Do we need decay-preserving error estimate for solving parabolic equations with initial singularity?

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joint work with Zhimin Zhang & Chengchao Zhao

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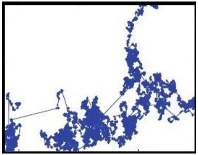
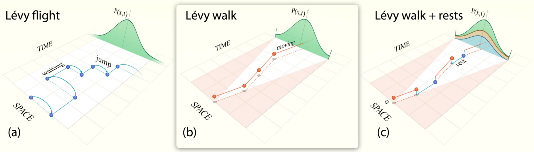
Outline

1. Why adaptive (nonuniform) time steps?
2. The α-robust error estimate for nonuniform time steps
3. Do we need decay-preserving error estimate for solving parabolic equations with initial singularity?

Why study the factional calculus?

- Fractional derivative characterizes the evolution of system depending on the history information.
- It is better to describe the experiment data using less parameters for certain phenomena.
- Abnormal diffusion, also known as non-brownian motion (Lévy process)





- We consider the computation for reaction-(sub)diffusion problem,

$$\begin{aligned} {}_0^{\mathrm{C}}\mathcal{D}_t^{\alpha} u &= \Delta u + f(x,t,u) && \text{for } x \in \Omega \text{ and } 0 < t \le T, \\ u &= u_0(x) && \text{for } x \in \Omega \text{ when } t = 0, \\ u &= 0 && \text{for } x \in \partial\Omega \text{ and } 0 < t < T. \end{aligned} \tag{1}$$

- ${}_0^{\mathrm{C}}\mathcal{D}_t^{\alpha}$ denotes the Caputo fractional derivative by

$$\begin{aligned} {}_0^{\mathrm{C}}\mathcal{D}_t^{\alpha} u &= \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial_s u(x,s)}{(t-s)^{\alpha}} \,\mathrm{d}s \\ &= \int_0^t \omega_{1-\alpha}(t-s)\partial_s u(x,s)\,\mathrm{d}s, \quad 0 < \alpha < 1, \end{aligned}$$

where the kernel $\omega_{\beta}(t) = \frac{t^{\beta-1}}{\Gamma(\beta)}, \quad t > 0.$

- ${}_0^{\mathrm{C}}\mathcal{D}_t^{\alpha} = \partial_t$ with $\alpha = 1$

Regularity of the solution (解的正则性)

- For $f = f(x,t)$, Sakamoto and Yamamoto in J. Math. Anal. Appl., 2011, show $\frac{\partial u}{\partial t} = O(1 + t^{\alpha-1})$ as $t \to 0$ for more general initial data u_0

- For nonlinear equation ${}_0^C\mathcal{D}_t^\alpha u = \Delta u + f(u)$: if f is Lipschitz continuous, Jin, Li and Zhou in SIUNM 2018, prove that the solution satisfies $\|\partial_t u(t)\|_{L^2(\Omega)} \le C_u t^{\alpha-1}$

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Blows-up or global existence of the solution (解爆破、全局存在性)

- Let us begin with a simple equation

$$\begin{aligned} u'(t) &= u^2, \qquad t > 0, \\ u(0) &= u_0 > 0. \end{aligned}$$

- The unique solution is given by

$$u(t) = \frac{u_0}{1 - u_0 t} \qquad \text{for } t < \frac{1}{u_0}.$$

- The solution blows up at the blow-up time $T_b = \dfrac{1}{u_0}$.

- Consider the following differential equation,

$$u'(t) = f(u), \qquad t > 0,$$
$$u(0) = u_0 > 0,$$

where $u_0 > 0$ is an initial value. To describe the blow-up behavior, we exchange the dependent and independent variables

$$\frac{\mathrm{d}t}{\mathrm{d}u} = \frac{1}{f(u)},$$

and the solution $u(t)$ satisfies

$$t = \int_{u_0}^{u(t)} \frac{1}{f(u)} \mathrm{d}u.$$

Theorem 1

Assume that $f(u)$ *is* positive *for all* $u > 0$. *Then all solutions blow up in finite time if and only if*

$$\int_u^\infty \frac{1}{f(x)}\mathrm{d}x < \infty \textit{ for all } u > 0, \tag{2}$$

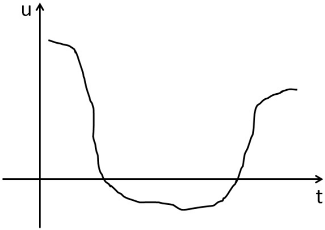
which is the Osgood's condition *found in 1898*.

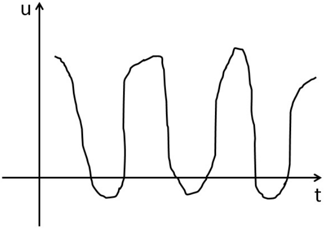
- Li et al. 2018 and Yang and Zhang, Zhao, 2019 show that fractional ODEs and PDEs have a finite time blow-up if and only if

$$\int_{u_0}^{\infty} \left(\frac{u}{f(u)}\right)^{1/\alpha} \frac{du}{u} < \infty.$$

Why adaptive time steps?

- The weak regularity of the solution at $t = 0$;
- The solution may grow fast far away from $t = 0$, such as blowup for nonlinear case.





Recent progress

- Numerous schemes are developed as L1 scheme (SW06, LX07), L2-type scheme (LX16,CXW14,K14-MC), Alikhanov's scheme (A15,LMZ21), and convolution quadrature (CQ) method (L88,JLZ18,JLZ19).
- Also, there has been an explosive growth in the numerical analysis
- Among the analysis, the error bounds generally contain a factor $1/(1-\alpha)$, which will blow up as $\alpha \to 1^-$.
- Jin-Li-Zhou-19-SINUM :"This phenomenon does not fully agree with the results for the continuous model ...and it is of interest to further refine the estimates to fill in the gap."

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Part I

The α-error estimate for L1 scheme on general nonuniform time step

General nonuniform time steps

- The time steps should be nonuniform because it fits for more general problems.
- Consider the time-step size $\tau_k = t_k - t_{k-1}$ for nonuniform time mesh $0 = t_0 < \cdots < t_{k-1} < t_k < \cdots < t_N = T$.
- Let $g^k = g(t_k)$ and difference operator $\nabla_\tau g^k = g^k - g^{k-1}$.
- The nonuniform L1 formula[1] of Caputo derivative with $v'(s) \approx \nabla_\tau v^k / \tau_k$ is given by

$$(\mathcal{D}_\tau^\alpha v)^n := \sum_{k=1}^{n} A_{n-k}^{(n)} \nabla_\tau v^k \quad \text{with} \quad A_{n-k}^{(n)} := \frac{1}{\tau_k} \int_{t_{k-1}}^{t_k} \omega_{1-\alpha}(t_n - s)\,\mathrm{d}s, \tag{3}$$

with (Liao et al 18' SINUM)

$$A_0^{(n)} > A_1^{(n)} > A_2^{(n)} > \cdots > A_{n-1}^{(n)} > 0 \quad \text{for } 1 \le n \le N, \tag{4}$$

[1] Sun and Wu, 06' and Lin & Xu, 07'

