Numerical Methods for Time-Fractional Diffusion

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Outline

Joint work with

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goal: robust numerical schemes for subdiff. via Laplace transform

problem setting

consider the initial boundary value problem for time fractional diffusion equation for $u(x,t)$:

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

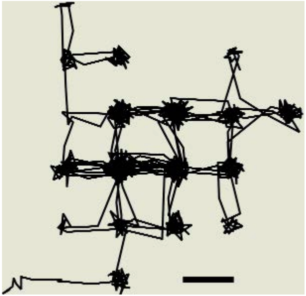
- Ω: bounded, convex polygonal domain in $\mathbb{R}^d$
- ∂_t^α: Caputo fractional derivative of order $\alpha \in (0,1)$ Djrbashian 1960s, Caputo 1967

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u'(s) \mathrm{d}s$$

- application: mathematical modeling of subdiffusion process, e.g., thermal diffusion in fractal domains, column experiments
- continuous time random walk $\Rightarrow$ pdf. satisfies $(*)$ (in $\mathbb{R}^d$)

diffusion of protein molecules in plasma membrane in live cells (A. Kusumi et al, 2005)

experimental trajectories (0.025 ms/frame)



simulation (100nm)

Fluorescent-molecule video imaging shows that the molecule spends relatively long times trapped between nanometre-sized compartments. ©: Klafter-Sokolov, 2005, Phys. Today

$$\langle x^2 \rangle \propto t^\alpha, \alpha < 1$$

Caputo fractional derivative

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u'(s)\mathrm{d}s$$

Laplace transform relation

$$\mathcal{L}[\partial_t^\alpha u](z) = \int_0^\infty e^{-zt} \partial_t^\alpha u(t)\mathrm{d}t = z^\alpha \hat{u}(z) - z^{\alpha-1} u(0)$$

$\Rightarrow$ allows specifying initial condition as usual ....

Riemann-Liouville fractional derivative

$$^R\partial_t^\alpha u(t) = \frac{\mathrm{d}}{\mathrm{d}t} \underbrace{\frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u(s)\mathrm{d}s}_{\text{Riemann-Liouville fractional integral } {}_0I_t^{1-\alpha}}$$

Laplace transform relation

$$\mathcal{L}[^R\partial_t^\alpha u](z) = z^\alpha \hat{u}(z) - ({}_0I_t^{1-\alpha} u)(0)$$

$\Rightarrow$ requires integral type initial condition !

regularity issue: the initial value problem with $\alpha \in (0, 1)$:

$$\partial_t^\alpha u + u = 0, \quad u(0) = 1$$

Laplace transform

$$z^\alpha \hat{u}(z) + \hat{u} = z^{\alpha-1} \quad \Rightarrow \quad \hat{u}(z) = \frac{z^{\alpha-1}}{z^\alpha + 1}$$

inverse Laplace transform $\Rightarrow$ the solution $u(t)$ is given by

$$u(t) = \mathcal{L}^{-1}\left[\frac{z^{\alpha-1}}{z^\alpha + 1}\right](t) = E_{\alpha,1}(-t^\alpha)$$

where Mittag-Leffler function 1903, 1905

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha + \beta)}$$

generalization of the exponential function

For $t \to 0$

$$u(t) = 1 - t^{\alpha}/\Gamma(1+\alpha) + O(t^{2\alpha}) \quad \text{and} \quad u'(t) \sim O(t^{\alpha-1})$$

Hence it fails to be $C^1[0,T] \Rightarrow$ limited smoothing property
$\alpha = 1$: $u(t) = E_{1,1}(-t) = e^{-t} \in C^{\infty}[0,1]$

Laplace transform ($A = -\Delta$)

$$z^\alpha \hat{u}(z) + A\hat{u}(z) = z^{\alpha-1} v + \hat{f}(z)$$
$$\Rightarrow \quad \hat{u}(z) = z^{\alpha-1}(z^\alpha + A)^{-1} v + (z^\alpha + A)^{-1}\hat{f}(z)$$

inverse Laplace transform

$$u(z) = F(t)v + \int_0^t E(t-s)f(s)\mathrm{d}s,$$

with

$$F(t) := \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt} z^{\alpha-1}(z^\alpha + A)^{-1}\,\mathrm{d}z$$
$$E(t) := \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt}(z^\alpha + A)^{-1}\,\mathrm{d}z$$

with contour $\Gamma_{\theta,\delta} \subset \mathbb{C}$ (oriented with an increasing imaginary part)

