Numerical Analysis for Time-Fractional Evolution Equations

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Outline

Problem Formulation

Initial-boundary value problem: $0 < \alpha < 1$, for $u(x,t)$ for $T \ge t > 0$:

$$\begin{aligned} \partial_t^\alpha u - \Delta u &= f, \quad \text{in } \Omega \quad && T \ge t > 0, \\ u &= 0, \quad \text{on } \partial\Omega \quad && T \ge t > 0, \\ u(0) &= v, \quad \text{in } \Omega. && \end{aligned} \tag{1}$$

Ω: a bounded and convex polygonal domain in $\mathbb{R}^d$ ($d = 1, 2, 3$).
∂_t^α: the left-sided Caputo fractional derivative of order α

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} \frac{d}{d\tau} u(\tau)\, d\tau.$$

The model equation (1) is known to capture well the dynamics of anomalous diffusion known as sub-diffusion.

Background

Standard (local) diffusion ($\alpha = 1$):
mean squared displacement of a particle is proportional to time, i.e., $\sigma_r^2 \propto t$.

Anomalous diffusion $\alpha \in (0, 1)$ or $(1, 2)$: $\sigma_r^2 \propto t^\alpha$

- $\alpha < 1$, sub-diffusion;
- $\alpha > 1$, super-diffusion.

Anomalous diffusion was found in several systems including

- ultra-cold atoms [16],
- single particle movements in cytoplasm [15],
- material with thermal memory [19],
- heartbeat intervals and DNA sequences [1],
- ...

Motivation

Goal:

- efficient numerical schemes (robust w.r.t weak data)
- theoretically verify the approximation

Challenge: limited smoothing properties in both time and space

Example:

$\partial_t^\alpha u(t) + \lambda u(t) = 0$, $\alpha \in (0,1)$, $\lambda > 0$ and $u(0) = 1$.

Solution:

$$u(t) = E_{\alpha,1}(-\lambda t^\alpha) = \sum_{k=0}^{\infty} \frac{(-1)^k \lambda^k t^{\alpha k}}{\Gamma(\alpha k + 1)} = 1 - \lambda t^\alpha / \Gamma(\alpha + 1) + O(t^{2\alpha}).$$

$\alpha = 1$: solution $u(t) = E_{1,1}(-\lambda t) = e^{-\lambda t}$.

Motivation

Moreover, the Mittag-Leffler function decays linearly :

$$|E_{\alpha,1}(-\lambda t^\alpha)| \le \frac{c}{1+\lambda t^\alpha}$$

Therefore, for any $\lambda > 0$ and fixed $t > 0$

$$|\lambda E_{\alpha,1}(-\lambda t^\alpha)| \le \frac{c\lambda}{1+\lambda t^\alpha} \le ct^{-\alpha}.$$

Standard diffusion ($\alpha = 1$)

$$|\lambda^m e^{-\lambda t}| \le t^{-m}|(\lambda t)^m e^{-\lambda t}| \le ct^{-m}.$$

Solution Representation

Go back to the FPDE:

$\{\lambda_j, \varphi_j\}$: eigenpairs of $-\Delta$ with homog. Dirichlet boundary condition.

Solution representation:

$$u(t) = E(t)v + \int_0^t \widetilde{E}(t-s)f(s)ds,$$

where operators $E(t)$ and $\widetilde{E}(t)$ are defined by

$$E(t)v = \sum_{j=1}^{\infty} E_{\alpha,1}(-\lambda_j t^\alpha)(v, \varphi_j)\varphi_j,$$

$$\widetilde{E}(t)v = \sum_{j=1}^{\infty} t^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j t^\alpha)(v, \varphi_j)\varphi_j.$$

Regularity

Fractional diffusion: ($f \equiv 0, \quad v \neq 0$):

$$\|(\partial_t^\alpha)^\ell u(t)\|_{\dot H^p(\Omega)} \le C t^{-\alpha(\ell + \frac{p-q}{2})} \|v\|_{\dot H^q(\Omega)},$$

where for $\ell = 0$, $q \le p$ and $0 \le p - q \le 2$ and for $\ell = 1$, $p \le q \le p + 2$.

Spatial regularity restriction (order 2)!!!

