CHAPTER 5

Numerical Methods for Solving the Robin Boundary Value Problem for a Generalized Diffusion Equation with a Non-smooth Solution.

5.1 Introduction

In the rectangle $H = \{(x,t) : 0 \leq x \leq 1, 0 \leq t \leq T\}$, consider the following Robin boundary value problem:

$$\partial_{0,t}^{\alpha,\omega(t)}\zeta = \frac{\partial}{\partial x}\left(m(x,t)\frac{\partial \zeta}{\partial x}\right) - p(x,t)\zeta + \phi(x,t), \quad x \in (0,1), \quad t \in (0,T], \tag{5.1}$$

$$\begin{aligned} -m(0,t)\zeta_x(0,t) &= \beta_1(t)\zeta(0,t) - \mu_1(t), \\ m(1,t)\zeta_x(1,t) &= \beta_2(t)\zeta(1,t) - \mu_2(t), \end{aligned} \tag{5.2}$$

$$\zeta(x,0) = \zeta_0(x). \tag{5.3}$$

where,

$$\partial_{0,t}^{\alpha,\omega(t)}\zeta(x,t) = \frac{1}{\Gamma(1-\alpha)}\int\limits_0^t \frac{\omega(t-\xi)}{(t-\xi)^\alpha}\frac{\partial\zeta}{\partial\xi}(x,\xi)\mathrm{d}\xi, \tag{5.4}$$

is the generalized Caputo fractional derivative of order $\alpha,\ 0<\alpha<1$ where $\omega(t)$ is the weight function with $\omega(t)\in C^2[0,T]$, $\omega(t)>0$ and $\omega'(t)\le 0$ for all $t\in[0,T]$, $0<c_1\le m(x,t)\le c_2$ and $p(x,t)\ge 0$ for all $(x,t)\in H$.

In this chapter we aim to develop stable L1 scheme on non-uniform mesh for the above model with Robin boundary conditions. The rest of the chapter is arranged as: Section 5.2 presents the approximation of the generalized Caputo derivative by L1 formula and also a difference scheme is developed. Stability and convergence of the scheme for non-smooth solution has been established in Section 5.3. Numerical experiments for the test example are performed in Section 5.4 which validates the theoretical results. Some final observations are made in Section 5.5.

5.2 Approximation and a difference scheme.

5.2.1 Formula derivation

Let $\zeta(x,t)$ be the exact solution of the problem (5.1)-(5.3). The interval $[0,T]$ is divided into sub-intervals with $0 = t_0 < t_1 \ldots < t_N = T$ and $\tau_n = t_n - t_{n-1}$, $1 \leq n \leq N$ where τ_n is the time step size. The formula for the approximation of the Caputo derivative $\partial_{0,t_n}^{\alpha,\omega(t)}\zeta(t)$ with $(0 < \alpha < 1,\ \omega(t) > 0,\ \omega'(t) \leq 0,\ \omega(t) \in C^2[0,T])$ is given as:

$$\partial_{0,t_n}^{\alpha,\omega(t)}\zeta(t) \approx \Delta_{0,t_n}^{\alpha,\omega(t)}\zeta = \sum_{s=0}^{n-1} c_s^n(\zeta(t_{s+1}) - \zeta(t_s)), \tag{5.5}$$

where,

$$c_s^n = \frac{1}{\Gamma(2-\alpha)}\left[\omega(t_n - t_s - \frac{\tau_{s+1}}{2})a_s^n + (\omega(t_n - t_{s+1}) - \omega(t_n - t_s))b_s^n\right],$$

with

$$a_s^n = \frac{(t_n - t_s)^{1-\alpha} - (t_n - t_{s+1})^{1-\alpha}}{\tau_{s+1}},$$
$$b_s^n = \frac{1}{\tau_{s+1}^2}\left(\frac{1}{2-\alpha}[(t_n - t_s)^{2-\alpha} - (t_n - t_{s+1})^{2-\alpha}] - \frac{\tau_{s+1}}{2}[(t_n - t_s)^{1-\alpha} + (t_n - t_{s+1})^{1-\alpha}]\right).$$

The details of the derivation can be found in the paper [69].