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

solution + resolvent estimate

$$\|(z+A)^{-1}\| \leq c|z|^{-1}, \quad \forall z \in \Sigma'_\theta$$

solution regularity Sakamoto-Yamamoto 2011; McLean 2011
Hilbert space $\dot{H}^s$: $\|v\|_{\dot{H}^s} = \sum_{j=1}^\infty \lambda_j^s (v, \varphi_j)^2$

- $f \equiv 0$, standard diffusion

$$\|(\partial_t)^\ell u(t)\|_{\dot{H}^p} \leq ct^{-(\ell+(p-q)/2)}\|v\|_{\dot{H}^q}, \;\; 0 \leq q \leq p, \ell \geq 0.$$

- $f \equiv 0$, fractional diffusion

$$\|(\partial_t^\alpha)^\ell u(t)\|_{\dot{H}^p} \leq ct^{-\alpha(\ell+(p-q)/2)}\|v\|_{\dot{H}^q}$$

for $\ell = 0$, $q \leq p$ and $0 \leq p - q \leq 2$ and for $\ell = 1$, $p \leq q \leq p + 2$

limited spatial smoothing property: maximum two order !!!

Galerkin FEM

Let $\mathcal{T}_h$ be a regular partition of the domain Ω into d-simplex

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

The semidiscrete Galerkin FEM: find $u_h(t) \in X_h$ s.t.

$$(\partial_t^\alpha u_h, \chi) + a(u_h, \chi) = (f, \chi) \quad \forall \chi \in X_h, t > 0$$

with $u_h(0) = v_h$ or

$$\partial_t^\alpha u_h - \Delta_h u_h = P_h f \quad \text{with } u_h(0) = v_h$$

- $a(u, w) = (\nabla u, \nabla w)$, $u, w \in H_0^1$
- $v_h \in X_h$ is a suitable approximation to the initial data v

solution representation

$$u_h(z) = F_h(t)v_h + \int_0^t E_h(t-s)P_hf(s)\mathrm{d}s$$

with

$$F_h(t) := \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt} z^{\alpha-1}(z^\alpha + A_h)^{-1}\, \mathrm{d}z$$
$$E_h(t) := \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt}(z^\alpha + A_h)^{-1}\, \mathrm{d}z$$

error representation for $f \equiv 0$

$$u_h(t) - u(t) = \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_{\theta,\delta}} e^{zt} z^{\alpha-1}[(z^\alpha + A_h)^{-1}v_h - (z^\alpha + A)^{-1}v]\mathrm{d}z$$

For $v \in L^2$, $z \in \Sigma'_\theta$, $w = (z^\alpha + A)^{-1} v$ and $w_h = (z^\alpha + A_h)^{-1} P_h v$,

$$\|w_h - w\|_{L^2} + h\|\nabla(w_h - w)\|_{L^2} \leq ch^2 \|v\|_{L^2}$$

for $v \in L^2$

$$\begin{aligned}\|e(t)\|_{L^2} &\leq c \int_{\Gamma_{\theta,\delta}} e^{\Re(z)t} |z|^{\alpha-1} \|(z^\alpha + A_h)^{-1} v_h - (z^\alpha + A)^{-1} v\|_{L^2} |\mathrm{d}z| \\ &\leq ch^2 \|v\|_{L^2} t^{-\alpha}.\end{aligned}$$

for $v \in D(A)$

$$\begin{aligned}\|e(t)\|_{L^2} &\leq c \int_{\Gamma_{\theta,\delta}} e^{\Re(z)t} |z|^{-1} \|(z^\alpha + A_h)^{-1} A_h R_h v_h - (z^\alpha + A)^{-1} A v\|_{L^2} |\mathrm{d}z| \\ &\leq ch^2 \|v\|_{L^2}\end{aligned}$$

Jin-Lazarov-Zhou SINUM 2013

(a) If $v \in \dot{H}^2$ and $v_h = R_h v$, then

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

identical with the classical diffusion equation

(b) If $v \in L^2$ and $v_h = P_h v$, then for $\ell_h = |\log h|$

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

different exponent: $t^{-\alpha}$

remarks

- similar results for lumped mass FEM/FVEM, but optimal estimates for $v \in L^2$ requires some restrictions on meshes

  Jin-Lazarov-Zhou 2013, Mustapha et al 2016

- One may also derive error estimates for $v \in \dot{H}^q$, $q \in (-1, 0)$
- similar results hold for inhomogeneous problems