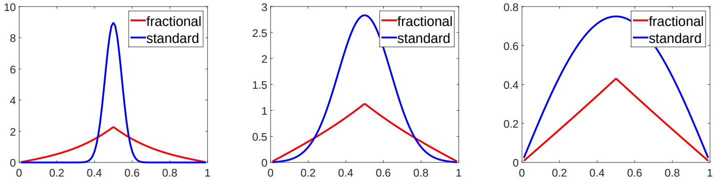
Standard diffusion: ($f \equiv 0, \quad v \neq 0$):

$$\|(\partial_t)^\ell u(t)\|_{\dot H^p(\Omega)} \le C t^{-(\ell + \frac{p-q}{2})} \|v\|_{\dot H^q(\Omega)}, \quad 0 \le q \le p, \ \ \ell \ge 0$$

Solution behavior

1-D example: $\partial_t^\alpha u - u_{xx} = 0$, $v(x) = \delta_{1/2}(x) \in \dot{H}^{-1/2-\epsilon}(\Omega)$

Plot of $u(t)$ at $t = 10^{-1}$, 10^{-2} and 10^{-3};



(a) $t = 10^{-3}$ (b) $t = 10^{-2}$ (c) $t = 10^{-1}$

$\alpha \in (0,1)$: continuous and piecewise smooth for all $t > 0$

$\alpha = 1$: infinitely differentiable for all $t > 0$

Outline

Galerkin FE Approx.

$\{\mathcal{T}_h\}_{0<h<1}$: family of regular partitions of Ω into d-simplexes.

$$X_h = \left\{\chi \in H_0^1(\Omega) : \ \chi \ \text{ is a linear function over } \ \tau, \ \ \forall \tau \in \mathcal{T}_h\right\}.$$

The semidiscrete Galerkin FEM: find $u_h(t) \in X_h$ such that

$$\begin{aligned} (\partial_t^\alpha u_h, \chi) + (\nabla u_h, \nabla \chi) &= (f, \chi), \quad \forall \chi \in X_h, \ T \geq t > 0, \\ u_h(0) &= v_h, \end{aligned} \tag{2}$$

where $v_h \in X_h$ is a given approximation of the initial data v. The choice of v_h will depend on the smoothness of the initial data v.

By defining $\Delta_h : X_h \to X_h$ s.t. $(\Delta_h \psi, \chi) = (\nabla \psi, \nabla \chi) \quad \forall \psi, \chi \in X_h$
Then we write the spatially discrete problem (2) as

$$\partial_t^\alpha u_h(t) - \Delta_h u_h(t) = f_h(t) \quad \text{for} \quad t \geq 0 \quad \text{with} \quad u_h(0) = v_h. \tag{3}$$

State of the Art: Available Numerical Methods and Tools

$$\partial_t u - \Delta u = 0, \quad \text{in } \Omega \quad u = 0 \ \text{ on } \partial\Omega \quad u(x,0) = v(x) \ \text{ in } \Omega. \tag{4}$$

Optimal estimates (see, monograph of Vidar Thomée [18]):

For smooth initial data, for $t \geq 0$:

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} + h\|\nabla(u_h(t) - u(t))\|_{L^2(\Omega)} \leq Ch^2\|v\|_{H^2(\Omega)}, \tag{5}$$

nonsmooth data, i.e. $v \in L^2(\Omega)$, for $t > 0$:

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} + h\|\nabla(u_h(t) - u(t))\|_{L^2(\Omega)} \leq Ch^2 t^{-1}\|v\|_{L^2(\Omega)}. \tag{6}$$

Our Main Results

In case of **smooth** initial data, $v \in H^2(\Omega) \cap H_0^1(\Omega)$, $t \geq 0$

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} + h\|\nabla(u_h(t) - u(t))\|_{L^2(\Omega)} \leq Ch^2\|v\|_{H^2(\Omega)},$$

In case of **nonsmooth** data, $v \in L^2(\Omega)$: for quasi-uniform meshes and $\ell_h = |\ln h|$, $t > 0$

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} + h\|\nabla(u_h(t) - u(t))\|_{L^2(\Omega)} \leq Ch^2\ell_h t^{-\alpha}\|v\|_{L^2(\Omega)}.$$

Error estimates for semidiscrete schemes

These estimates follows from a novel argument which utilizes

- Duhamel's principle of the model.
- solution regularity pickup from $\dot{H}^s(\Omega)$ to $\dot{H}^{s+2}(\Omega)$.
- properties L^2-projection, inverse inequality...

The argument is powerful and can be extended to

- lumped mass FEM. However, the optimal estimate in case of $v \in L^2(\Omega)$ requires some restrictions on meshes
- weaker data $v \in \dot{H}^q(\Omega)$ with $q \in (-1, 0)$
- inhomogeneous source data $f \in L^\infty(0, T; \dot{H}^q(\Omega))$, $q \in (-1, 0]$
- multi-term model, distributed-order model, diffusion-wave...

