θ schemes for finite element discretization of the space-time fractional diffusion equations

Qingguang Guan Advisor: Max Gunzburger

Florida State University

Abstract

The numerical solution of a space-time fractional diffusion equation used to model the anomalous diffusion is considered. Spatial discretization is effected using a finite element method whereas the θ-scheme is used for temporal discretization. The fully discrete scheme is analyzed for all $0 \le \theta \le 1$ to determine conditional and unconditional stability regimes for the scheme and also to obtain error estimates for the approximate solution. The analysis is facilitated by making use of a variational formulation of the equations that is based on a recently developed nonlocal calculus. One-dimensional numerical examples are provided that illustrate the theoretical stability and convergence results.

Introduction

Space-time fractional diffusion equations are used as models for anomalous transport in many disciplines such as hydrogeology, biology, etc. For flow in porous media, the space fractional derivative comes from particles having large movements through fractures in the media, and time fractional derivative comes from particles remaining stationary for long time. In this paper, we consider the space-time fractional diffusion equation

$$\begin{aligned} &\frac{\partial^\alpha u}{\partial t^\alpha} = -c^2\mathcal{L}u + f(x,t), \quad x \in \Omega_I \\ &u(x,t) = 0, \ x \in \Omega_B, \quad t \in [0,T] \\ &u(x,0) = u_0(x), \quad x \in \Omega_I, \end{aligned} \tag{1}$$

where $\mathcal{L}$ denotes the space-fractional operator

$$\mathcal{L}u = \int_{B(x,\delta)} \frac{u(x,t)-u(y,t)}{|x-y|^{d+2s}}\,\mathrm{d}y, \quad 0<s<1,$$

where $\delta > 0$, and where $\Omega_I \subset \mathbb{R}^d$ is a convex open bounded subset with piecewise smooth boundary, $\Omega = \{x \in \mathbb{R}^d \,|\, d(x,\Omega_I) \le \delta\}$, $\Omega_B = \Omega/\Omega_I$, and $Q = \Omega_I \times (0,T]$.
There are several definitions available for time-fractional derivatives, we use the Caputo fractional derivative of order α defined by

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial u(x,\eta)}{\partial \eta}\frac{\mathrm{d}\eta}{(t-\eta)^\alpha}, \quad 0<\alpha<1, \tag{2}$$

where $\Gamma(\cdot)$ denotes the gamma function. Letting $\Delta t = T/N$, $t_n = n\Delta t$ for $n = 0,1,\dots,N$, and $D_t u(x,t_n) = u(x,t_{n+1}) - u(x,t_n)$, an approximation to the factional derivative is given by

$$\begin{aligned} \frac{\partial^\alpha u(x,t_{n+1})}{\partial t^\alpha} &= \frac{1}{\Gamma(1-\alpha)}\sum_{i=0}^{n}\int_{t_i}^{t_{i+1}} (t_{n+1}-\eta)^{-\alpha}\frac{\partial u(x,\eta)}{\partial\eta}\mathrm{d}\eta \\ &\approx \frac{1}{\Gamma(1-\alpha)}\sum_{i=0}^{n}\frac{D_t u(x,t_i)}{\Delta t}\int_{t_i}^{t_{i+1}}(t_{n+1}-\eta)^{-\alpha}\mathrm{d}\eta + O(\Delta t) \\ &= \frac{\Delta t^{-\alpha}}{\Gamma(2-\alpha)}\sum_{i=0}^{n} b_i D_t u(x,t_{n-i}) + O(\Delta t), \end{aligned} \tag{3}$$

where $b_i = (i+1)^{1-\alpha} - i^{1-\alpha}$ for $i = 0,1,\cdots,n$.
Here, we provide a stability analysis of fully discrete approximations of (1) for which θ schemes and finite element methods are used for temporal and spatial discretizations, respectively. If $\theta = 0$, the θ scheme becomes an explicit scheme. Additionally, we provide convergence analyses. In contrast with the classical diffusion equation, we see from (3) that $u(x,t_{n+1})$ not only depends on $u(x,t_n)$, but also depends on all former $u(x,t_i)$, $i = 0,\cdots,n-1$. This poses some difficulties in obtaining stability results. However, for implicit schemes, using the classical method described in [1] does allow us to obtain the unconditional stability result. However, that approach is not useful for θ schemes. Instead, using the matrix analysis given in [2], we develop a new method to solve the stability problem.

Stability of the θ schemes

We subdivide the spatial domain Ω_I by a quasi-uniform triangulation $\mathcal{T}_h$ and use the corresponding continuous piecewise-linear finite element

$$V_h := \{v_h \in C^0(\Omega), \ \ v_h|_{\Omega_B} = 0, \ \text{ and } \ v_h|_\tau \in P_1 \ \forall\, \tau \in \mathcal{T}_h\}.$$

Then, with $\{\phi_j\}_{j=1}^J$ denoting the usual linear basis function for V_h, we have the approximations

$$u_h(t,x) = \sum_{j=1}^{J} u_j(t)\phi_j(x) \quad \text{and} \quad u_h^n = \sum_{j=1}^{J} u_j(t_n)\phi_j(x).$$

Let $\beta = c^2\Gamma(2-\alpha)$ and

$$u_h^{n+\theta} = \theta u_h^{n+1} + (1-\theta)u_h^n, \quad 0 \le \theta \le 1.$$