  Jin-Lazarov-Pasciak-Zhou 2015

semidiscrete Galerkin FEM for $v = \chi_{[0,1/2]}$.

t	h	1/8	1/16	1/32	1/64	1/128	rate
0.005	L^2	8.54e-3	2.13e-3	5.33e-4	1.33e-4	3.33e-5	2.01 (2.00)
	H^1	2.67e-1	1.24e-2	6.18e-2	3.09e-2	1.54e-2	1.01 (1.00)
0.01	L^2	6.51e-3	1.63e-3	4.06e-4	1.02e-4	2.54e-5	2.00 (2.00)
	H^1	1.84e-1	9.20e-2	4.60e-2	2.30e-2	1.15e-2	1.00 (1.00)
1	L^2	8.00e-4	2.00e-4	5.00e-5	1.25e-5	3.13e-6	2.00 (2.00)
	H^1	2.05e-2	1.03e-2	5.13e-3	2.56e-3	1.28e-3	1.00 (1.00)

- The estimate is robust for small t and nonsmooth data.
- the error increases as $t \to 0$, with the correct exponent

Time stepping schemes: challenges in fully discrete schemes

- history mechanism: storage issue
  Ford, Lubich, Banjai, McLean, Hesthaven, Jiang, ...
- limited smoothing property $\rightarrow$ lack of robustness

two popular schemes

- convolution quadrature Lubich NM 1986 ...
- L1 scheme Lin-Xu JCP 2007, Sun-Wu ANM 2006
- many other approaches, including spectral type methods ...

Focus: uniform grid on $[0, T]$ with $\tau = T/N$, $t_n = n\tau$, $n = 0, \dots, N$
nonuniform mesh is much more challenging

convolution quadrature for the Riemann-Liouville derivative ${}^R\partial_t^\alpha \varphi$

$$\begin{aligned}
{}^R\partial_t^\alpha \varphi(t) &= \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \frac{s^{-\alpha}}{\Gamma(1-\alpha)}\varphi(t-s)\mathrm{d}s \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\int_0^t \left(\frac{1}{2\pi\mathrm{i}}\int_\Gamma e^{zs} z^{\alpha-1}\mathrm{d}z\right)\varphi(t-s)\mathrm{d}s \\
&= \frac{1}{2\pi\mathrm{i}}\int_\Gamma z^{\alpha-1}\underbrace{\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t e^{zs}\varphi(t-s)\mathrm{d}s}_{:=y(t)}\,\mathrm{d}z
\end{aligned}$$

$y(t)$ solves

$$y' = zy + \varphi \quad \text{with} \quad y(0) = 0.$$

linear multistep method for the ODE with characteristic functions

$$\sigma(\xi) = a_k \xi^k + \ldots + a_0 \quad \text{and} \quad \rho(\xi) = b_k \xi^k + \ldots + b_0$$

i.e., given for $n \geq 0$

$$\sum_{j=0}^{k} a_j y_{n+j-k} = \tau \sum_{j=0}^{k} b_j (z y_{n+j-k} + \varphi_{n+j-k})$$

with starting values $y_{-k} = \ldots = y_{-1} = 0$ and $\varphi_{-k} = \ldots = \varphi_{-1} = 0$.
multiplying the scheme by ξ^n and summing over n from 0 to ∞

$$(a_0 \xi^k + \ldots + a_k) \widetilde{y}(\xi) = \tau (b_0 \xi^k + \ldots + b_k)(z \widetilde{y}(\xi) + \widetilde{\varphi}(\xi)),$$

with the generating series

$$\widetilde{y}(\xi) = \sum_{n=0}^{\infty} y_n \xi^n \quad \text{and} \quad \widetilde{\varphi}(\xi) = \sum_{n=0}^{\infty} \varphi_n \xi^n$$

rearranging the terms gives

$$\widetilde{y}(\xi) = (\tau^{-1}\delta(\xi) - z)^{-1}\widetilde{\varphi}(\xi), \quad \text{with } \delta(\xi) = \frac{\sigma(\xi^{-1})}{\rho(\xi^{-1})}$$

$$\widetilde{y}'(\xi) = (\tau^{-1}\delta(\xi))\widetilde{y}(\xi) = (\tau^{-1}\delta(\xi))(\tau^{-1}\delta(\xi) - z)^{-1}\widetilde{\varphi}(\xi)$$

substituting back

$$\frac{1}{2\pi \mathrm{i}}\int_\Gamma z^{\alpha-1}(\tau^{-1}\delta(\xi))(\tau^{-1}\delta(\xi) - z)^{-1}\widetilde{\varphi}(\xi)\mathrm{d}z = (\tau^{-1}\delta(\xi))^\alpha\widetilde{\varphi}(\xi)$$