Error estimates for semidiscrete schemes

As an example, we consider the multi-term fractional diffusion model:

$$\partial_t^{\alpha} + \sum_{i=1}^{m} b_i \partial_t^{\alpha_i} u - \Delta u = f, \quad \text{in } \Omega, \quad u = 0 \;\text{ on } \partial\Omega, \quad u(x,0) = v(x) \;\text{ in } \Omega. \quad (7)$$

where $0 < \alpha_m \leq ... \leq \alpha_1 < \alpha < 1$ and $b_i > 0$, $i = 1, 2, ..., m$.

The solution operator involves multinomial Mittag-Leffler function.

$v \in L^2(\Omega)$, $f \equiv 0$: for quasi-uniform meshes and $\ell_h = |\ln h|$, $t > 0$

$$\|u_h(t) - u(t)\|_{L^2(\Omega)} + h\|\nabla(u_h(t) - u(t))\|_{L^2(\Omega)} \leq Ch^2 \ell_h t^{-\alpha} \|v\|_{L^2(\Omega)}.$$

Numerical experiments

(a) Smooth initial data: $v(x) = x(1-x) \in H^2(\Omega) \cap H_0^1(\Omega)$

(b) Nonsmooth initial data: $v(x) = \chi_{[0,\frac{1}{2}]}$.

Table: Standard Galerkin FEM for nonsmooth initial data, example (b) with $\alpha = 0.5$.

t	h	1/16	1/32	1/64	1/128	rate
0.005	L^2	2.13e-3	5.33e-4	1.33e-4	3.33e-5	$\approx$ 2.01 (2.00)
	H^1	1.24e-2	6.18e-2	3.09e-2	1.54e-2	$\approx$ 1.01 (1.00)
0.01	L^2	1.63e-3	4.06e-4	1.02e-4	2.54e-5	$\approx$ 2.00 (2.00)
	H^1	9.20e-2	4.60e-2	2.30e-2	1.15e-2	$\approx$ 1.00 (1.00)
1	L^2	2.00e-4	5.00e-5	1.25e-5	3.13e-6	$\approx$ 2.00 (2.00)
	H^1	1.03e-2	5.13e-3	2.56e-3	1.28e-3	$\approx$ 1.00 (1.00)

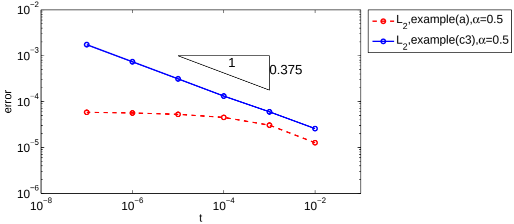
The scheme is robust for small t and nonsmooth data.

Numerical experiments

$$\text{interpolation} \Rightarrow \|(u-u_h)(t)\|_{L^2(\Omega)} \le ch^2 t^{-\alpha\left(1-\frac{q}{2}\right)} \|v\|_{\dot H^q(\Omega)}.$$

Table: L^2-error with $\alpha = 0.5$ and $h = 2^{-7}$ for $t \to 0$ for (a) and (b), initial data.

t	1e-3	1e-4	1e-5	1e-6	1e-7	order
(a)	3.07e-5	4.53e-5	5.28e-5	5.65e-5	5.85e-5	≈ -0.02
(b)	6.00e-5	1.32e-4	3.13e-4	7.39e-4	1.74e-3	≈ -0.37



Outline

L1 scheme: derivation of the scheme

The L1 scheme was first mentioned by Oldham and Spanier [14].

Consider uniform grid on $[0, T]$: $0 = t_0 < t_1 < \ldots < t_N = T$ and $t_n = n\tau$,

$$
\begin{aligned}
\partial_t^\alpha u(x, t_n) &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \int_{t_j}^{t_{j+1}} \frac{\partial u(x, s)}{\partial s} (t_n - s)^{-\alpha}\, ds \\
&\approx \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{n-1} \frac{u(x, t_{j+1}) - u(x, t_j)}{\tau} \int_{t_j}^{t_{j+1}} (t_n - s)^{-\alpha} ds \\
&= \tau^{-\alpha}[b_0 u(x, t_n) - b_n u(x, t_0) + \sum_{j=1}^{n} (b_j - b_{j-1}) u(x, t_{n-j})] =: L_1^n(u).
\end{aligned}
$$

where the weights b_j are given by

$$
b_j = ((j+1)^{1-\alpha} - j^{1-\alpha})/\Gamma(2-\alpha),\ j = 0, 1, \ldots, n-1.
$$

L1 scheme

local truncation error: $O(\tau^{2-\alpha})$, provided that $u \in C^2([0,T], \dot{H}^2(\Omega))$.

