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Reconstruction of a solely time-dependent source in a time-fractional diffusion equation with non-smooth solutions

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Outline

Introduction

Uniqueness of a solution to the ISP

Existence of a solution to the ISP (for exact data)

Numerical experiments

Further research

Problem setting I

- $\Omega \subset \mathbb{R}^d$, $d \in \mathbb{N}$: bounded Lipschitz domain with boundary $\partial\Omega$
- T: final time
- $Q_T := \Omega \times (0, T]$ and $\Sigma_T := \partial\Omega \times (0, T]$
- Consider a general second-order linear differential operator given by

$$L(\mathbf{x}, t)u(\mathbf{x}, t) = -\nabla \cdot (\boldsymbol{A}(\mathbf{x}, t)\nabla u(\mathbf{x}, t)) + c(t)u(\mathbf{x}, t),$$

where $((\mathbf{x}, t) \in Q_T)$

$$\boldsymbol{A}(\mathbf{x}, t) = \left(a_{i,j}(\mathbf{x}, t)\right)_{i,j=1,\ldots,d}, \quad \boldsymbol{A}^\top = \boldsymbol{A}$$

- $\partial_t^\beta u$ denotes the Caputo derivative of order $\beta \in (0, 1)$ defined by

$$\left(\partial_t^\beta u\right)(\mathbf{x}, t) = \partial_t \int_0^t \frac{(t-s)^{-\beta}}{\Gamma(1-\beta)} \left[u(\mathbf{x}, s) - u(\mathbf{x}, 0)\right] \, ds, \qquad (\mathbf{x}, t) \in Q_T,$$

where Γ denotes the Gamma function

Problem setting II

- Goal: determine the couple $\{h(t), u\}$ such that

$$
\begin{cases}
\left(\partial_t^{\beta} u\right)(\mathbf{x}, t) + (Lu)(\mathbf{x}, t) & \\
\qquad = h(t) f(\mathbf{x}) + \int_0^t F(\mathbf{x}, s, u(\mathbf{x}, s))\, \mathrm{d}s & (\mathbf{x}, t) \in Q_T, \\
(-\boldsymbol{A}(\mathbf{x}, t) \nabla u(\mathbf{x}, t)) \cdot \nu(\mathbf{x}) = g(\mathbf{x}, t) & (\mathbf{x}, t) \in \Sigma_T, \\
u(\mathbf{x}, 0) = \tilde{u}_0(\mathbf{x}) & \mathbf{x} \in \Omega,
\end{cases}
$$

and the following integral measurement are satisfied

$$
\int_\Omega u(\mathbf{x}, t)\, \mathrm{d}\mathbf{x} = m(t)
$$

Literature overview: classical heat equation I

- Finding the evolution parameter $h(t)$ from the condition of overdetermination

$$\begin{cases} \partial_t u - \Delta u = h(t) f(\mathbf{x}) & \text{in } Q_T, \\ u = 0 \text{ or } -\nabla u \cdot \boldsymbol{\nu} = g & \text{on } \Sigma_T, \\ u(\mathbf{x}, 0) = \tilde{u}_0(\mathbf{x}) & \text{for } \mathbf{x} \in \Omega, \\ \int_\Omega \omega(\mathbf{x}) u(\mathbf{x}, t) \, \mathrm{d}\mathbf{x} = E(t) & \text{for } t \in [0, T] \end{cases}$$

- Idea: measure equation, assume that $\int_\Omega f(\mathbf{x})\omega(\mathbf{x}) \, \mathrm{d}\mathbf{x} \neq 0$
- [Cannon and Lin, 1988] for $-\nabla u \cdot \boldsymbol{\nu} = g$ on Σ_T:

$$h(t) = \frac{E'(t) + \int_\Omega \nabla u \cdot \nabla \omega \, \mathrm{d}\mathbf{x} + \int_{\partial\Omega} g\omega \, \mathrm{d}\Omega}{\int_\Omega f\omega \, \mathrm{d}\mathbf{x}}, \quad \omega \in \mathrm{H}^1(\Omega)$$

- [Prilepko et al., 2000] for $u = 0$ on Σ_T:

$$h(t) = \begin{cases} \frac{E'(t) + \int_\Omega \nabla u \cdot \nabla \omega \, \mathrm{d}\mathbf{x}}{\int_\Omega f\omega \, \mathrm{d}\mathbf{x}} & \omega \in \mathrm{H}_0^1(\Omega) \\ \frac{E'(t) - \int_\Omega u \Delta \omega \, \mathrm{d}\mathbf{x}}{\int_\Omega f\omega \, \mathrm{d}\mathbf{x}} & \omega \in \mathrm{H}^2(\Omega) \cap \mathrm{H}_0^1(\Omega) \end{cases}$$

