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2017

Li, X., & Wong, P. J. Y. (2017). Nonpolynomial numerical scheme for fourth-order fractional sub-diffusion equations. AIP Conference Proceedings, 1863, 190002-.
doi:10.1063/1.4992370

<https://hdl.handle.net/10356/88959>

<https://doi.org/10.1063/1.4992370>

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Nonpolynomial Numerical Scheme for Fourth-Order Fractional Sub-diffusion Equations

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Abstract. We shall develop a high order numerical scheme for a fourth-order fractional sub-diffusion problem. Theoretical results will be established in maximum norm and it is shown that the convergence order is *higher* than some earlier work done. Numerical experiments will be carried out to demonstrate the efficiency of the proposed scheme as well as to compare with other methods.

INTRODUCTION

Fractional diffusion equation (FDE) is obtained from the classical diffusion or wave equation by replacing the first-order or second-order time derivative by a fractional derivative of order $\gamma > 0$, see [1] for details. The classical diffusion equation contains second-order space derivative, but a fourth-order space derivative may be necessary in some models, e.g. transverse vibration of beams [2].

There is abundant interest on FDEs involving *fourth-order* space derivatives. Agrawal [3] has presented the general solution for fourth-order diffusion-wave problems but no numerical considerations. Thereafter, numerical methods such as decomposition method [4], homotopy perturbation method [5], quintic B-spline method [6], finite element [7], finite difference [8] and compact finite difference [9] – which achieves the *best spatial convergence* of $O(h^4)$ (where h is the spatial step size), have been applied successfully.

Motivated by the above research, in this paper we shall discuss the numerical treatment of a *fourth-order* fractional sub-diffusion problem which has also been considered in [8]. The sub-diffusion problem is stated as follows:

$$\begin{cases} {}^C_0D_t^\gamma u(x, t) + b^2 \frac{\partial^4 u}{\partial x^4} = f(x, t), & x \in [0, L], t \in [0, T] \\ u(x, 0) = \phi(x), & x \in [0, L] \\ u(0, t) = g_1(t), \quad u(L, t) = g_2(t), \quad \frac{\partial^2 u(0, t)}{\partial x^2} = g_3(t), \quad \frac{\partial^2 u(L, t)}{\partial x^2} = g_4(t), & t \in [0, T] \end{cases} \quad (1)$$

where $0 < \gamma < 1$, ${}^C_0D_t^\gamma u(x, t)$ is in Caputo sense, b, L, T are positive constants, $f(x, t)$, $\phi(x)$, $g_1(t)$, $g_2(t)$, $g_3(t)$ and $g_4(t)$ are known continuous functions with $\phi(0) = g_1(0)$ and $\phi(L) = g_2(0)$.

NONPOLYNOMIAL NUMERICAL SCHEME

In tackling (1), we shall introduce a parametric quintic spline method [10] in the spatial dimension and a higher order $L2 - 1_\sigma$ [11] approximation for Caputo fractional derivatives.

To begin, let $P : 0 = x_0 < x_1 < \dots < x_K = L$ and $P' : 0 = t_0 < t_1 < \dots < t_N = T$ be the uniform meshes in the spatial and temporal dimensions respectively, with spatial and temporal step sizes $h = \frac{L}{K}$ and $\tau = \frac{T}{N}$. For any function $u(x, t)$, denote the function value $u(x_j, t_n)$ by u_j^n . For any $v = (v_0, v_1, \dots, v_K)$, define $\delta_x v_{j+\frac{1}{2}} = (v_{j+1} - v_j)/h$,

$\delta_x^2 v_j = (\delta_x v_{j+\frac{1}{2}} - \delta_x v_{j-\frac{1}{2}})/h$, $\delta_x^3 v_{j+\frac{1}{2}} = (\delta_x^2 v_{j+1} - \delta_x^2 v_j)/h$ and $\delta_x^4 v_j = (\delta_x^3 v_{j+\frac{1}{2}} - \delta_x^3 v_{j-\frac{1}{2}})/h$. Next, we state the $L2 - 1_\sigma$ formula [11] and give the definition of parametric quintic spline. (A similar definition is also given in [10].)

Lemma 1. [11] Let $u(x, t) \in C^{8,3}([0, L] \times [0, T])$. The following holds for $0 < \gamma < 1$, $\sigma = 1 - \frac{\gamma}{2}$ and $t_{n+\sigma} = (n + \sigma)\tau$:

$${}_0^C D_t^\gamma u(x_j, t_{n+\sigma}) = \frac{1}{\Gamma(2 - \gamma)\tau^\gamma} \left[r_0 u_j^{n+1} - \sum_{k=1}^n (r_{n-k} - r_{n-k+1}) u_j^k - r_n u_j^0 \right] + O(\tau^{3-\gamma}), \quad (2)$$

where the coefficients r_i 's are given in (28) of [11].