The nonuniform L1 scheme

One has a nonuniform L1 scheme for the problem (1)

$$\begin{aligned} (\mathcal{D}_\tau^\alpha u_i)^n - \Delta_h u_i^n =& \kappa u_i^n, \ 1 \le n \le N, \\ u_i^n =& u_b(x_i, t_n), \quad x_i \in \partial\Omega_h, \ 1 \le n \le N, \\ u_i^0 =& u^0(x_i), \quad x_i \in \bar{\Omega}_h \,. \end{aligned} \tag{5}$$

Stability analysis for subdiffusion equation (1)

$$ {}_0^C\mathcal{D}_t^\alpha u = \Delta u + \kappa u. $$

- Stability analysis by using the inequality $\frac{1}{2}{}_0^C\mathcal{D}_t^\alpha u^2 \le u {}_0^C\mathcal{D}_t^\alpha u$,

$$ \frac{1}{2}{}_0^C\mathcal{D}_t^\alpha \|u\|^2 \le \kappa\|u\|^2. $$

- The semigroup property of RL integral that $\mathcal{I}^\alpha\mathcal{I}^\beta u = \mathcal{I}^{\alpha+\beta}u$ implies

$$ \mathcal{I}^\alpha {}_0^C\mathcal{D}_t^\alpha u := \mathcal{I}^\alpha\mathcal{I}^{1-\alpha}u' = \int_0^t u'(s)\,\mathrm{d}s. $$

It is easy to have

$$ \|u\|^2 \le \|u_0\|^2 + \kappa\int_0^t \omega_\alpha(t-s)\|u\|^2(s)ds. $$

- If $\kappa \le 0$, we arrive at

$$ \|u\|^2 \le \|u_0\|^2. $$

- For $\kappa > 0$, standard integral-type Grönwall inequality produces

$$ \|u\|^2 \le E_\alpha(2\kappa t^\alpha)\|u_0\|^2. $$

Stability analysis for $L1$ scheme (5)

$$ (\mathcal{D}_\tau^\alpha u_i)^n - \Delta_h u_i^n = \kappa u_i^n. $$

The inequality $u^n(\mathcal{D}_\tau^\alpha u)^n \ge \frac{1}{2}(\mathcal{D}_\tau^\alpha u^2)^n,\ \forall\{u^k\}_{k=0}^n$ holds if and only if $A_0^{(n)} \ge A_1^{(n)} \ge \cdots \ge A_{n-1}^{(n)} \ge 0$

$$ \Longrightarrow \frac{1}{2}(\mathcal{D}_\tau^\alpha\|u\|^2)^n \le \kappa\|u\|^2. \qquad (6) $$

Challenges:

- The discrete RL integral generally does not hold the semi-group property.
- What and how to establish the discrete Grönwall inequality?

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Discrete complementary convolution (DCC) kernels

The semigroup property of RL derivative is derived by the fact that $\omega_\alpha * \omega_\beta = \omega_{\alpha+\beta}$, i.e.,

$$\mathcal{I}^\alpha \mathcal{I}^\beta v(t) = \omega_\alpha * (\omega_\beta * v) = \omega_{\alpha+\beta} * v = \mathcal{I}^{\alpha+\beta} v(t), \quad \forall \alpha, \beta > 0, \tag{7}$$

In analogy of $\omega_\alpha * \omega_{1-\alpha} = 1$, the DCC kernels $p_{n-j}^{(n)}$ is defined by

$$\sum_{j=m}^{n} p_{n-j}^{(n)} A_{j-m}^{(j)} \equiv 1 \quad \text{for } 1 \le m \le n \le N. \tag{8}$$

The DCC kernels may be calculated by [Liao, li and Z. '18, SINUM]

$$p_{n-k}^{(n)} = \frac{1}{A_0^{(k)}} \begin{cases} 1\,, & k = n, \\ \sum_{j=k+1}^{n} \left(A_{j-k-1}^{(j)} - A_{j-k}^{(j)}\right) p_{n-j}^{(n)}\,, & 1 \le k \le n-1. \end{cases} \tag{9}$$

Discrete complementary convolution (DCC) kernels

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- From (9), the DCC kernels $p_{n-j}^{(n)} \geq 0$ if the coefficients are monotonous $A_0^{(n)} \geq A_1^{(n)} \geq \cdots \geq A_{n-1}^{(n)} \geq 0$.
- the definition of DCC kernels $p_{n-j}^{(n)}$ (8) implies

$$\begin{aligned} \sum_{j=1}^{n} p_{n-j}^{(n)} \mathcal{D}_\tau^\alpha v^j &= \sum_{j=1}^{n} p_{n-j}^{(n)} \sum_{k=1}^{j} A_{j-k}^{(j)} \nabla_\tau v^k \\ &= \sum_{k=1}^{n} \nabla_\tau v^k \sum_{j=k}^{n} p_{n-j}^{(n)} A_{j-k}^{(j)} \; = \; v^n - v^0, \quad n \geq 1. \end{aligned} \tag{10}$$

- which is in analog of

$$\mathcal{I}_0^\alpha {}^C_0\mathcal{D}_t^\alpha u := \mathcal{I}^\alpha \mathcal{I}^{1-\alpha} u' = \int_0^t v'(s)\,\mathrm{d}s = v(t) - v_0. \tag{11}$$

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Stability analysis for linear reaction–subdiffusion equation (1) (${}_0^C\mathcal{D}_t^\alpha u = \Delta u + \kappa u$.)

- Stability analysis by using the inequality $\frac{1}{2}{}_0^C\mathcal{D}_t^\alpha u^2 \le u{}_0^C\mathcal{D}_t^\alpha u$,

$$\frac{1}{2}{}_0^C\mathcal{D}_t^\alpha \|u\|^2 \le \kappa\|u\|^2.$$

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$$\mathcal{I}^\alpha{}_0^C\mathcal{D}_t^\alpha u := \mathcal{I}^\alpha\mathcal{I}^{1-\alpha}u' = \int_0^t v'(s)\,\mathrm{d}s. \quad (12)$$

It is easy to have

$$\|u\|^2 \le \|u_0\|^2 + \kappa\int_0^t \omega_\alpha(t-s)\|u\|^2(s)ds.$$

- If $\kappa \le 0$, we arrive at

$$\|u\|^2 \le \|u_0\|^2.$$

- For $\kappa > 0$, standard integral-type Grönwall inequality produces

$$\|u\|^2 \le E_\alpha(2\kappa t^\alpha)\|u_0\|^2.$$

Stability analysis for $L1$ scheme (5) ($(\mathcal{D}_\tau^\alpha u_i)^n - \Delta_h u_i^n = \kappa u_i^n$.)

- The inequality $u^n(\mathcal{D}_\tau^\alpha u)^n \ge \frac{1}{2}(\mathcal{D}_\tau^\alpha u^2)^n,\ \forall\{u^k\}_{k=0}^n$ holds if and only if $A_0^{(n)} \ge A_1^{(n)} \ge \cdots \ge A_{n-1}^{(n)} \ge 0$

$$\Longrightarrow \frac{1}{2}(\mathcal{D}_\tau^\alpha\|u\|^2)^n \le \kappa\|u\|^2.$$

- For $\kappa \le 0$, using the DCC kernels $p_{n-k}^{(n)}$, one has

$$\|u^n\| \le \|u^0\|.$$

- For $\kappa > 0$, the discrete Grönwall inequality can be established as follows.