$\Rightarrow$ Cauchy integral formula: the *n*th coefficient is given by

$${}^R\partial_t^\alpha \varphi(t_n) \approx \sum_{j=0}^{n} \omega_j \varphi^{n-j} := \bar{\partial}_\tau^\alpha \varphi^n.$$

with quadrature weights $\{\omega_j\}_{j=0}^\infty$ given by

$$\tau^{-\alpha}\sum_{j=0}^{\infty} \omega_j \xi^j = (\tau^{-1}\delta(\xi))^\alpha$$

approximate ${}^R\partial_t^\alpha \varphi(t_n)$ by

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

where the quadrature weights $\{\omega_j\}_{j=0}^\infty$ are determined by

$$\tau^{-\alpha} \sum_{j=0}^{\infty} \omega_j \xi^j = (\tau^{-1}\delta(\xi))^\alpha$$

$\delta(\xi)$: the characteristic polynomial of linear multistep methods
Ex (backward Euler) $\delta(\xi) = 1 - \xi$

$$(1-\xi)^\alpha = \sum_{j=0}^{\infty} \omega_j \xi_j, \qquad \omega_j = (-1)^j \frac{\alpha(\alpha-1)\ldots(\alpha-j+1)}{j!}$$

Grunwald-Letnikov formula 1867,68

relation between (regularized) Caputo and Riemann-Liouville fractional derivatives ($0 < \alpha < 1$)

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

spatial semidiscrete scheme

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

fully discrete scheme reads: find $U_h^n \in X_h$ s.t.

$$\bar{\partial}_\tau^\alpha (U_h^n - v_h) = \Delta_h U_h^n + P_h f(t_n), \quad \text{with} \quad U_h^0 = v_h.$$

Jin-Lazarov-Zhou SISC 2016

For the BE, $v \in \dot{H}^q$, $q \in [0,2]$, $U_h^0 = P_h v$ and $f \equiv 0$, there holds

$$\|u(t_n) - U_h^n\|_{L^2} \le c(\tau t_n^{\alpha q/2-1} + h^2 t_n^{-\alpha(1-q/2)})\|v\|_{\dot{H}^q}$$

- proof by discrete Laplace transform Lubich-Sloan-Thomee 1996
- for fixed $t_n > 0$, the rate is $O(\tau)$ and $O(h^2)$ in $L^2(\Omega)$
- no condition on u directly, but on v
- the error deteriorates for $t_n \to 0$ (cf. regularity) $\Rightarrow$ low uniform rate !!

- BDFk, $k \geq 2$, requires initial correction, for $O(\tau^k)$ rate

BDF2: the scheme is only $O(\tau)$ if $\varphi(0) \neq 0$

How to recover $O(\tau^2)$ rate ?

splitting $f_h = f_{h,0} + \tilde{f}_h$, with $f_{h,0} = f_h(0)$ and $\tilde{f}_h = f_h - f_{h,0}$

$$
\begin{aligned}
u_h(t) &= v_h - (\partial_t^\alpha + A_h)^{-1} A_h v_h + (\partial_t^\alpha + A_h)^{-1}(f_{h,0} + \tilde{f}_h) \\
&= v_h - (\partial_t^\alpha + A_h)^{-1} \partial_t \partial_t^{-1} A_h v_h + (\partial_t^\alpha + A_h)^{-1}(\partial_t \partial_t^{-1} f_{h,0} + \tilde{f}_h).
\end{aligned}
$$

Now with $\bar{\partial}_\tau^\alpha$ BDF2 CQ

$$
U_h^n = v_h - (\bar{\partial}_\tau^\alpha + A_h)^{-1} \bar{\partial}\tau \partial_t^{-1} A_h v_h + (\bar{\partial}_\tau^\alpha + A_h)^{-1}(\bar{\partial}_\tau \partial_t^{-1} f_{h,0} + \tilde{f}_h).
$$

Cuesta-Lubich-Palencia 2006

$$\bar{\partial}_\tau \partial_t^{-1} 1 = (0, 3/2, 1, \ldots) := 1_\tau$$

$$(\bar{\partial}_\tau^\alpha + A_h)(U_h^n - v_h) = -1_\tau A_h v_h + 1_\tau f_{h,0} + \tilde{f}_h.$$

corrected BDF2 CQ scheme: find U_h^n s.t.