Definition 1. Let $t = t_n$, $1 \leq n \leq N$ be fixed. We say $Q(x, t_n; \xi) \in C^{(4)}[0, L]$ is the *parametric quintic spline with parameter $\xi > 0$* (with respect to mesh P) if its restriction $Q_j(x, t_n; \xi) \equiv Q_j(x, t_n)$ in $[x_{j-1}, x_j]$, $1 \leq j \leq K$ satisfies $Q_j^{(4)}(x, t_n) + \xi^2 Q_j''(x, t_n) = (F_j^n + \xi^2 M_j^n)(x - x_{j-1})/h + (F_{j-1}^n + \xi^2 M_{j-1}^n)(x_j - x)/h$, with $Q_j(x_i, t_n) = u_i^n$, $Q_j'(x_i, t_n) = M_i^n$, $Q_j^{(4)}(x_i, t_n) = F_i^n$, $i = j - 1, j$.

By continuity of the first and third derivatives of the spline, we obtain an equation which connects the fourth derivatives and the function values

$$HF_j^n := p(F_{j-2}^n + F_{j+2}^n) + q(F_{j-1}^n + F_{j+1}^n) + sF_j^n = \delta_x^4 u_j^n, \quad 2 \leq j \leq K - 2.$$

(See [10] for the expressions of p , q , s .) Further, two more equations are derived as

$$HF_1^n := \frac{1}{360} (28F_0^n + 245F_1^n + 56F_2^n + F_3^n) = \delta_x^4 u_1^n, \quad HF_{K-1}^n := \frac{1}{360} (28F_K^n + 245F_{K-1}^n + 56F_{K-2}^n + F_{K-3}^n) = \delta_x^4 u_{K-1}^n.$$

Let $\sigma = 1 - \frac{\gamma}{2}$ and $t_{n+\sigma} = (n + \sigma)\tau$. At the node $(x_j, t_{n+\sigma})$, it follows from (1) that

$$\frac{1}{b^2} [f_j^{n+\sigma} - {}_0^C D_t^\gamma u(x_j, t_{n+\sigma})] = \frac{\partial^4 u(x_j, t_{n+\sigma})}{\partial x^4} = \sigma \frac{\partial^4 u(x_j, t_{n+1})}{\partial x^4} + (1 - \sigma) \frac{\partial^4 u(x_j, t_n)}{\partial x^4} + O(\tau^2) \quad (3)$$

Let $F_j^n \approx D_x^4 u(x_j, t_n)$. We apply H on both sides of (3) and employ $L2 - 1_\sigma$ approximation (Lemma 1) for the Caputo derivative. After omitting the small terms, we get the *parametric quintic spline (PQS) scheme*:

$$\frac{1}{b^2 \Gamma(2 - \gamma) \tau^\gamma} H \left[r_0 u_j^{n+1} - \sum_{k=1}^n (r_{n-k} - r_{n-k+1}) u_j^k - r_n u_j^0 \right] + \sigma \delta_x^4 u_j^{n+1} + (1 - \sigma) \delta_x^4 u_j^n = \frac{1}{b^2} H f_j^{n+\sigma}, \quad 1 \leq j \leq K - 1 \quad (4)$$

with $u_j^0 = \phi(x_j)$, $0 \leq j \leq K$ and $u_0^n = g_1(t_n)$, $u_K^n = g_2(t_n)$, $\delta_x^2 u_0^n = g_3(t_n)$, $\delta_x^2 u_K^n = g_4(t_n)$, $0 \leq n \leq N$.

STABILITY, SOLVABILITY, CONVERGENCE

In this section, we shall first analyze the local truncation error of the PQS scheme and then establish the stability, solvability and convergence in maximum norm.

The local truncation error of the PQS scheme can be obtained easily by first replacing u_j^n in formula (4) by exact value $u(x_j, t_n)$ and then carrying out Taylor expansion at $x = x_j$.

Lemma 2. Let T_j^{n+1} be the local truncation error of the j -th equation in the PQS scheme (4). We have $T_j^{n+1} = O(h^4 + \tau^2)$, $j = 1, K - 1$ and $T_j^{n+1} = -Z_1 D_x^4 u(x_j, t_{n+\sigma}) - h^2 Z_2 D_x^6 u(x_j, t_{n+\sigma}) - h^4 Z_3 D_x^8 u(x_j, t_{n+\sigma}) + O(h^6 + \tau^2)$, $2 \leq j \leq K - 2$ where $Z_1 = 2p + 2q + s - 1$, $Z_2 = 4p + q - \frac{1}{6}$ and $Z_3 = \frac{4}{3}p + \frac{1}{12}q - \frac{1}{80}$.