Lemma 2 (Liao, Li and Z. ’18, SINUM)

The discrete coefficient $p_{n-k}^{(n)}$ *with property* $\sum_{j=m}^{n} p_{n-j}^{(n)} A_{j-m}^{(j)} \equiv 1$ *holds:*

(i) $0 < p_{n-k}^{(n)} \leq \Gamma(2-\alpha)\tau_k^{\alpha}\,, \quad 1 \leq k \leq n.$

(ii) *For any nonnegative integer* $0 \leq m \leq \lfloor 1/\alpha \rfloor$,

$$\sum_{j=1}^{n} p_{n-j}^{(n)} \omega_{1+m\alpha-\alpha}(t_j) \leq \omega_{1+m\alpha}(t_n)\,, \quad n \geq 1.$$

(iii) *For any integer* $m \geq 1$,

$$\sum_{j=1}^{n-1} p_{n-j}^{(n)} \omega_{1+m\alpha-\alpha}(t_j) \leq \omega_{1+m\alpha}(t_n)\,, \quad n \geq 1.$$

Properties of discrete convolution kernel

Recalling the Mittag-Leffler function

$$E_\alpha(\mu t^\alpha) = \sum_{k=0}^{\infty} \frac{\mu^k t^{k\alpha}}{\Gamma(1+k\alpha)} = \sum_{k=0}^{\infty} \mu^k \omega_{k\alpha}(t),$$

where the series is absolutely convergent for any $0 < \alpha < 1$.

Lemma 3 (Liao, Li and Z. '18, SINUM)

Let $\mu > 0$ *be a constant. It holds that*

$$\mu \sum_{j=1}^{n-1} p_{n-j}^{(n)} E_\alpha(\mu t_j^\alpha) \le E_\alpha(\mu t_n^\alpha) - 1\,, \quad n \ge 1, \quad \mu > 0. \tag{13}$$

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It is easy to have

$$\|u\|^2 \leq \|u_0\|^2 + \kappa \int_0^t \omega_\alpha(t-s)\|u\|^2(s)ds.$$

- If $\kappa \leq 0$, we arrive at

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$$\Longrightarrow \frac{1}{2}(\mathcal{D}_\tau^\alpha \|u\|^2)^n \leq \kappa \|u\|^2. \tag{15}$$

- For $\kappa \leq 0$, using the DCC kernels $p_{n-k}^{(n)}$, one has

$$\|u^n\| \leq \|u^0\|.$$

- For $\kappa > 0$, the discrete Grönwall inequality produces

$$\|u^n\| \leq C_u E_\alpha(4\kappa t_n^\alpha)\|u^0\|. \tag{16}$$

.

Convergence analysis

To analyze the convergence of the scheme (5), we introduce the error function $e_i^n = U_i^n - u_i^n$ for $x_i \in \bar{\Omega}_h$, $0 \le n \le N$, which satisfies the initial error $e_i^0 = 0$ and governing equation

$$\left(\mathcal{D}_\tau^\alpha - \Delta_h - \kappa\right) e_i^n = (R_t)_i^n + (R_s)_i^n, \quad x_i \in \Omega_h,$$

where $(R_t)_i^n$ and $(R_s)_i^n$ represent the truncation errors in time and space as

$$(R_t)_i^n = {}_0^{\mathrm{C}}\mathcal{D}_t^\alpha u(x_i, t_n) - \mathcal{D}_\tau^\alpha u(x_i, t_n),$$
$$(R_s)_i^n = \Delta u(x_i, t_n) - \Delta_h u_i^n.$$

Theorem 4 (Discrete fractional Grönwall inequality, SINUM 2018)

For any finite time $t_N = T > 0$ and $\kappa \geq 0$, the error satisfies

$$\mathcal{D}_\tau^\alpha \left\|e^n\right\|^2 \leq 2\kappa \left\|e^n\right\|^2 + 2\left\|e^n\right\| \left(\left|(R_t)^n\right| + \left|(R_s)^n\right|\right), \quad n \geq 1.$$

If the maximum time-step size $\tau_N \leq \sqrt[\alpha]{\frac{1}{4\kappa\Gamma(2-\alpha)}}$ and $\kappa > 0$, it holds

$$\left\|e^n\right\| \leq C_u E_\alpha(4\kappa t_n^\alpha) \left(\max_{1 \leq j \leq n} \sum_{l=1}^{j} p_{j-l}^{(j)} \left|(R_t)^l\right| + \omega_{1+\alpha}(t_n) \max_{1 \leq k \leq n} \left|(R_s)^n\right| \right).$$

It can be proved by mathematical induction!!!

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It can be proved by mathematical induction!!!

Local consistency error

- Under the regularity assumption $\left\|\partial_x^{(4)} u(t)\right\|_{L^2} \le C_u$, the spacial truncation error satisfies $\left|((R_s))^n\right| \le C_u h^2$.
- Rewrite the definition of L1 scheme as

$$(\mathcal{D}_\tau^\alpha v)^n = A_0^{(n)} v^n - \sum_{k=1}^{n-1} \left(A_{n-k-1}^{(n)} - A_{n-k}^{(n)}\right) v^k - A_{n-1}^{(n)} v^0 ,$$

- The temporal mesh grid information is unknown.
- Our finding: $(R_t)^j$ is bounded by a discrete convolution form,

$$\text{(ECS estimate)} \qquad \left|(R_t)^n\right| \le A_0^{(n)} G_{\text{loc}}^n + \sum_{k=1}^{n-1} \left(A_{n-k-1}^{(n)} - A_{n-k}^{(n)}\right) G_{\text{his}}^k,$$

where $G_{\text{loc}}^n = G_{\text{his}}^n$ with

$$G_{\text{his}}^k \triangleq \int_{t_{k-1}}^{t_k} (\mu - t_{k-1}) \left|g''(\mu)\right| \, \mathrm{d}\mu , \quad 1 \le k \le n-1.$$

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Global consistency error

- Global consistency error (Liao, Li, Z., SINUM, '18)

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\begin{aligned}
\sum_{j=1}^{n} p_{n-j}^{(n)} \left|(R_t)^j\right| &\le \sum_{k=1}^{n} p_{n-k}^{(n)} A_0^{(k)} G_{\mathrm{loc}}^k + \sum_{k=1}^{n} p_{n-k}^{(n)} \sum_{j=1}^{k-1} \left(A_{k-j-1}^{(k)} - A_{k-j}^{(k)}\right) G_{\mathrm{his}}^j \\
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&\le 2 \sum_{k=1}^{n} p_{n-k}^{(n)} A_0^{(k)} G_{\mathrm{loc}}^k .
\end{aligned}
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Note that, the cyan term denotes the global consistency error of local part in $[t_{j-1}, t_j]$, and the red term is the global consistency error of historical part over $[t_0, t_{j-1}]$.

