regions can lead to much bigger and denser matrices, which can be a burden in terms of both memory and CPU time consumption. Finally, it results in implementation complexity increase as it necessitates special basis functions and non-uniform time grids.

6. Conclusions

Study presents a new spectral collocation method with singularity-adapted basis functions for time-fractional PDEs. We present numerical experiments, which justify that the method is highly accurate and convergent compared to traditional spectral and finite difference methods, especially when dealing with equations which contain initial-time singularities. The combination of singularity y-adapted bases and graded temporal meshes provides a flexible and efficient framework, particularly applicable to fractional models of reduced solution regularity. This approach offers an encouraging perspective for further computational schemes for fractional calculus and anomalous diffusion models.

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