5.2.2 Difference scheme

In the rectangle H consider the mesh as $\chi_{h\tau} = \chi_h \times \chi_\tau$ with,

$\chi_h = \{x_i = ih : i = 0, 1, \ldots, M, hM = l\}$ and $\chi_\tau = \{t_n : 0 = t_0 < t_1 < t_2 < \ldots < t_{N-1} < t_N = T\}$,

the assigned difference scheme to the model (5.1)-(5.3) is:

$$\Delta_{0,t_n}^{\alpha,\omega(t)} \varpi_i = \wedge \varpi_i^n + \phi_i^n, \quad n = 1, \ldots, N, \ i = 0, 1, 2, \ldots, M, \tag{5.6}$$

$$\varpi(x, 0) = \zeta_0(x) \quad i = 0, 1, 2, \ldots, M, \tag{5.7}$$

where

$$\wedge \varpi = \begin{cases} \frac{2}{h}(a_1 \varpi_x - \kappa_1 \varpi), \quad i = 0, \\ a(\varpi_{\bar{x}})_x - d\varpi, \quad 1 \leq i \leq M-1, \\ -\frac{2}{h} a_M \varpi_x + \kappa_2 \varpi, \quad i = M, \end{cases}$$

and

$$\phi = \begin{cases} \frac{2}{h}\bar{\mu}_1, \ i = 0, \\ f, \ 1 \leq i \leq M-1, \\ \frac{2}{h}\bar{\mu}_2, \ i = M. \end{cases}$$

with $a(\varpi_{\bar{x}})_x - d(\varpi)_i = \dfrac{a_{i+1}\varpi_{i+1} - (a_{i+1} + a_i)\varpi_i + a_i \varpi_{i-1}}{h^2} - d_i \varpi_i, \quad i = 1, \ldots, M-1,$

$$\varpi_{\bar{x},i} = \frac{\varpi_i - \varpi_{i-1}}{h}, \ \varpi_{x,i} = \frac{\varpi_{i+1} - \varpi_i}{h}, \ a_i^n = m(x_{i-1/2}, t_n), \ d_i^n = p(x_i, t_n),$$

$$\kappa_1 = \beta_1 + 0.5hd_0, \quad \kappa_2 = \beta_2 + 0.5hd_M, \quad \bar{\mu_1} = \mu_1 + 0.5hf_0, \quad \bar{\mu_2} = \mu_2 + 0.5hf_M.$$

The non-uniform mesh used here for the case of non-smooth solution is defined by $t_n = T(n/N)^r$ for $n = 0, 1, \ldots, N$, where the constant mesh grading is being chosen by the user. When $r = 1$, the mesh is uniform. Also, $\tau_n = t_n - t_{n-1}$ for $n = 1, 2, \ldots, N$.

5.3 Stability

In this section it is proved that the difference scheme has the order of approximation as $\mathcal{O}(N^{\alpha-2} + h^2)$.

Lemma 5.3.1. [37, 69, 101] For $n \in \mathbb{N}$, $\{a_s^n | 0 \leq s \leq n-1\}$ *and* $\alpha \in (0,1)$, the following result holds:

$$a_{n-1}^n > a_{n-2}^n > \ldots > a_s^n > a_{s-1}^n > \ldots a_0^n > \frac{1-\alpha}{(t_n - t_0)^\alpha},$$

and

$$b_{n-1}^n > b_{n-2}^n > \ldots > b_s^n > b_{s-1}^n > \ldots > b_0^n > 0.$$

Corollary 5.3.1. [69] For $n \in \mathbb{N}$, $\{c_s^n | 0 \leq s \leq n-1\}$, $\alpha \in (0,1)$ *and* $\omega(t) \in C^2[0,T]$, where $\omega(t) > 0$, $\omega'(t) \leq 0\ \forall t \in [0,T]$, the following results hold:

$$c_{n-1}^n > c_{n-2}^n > \ldots > c_s^n > c_{s-1}^n > \ldots c_0^n > \frac{\omega(t_n - t_0 - \frac{\tau_1}{2})}{\Gamma(1-\alpha)(t_n - t_0)^\alpha} > \frac{\omega(T)}{\Gamma(1-\alpha)T^\alpha}.$$

Proof. For the proof of this Theorem please refer to the paper [69]. □

Theorem 5.3.1. The difference scheme (5.6)-(5.7) is unconditionally stable and its solution satisfies the following inequality:

$$||\varpi^n||_0^2 \leq ||\varpi^0||_0^2 + \frac{\Gamma(1-\alpha)T^\alpha}{\omega(T)4c_1} \max_{0\leq n\leq N-1}\left(||f^{n+1}||_0^2 + \bar{\mu_1}^2(t_{n+1}) + \bar{\mu_2}^2(t_{n+1})\right), \quad (5.8)$$

where $[\varpi, v] = \sum_{i=1}^{M-1} \varpi_i v_i h + 0.5(\varpi_0 v_0 h + 0.5\varpi_M v_M h),\ ||\varpi||_0^2 = [\varpi, \varpi]$.