However, it fails to achieve this desired uniform convergence rate.

$\partial_t^\alpha u(t) + u(t) = 0$, $\alpha \in (0,1)$, and $u(0) = 1$. $u(t) = E_{\alpha,1}(-t^\alpha)$

The L1 scheme:

$$L_1^n(U) + U^n = 0, \quad \text{with} \;\; U^0 = 0.$$

at the first step:

$$U^1 = (1 + \Gamma(2-\alpha)\tau^\alpha)^{-1} = 1 + \sum_{n=1}^{\infty} (-1)^n (\Gamma(2-\alpha)\tau^\alpha)^n.$$

The difference between U^1 and $u(\tau)$:

$$u(\tau) - U^1 = (\Gamma(2-\alpha) - \Gamma(\alpha+1)^{-1})\tau^\alpha + c_\tau \tau^{2\alpha},$$

with $c_\tau = \sum_{n=2}^{\infty} (-1)^n (\Gamma(n\alpha+1)^{-1} - \Gamma(2-\alpha)^n)\tau^{(n-2)\alpha}$.

L1 scheme

The initial singularity even pollutes the approximation error for large t.

Numerical experiment: $\partial_t^\alpha u + u = 0$, $u(0) = 1$.

Table: $|e^N = U^N - u(t_N)|$, pointwise error at $T = t_N = 1$

$\alpha \backslash N$	10	20	40	80	160	order
0.25	3.41e-3	1.65e-3	8.09e-4	3.97e-4	1.94e-4	$\approx$ 1.04
0.5	7.87e-3	3.75e-3	1.81e-3	8.81e-4	4.27e-4	$\approx$ 1.05
0.75	1.43e-2	6.92e-3	3.36e-3	1.63e-3	7.85e-4	$\approx$ 1.05

Pointwise error is of order $O(\tau)$.

L1 scheme

Mathematical Understanding: consider $w := u - u(0) = u - 1$

$$\partial_t^\alpha w + w = -1, \quad w(0) = 0.$$

Applying Laplace transform:

$$z^\alpha \widehat{w}(z) + \widehat{w}(z) = -z^{-1} \to \widehat{w}(z) = -z^{-1}(z^\alpha + 1)^{-1}.$$

Then the inverse Laplace transform gives

$$w(t) = -\frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt} z^{-1}(z^\alpha + 1)^{-1} dz$$

Here the contour $\Gamma_{\theta,\delta}$ is given by

$$\Gamma_{\theta,\delta} = \{z \in \mathbb{C} : |z| = \delta, |\arg z| \le \theta\} \cup \{z \in \mathbb{C} : z = \rho e^{\pm i\theta}, \rho \ge \delta\}.$$

L1 scheme

Representation for $W^n = U^n - U^0$:

$$L_1^n(W) + W^n = -1, \quad W^0 = 0.$$

Next multiplying both sides of the equation by ξ^n

$$L_1^n(W)\xi^n + W^n\xi^n = -\xi^n.$$

summing from 1 to ∞

$$\sum_{n=1}^{\infty} L_1^n(W)\xi^n + \widetilde{W}(\xi) = -\frac{\xi}{1-\xi}.$$

where

$$\widetilde{W}(\xi) = \sum_{j=0}^{\infty} W^n\xi^n$$

is called the generating function of W^n.

L1 scheme

Moreover, we have

$$\sum_{n=1}^{\infty} L_1^n(W)\xi^n = \frac{(1-\xi)^2 \mathrm{Li}_{\alpha-1}(\xi)}{\xi\Gamma(2-\alpha)\tau^\alpha}\widetilde{W}(\xi).$$

with the polylogarithm function: $\mathrm{Li}_p(z) = \sum_{j=1}^\infty z^j/j^p$. ($z = 1 \Rightarrow$ Riemann zeta)

$$\widetilde{W}(\xi) = -\frac{\xi}{1-\xi}\left(\frac{(1-\xi)^2}{\xi\tau^\alpha\Gamma(2-\alpha)}\mathrm{Li}_{\alpha-1}(\xi)+1\right)^{-1}.$$