$$\bar{\partial}_\tau^\alpha U_h^1 + A_h U_h^1 + \tfrac{1}{2} A_h U_h^0 = \bar{\partial}_\tau^\alpha U_h^0 + F_h^1 + \tfrac{1}{2} F_h^0,$$
$$\bar{\partial}_\tau^\alpha U_h^n + A_h U_h^n = \bar{\partial}_\tau^\alpha U_h^0 + F_h^n, \quad n = 2, \ldots, N.$$

Jin-Lazarov-Zhou SISC 2016

For the BDF2, $v \in \dot{H}^q$, $q \in [0,2]$, $U_h^0 = P_h v$ and $f \equiv 0$, there holds

$$\|u(t_n) - U_h^n\|_{L^2} \le c(\tau^2 t_n^{\alpha q/2 - 2} + h^2 t_n^{-\alpha(1-q/2)})\|v\|_{\dot{H}^q}$$

without correction, it is only $O(\tau)$!

(a) $\Omega = (0,1)^2$, and $v = xy(1-x)(1-y) \in \dot{H}^2$;

(b) $\Omega = (0,1)^2$, and $v = \chi_{(0,1/2]\times(0,1)} \in \dot{H}^{1/2-\epsilon}$ with $\epsilon \in (0,1/2)$

The L2 error for $t = 0.1$, $\alpha = 0.5$, and $h = 2^{-9}$.

N	method	5	10	20	40	80	rate
(a)	BE	7.00e-3	3.34e-3	1.63e-3	8.05e-4	4.00e-4	1.00 (1.00)
	BDF2	2.00e-3	4.20e-4	9.79e-5	2.42e-5	6.54e-6	1.98 (2.00)
(b)	BE	4.39e-3	2.09e-3	1.02e-3	5.05e-4	2.51e-4	1.01 (1.00)
	BDF2	1.25e-3	2.64e-4	6.13e-5	1.49e-5	3.79e-6	2.05 (2.00)

correction type schemes

- Jin-Li-Zhou 2017 high-order BDF schemes
- Jin-Li-Zhou 2018 Crank-Nicolson scheme (two-step correction)
- Wang et al 2020 Crank-Nicolson scheme (single step correction)
- ...

L1 scheme approximates $\partial_t^\alpha u(t_n)$ by Lin-Xu 2007, Sun-Wu 2006, Stynes 2021

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

where the weights b_j are given by

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

UCL CENTRE FOR INVERSE PROBLEMS

fully discrete scheme: find U_h^n for $n = 1, 2, \dots, N$

$$(b_0 I - \tau^\alpha \Delta_h) U_h^n = b_n U_h^0 + \sum_{j=1}^{n} (b_{j-1} - b_j) U_h^{n-j} + \tau^\alpha F_h^n$$

with $U_h^0 = v_h$ and $F_h^n = P_h f(t_n)$

- $u \in C^2([0, T], \dot{H}^2(\Omega)) \Rightarrow O(\tau^{2-\alpha})$ rate Lin-Xu 2007, Sun-Wu 2006
- if the assumption fails $\Rightarrow$ NO $O(\tau^{2-\alpha})$ rate

Jin-Lazarov-Zhou IMAJNA 2016

For the L1 scheme, there hold

(a) If $v \in \dot{H}^2$ and $v_h \in R_h v$, then

$$\|U_h^n - u_h(t_n)\|_{L^2} \le c\tau t_n^{\alpha-1}\|v\|_{\dot{H}^2}$$

(b) If $v \in L^2$ and $v_h = P_h v$, then

$$\|U_h^n - u_h(t_n)\|_{L^2} \le c\tau t_n^{-1}\|v\|_{L^2}$$

- even for $v \in D(A)$: the rate is below $O(\tau^{2-\alpha})$

$$\|U_h^n - u_h(t_n)\|_{L^2} \le c\tau t_n^{\alpha-1}\|v\|_{\dot{H}^2} \le c\tau(n\tau)^{\alpha-1}\|v\|_{\dot{H}^2} \le c\tau^{\alpha}\|v\|_{\dot{H}^2}$$