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Global convergence

Lemma 5 (Liao, Li, Z., SINUM, '18)

Assume $u \in C^2((0,T])$ *and there exists a constant* $C_u > 0$ *such that*

$$\left|u''(t)\right| \le C_u(1+t^{\sigma-2}), \quad 0 < t \le T, \tag{17}$$

where $\sigma \in (0,1) \cup (1,2)$ *is a regularity parameter. Then*

$$\sum_{j=1}^{n} p_{n-j}^{(n)} \left|(R_t)^j\right| \le C_u\Big(\tau_1^{\sigma}/\sigma + \frac{1}{1-\alpha} \max_{2\le k\le n} (t_k - t_1)^{\alpha} t_{k-1}^{\sigma-2} \tau_k^{2-\alpha}\Big).$$

Global convergence (Liao, Li, Z., SINUM, '18)

- **Uniform mesh:** Taking $\tau = TN^{-1}$ and $t_k = k\tau$, we have

$$\sum_{j=1}^{n} p_{n-j}^{(n)} \left|(R_t)^j\right| \leq C_g \left(\tau^\sigma/\sigma + \frac{1}{1-\alpha} T^{\sigma - \min\{\sigma, 2-\alpha\}} \tau^{\min\{\sigma, 2-\alpha\}} \right).$$

- As expected, the convergence order increases when the initial regularity of solution improves for $\sigma \leq 2 - \alpha$
- but the accuracy barrier is of order $O(\tau^{2-\alpha})$.

Global convergence (Liao, Li, Z., SINUM, '18)

- Nonuniform mesh (Graded mesh): $t_k = T\left(k/N\right)^{\gamma}$ with the parameter $\gamma > 1$, we have

$$\sum_{j=1}^{n} p_{n-j}^{(n)} \left|(R_t)^j\right| \le C_g T^{\sigma}\left(\frac{1}{\sigma} N^{-\gamma\sigma} + \frac{\gamma^2 4^{\gamma-1}}{1-\alpha} N^{-\min\{\gamma\sigma, 2-\alpha\}}\right).$$

- The accuracy barrier is $O(N^{\alpha-2})$
- The accuracy is $O(N^{-\min(\sigma\gamma, 2-\alpha)})$

The α-blow-up phenomenon

- The most error bounds contain a factor $\frac{1}{1-\alpha} \to \infty$ as $\alpha \to 1^-$.
- This is the so-called α-blowup phenomenon
- Jin, Li and Zhou, SINUM 2019 :
  "This phenomenon does not fully agree with the results for the continuous model ...and it is of interest to further refine the estimates to fill in the gap."

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- However, the existing analysis depends on the precise form of graded mesh $t_n = (k/N)^\gamma$ with $\gamma \geq 1$.
- Although efforts have been made to avoid the factor blow-up phenomenon, a robust analysis of error estimates still remains incomplete for with general nonuniform time steps.

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The α-robust error estimate on general nonuniform mesh

Lemma 6 (Z., Zhang and Zhao, 2022[2])

Assume $u \in C^2((0,T])$ *and there exists a constant* $C_u > 0$ *such that*

$$\left|u''(t)\right| \le C_u(1+t^{\sigma-2}), \quad 0 < t \le T, \tag{18}$$

where $\sigma \in (0,1)\cup(1,2)$ *is a regularity parameter. Then*

$$\sum_{j=1}^{n} p_{n-j}^{(n)} \left|(R_t)^j\right| \le C_u\Big(\frac{\tau_1^{\sigma}}{\sigma} + \Gamma(2-\alpha)\sum_{j=2}^{n}\tau_j \max_{j\le k\le n} t_k^{\alpha-1} t_{k-1}^{\sigma-2}\tau_k^{2-\alpha}\Big).$$

[2] Z., Zhang and Zhao, α-robust error estimates of general non-uniform time-step numerical schemes for reaction-subdiffusion problems, 2022

Typical widely-used meshes

- Uniform mesh: Taking the time step: $\tau = TN^{-1}$ and $t_k = k\tau$
- Graded mesh: $t_k = T(k/N)^{\gamma}$ with the parameter $\gamma \geq 1$
- The general graded mesh

  M1. There is a constant C_1, C_γ such that $\tau_1 \geq C_1\tau^{\gamma}$ and $\tau_k \leq C_\gamma \tau \min\{1, t_k^{1-1/\gamma}\}$ for $1 \leq k \leq N$, $t_k \leq C_\gamma t_{k-1}$ and $\tau_k \leq C_\gamma \tau_{k-1}$ for $2 \leq k \leq N$.

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  M1. There is a constant C_1, C_γ such that $\tau_1 \geq C_1\tau^{\gamma}$ and $\tau_k \leq C_\gamma \tau \min\{1, t_k^{1-1/\gamma}\}$ for $1 \leq k \leq N$, $t_k \leq C_\gamma t_{k-1}$ and $\tau_k \leq C_\gamma \tau_{k-1}$ for $2 \leq k \leq N$.

Typical widely-used meshes

- **Uniform mesh:** Taking the time step: $\tau = TN^{-1}$ and $t_k = k\tau$
- **Graded mesh:** $t_k = T(k/N)^{\gamma}$ with the parameter $\gamma \geq 1$
- **The general graded mesh**

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Convergence of L1 scheme

Theorem 7 (Z., Zhang and Zhao, '22)

The error estimate in L^2-norm with $C = E_\alpha(4\max\{1,\rho\}\kappa_+ t_n^\alpha)$ is that:

- *if graded mesh is used, then it holds that*

$$\|e_h^n\| \le C_u C \left(\|e_h^0\| + (\frac{1}{\sigma} + \varsigma_{n,\gamma}^L) T^\sigma N^{-\max\{\sigma\gamma, 2-\alpha\}} + t_n^\alpha h^2 \right), \quad \sigma < 1,$$

- *if* M1 *holds, then it holds with $n^* = (\frac{t_n}{\tau_1})^{\frac{1}{\gamma}}$ that*

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- *By choosing $\gamma_{opt} = \max\{1, (2-\alpha)/\sigma\}$, one can achieve the (quasi-)optimal convergence $\mathcal{O}(N^{\alpha-2}\log N)$ as $\alpha \to 1^-$.*

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L1 scheme	$\sigma\gamma < 2-\alpha$	$\sigma\gamma = 2-\alpha$	$\sigma\gamma > 2-\alpha$
Uniform mesh ($\gamma = 1$) Graded mesh ($\gamma \geq 1$)	$\frac{1-n^{\sigma\gamma+\alpha-2}}{2-\alpha-\sigma\gamma}$	$\ln n$	$\frac{1-n^{2-\alpha-\sigma\gamma}}{\alpha-2+\sigma\gamma}$
General graded mesh ($\gamma \geq 1$)	$\frac{1-(\frac{t_n}{\tau_1})^{\sigma+\frac{\alpha-2}{\gamma}}}{2-\alpha-\sigma\gamma}$	$\ln\frac{t_n}{\tau_1}$	$\frac{1-(\frac{t_n}{\tau_1})^{\frac{2-\alpha}{\gamma}-\sigma}}{\alpha-2+\sigma\gamma}$

Table: $\sigma \in (0,1)$:The formula of factor $\varsigma_{n,\gamma}^{L}$ for L1 w.r.t. fractional order α, regularity parameter σ, the grading parameter γ and time step n.

Noting that$\varsigma_{n,\gamma}^{L}$ is uniformly bounded by $(T+1)\log n$ as $\alpha \to 1^{-}$.