Cauchy theorem implies that for ϱ small enough, there holds

$$W^n = -\frac{1}{2\pi\mathrm{i}}\int_{|\xi|=\varrho}\frac{1}{(1-\xi)\xi^n}\left(\frac{(1-\xi)^2}{\xi\tau^\alpha\Gamma(2-\alpha)}\mathrm{Li}_{\alpha-1}(\xi)+1\right)^{-1}\,d\xi.$$

L1 scheme

Upon changing variable $\xi = e^{-z\tau}$

$$W^n = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma^0} e^{zt_n} \frac{\tau e^{-z\tau}}{1 - e^{-z\tau}} \left(\frac{(1 - e^{-z\tau})^2}{e^{-z\tau}\tau^\alpha \Gamma(2-\alpha)} \mathrm{Li}_{\alpha-1}(e^{-z\tau}) + 1 \right)^{-1} dz,$$

with $\Gamma^0 := \{z = -\ln(\varrho)/\tau + \mathrm{i}y : |y| \le \pi/\tau\}$.

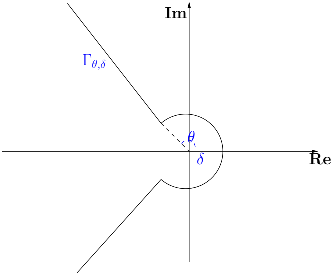
By deforming the contour Γ^0 to $\Gamma_\tau := \{z \in \Gamma_{\theta,\delta} : |\Im(z)| \le \pi/\tau\}$ and using the periodicity of the exponential function

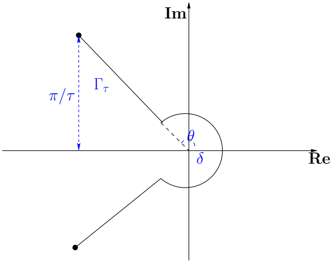
$$W^n = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_\tau} e^{zt_n} \frac{\tau e^{-z\tau}}{1 - e^{-z\tau}} \left(\frac{(1 - e^{-z\tau})^2}{e^{-z\tau}\tau^\alpha \Gamma(2-\alpha)} \mathrm{Li}_{\alpha-1}(e^{-z\tau}) + 1 \right)^{-1} dz,$$

L1 scheme

$$w(t_n) = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt_n} z^{-1} (z^\alpha + 1)^{-1} dz$$

$$W^n = -\frac{1}{2\pi \mathrm{i}} \int_{\Gamma_\tau} e^{zt_n} \frac{\tau e^{-z\tau}}{1 - e^{-z\tau}} \left(\frac{(1 - e^{-z\tau})^2}{e^{-z\tau} \tau^\alpha \Gamma(2-\alpha)} \mathrm{Li}_{\alpha-1}(e^{-z\tau}) + 1 \right)^{-1} dz,$$





L1 scheme

- on $\Gamma_{\theta,\delta}\backslash\Gamma_\tau$, $|e^{zt}K(z)| \leq c|z|^{-1}e^{-c|z|t}$, it decays very fast as $|z| \to \infty$;
- let $\chi(z) = \tau^{-1}(e^{z\tau} - 1)$ and $\psi(z) = \frac{e^z - 1}{\Gamma(2-\alpha)}\mathrm{Li}_{\alpha-1}(e^{-z})$. Then on Γ_τ,

$$|z^{-1} - \chi(z)^{-1}| \sim c\tau \qquad \text{and} \qquad |z^\alpha - \frac{1 - e^{-z\tau}}{\tau^\alpha}\psi(z\tau)| \leq c\tau^{2-\alpha}|z|^2.$$

As a result, the best result we can get is $|U^N - u(t_N)| \leq c\tau t_N^{\alpha-1}$.

This argument can be exploited directly to the FPDE with $v \in H^2(\Omega) \cap H_0^1(\Omega)$.

$$\|U^N - u(t_N)\|_{L^2(\Omega)} \leq c\tau t_N^{\alpha-1}\|\Delta v\|_{L^2}.$$

Moreover, for $N = 1$, we have

$$\|U^1 - u(\tau)\|_{L^2(\Omega)} \leq c\tau^\alpha\|\Delta v\|_{L^2}.$$

Convolution Quadrature

The convolution quadrature is developed first by C. Lubich [13, 12].