Setting $Z_1 = Z_2 = Z_3 = 0$ yields $p = -\frac{1}{720}$, $q = \frac{31}{180}$ and $s = \frac{79}{120}$ which will be used throughout the paper.

Next, we use energy method to establish the stability. This involves introducing a suitable inner product and a norm. Let $V_h = \{v = (v_0, v_1, \dots, v_K) \mid v_0 = v_K = 0\}$. For any $v, w \in V_h$, define $\|v\|_\infty = \max_{1 \leq j \leq K-1} |v_j|$,

$$(w, v) = h \sum_{j=1}^{K-1} w_j v_j, \quad \langle w, v \rangle = h \sum_{j=1}^{K-1} (\delta_x^2 w_j) (\delta_x^2 v_j) - \frac{h^3}{6} \sum_{j=0}^{K-1} (\delta_x^3 w_{j+\frac{1}{2}}) (\delta_x^3 v_{j+\frac{1}{2}}) - \frac{h^5}{720} \sum_{j=1}^{K-1} l_j (\delta_x^4 w_j) (\delta_x^4 v_j)$$

where $l_j = -2$, $j = 1, K-1$ and $l_j = 1$, $2 \leq j \leq K-2$. Clearly, $\|v\| = (v, v)^{\frac{1}{2}}$ is a norm.

Now, let v_j^{n+1} be the solution of scheme (4) with $f_j^{n+\sigma}$ and $\phi(x_j)$ replaced by $\tilde{f}_j^{n+\sigma}$ and $\phi(x_j) + \theta_j$ respectively. Let $\epsilon_j^n = v_j^n - u_j^n$, $0 \leq j \leq K$, $0 \leq n \leq N$. Obviously, ϵ_j^n satisfies

$$\frac{1}{b^2 \Gamma(2-\gamma) \tau^\gamma} H \left[r_0 \epsilon_j^{n+1} - \sum_{k=1}^n (r_{n-k} - r_{n-k+1}) \epsilon_j^k - r_n \epsilon_j^0 \right] + \sigma \delta_x^4 \epsilon_j^{n+1} + (1-\sigma) \delta_x^4 \epsilon_j^n = \frac{1}{b^2} H g_j^{n+\sigma}, \quad 1 \leq j \leq K-1 \quad (5)$$

where $g_j^{n+\sigma} = \tilde{f}_j^{n+\sigma} - f_j^{n+\sigma}$, with $\epsilon_j^0 = \theta_j$, $0 \leq j \leq K$ and $\epsilon_0^n = \epsilon_K^n = \delta_x^2 \epsilon_0^n = \delta_x^2 \epsilon_K^n = 0$, $0 \leq n \leq N$. By energy method, we obtain the stability result.

Theorem 1. (Stability) The PQS scheme (4) is unconditionally stable in maximum norm. In fact, we have

$$\|\epsilon^{n+1}\|_\infty^2 \leq \frac{45}{224} L^3 \left[\langle \epsilon^0, \epsilon^0 \rangle + \frac{\Gamma(1-\gamma) T^\gamma}{b^2} \max_{0 \leq n \leq N-1} \|H g^{n+\sigma}\|^2 \right], \quad 0 \leq n \leq N-1. \quad (6)$$

From (6), it follows that the corresponding homogeneous system of (4) (with zero initial and boundary conditions and nonlinear term $f \equiv 0$) has only the trivial solution. This leads to the next result.

Theorem 2. (Solvability) The PQS scheme (4) is uniquely solvable.

Let u_j^n be the numerical solution of (1) at (x_j, t_n) obtained via (4) and U_j^n be the corresponding exact solution of (1). Let $e_j^n = U_j^n - u_j^n$ be the error. By energy method again, the convergence of the PQS scheme (4) is established.

Theorem 3. (Convergence) Let $u(x, t) \in C^{8,3}([0, L] \times [0, T])$. Then, we have $\|e^n\|_\infty \leq O(\tau^2 + h^{4.5})$, $1 \leq n \leq N$.

Remark 1. We conclude by Theorem 3 that the PQS scheme (4) achieves $O(h^{4.5})$ in the spatial dimension – this is higher than *finite difference method* ($O(h^2)$, see [8]) and *compact finite difference scheme* ($O(h^4)$, see [9]).

Remark 2. In practice, it is possible to get a higher convergence order than the *theoretical* $O(h^{4.5})$ in Theorem 3.