The α-robust estimate for Alikhanov's scheme

The general α-robust error estimate

Theorem 8 (Z., Zhang and Zhao, 2022[3])

Assume A1–A3 *holds, there exists a constant* $C_u > 0$ *such that*

$$\left|u''(t)\right| \leq C_u(1 + t^{\sigma-2}), \quad 0 < t \leq T, \ \sigma \in (0,1) \cup (1,2). \tag{19}$$

For $C = C_u E_\alpha(4\max(1,\rho)\pi_A \kappa t_n^\alpha)$

$$\|e_h^n\| \leq C\left(\|e_h^0\| + \frac{\tau_1^{\sigma+\alpha}}{\sigma} + t_n^\alpha h^2 + t_n^\alpha \max_{2\leq k\leq n} t_{k-1}^{\sigma-2}\tau_k^2 + (\rho+1)\max_{1\leq k\leq n} \Xi_t^k\right),$$

where $\Xi_t^k = \Gamma(2-\alpha)\pi_A\left(\sum_{j=2}^n \tau_j \max_{j\leq k\leq n} t_k^{\alpha-1}\mathcal{G}^k + \tau_1^\alpha \mathcal{G}^1\right)$.

[3] Z., Zhang and Zhao, α-robust error estimates of general non-uniform time-step numerical schemes for reaction-subdiffusion problems, 2022

Theorem 9 (Z., Zhang and Zhao, 2022[4])

The L^2-error estimate is bounded by:

- *for graded mesh, it holds with $C = C_u C_{\gamma,T} E_\alpha(20\kappa_+ t_n^\alpha)$ that*

$$\|e_h^n\| \leq C\left(\|e_h^0\| + (1/\sigma + \varsigma_{n,\gamma}^A)N^{-\min\{\sigma\gamma,2\}} + t_n^\alpha h^2\right), \quad 0 < \sigma < 1,$$

- *if* M1 *also holds, then it holds with $C = C_u C_{\gamma,\rho,T} E_\alpha(20\kappa_+ t_n^\alpha)$ that*

$$\|e_h^n\| \leq C\left(\|e_h^0\| + (1/\sigma + \varsigma_{n^*,\gamma}^A)N^{-\min\{\sigma\gamma,2\}} + t_n^\alpha h^2\right), \quad 0 < \sigma < 1,$$

where $n^* = (\frac{t_n}{\tau_1})^{\frac{1}{\gamma}}$.

[4] Z., Zhang and Zhao, α-robust error estimates of general non-uniform time-step numerical schemes for reaction-subdiffusion problems, 2022

The dependence of factor $\tilde{\varsigma}_n^*$ on α in error bounds [5]

Alikhanov's scheme	$\sigma\gamma < 3-\alpha$	$\sigma\gamma = 3-\alpha$	$\sigma\gamma > 3-\alpha$
Uniform mesh ($\gamma = 1$) Graded mesh ($\gamma > 1$)	$\frac{1-n^{\sigma\gamma+\alpha-3}}{3-\alpha-\sigma\gamma}$	$\ln n$	$\frac{1-n^{3-\alpha-\sigma\gamma}}{\alpha-3+\sigma\gamma}$
General mesh ($\gamma \geq 1$)	$\frac{1-(\frac{t_n}{\tau_1})^{\sigma+\frac{\alpha-3}{\gamma}}}{3-\alpha-\sigma\gamma}$	$\ln\frac{t_n}{\tau_1}$	$\frac{1-(\frac{t_n}{\tau_1})^{\frac{3-\alpha}{\gamma}-\sigma}}{\alpha-3+\sigma\gamma}$

Table: The formula of factor ς_n^* for Alikhanov's schemes w.r.t fractional order α, regularity parameter σ, the grading parameter γ and time step n.

Again, $\varsigma_{n,\gamma}^L$ is uniformly bounded by $(T+1)\log n$ as $\alpha \to 1^-$.

[5] Z., Zhang and Zhao, α-robust error estimates of general non-uniform time-step numerical schemes for reaction-subdiffusion problems, preprint, 2022

Part II

Do we need decay-preserving error estimate for solving parabolic equations with initial singularity?

Motivation

- Consider

$$\partial_t^\alpha u - \Delta u = \kappa u + f, \quad x \in \Omega, \ t \in (0, T], \tag{20}$$

- Under the regularity condition

$$\|\partial_t u(t)\|_{L^2(\Omega)} \leq C t^{\alpha - 1}.$$

- The above α-error estimate for L1 scheme on uniform mesh holds

$$\|e\|_\infty := \max_{1 \leq n \leq N} \|e^n\| \leq C\tau^\alpha.$$

- But, sometimes, one is interesting in error $\|e^N\|$ at time level N.
- The point-wise error $\|e^n\| \leq C\tau t_n^{\alpha-1}$ (see Jin, Li and Zhou and Qin, Li and Z., JCM 23 [6])
- One can observe the following interesting phenomena.

[6] Hongyu Qin, Dongfang Li and Jiwei Zhang, Sharp Pointwise-in-time Error Estimate of L1 Scheme for Nonlinear Subdiffusion Equations, JCM, 23'

Example for subdiffusion equation with L1 scheme

- Assume the regularity: $\|\partial_t u(t)\|_{L^2(\Omega)} \leq Ct^{\alpha-1}$
- Set $\Omega = (0, L)$ and exact solution $u = t^\alpha \sin(\pi x/L)$ with $\alpha = 0.5$

Table: Convergence rates of L1 scheme by taking various L, κ and T,.

	N	$L=1$			$L=\pi$		
		$\kappa=1$	$\kappa=0$	$\kappa=-8$	$\kappa=1$	$\kappa=0$	$\kappa=-8$
$T=1$	64	1.28	1.29	1.36	1.00	1.06	1.28
	128	1.24	1.25	1.32	1.00	1.05	1.24
	256	1.19	1.20	1.28	1.00	1.03	1.19
	512	1.15	1.16	1.23	1.00	1.02	1.15
$T=10$	64	1.40	1.41	1.45	1.00	1.16	1.40
	128	1.37	1.38	1.43	1.00	1.12	1.37
	256	1.33	1.34	1.40	1.00	1.09	1.33
	512	1.30	1.31	1.37	1.00	1.07	1.29

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Example for subdiffusion equation with L1 scheme

- The above shows various convergence rates for different model parameters (i.e., Ω, T, and reaction coefficient κ).
- This elusive phenomena cannot be explained by error estimates in previous literatures as their theory does not involve the influence of model parameters.
- This inconsistence between numerical experiments and theoretical analysis has been puzzling us for a long time, and motivating us to find what goes on behind scenes and to uncover the mystery.
- The similar behavior happens to the classical model?

$$\partial_t u - \Delta u = \kappa u + f, \quad x \in \Omega, \; t \in (0, T], \tag{21}$$

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Example for classical diffusion equation with Euler scheme

Table: Convergence rates of implicit Euler with $\alpha = 0.5$ for exact solution.