The idea is to approximate the Riemann-Liouville derivative ${}^R\partial_t^\alpha$

$$ {}^R\partial_t^\alpha \varphi(t) = \frac{d}{dt}\int_0^t \frac{s^{-\alpha}}{\Gamma(1-\alpha)}\varphi(t-s)\,ds, $$

using

$$ {}^R\partial_t^\alpha \varphi(t_n) \approx \sum_{j=0}^{n} \omega_j \varphi(t_n - j\tau) := \bar\partial_\tau^\alpha \varphi(t_n), \quad n \geq 0, \tag{8} $$

where $\{\omega_j\}_{j=0}^\infty$ are determined by $\sum_{j=0}^\infty \omega_j \xi^j = (\delta(\xi)/\tau)^\alpha$.

- $k=1$, $\delta(\xi) = 1-\xi$
- $k=2$, $\delta(\xi) = 3/2 - 2\xi + \xi^2/2$
- $k=3$, $\delta(\xi) = 11/6 - 3\xi + 3/2\xi^2 - 1/3\xi^3$
- $k=4$, $\delta(\xi) = 25/12 - 4\xi + 3\xi^2 - 4/3\xi^3 + 1/4\xi^4$
- $k=5$, $\delta(\xi) = 137/60 - 5\xi + 5\xi^2 - 10/3\xi^3 + 5/4\xi^4 - 1/5\xi^5$
- $k=6$, $\delta(\xi) = 49/20 - 6\xi + 15/2\xi^2 - 20/3\xi^3 + 15/4\xi^4 - 6/5\xi^5 + 1/6\xi^6$

Convolution Quadrature

Go back to the FPDE.

By the relation between the Caputo and R-L fractional derivatives

$$\partial_t^\alpha \varphi(t) := {}^R\partial_t^\alpha \left[\varphi(t) - \sum_{k=0}^{n-1} \frac{\varphi^{(k)}(0)}{k!} t^k \right] \quad \text{for } \ n-1 < \alpha < n.$$

In particular, for subdiffusion ($0 < \alpha < 1$) we have

$$\partial_t^\alpha \varphi = \partial_t^\alpha (\varphi(t) - \varphi(0)) = {}^R\partial_t^\alpha (\varphi(t) - \varphi(0)).$$

The spatial semidiscrete scheme (3) can be rewritten as

$${}^R\partial_t^\alpha (u_h - v_h)(t) - \Delta_h u_h = f_h.$$

Then the fully discrete scheme reads: to find U_h^n such that

$$\bar\partial_\tau^\alpha (U_h^n - v_h) - \Delta_h U_h^n = f_h^n, \quad \text{with } \ U_h^0 = v_h. \tag{9}$$

Convolution Quadrature

Let's start with the second order BDF, i.e., $\delta(\xi) = 3/2 - 2\xi + \xi^2/2$.

Let $W_h^n := U_h^n - U_h^0 = U_h^n - v_h$.

discrete Laplace transform + Cauchy's integral formula:

$$W_h^n = \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_\tau} e^{zt_n} \frac{3e^{-z\tau} - e^{-2z\tau}}{2} (\delta(e^{-z\tau})/\tau)^{-1} \left(\delta(e^{-z\tau})^\alpha/\tau^\alpha - \Delta_h\right)^{-1} \Delta_h v_h \, dz,$$

Recall that:

$$w_h(t_n) = \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt_n} z^{-1} (z^\alpha - \Delta_h)^{-1} \Delta_h v_h dz$$

Observation: $\delta(e^{-z\tau})/\tau$ is a good approximation to z.

Trouble maker: the leading term:

$$\mu(\xi) = \frac{3\xi - \xi^2}{2}. \qquad |\mu(e^{-z\tau}) - 1| \le c\tau|z|.$$

Convolution Quadrature

As a result, the error at t_N satisfies:

$$\|U_h^N - u_h(t_N)\|_{L^2(\Omega)} \le c\tau t_N^{\alpha-1}\|\Delta v\|_{L^2(\Omega)}$$

only first order!!!!

Question: Shall we restore the optimal order by a simple correction?

My answer: Yes. Just by changing the leading polynomial $\mu(\xi)$.

Criterion 1: choose $\mu(\xi)$ such that

$$|\mu(e^{-z\tau}) - 1| \le c\tau^2|z|^2.$$

However, an arbitary choice may break the structure of the scheme...