- The scheme can be corrected to $O(\tau^{2-\alpha})$ order Yan et al 2016

let $w_h = u_h - v_h$, $W_h^n = U_h^n - v_h$
w_h satisfies the problem (with $A_h = -\Delta_h$)

$$\partial_t^\alpha w_h + A_h w_h = -A_h v_h, \quad w_h(0) = 0$$

Laplace transform $\Rightarrow$

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

representing the semidiscrete solution

$$w_h(t) = -\frac{1}{2\pi i}\int_{\Gamma_{\theta,\delta}} e^{zt} z^{-1} (z^\alpha I + A_h)^{-1} A_h v_h \mathrm{d}z$$

with $\Gamma_{\theta,\delta} = \{z \in \mathbb{C} : |z| = \delta, |\arg(z)| \leq \theta\} \cup \{z \in \mathbb{C} : z = \rho e^{\pm i\theta}, \rho \geq \delta\}$.

fully discrete problem

$$L_1^n(W_h) + A_h W_h^n = -A_h v_h, \quad \text{with } W_h^0 = 0$$

multiplying by ξ^n and summing from 1 to $\infty \Rightarrow$

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

the definition of the difference operator L_1^n

$$\begin{aligned}
\sum_{n=1}^{\infty} L_1^n(W_h)\xi^n &= \tau^{-\alpha} \sum_{n=1}^{\infty} \left(b_0 W_h^n + \sum_{j=1}^{n-1} (b_j - b_{j-1}) W_h^{n-j} \right) \xi^n \\
&= \tau^{-\alpha} \sum_{n=1}^{\infty} \left(\sum_{j=0}^{n-1} b_j W_h^{n-j} \right) \xi^n - \tau^{-\alpha} \sum_{n=1}^{\infty} \left(\sum_{j=1}^{n-1} b_{j-1} W_h^{n-j} \right) \xi^n \\
&:= I - II.
\end{aligned}$$

$W_h^0 = 0$ + the convolution rule

$$I = \tau^{-\alpha} \sum_{n=1}^{\infty} (\sum_{j=0}^{n} b_j W_h^{n-j}) \xi^n = \tau^{-\alpha} \widetilde{b}(\xi) \widetilde{W_h}(\xi)$$

$$II = \tau^{-\alpha} \sum_{n=1}^{\infty} (\sum_{j=1}^{n} b_{j-1} W_h^{n-j}) \xi^n = \tau^{-\alpha} \xi \widetilde{b}(\xi) \widetilde{W_h}(\xi).$$

$\Rightarrow$

$$\sum_{n=1}^{\infty} L_1^n(W_h) \xi^n = \tau^{-\alpha} (1 - \xi) \widetilde{b}(\xi) \widetilde{W_h}(\xi).$$

proper representation for $\widetilde{b}(\xi)$:

$$\widetilde{b}(\xi) = \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{\infty} ((j+1)^{1-\alpha} - j^{1-\alpha})\xi^j$$

$$= \frac{1-\xi}{\xi\Gamma(2-\alpha)} \sum_{j=1}^{\infty} j^{1-\alpha}\xi^j = \frac{(1-\xi)\mathrm{Li}_{\alpha-1}(\xi)}{\xi\Gamma(2-\alpha)}$$

polylogarithmic function $\mathrm{Li}_p(z)$ Flajolet 1999

$$\mathrm{Li}_p(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^p}$$

the fully discrete solution $\widetilde{W}_h(\xi)$

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

$\widetilde{W}_h(\xi)$ is analytic at $\xi = 0$ + Cauchy theorem $\Rightarrow$ for ϱ small enough

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

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

$$W_h^n = -\frac{1}{2\pi\mathrm{i}} \int_{\Gamma_\tau} e^{zt_{n-1}} \frac{\tau}{1-e^{-z\tau}} \left(\frac{(1-e^{-z\tau})^2}{e^{-z\tau}\tau^\alpha\Gamma(2-\alpha)} \mathrm{Li}_{\alpha-1}(e^{-z\tau}) + A_h \right)^{-1} A_h v_h \mathrm{d}z$$

with

$$\Gamma_\tau := \{ z \in \Gamma_{\theta,\delta} : |\Im(z)| \le \pi/\tau \}$$

- representing the semidiscrete solution

$$w_h(t) = -\frac{1}{2\pi i}\int_{\Gamma_{\theta,\delta}} e^{zt} z^{-1}(z^\alpha I + A_h)^{-1} A_h v_h \mathrm{d}z$$