	N	$L = 1$			$L = \pi$		
		$\kappa = 1$	$\kappa = 0$	$\kappa = -1$	$\kappa = 1$	$\kappa = 0$	$\kappa = -1$
$T = 1$	64	1.03	1.03	1.02	0.47	0.50	0.56
	128	1.00	1.01	1.01	0.48	0.50	0.54
	256	0.98	0.99	1.00	0.49	0.50	0.53
	512	0.96	0.98	1.00	0.49	0.50	0.52
$T = 10$	64	1.01	1.01	1.01	0.47	1.03	1.01
	128	1.01	1.01	1.01	0.48	1.01	1.01
	256	1.00	1.00	1.00	0.49	1.00	1.00
	512	1.00	1.00	1.00	0.49	0.99	1.00

- Again, the existing theory cannot explain why we see different convergence rates with different model parameters.
- This motivates us to express various convergence regimes ranging from lower order to high order.
- To the end, we first eliminate the effect of the spatial domain to consider an ODE also with initial weak singularity:

$$u_t = \kappa u + f, \quad t > 0 \tag{22}$$

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- Uniform mesh: $t_n = n\tau, n = 0, 1, \ldots, N, \tau = T/N$.
- Denote

$$v^{n-\frac{1}{2}} = \frac{1}{2}(v^n + v^{n-1}), \quad D_2 v^n := \frac{3v^n - 4v^{n-1} + v^{n-2}}{2\tau}.$$

- The discretizations are given by

$$\frac{1}{\tau}\nabla_\tau U^n = \kappa U^n + f^n, \qquad \text{Implicit Euler scheme} \tag{23}$$

$$\frac{1}{\tau}\nabla_\tau U^n = \kappa U^{n-\frac{1}{2}} + f^{n-\frac{1}{2}}, \qquad \text{C-N scheme} \tag{24}$$

$$D_2 U^n = \kappa U^n + f^n, \quad n \geq 2, \qquad \text{BDF2 scheme} \tag{25}$$

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- Noting BDF2 needs two starting values, we here use IE scheme to compute U^1.

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A decay-preserving error estimate for ODEs

- A point-wise decay-preserving ($\kappa < 0$) error estimate for ODEs:

$$|e^n| \le e^{C\kappa t_n}|e^0| + C_u\left(e^{C\kappa t_n}\tau^{\alpha} + Ct_{n-1}^{\alpha-1}\tau^{k}\right),$$

  where $k = 1$ indicates implicit Euler scheme and $k = 2$ indicates C-N or BDF2 scheme.
- From a theoretical point of view, τ^{α} is the leading order as $\tau \to 0$.
- However, due to limited computational resources, we can only take a finite N in practice.
- Once N is finite (i.e., τ is not infinitesimal), the coefficients of τ^{α} and τ^{k} will play an important role to determine which is dominant.
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We present the qualitative analysis as follows:

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$$|e^n| \leq e^{C\kappa t_n}|e^0| + C_u\left(e^{C\kappa t_n}\tau^{\alpha} + Ct_{n-1}^{\alpha-1}\tau^k\right).$$

- Case 1: $\kappa \geq 0$. Coefficient $e^{C\kappa T}$ exponentially increases. Hence, the convergence rate always performs as α-order.
- Case 2: $\kappa < 0$. The coefficient $e^{C\kappa T}$ exponentially decays.
- If $e^{C\kappa T}\tau^{\alpha} \ll T^{\alpha-k}\tau^k$ for $\tau \geq \tau_0$, it has $\|e^N\| \leq C\tau^k$.
- If coefficients $e^{C\kappa T}$ and $T^{\alpha-k}$ are in the same scale, it has $\|e^N\| \leq C\tau^{\alpha}$, $\forall \tau > 0$.

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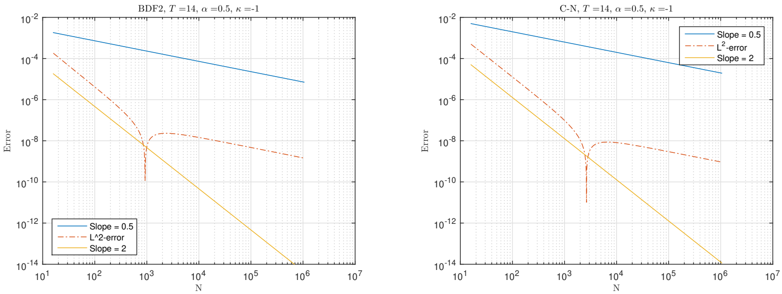
- If coefficients $e^{C\kappa T}$ and $T^{\alpha-k}$ are in the same scale, it has $\|e^N\| \le C\tau^\alpha,\ \forall\tau > 0$.

Numerical simulations

Table: (Example for ODEs) The convergence rates with various $\kappa \geq 0$ and T.

	N	$\kappa = 0$		$\kappa = 0.5$	
		$T = 1$	$T = 5$	$T = 1$	$T = 5$
IE	512	0.49	0.49	0.49	0.49
	1024	0.49	0.49	0.49	0.49
	2048	0.50	0.50	0.49	0.49
C-N	512	0.50	0.50	0.50	0.50
	1024	0.50	0.50	0.50	0.50
	2048	0.50	0.50	0.50	0.50
BDF2	512	0.50	0.50	0.50	0.50
	1024	0.50	0.50	0.50	0.50
	2048	0.50	0.50	0.50	0.50

Numerical simulations



(a) BDF2 scheme (b) C-N scheme

图: Absolute errors with parameters $T = 14, \alpha = 0.5, \kappa = -1$.

2. The decay-preserving error estimates for PDEs

$$
\begin{aligned}
\partial_t u - \Delta u &= \kappa u + f, && x \in \Omega,\ t \in (0, T], \\
u(x,t) &= 0, && x \in \partial\Omega,\ t \in [0, T], \\
u(x,0) &= u_0(x), && x \in \bar{\Omega}.
\end{aligned}
$$

- The discretizations are given by

$$\frac{1}{\tau}\nabla_\tau U^n = \Delta U^n + \kappa U^n + f^n, \qquad \text{IE scheme}$$

$$\frac{1}{\tau}\nabla_\tau U^n = \Delta U^{n-\frac{1}{2}} + \kappa U^{n-\frac{1}{2}} + f(t_{n-\frac{1}{2}}), \qquad \text{C-N scheme}$$

$$D_2 U^n = \Delta U^n + \kappa U^n + f^n, \quad n \geq 2, \qquad \text{BDF2 scheme}$$

- We introduce the associate eigenvalue problem

$$-\Delta\omega = \lambda\omega, \qquad \text{with } \omega = 0 \text{ on } \partial\Omega$$

- If $\Omega = (0, L)$, the eigenvalues and eigenvectors are given as

$$\lambda_k = (k\pi/L)^2, \quad \omega_k(x) = \sin(k\pi x/L), \qquad k = 1, 2, \cdots.$$

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A decay-preserving error estimate for PDEs

- A point-wise decay-preserving error estimate:

$$|||e^N|| \leq C(e^{-C(\lambda_1-\kappa)T}\tau^{\alpha} + T^{\alpha-k}\tau^{k}),$$

where $k = 1$ for IE scheme and $k = 2$ for C-N or BDF2 scheme.

- Given a lower bound of time steps τ_0 and letting $\tau \geq \tau_0$, then
  - (C1) for sufficiently small $\lambda_1 - \kappa$ (relative large κ or small λ_1) and T, the convergence order is $\mathcal{O}(\tau^{\alpha})$;
  - (C2) for sufficiently large $\lambda_1 - \kappa$ (relative small κ or large λ_1) and T, the convergence order is $\mathcal{O}(\tau^{k})$.
- Given the model parameters κ, λ_1 and T, then
  - (C3) for sufficiently small τ, the convergence order is $\mathcal{O}(\tau^{\alpha})$.

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Numerical simulations for PDEs

Table: (PDEs) Convergence rates with $T = 1, L = \pi$ for various κ.