Convolution Quadrature

Criterion 2: choose the polynomial with the form

$$\mu(\xi) = p(\xi)\left[\frac{\xi}{1-\xi}\delta(\xi)\right].$$

Now the simplest choice is

$$p(\xi) = 3/2 - \xi/2.$$

Then the resulting modified time stepping scheme reads ($f \equiv 0$):

$$\bar\partial_\tau^\alpha (U_h)^1 - \Delta_h U_h^1 - \frac{1}{2}\Delta_h v_h = \bar\partial_\tau^\alpha (v_h)^1,$$
$$\bar\partial_\tau^\alpha (U_h)^n - \Delta_h U_h^n = \bar\partial_\tau^\alpha (v_h)^n, \quad n \geq 2.$$

Hence we restore the second order convergence: [8]

$$\|U_h^n - u_h(t_n)\| \leq c\tau^2 t_n^{\alpha-2}\|\Delta v\|_{L^2(\Omega)}, \quad v \in H^2(\Omega)\cap H_0^1(\Omega)$$
$$\|U_h^n - u_h(t_n)\| \leq c\tau^2 t_n^{-2}\|v\|_{L^2(\Omega)}, \quad v \in L^2(\Omega)$$

Convolution Quadrature

Argument for the nonhomogeneous source problem is quite similar.

Observation: the second order scheme works well for smooth f with $f(0) = 0$.

Hence we consider the splitting:

$$f = f(0) + (f - f(0)) = f(0) + \big(tf'(0) + (t * f'')(t)\big) .$$

Repeating the similar argument, we obtain the modified scheme:

$$\begin{aligned} \bar\partial_\tau^\alpha (U_h)^1 - \Delta_h U_h^1 - \frac{1}{2}\Delta_h v_h &= \bar\partial_\tau^\alpha (v_h)^1 + \frac{1}{2}F_h^0 + F_h^n, \\ \bar\partial_\tau^\alpha (U_h)^n - \Delta_h U_h^n &= \bar\partial_\tau^\alpha (v_h)^n + F_h^n, \quad n \geq 2. \end{aligned}$$

Suppose $v \equiv 0$, then we have the error estimate

$$\begin{aligned} \|U_h^n - u_h(t_n)\| \leq c\tau^2 t_n^{\alpha-2} \|f(0)\|_{L^2(\Omega)} &+ c\tau^2 t_n^{\alpha-1} \|f'(0)\|_{L^2(\Omega)} \\ &+ c\tau^2 \int_0^t (t_n - s)^{\alpha-1} \|f''(t)\|_{L^2(\Omega)}\, dt. \end{aligned}$$

Convolution Quadrature

This argument may help to reinstate other high order schemes.

e.g., we can extend the above argument to CQ with $k = 3, ..., 6$.

Advantage:

- keep the structure of the original schemes, only change the starting $k - 1$ steps for a k-th order scheme;
- restore k-th order, robust w.r.t. the nonsmooth data.

Numerical experiments

Consider the problem with $f \equiv 0$ and the nonsmooth initial data:

- $\Omega = (0,1)$, and $v = x^{-1/4} \in H^{1/4-\epsilon}(\Omega)$, with $\epsilon \in (0, 1/4)$.

Table: The L^2-norm of the error $\|U^N - u(t_N)\|_{L^2(\Omega)}$ at $t_N = 1$, computed the fully discrete scheme without initial correction, $h = 1/100$.

α	N	50	100	200	400	rate
	BDF2	5.01e-3	2.50e-3	1.26e-3	6.20e-4	$\approx$ 1.00
	BDF3	4.98e-3	2.48e-3	1.24e-3	6.19e-4	$\approx$ 1.00
	BDF4	4.97e-3	2.48e-3	1.24e-3	6.19e-4	$\approx$ 1.00
0.5	BDF5	4.97e-3	2.48e-3	1.24e-3	6.19e-4	$\approx$ 1.00
	BDF6	4.94e-3	2.48e-3	1.24e-3	6.19e-4	$\approx$ 1.00
	L1	5.10e-3	2.52e-3	1.25e-3	6.24e-4	$\approx$ 1.04

Numerical experiments

Table: The L^2-norm of the error $\|U^N - u(t_N)\|_{L^2(\Omega)}$ at $t_N = 1$, computed the fully discrete scheme with initial correction, $h = 1/100$.