Proof. Taking the inner product of (5.6) with ϖ^n, we get

$$[\varpi^n, \Delta_{0,t_n}^{\alpha,\omega(t)}\varpi] - [\wedge\varpi^n, \varpi^n] = [\varpi^n, \phi], \quad (5.9)$$

Since,

$$[\varpi^n, \Delta_{0,t_n}^{\alpha,\omega(t)}\varpi] \geq \frac{1}{2}\Delta_{0,t_n}^{\alpha,\omega(t)}||\varpi||_0^2,$$

On solving $[\wedge\varpi^n, \varpi^n]$ and $[\varpi^n, \phi]$ and using in (5.9) we get

$$\frac{1}{2}\Delta_{0,t_n}^{\alpha,\omega(t)}||\varpi||_0^2 + c_1||\varpi_{\bar{x}}||_0^2 + \kappa_1(\varpi_0^n)^2 + \kappa_2(\varpi_M^n)^2 \leq \epsilon||\varpi_0||^2 + \epsilon(\varpi_0^n)^2 + \epsilon(\varpi_M^n)^2 + \frac{1}{4\epsilon}\left(||f||_0^2 + \bar{\mu_1}^2 + \bar{\mu_2}^2\right),$$

Taking $2\epsilon_0 = min(c_1, \kappa_1, \kappa_2)$ we get

$$\Delta_{0,t_n}^{\alpha,\omega(t)}||\varpi||_0^2 \leq \frac{1}{\epsilon_0}\left(||f||_0^2 + \bar{\mu_1}^2 + \bar{\mu_2}^2\right). \quad (5.10)$$

The inequality (5.10) can be written in the form

$$c_{n-1}^n||\varpi^n||_0^2 \leq \sum_{s=1}^{n-1}(c_s^n - c_{s-1}^n)||(\varpi^s||_0^2 + c_0^n||(\varpi^0||_0^2 + \frac{1}{\epsilon_0}\left(||f||_0^2 + \bar{\mu_1}^2 + \bar{\mu_2}^2\right),$$

From Corollary 5.3.1 we have $c_0^n \geq \dfrac{\omega(T)}{\Gamma(1-\alpha)T^\alpha} = m_2$ (*let*), we get

$$c_{n-1}^n ||\varpi^n||_0^2 \leq \sum_{s=1}^{n-1}(c_s^n - c_{s-1}^n)||\varpi^s||_0^2 + c_0^n\left(||\varpi^0||_0^2 + \frac{1}{m_2\epsilon_0}\left(||f||_0^2 + \bar{\mu_1}^2 + \bar{\mu_2}^2\right)\right),$$

By using induction we arrive at the inequality:

$$||\varpi^n||_0^2 \leq ||\varpi^0||_0^2 + \frac{1}{m_2\epsilon_0}\max_{0\leq n\leq N-1}\left(||f^{n+1}||_0^2 + \bar{\mu_1}^2(t_{n+1}) + \bar{\mu_2}^2(t_{n+1})\right),$$

we get $(-\wedge\varpi,\varpi) \geq 4c_1||\varpi||_0^2$, for the difference operator $\wedge$, using Green's first difference formula and the embedding theorem [102] for the functions vanishing at $x=0$ and $x=1$, that is, we take $\epsilon_0 = 4c_1$ for this operator. As a result

$$||\varpi^n||_0^2 \leq ||\varpi^0||_0^2 + \frac{\Gamma(1-\alpha)T^\alpha}{\omega(T)4c_1}\max_{0\leq n\leq N-1}\left(||f^{n+1}||_0^2 + \bar{\mu_1}^2(t_{n+1}) + \bar{\mu_2}^2(t_{n+1})\right).$$

Hence, the theorem is proved. □

From the a priori estimate (5.8) it follows that the solution of the difference scheme (5.6)-(5.7) converges to the solution of the mathematical problem (5.1)-(5.3) with the rate equal to the approximation error order $\mathcal{O}(N^{\alpha-2} + h^2)$.

5.4 Numerical results

In this section, the maximum error and the convergence order (CO) for the domain have been calculated using the following norm $||.||_{H(\chi_{h\tau})}$, where $||w||_{H(\chi_{h\tau})} = \max\limits_{(x_i,t_j)\in\chi_{h\tau}} |w|$ and $w = \varpi - \zeta$ is the error, where ϖ is the approximate solution. In time the CO= $\log_{\frac{\mathrm{N}_1}{\mathrm{N}_2}} \frac{||w_1||}{||w_2||}$ and in space the CO= $\log_{\frac{h_1}{h_2}} \frac{||w_1||}{||w_2||}$. $||\cdot||_0$ is the definition of the L_2-norm.