Then, using (3), we define the full space-time discretization of (1) by

$$\Big(\sum_{i=0}^{n} b_i D_t u_h^{n-i}, v_h\Big) = -\beta\Delta t^\alpha a(u_h^{n+\theta}, v_h) + \Gamma(2-\alpha)\Delta t^\alpha (f^{n+\theta}, v_h) \tag{4}$$

for all $v_h \in V_h$ and for $n = 0,\dots,N-1$ along with the initial condition approximation

$$a(u_h^0, v_h) = a(u_0, v_h),$$

where letting

$$\gamma(x,y) = \begin{cases} \dfrac{1}{|y-x|^{d+2s}}, & |y-x| \le \delta \\ 0, & |y-x| > \delta, \end{cases}$$

the bilinear form

$$a(u,v) = \frac{1}{2}\int_\Omega\int_\Omega \gamma(x,y)(u(x)-u(y))(v(x)-v(y))\mathrm{d}y\mathrm{d}x.$$

and $f^{n+\theta} = \theta f(t_{n+1},x) + (1-\theta)f(t_n,x)$.
In the sequel, we denote the L^2 norm by $\|\cdot\|$. Also, $\mathbb{M}$ and $\mathbb{K}$ denote the symmetric, positive definite mass and stiffness matrices associated with (4), i.e., we have that $\mathbb{M}_{jj'} = (\phi_j, \phi_{j'})$ and $\mathbb{K}_{jj'} = a(\phi_j, \phi_{j'})$ for $j, j' = 1,\dots,J$. The eigenvalues of $\mathbb{M}$ and $\mathbb{K}$ can be evaluated by Gershgorin circle theorem. We then have the following stability result.

Theorem 1. *The scheme* (4) *is unconditionally stable for $\theta \ge 1/(2-b_1)$. For $\theta < 1/(2-b_1)$, it is stable if*

$$\Delta t^\alpha \le \frac{2-2b_1}{1-(2-b_1)\theta}\cdot\frac{1}{\beta}\cdot\frac{\lambda_{\min}(\mathbb{M})}{\lambda_{\max}(\mathbb{K})},$$

where $b_1 = 2^{1-\alpha} - 1$ and $\beta = c^2\Gamma(2-\alpha)$.

Remark 1. *As in* [4], *for the one-dimensional case and a sufficiently small uniform mesh size h, we have the stability condition for the explicit scheme $\theta = 0$ given by $\Delta t^\alpha / h^{2s} = O(1)$.*

Convergence of the θ schemes

Here we use a variant of the discrete θ scheme (see (4)) given by

$$\left(\frac{\Delta t^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{i=0}^{n} b_i \frac{D_t u_h^{n-i}}{\Delta t}, v_h\right) = -c^2 a(u_h^{n+\theta}, v_h) + (f^{n+1}, v_h) \tag{5}$$

for $n = 0,\dots,N-1$; note that we have merely replaced $f^{n+\theta}$ in (4) by f^{n+1}. Also, recall that $u(x,t_n)$ denotes the solution of (1) evaluated at $t = t_n$, we have the following convergence result.

Theorem 2. *Assume that u is sufficiently smooth and, if Δt satisfies the stability conditions in Theorem 1. Then,*

$$\max_{1\le n\le N}\|u(\cdot,t_n) - u_h(\cdot,t_n)\| \le C(\Delta t + h^2),$$

where $C > 0$ does not depend on Δt or h.

Remark 2. *For $\theta = 1$, as in* [3], *we obtain*

$$\max_{1\le n\le N}\|u(\cdot,t_n) - u_h(\cdot,t_n)\| \le C(\Delta t^{2-\alpha} + h^2),$$

where C does not depend on Δt or h.

Remark 3. *The stability and convergence analysis given above can also be applied to the time-fractional diffusion equation*

$$\frac{\partial^\alpha u}{\partial t^\alpha} = -c^2\Delta u + f(x,t). \tag{6}$$

In particular, we obtain the stability result for $0 \le \theta < 1$ that, to our knowledge, has not previously been given in the literature.

Numerical Results in 1-D

Take equation (6) as an example, where $u(x,t) = t^2(-x^4 + x^3)$, $c^2 = 1$ using scheme (5), we have
a) Errors and convergence rates at the final time $T = 1$ for the model parameters $h = 1/17$ and $\theta = 0$

α	Δt	L^2 error	Δt	L^2 error	Prediction Δt
0.9	1/3900	6.2221e-05	1/3800	5.9529e+22	1/3968
0.99	1/1820	9.9938e-05	1/1800	6.2537e+05	1/1825
0.999	1/1700	1.0501e-04	1/1690	2.6022e+08	1/1704

b) Errors and convergence rates at the final time $T = 1$ for the model parameters $\alpha = 0.6$ and $\theta = 1$

h	Δt	L_2 norm error	rate
1/512	1/4	3.7920e-04	-
1/512	1/8	1.4732e-04	1.3640
1/512	1/16	5.6714e-05	1.3772
1/512	1/32	2.1721e-05	1.3846
1/512	1/64	8.3000e-06	1.3879

References

[1] E. Süli, Lecture Notes on Finite Element. Methods for Partial Differential. Equations. Mathematical Institute. University of Oxford. 2012

[2] L. Zhu and Q. Du, Mesh dependent stability and condition number estimates for finite element approximations of parabolic problems, Mathematics of Computation. **83** (2014), 37–64.

[3] Y. Jiang and J. Ma, High-order finite element methods for time-fractional partial differential equations, Journal of Computational and Applied Mathematics. **235** (2011), 3285–3290.

[4] Q. Guan and M. Gunzburger, Stability and convergence of time-stepping methods for a nonlocal model for diffusion, to appear in DCDS-B.