- representing fully discrete solution W_h^n

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

the polylogarithm function

$$\mathrm{Li}_p(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^p}$$

idea of error analysis

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

$$z \sim \chi(z) \quad \text{and} \quad z^\alpha \sim \frac{1 - e^{-z\tau}}{\tau^\alpha}\psi(z\tau) \quad z \in \Gamma_\tau$$

technical lemmas

For $z \in \Gamma_\tau$, the following estimates hold

- $|\chi(z) - z| \leq c|z|^2\tau$ and $c_1|z| \leq |\chi(z)| \leq c_2|z|$, for some $c_1, c_2 > 0$
- $|\frac{1-e^{-z\tau}}{\tau^\alpha}\psi(z\tau) - z^\alpha| \leq c|z|^2\tau^{2-\alpha}$, for $\theta \in (\pi/2, 5\pi/6)$
- $|\psi(z\tau)| \geq c > 0$, for any θ close to $\pi/2$ and $\delta < \pi/2\tau$
- there exists $\theta_0 \in (\pi/2, \pi)$ s.t. $\frac{1-e^{-z\tau}}{z^\alpha}\psi(z\tau) \in \Sigma_{\theta_0}$ for $z \in \Sigma_\theta$

The only difference in the analysis of the two schemes is the kernel

- convolution quadrature: $z^\alpha \approx (1 - e^{-z\tau})^\alpha / \tau^\alpha$
- L1 scheme: $z^\alpha \sim$ complex function involving $\mathrm{Li}_p(z)$

numerical experiments: L1 scheme

(a) $\Omega = (0,1)$, and $v = \sin(2\pi x) \in \dot{H}^2$

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

The L^2-error at $t = 0.1$ with $h = 2^{-13}$, $\tau = 1/N$

t	N	20	40	80	160	320	rate
0.1	(a)	7.18e-5	3.55e-5	1.77e-5	8.82e-6	4.40e-6	1.01 (1.00)
	(b)	1.93e-4	9.57e-5	4.76e-5	2.38e-5	1.19e-5	1.00 (1.00)
0.5	(a)	5.89e-4	2.88e-4	1.43e-4	7.08e-5	3.52e-5	1.01 (1.00)
	(b)	1.73e-3	8.36e-4	4.09e-4	2.02e-4	1.00e-4	1.02 (1.00)
0.9	(a)	3.05e-3	1.39e-3	6.53e-4	3.12e-4	1.50e-4	1.07 (1.00)
	(b)	7.67e-3	3.79e-3	1.87e-3	9.23e-4	4.55e-4	1.02 (1.00)

- nonlinear problem

$$\begin{cases} \partial_t^\alpha u - \Delta u = f(u) & \text{in } \Omega \times (0,T), \\ u = 0 & \text{on } \partial\Omega \times (0,T), \\ u = u_0 & \text{in } \Omega \times \{0\}, \end{cases}$$

with $u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$ and $|f(s) - f(t)| \le L|s-t|$ for all $s, t \in \mathbb{R}$

- linearized time stepping scheme

$$\bar\partial_\tau^\alpha (u_h^n - u_h^0) - \Delta_h u_h^n = P_h f(u_h^{n-1}),$$

Tools: regularity + maximal ℓ^p regularity + Gronwall's inequality maximal L^p-regularity

$$\partial_t^\alpha u(t) = Au(t) + f \quad \forall t > 0, \quad \text{with } u(0) = 0,$$

The solution satisfies: for any $1 < p < \infty$ Bazhlekova 2002, 2003

$$\|\partial_t^\alpha u\|_{L^p(\mathbb{R}^+;X)} + \|Au\|_{L^p(\mathbb{R}^+;X)} \le c_{p,X}\|f\|_{L^p(\mathbb{R}^+;X)} \quad \forall f \in L^p(\mathbb{R}^+;X)$$

What about the discrete analogues ?

Jin-Li-Zhou Numer. Math. 2018

The discrete analogue holds for CQ generated by BDF1, BDF2, L1 ...

maximal ℓ^p regularity for L1 scheme Jin-Li-Zhou Numer. Math. 2016

Let X be a UMD space, $0 < \alpha < 1$, and let A be R-sectorial on X of angle $\alpha\pi/2$. Then the L1 scheme satisfies

$$\|(\bar\partial_\tau^\alpha u^n)_{n=1}^N\|_{\ell^p(X)} + \|(Au^n)_{n=1}^N\|_{\ell^p(X)} \leq c_{p,X} c_R \|(f^n)_{n=1}^N\|_{\ell^p(X)}$$

where $c_{p,X}$ is independent of N, τ and A.