	N	$\kappa = 0$	$\kappa = -5$	$\kappa = -10$	$\kappa = -15$	$\kappa = -20$
IE	512	0.50	0.75	1.00	1.00	1.00
	1024	0.50	0.70	0.99	1.00	1.00
	2048	0.50	0.66	0.98	1.00	1.00
C-N	512	0.50	0.48	1.36	2.01	2.00
	1024	0.50	0.49	-0.50	2.03	2.00
	2048	0.50	0.50	0.26	2.10	2.00
BDF2	512	0.50	0.48	-0.22	2.08	2.01
	1024	0.50	0.49	0.31	2.24	2.04
	2048	0.50	0.50	0.44	3.01	2.08

Table: (PDEs) Convergence rates with $\kappa = 0, T = 10$ for various L.

	N	$L = 1$ ($\lambda_1 \approx 9.87$)	$L = 2$ ($\lambda_1 \approx 2.47$)	$L = 3$ ($\lambda_1 \approx 1.10$)	$L = 4$ ($\lambda_1 \approx 0.62$)	$L = 5$ ($\lambda_1 \approx 0.39$)
IE	512	1.00	1.00	1.00	0.77	0.59
	1024	1.01	1.00	0.99	0.72	0.57
	2048	1.01	1.00	0.98	0.67	0.55
C-N	512	1.98	1.99	1.18	0.48	0.49
	1024	1.93	1.99	-0.45	0.49	0.50
	2048	1.86	1.98	0.27	0.50	0.50
BDF2	512	1.05	2.26	-0.15	0.48	0.49
	1024	3.77	1.28	0.33	0.49	0.50
	2048	-1.94	0.64	0.39	0.50	0.50

Numerical simulations for PDEs

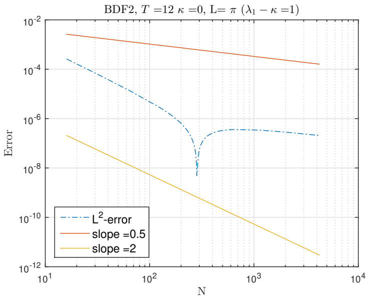
Table: (PDEs) Convergence rates with $\kappa = 0, L = \pi$ for various T.

	N	$T = 1$	$T = 5$	$T = 10$	$T = 15$	$T = 20$
IE	512	0.50	0.66	0.99	1.00	1.00
	1024	0.50	0.62	0.97	1.00	1.00
	2048	0.50	0.59	0.96	1.00	1.00
C-N	512	0.50	0.49	-0.63	2.03	2.00
	1024	0.50	0.50	0.24	2.10	2.01
	2048	0.50	0.50	0.42	2.37	2.07
BDF2	512	0.50	0.49	0.27	2.39	2.31
	1024	0.50	0.50	0.43	3.53	1.37
	2048	0.50	0.50	0.45	1.79	0.75

Table: (PDEs) Convergence rates with $T = 5$ and different $\kappa \geq \lambda_1$ and L.

	N	$\kappa = 1$		$\kappa = 1.5$	
		$L = \pi$ ($\lambda_1 = 1$)	$L = 4$ ($\lambda_1 \approx 0.62$)	$L = \pi$ ($\lambda_1 = 1$)	$L = 4$ ($\lambda_1 \approx 0.62$)
IE	512	0.49	0.49	0.49	0.50
	1024	0.49	0.49	0.49	0.50
	2048	0.50	0.49	0.49	0.50
C-N	512	0.50	0.50	0.50	0.50
	1024	0.50	0.50	0.50	0.50
	2048	0.50	0.50	0.50	0.50
BDF2	512	0.50	0.50	0.50	0.50
	1024	0.50	0.50	0.50	0.50
	2048	0.50	0.50	0.50	0.50

Numerical simulations



(a) BDF2 scheme for PDEs (b) C-N scheme for PDEs

图: Errors with fixed model parameters T, κ, λ_1.

Subdiffusion equations

- The L1 scheme for subdiffusion equations:

$$\mathcal{D}_\tau^\alpha U^n = \Delta U^n + \kappa U^n + f^n, \tag{29}$$

- Conjecture: the decay-preserving error estimate is given as

$$\|e^N\| \leq C(E'_\alpha(-C(\lambda_1 - \kappa)T^\alpha)\tau + \tau^{2-\alpha}).$$

- The conjecture shows that:
  - (E1) for sufficient small $\lambda_1 - \kappa$ (relative large κ or small λ_1) and T, the convergence order is $\mathcal{O}(\tau)$;
  - (E2) for sufficiently large $\lambda_1 - \kappa$ (relative small κ or large λ_1) and T, the convergence order is $\mathcal{O}(\tau^{2-\alpha})$.

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Numerical simulations for subdiffusion equations

Table: Convergence rate with $T = 1, L = \pi$ and various κ.

N	$\kappa = 0$	$\kappa = -5$	$\kappa = -10$	$\kappa = -20$	$\kappa = -50$
128	1.05	1.19	1.26	1.34	1.42
256	1.03	1.15	1.22	1.30	1.39
512	1.02	1.11	1.18	1.25	1.36

Table: Convergence rate with $\kappa = 0, T = 10$ and various L.

N	$L = 1$ ($\lambda_1 \approx 9.87$)	$L = 2$ ($\lambda_1 \approx 2.47$)	$L = 3$ ($\lambda_1 \approx 1.10$)	$L = 4$ ($\lambda_1 \approx 0.62$)	$L = 5$ ($\lambda_1 \approx 0.39$)
128	1.38	1.22	1.13	1.08	1.06
256	1.34	1.18	1.10	1.06	1.04
512	1.31	1.14	1.07	1.04	1.03

Numerical simulations for subdiffusion equations

Table: Convergence rate with $\kappa = 0, L = \pi$ and various T.

N	$T = 1$	$T = 10$	$T = 20$	$T = 50$	$T = 100$
128	1.05	1.12	1.15	1.21	1.25
256	1.03	1.09	1.12	1.17	1.21
512	1.02	1.07	1.09	1.13	1.17

Table: Convergence rate with $T = 5, \kappa \geq \lambda_1$ and various L.

N	$\kappa = 1$		$\kappa = 1.5$	
	$L = \pi$ ($\lambda_1 = 1$)	$L = 4$ ($\lambda_1 \approx 0.62$)	$L = \pi$ ($\lambda_1 = 1$)	$L = 4$ ($\lambda_1 \approx 0.62$)
128	1.00	0.96	0.94	0.92
256	1.00	0.97	0.96	0.93
512	1.00	0.98	0.97	0.95

Conclusion

- We provide a new decay-preserving error estimate to study numerical behavior of widely used IE, C-N and BDF2 schemes.
- The error estimate consists of two components: $e^{-C(\lambda_1-\kappa)T}\tau^{\alpha}$ and $T^{\alpha-k}\tau^{k}$, where λ_1 is the minimal eigenvalue.
- The estimate shows various convergence rates are caused by the trade-off between two components in different model parameter regimes.
- Our decay-preserving error estimates succeed to capture the different states of convergence rate where the traditional error estimates fail because we take the model parameters into account and thus retain more properties of continuous equations.
- We only present a conjecture on the decay-preserving error estimate of L1 scheme for sub-diffusion equations!!!

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- We only present a conjecture on the decay-preserving error estimate of L1 scheme for sub-diffusion equations!!!