α	$k\backslash N$	100	200	400	800	rate
0.25	2	1.40e-5	3.47e-6	8.64e-7	2.16e-7	$\approx$ 2.00 (2.00)
	3	2.76e-7	3.39e-8	4.20e-9	5.23e-10	$\approx$ 3.01 (3.00)
	4	8.34e-9	5.04e-10	3.10e-11	1.92e-12	$\approx$ 4.02 (4.00)
	5	3.41e-10	1.01e-11	3.07e-13	9.46e-15	$\approx$ 5.03 (5.00)
	6	1.60e-9	2.55e-13	3.82e-15	5.83e-17	$\approx$ 6.04 (6.00)
0.75	2	1.18e-4	2.93e-5	7.30e-6	1.82e-6	$\approx$ 2.00 (2.00)
	3	3.04e-6	3.72e-7	4.59e-8	5.71e-9	$\approx$ 3.01 (3.00)
	4	1.11e-7	6.68e-9	4.09e-10	2.53e-11	$\approx$ 4.02 (4.00)
	5	5.29e-9	1.55e-10	4.70e-12	1.45e-13	$\approx$ 5.03 (5.00)
	6	3.01e-7	4.53e-12	6.60e-14	1.00e-15	$\approx$ 6.07 (6.00)

Numerical experiments

Consider the problem with $v \equiv 0$ and the nonhomogeneous source term:

- $\Omega = (0, 1)$, and $f(x, t) = \cos(t)(1 + \chi_{(0,1/2)}(x))$.

Table: The L^2-norm of the error $\|U^N - u(t_N)\|_{L^2(\Omega)}/\|u(t_N)\|_{L^2(\Omega)}$ at $t_N = 1$, computed the fully discrete scheme without initial correction, $h = 1/100$.

α	N	100	200	400	800	rate
	BDF2	2.57e-4	1.29e-4	6.45e-5	3.22e-5	≈ 1.00
	BDF3	2.59e-4	1.29e-4	6.45e-5	3.23e-5	≈ 1.00
	BDF4	2.59e-4	1.29e-4	6.45e-5	3.23e-5	≈ 1.00
0.5	BDF5	2.59e-4	1.29e-4	6.45e-5	3.23e-5	≈ 1.00
	BDF6	2.59e-4	1.29e-4	6.45e-5	3.23e-5	≈ 1.00
	L1	2.86e-4	1.39e-4	6.80e-5	3.35e-5	≈ 1.02
	L1-2	1.80e-4	8.76e-4	4.25e-5	2.07e-5	≈ 1.04

Numerical experiments

Table: The L^2-norm of the error $\|U^N - u(t_N)\|_{L^2(\Omega)}$ at $t_N = 1$, computed the fully discrete scheme with initial correction, $h = 1/100$.

α	$k\backslash N$	100	200	400	800	rate
0.25	2	1.65e-6	4.10e-7	1.02e-7	2.55e-8	$\approx$ 2.00 (2.00)
	3	3.20e-8	3.91e-9	4.83e-10	6.00e-11	$\approx$ 3.01 (3.00)
	4	1.25e-9	7.57e-11	4.65e-12	2.88e-13	$\approx$ 4.02 (4.00)
	5	5.11e-11	1.51e-12	4.61e-14	1.42e-15	$\approx$ 5.03 (5.00)
	6	2.40e-10	3.79e-14	5.68e-16	8.67e-18	$\approx$ 6.05 (6.00)
0.75	2	7.47e-6	1.86e-6	4.63e-7	1.16e-7	$\approx$ 2.00 (2.00)
	3	1.31e-7	1.59e-8	1.96e-9	2.43e-10	$\approx$ 3.01 (3.00)
	4	5.72e-9	3.43e-10	2.10e-11	1.30e-12	$\approx$ 4.02 (4.00)
	5	2.81e-10	8.24e-12	2.50e-13	7.68e-15	$\approx$ 5.03 (5.00)
	6	1.61e-8	2.40e-13	3.50e-15	5.33e-17	$\approx$ 6.07 (6.00)

Outline

Extensions and Future works

Some extensions:

(1) modify other schemes, e.g. L1 scheme or Crank-Nicolson;

(2) diffusion-wave: $\alpha \in (1, 2)$;

(3) multi-term: $\partial_t^\alpha u + \sum_{k=1}^m b_m \partial_t^{\beta_k} u - \Delta u = f$;

(4) distributed order: $\partial_t^{[\mu]} u - \Delta u = f$ with $\partial_t^{[\mu]} u = \int_0^1 (\partial_t^\alpha u)\mu(\alpha) d\alpha$;

Future works:

(1) fast algorithm to solve fractional model;

(2) fully discrete schemes with variable time step;

(3) nonlinear problem.

Thank you for your attention !!!

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