- representation of the scheme in Laplace domain
- discrete Fourier multiplier theorem of Blunck

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Grönwall's inequality for fractional differential inequalities

For $\alpha \in (0,1)$ and $p \in (1/\alpha, \infty)$, if $u \in C([0,T];X)$ satisfies $\partial_t^\alpha u \in L^p(0,T;X)$, $u(0) = 0$ and

$$\|\partial_t^\alpha u\|_{L^p(0,s;X)} \le \kappa \|u\|_{L^p(0,s;X)} + \sigma, \quad \forall s \in (0,T],$$

for $\kappa, \sigma > 0$, then

$$\|u\|_{C([0,T];X)} + \|\partial_t^\alpha u\|_{L^p(0,s;X)} \le c\sigma$$

where the constant c is independent of σ, u and X.

discrete Gronwall's inequality Jin-Li-Zhou SINUM 2018

Let X be a UMD space. If $\alpha \in (0,1)$ and $p \in (1/\alpha, \infty)$, and a sequence $v^n \in X$ satisfies

$$\|(\bar\partial_\tau^\alpha v^n)_{n=1}^m\|_{\ell^p(X)} \le \kappa \|(v^n)_{n=1}^m\|_{\ell^p(X)} + \sigma, \quad \forall\, 1 \le m \le N,$$

for $\kappa, \sigma > 0$, then there exists a $\tau_0 > 0$ s.t. for any $\tau < \tau_0$ there holds

$$\|(v^n)_{n=1}^N\|_{\ell^\infty(X)} + \|(\bar\partial_\tau^\alpha v^n)_{n=1}^N\|_{\ell^p(X)} \le c\sigma,$$

where c and τ_0 are independent of σ, τ, N and v^n.

- linearized time stepping scheme

$$\bar{\partial}_\tau^\alpha(u_h^n - u_h^0) - \Delta_h u_h^n = P_h f(u_h^{n-1}),$$

- $u_0 \in H_0^1(\Omega) \cap H^2(\Omega)$ and $|f(s) - f(t)| \leq L|s - t|$ for all $s, t \in \mathbb{R} \Rightarrow$

$$\max_{0 \leq t \leq T} \|u(t) - u_h(t)\|_{L^2(\Omega)} \leq c\ell_h^2 h^2$$
$$\max_{1 \leq n \leq N} \|u_h(t_n) - u_h^n\|_{L^2(\Omega)} \leq c\tau^\alpha$$

  uniformly $O(\tau^\alpha)$ rate

- Outlook: strongly nonlinear problems ?

$f = \sqrt{1+u^2}$, and $v = x(1-x)y(1-y)$

Numerical results: the spatial error e_s with $T = 1$.

$\alpha \backslash M$	5	10	20	40	80	rate
0.4	6.89e-2	2.00e-2	5.34e-3	1.37e-3	3.31e-4	$\approx$ 2.01 (2.00)
0.6	7.06e-2	2.05e-2	5.58e-3	1.42e-3	3.44e-4	$\approx$ 2.01 (2.00)
0.8	7.59e-2	2.18e-2	5.80e-3	1.48e-3	3.57e-4	$\approx$ 2.01 (2.00)

Numerical results: the temporal error e_t with $T = 1$, $N = k \times 10^4$.

α	k	1	2	4	8	16	rate
0.4	BE	1.16e-3	8.88e-4	6.79e-4	5.19e-4	3.86e-4	$\approx$ 0.39 (0.40)
	L1	2.06e-3	1.59e-3	1.22e-3	9.34e-4	7.15e-4	$\approx$ 0.38 (0.40)
0.6	BE	1.79e-4	1.18e-4	7.75e-5	5.10e-5	3.36e-5	$\approx$ 0.60 (0.60)
	L1	3.05e-4	2.02e-4	1.33e-4	8.80e-5	5.81e-5	$\approx$ 0.60 (0.60)
0.8	BE	1.73e-5	9.87e-6	5.65e-6	3.24e-6	1.86e-6	$\approx$ 0.80 (0.80)
	L1	3.91e-5	2.24e-5	1.29e-5	7.38e-6	4.24e-6	$\approx$ 0.80 (0.80)

references

- B. Jin, R. Lazarov, Z. Zhou. Comput. Methods Appl. Mech. Eng., 2019 (review)
- B. Jin. Fractional Differential Equations, textbook, submitted to Springer

THANK YOU