$\alpha \to 1^-$ VS $\alpha \to 0^+$

Fast algorithm

- Using the identity $\frac{1}{t^\alpha} = \frac{1}{\Gamma(\alpha)} \int_0^\infty e^{-t \cdot s} s^{\alpha-1} ds$
- we use SOE to approximate the power function:

$$\left| \frac{1}{t^\alpha} - \sum_{i=1}^{N_{\exp}} \omega_i e^{-s_i t} \right| \leq \varepsilon, \quad t \in [\delta, T]. \tag{30}$$

Table: # of exponentials needed to approximate $t^{-\alpha}$.

	$\alpha = 0.06$				$\alpha = 0.006$			
$\varepsilon \backslash \delta$	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
10^{-3}	10	14	15	17	6	9	12	13
10^{-3}	5	7	8	10	4	6	7	7
10^{-6}	22	25	27	35	22	25	32	34
10^{-6}	11	14	18	22	10	12	14	16
10^{-9}	32	35	39	49	26	40	44	48
10^{-9}	16	21	25	30	15	19	23	28

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10^{-3}	5	7	8	10	4	6	7	7
10^{-6}	22	25	27	35	22	25	32	34
10^{-6}	11	14	18	22	10	12	14	16
10^{-9}	32	35	39	49	26	40	44	48
10^{-9}	16	21	25	30	15	19	23	28

应用一：粘弹性地质下的P-SV地震波传播

分数阶Caputo算子用于描述地震波在真实介质中传播的衰减性

- 动量守恒

$$\rho\frac{\partial}{\partial t}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x_1}\sigma_{11} \\ \frac{\partial}{\partial x_2}\sigma_{22} \\ \frac{\partial}{\partial x_3}\sigma_{33} \end{pmatrix} + \begin{pmatrix} \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} & 0 \\ \frac{\partial}{\partial x_1} & 0 & \frac{\partial}{\partial x_3} \\ 0 & \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} \end{pmatrix}\begin{pmatrix} \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix} + \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix}$$

- 正应力-应变关系

$$\frac{1}{\rho}\frac{\partial}{\partial t}\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \end{pmatrix} = \begin{pmatrix} C_P D_t^{2\gamma_P}\frac{\partial v_{11}}{\partial x_1} + (C_P D_t^{2\gamma_P} - C_S D_t^{2\gamma_S})(\frac{\partial v_{22}}{\partial x_2} + \frac{\partial v_{33}}{\partial x_3}) \\ C_P D_t^{2\gamma_P}\frac{\partial v_{22}}{\partial x_2} + (C_P D_t^{2\gamma_P} - C_S D_t^{2\gamma_S})(\frac{\partial v_{11}}{\partial x_1} + \frac{\partial v_{33}}{\partial x_3}) \\ C_P D_t^{2\gamma_P}\frac{\partial v_{33}}{\partial x_3} + (C_P D_t^{2\gamma_P} - C_S D_t^{2\gamma_S})(\frac{\partial v_{11}}{\partial x_1} + \frac{\partial v_{22}}{\partial x_2}) \end{pmatrix}$$

- 剪切应力-应变关系

$$\frac{1}{\rho}\frac{\partial}{\partial t}\begin{pmatrix} \sigma_{12} \\ \sigma_{13} \\ \sigma_{23} \end{pmatrix} = \begin{pmatrix} C_S D_t^{2\gamma_S}(\frac{\partial v_{12}}{\partial x_1} + \frac{\partial v_{12}}{\partial x_2}) \\ C_S D_t^{2\gamma_S}(\frac{\partial v_{13}}{\partial x_3} + \frac{\partial v_{13}}{\partial x_1}) \\ C_S D_t^{2\gamma_S}(\frac{\partial v_{23}}{\partial x_2} + \frac{\partial v_{23}}{\partial x_3}) \end{pmatrix}$$

数值挑战：长记忆困难

- 实际地球物理应用中，分数阶非常小，通常在0.006-0.06量级
- Abel核非常平坦，常规离散方法有“长记忆”困难
- 我们的贡献:
  - 设计了基于SOE快速格式，克服了“长记忆”挑战
    - 已有格式需要保留500层记忆，对于256^3的空间网格规模需内存超过500多GB, 且长时间模拟精度难以保证
    - 我们只需存(小于等于)10层中间变量就可以实现10^{-3}量级的相对误差，对于256^3的空间网格规模需内存为10GB
  - 结合多尺度Strang分裂格式，实现了三维地震波方程的高效求解

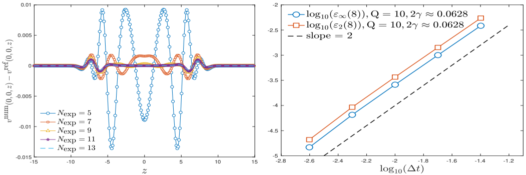

图: 与参考解定量验证(左)，在时间方向严格二阶收敛(右)

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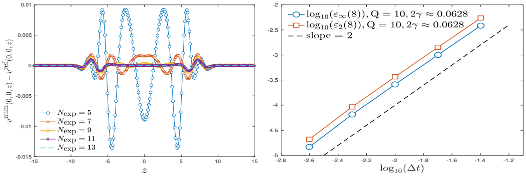
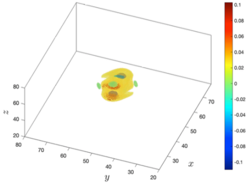
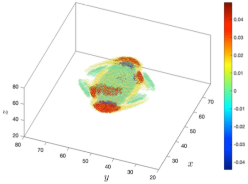


图: 与参考解定量验证(左)，在时间方向严格二阶收敛(右)

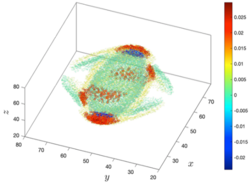
弹性波的传播过程



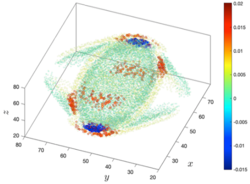
(a) $t = 2.5$.



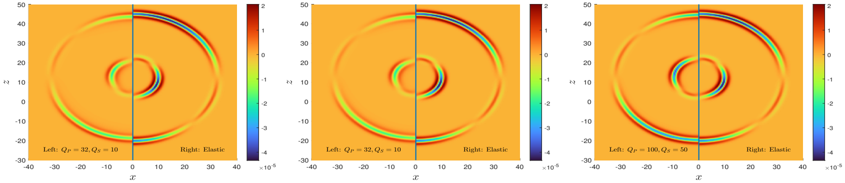
(b) $t = 5$.



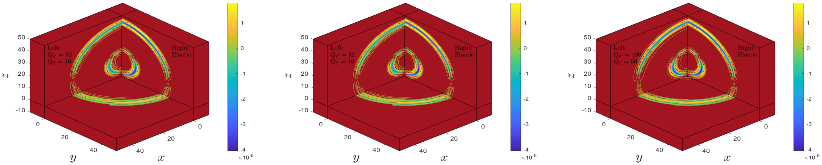
(c) $t = 7.5$.



(d) $t = 10$.



(a) $t = 10$s. (left: Elastic, midde: $Q_P = 100, Q_S = 50$, right: $Q_P = 32, Q_S = 10$).



(b) $t = 10$s. (left: Elastic, midde: $Q_P = 100, Q_S = 50$, right: $Q_P = 32, Q_S = 10$).

图: Snapshots of the propagation of wavefield v_3. The viscoelasticity influences the amplitude and causes the lag in the first arrival time of the seismic signals.

Thanks for your attention!