NUMERICAL SIMULATION

We shall present simulation results to verify the efficiency of the PQS scheme (4) and also to compare the performance with compact finite difference (CFD) method and finite difference (FD) method. To have proper comparison, we shall solve the same problem using $L2-1_\sigma$ formula (Lemma 1) to approximate the Caputo derivative while employing one of the three methods (PQS, CFD, FD) in the spatial dimension.

In our experiment, for a fixed (τ, h) we shall compute the maximum absolute error at $t = t_N = T$, i.e., $\|e^N\|_\infty = \max_{1 \leq j \leq K-1} |U_j^N - u_j^N|$.

Example 1. [8] Consider problem (1) with $b = L = T = 1$, $f(x, t) = e^x \left[\frac{\Gamma(\gamma+4)}{6} t^3 + t^{3+\gamma} \right]$, $\phi(x) = 0$, $g_1(t) = g_3(t) = t^{3+\gamma}$ and $g_2(t) = g_4(t) = e t^{3+\gamma}$. The exact solution is given as $u(x, t) = e^x t^{3+\gamma}$.

To observe the spatial convergence order (x -order) of PQS method, we fix the temporal step size $\tau = \frac{1}{200000}$ and let the spatial step size h vary; likewise to observe the temporal convergence order (t -order), we fix $h = \frac{1}{100}$ and let τ vary. The maximum absolute errors $\|e^N\|_\infty$ and the convergence orders are displayed in Tables 1 and 2. From Table 1, it is observed that the spatial convergence order of PQS scheme is more than 4.5 – the *theoretical* order obtained in Theorem 3. As indicated in Remark 2, a higher convergence order is possible in practice. The simulation results in Table 2 verify that the temporal convergence order of PQS scheme is 2 – same as the theoretical result given in Theorem 3.

TABLE 1. Spatial convergence order of PQS method ($\tau = \frac{1}{200000}$)

h	$\gamma = 0.1$	x -order	$\gamma = 0.5$	x -order	$\gamma = 0.9$	x -order
1/5	5.28E-08		5.24E-08		5.16E-08	
1/10	8.71E-10	5.9232	8.67E-10	5.9180	8.56E-10	5.9137
1/20	1.47E-11	5.8870	1.88E-11	5.5233	2.07E-11	5.3725

TABLE 2. Temporal convergence order of PQS method ($h = \frac{1}{100}$)

τ	$\gamma = 0.1$	t -order	$\gamma = 0.5$	t -order	$\gamma = 0.9$	t -order
1/10	3.11E-04		1.64E-03		2.73E-03	
1/20	7.93E-05	1.9722	4.18E-04	1.9749	6.89E-04	1.9882
1/40	2.00E-05	1.9856	1.05E-04	1.9858	1.73E-04	1.9928

Finally, we shall compare the performance of PQS, CFD and FD methods, which have *theoretical* spatial convergence order of $O(h^{4.5})$, $O(h^4)$ and $O(h^2)$ respectively. Here, we fix $\tau = \frac{1}{200000}$ and let h vary. Table 3 presents the maximum absolute errors $\|e^N\|_\infty$ and convergence orders. Clearly, the simulation results indicate that PQS method *outperforms* in terms of convergence and also achieves the *smallest* absolute error in all cases.

TABLE 3. Comparison of PQS, CFD and FD methods ($\tau = \frac{1}{200000}$)

γ	h	PQS	x -order	CFD	x -order	FD	x -order
0.3	1/5	5.27E-08		8.20E-08		6.12E-04	
	1/10	8.69E-10	5.9206	3.60E-09	4.5107	1.54E-04	1.9882
	1/20	1.79E-11	5.6047	2.00E-10	4.1660	3.90E-05	1.9860
0.6	1/5	5.23E-08		8.14E-08		6.07E-04	
	1/10	8.65E-10	5.9167	3.57E-09	4.5098	1.53E-04	1.9882
	1/20	2.15E-11	5.3292	2.01E-10	4.1484	3.87E-05	1.9856
0.9	1/5	5.16E-08		8.04E-08		6.00E-04	
	1/10	8.56E-10	5.9137	3.53E-09	4.5093	1.51E-04	1.9881
	1/20	2.07E-11	5.3725	2.01E-10	4.1376	3.82E-05	1.9850

CONCLUSION

In this paper, we have developed a numerical method for a fourth-order fractional sub-diffusion problem. Our method is built on deploying a parametric quintic spline scheme in the spatial dimension and a higher order non-uniform approximation for Caputo derivatives. The solvability, convergence and stability can be proved using energy method. It is shown that the proposed method has the convergence order of $O(\tau^2 + h^{4.5})$, which improves the earlier work done to date. Finally, through some numerical simulations, we confirm the theoretical accuracy and also demonstrate the outperformance of the proposed method over compact finite difference and finite difference methods.

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