Example 5.4.1. We examine a test problem with non-smooth solution. Let $\zeta(x,t) = t^{\beta}\sin(\pi x)e^{-bt}$ be the exact solution of (5.1)-(5.3) with $\omega(t) = e^{-5t}$, $0 < \beta < 1$, the coefficients $p(x,t) = 1 - \sin(xt)$, $m(x,t) = 2 - \cos(xt)$, $T = 1$, $\mu_1(t) = -\pi t^{\beta}e^{-bt}$, $\mu_2(t) = \pi t^{\beta}e^{-bt}(\cos(t) - 2)$, $\beta_1(t) = 2 - \sin(t)$ and $\beta_2(t) = 2 - \cos(3t)$.

The numerical results of this example are shown and illustrated below.

- Due to the presence of a singularity in the first derivative of the solution at $t = 0$, the exact solution is non-smooth. As can be seen in Table 5.1, a uniform mesh yields poor outcome in this scenario.
- For different values of α and β with fixed $h = 1/1000$ in the temporal direction, maximum norm error and CO estimated in the domain are provided in Table 5.1.
- The results for uniform and non-uniform meshes are compared, revealing that the non-uniform grid produces CO about $\mathcal{O}(N^{\alpha-2})$, confirming the theoretical findings.
- Table 5.2 shows the maximum norm error and CO in space for Ex. 5.4.1 when $N = 5000$ is fixed and $h = 1/M$ is varied.

			Uniform		**Non-Uniform**	
α	β	N	$\|\|w\|\|_{H(\chi_{h\tau})}$	CO	$\|\|w\|\|_{H(\chi_{h\tau})}$	CO
0.3	0.3	40	2.23e-02	-	7.7439e-04	-
		80	1.93e-02	0.2133	2.7586e-04	1.4891
		160	1.69e-02	0.1885	9.3904e-05	1.5547
		320	1.49e-02	0.1779	3.1225e-05	1.5885
0.5	0.5	40	1.85e-02	-	1.3000e-03	-
		80	1.43e-02	0.3787	5.4202e-04	1.2866
		160	1.10e-02	0.3761	2.1228e-04	1.3524
		320	8.40e-03	0.3818	8.0175e-05	1.4047
0.9	0.9	40	6.0000e-03	-	4.0000e-03	-
		80	3.1000e-03	0.9324	2.0000e-03	1.0045
		160	1.6000e-03	0.9597	9.7184e-04	1.0315
		320	8.2134e-04	0.9664	4.6964e-04	1.0492

TABLE 5.1: For $h = 1/1000$, CO and maximum norm error calculated in the domain for Ex. 5.4.1 .

Table 2

α	β	h	$\max_{0\le n\le N} \|\|w^n\|\|_0$	CO in $\|\|\cdot\|\|_0$	$\|\|w\|\|_{H(\chi_{h\tau})}$	CO in $\|\|\cdot\|\|_{H(\chi_{h\tau})}$
0.3	0.3	1/10	1.5000e-03	-	2.1000e-03	-
		1/20	3.7356e-04	2.0030	5.2828e-04	2.0030
		1/40	9.3540e-05	1.9977	1.3229e-04	1.9977
0.5	0.5	1/10	9.0001e-04	-	1.3000e-03	-
		1/20	2.2424e-04	2.0049	3.1712e-04	2.0048
		1/40	5.5856e-05	2.0052	7.9006e-05	2.0050
0.9	0.9	1/10	4.0138e-04	-	5.6910e-04	-
		1/20	9.5084e-05	2.0777	1.3532e-04	2.0723
		1/40	2.0064e-05	2.2446	2.8843e-05	2.2301

TABLE 5.2: For $N = 5000$, L_2-norm, maximum norm error and CO in space calculated in the domain.

5.5 Conclusion

A scheme for a generalized diffusion problem with a non-smooth solution and Robin boundary conditions is presented in this chapter. The major goal of this study is to demonstrate that a non-uniform mesh is needed to handle the singularity in the derivative of a solution at $t = 0$. It is clear that a non-uniform grid achieves significantly better outcome than a uniform mesh. For the non-smooth solution with respect to the L_2-norm, the stability and CO of $\mathcal{O}(N^{\alpha-2})$ has been devised. A second order of convergence has been developed in the spatial direction. Theoretical results are validated by numerical test example.

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