Literature overview: classical heat equation II

- Uniqueness via variational/energy estimate approach ($u = 0$ on Σ_T):
  - linear problem: $E = 0$ and $\tilde{u}_0 = 0 \quad \Rightarrow \quad u = 0$ and $h = 0$
  - $|h(t)| \leqslant C \|\nabla u\|$ or $|h(t)| \leqslant C \|u\|$ depending on condition on ω
  - Using the solution as a test function gives

$$\int_0^\eta (\partial_t u(t), u(t))\,\mathrm{d}t + \int_0^\eta \|\nabla u(t)\|^2\,\mathrm{d}t = \int_0^\eta h(t)\,(f, u(t))\,\mathrm{d}t$$

  - Hence (assume $f \in \mathrm{L}^2(\Omega)$)

$$\frac{\|u(\eta)\|^2}{2} + \int_0^\eta \|\nabla u(t)\|^2\,\mathrm{d}t \leqslant \varepsilon \int_0^\eta |h(t)|^2\,\mathrm{d}t + C_\varepsilon \int_0^\eta \|u(t)\|^2\,\mathrm{d}t$$

  - Grönwall lemma implies that $u = 0$ a.e. in Q_T
  - Therefore, $h = 0$
  - Also valid in case of NBC ($g = 0$ on Σ_T)
- Global (in time) solvability of the problem including numerical scheme for computations is studied in [Grimmonprez and Slodička, 2015] for $\omega = 1$ and DBC

Literature overview: classical heat equation III

- Uniqueness for an autonomous heat equation $\partial_t u + Lu = h(t)f(\mathbf{x})$
  - Let L be a linear elliptic operator:
    $Lu = -\nabla \cdot (\mathbf{A}(\mathbf{x})\nabla u(\mathbf{x}, t)) + c(\mathbf{x})u(\mathbf{x}, t), \quad \mathrm{dom}(L) = \mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega) \subset \mathrm{L}^2(\Omega)$
  - Assume that $\mathbf{A}^T = \mathbf{A}$ such that $L = L^*$
  - Semigroup theory [Pazy, 1983] gives on closed formula for the solution:
    $u(t) = \mathrm{e}^{-Lt}u(0) + \int_0^t \mathrm{e}^{-L(t-s)}h(s)f \, \mathrm{d}s$
  - We have that

$$f(\mathbf{x})h(t) - \partial_t u(\mathbf{x}, t) = Lu(\mathbf{x}, t) = L\mathrm{e}^{-Lt}u(0) + \int_0^t h(s)L\mathrm{e}^{-L(t-s)}f \, \mathrm{d}s$$

  - Multiply the equation with $\omega(\mathbf{x})$ and integrate over the domain

$$h(t)\int_\Omega f(\mathbf{x})\omega(\mathbf{x}) \, \mathrm{d}\mathbf{x} = E'(t) + \left(\mathrm{e}^{-Lt}u(0), L\omega\right) + \int_0^t h(s)\left(\mathrm{e}^{-L(t-s)}f, L\omega\right) \, \mathrm{d}s$$

  - If $\int_\Omega f(\mathbf{x})\omega(\mathbf{x}) \, \mathrm{d}\mathbf{x} \neq 0$, then we have a Volterra integral equation of the second kind
  - There exists a unique h if $E \in \mathrm{C}^1([0, T])$, $u_0, f \in \mathrm{L}^2(\Omega)$, $\omega \in \mathrm{H}^2(\Omega) \cap \mathrm{H}^1_0(\Omega)$
  - $E = 0$ and $\tilde{u}_0 = 0 \Rightarrow h = 0 \Rightarrow u = 0$
  - [Slodička, 2013]: $h(t)$ can also be recovered from the measurement $u(\mathbf{y}, t)$ for $t \in [0, T]$ at a single interior point $\mathbf{y}$ if $f(\mathbf{y}) \neq 0$

Literature overview: fractional diffusion equation I

- [Sakamoto and Yamamoto, 2011]:
  - $Lu = -\nabla \cdot (\mathbf{A}(\mathbf{x})\nabla u(\mathbf{x}, t)) + c(\mathbf{x})u(\mathbf{x}, t), \quad \text{dom}(L) = \mathrm{H}^2(\Omega) \cap \mathrm{H}_0^1(\Omega) \subset \mathrm{L}^2(\Omega)$
  - Stability estimate (and thus uniqueness) for inverse source problem of determining $h(t)$ by observation $u(\mathbf{y}, t)$ at one point $\mathbf{y}$ over $t \in [0, T]$ with $f(\mathbf{y}) \neq 0$
- [Wei and Zhang, 2013]:
  - $Lu = -u_{xx}$ with $\Omega = (0, 1)$, $u(0) = u(1) = 0$
  - Determine $h(t)$ from $u(y, t), t \in [0, T]$ with $y \in (0, 1)$
  - Analysis is based on the separation of variables and Duhamel's principle
  - Inverse source problem is transformed into a first kind Volterra integral equation
  - Boundary element method combined with Tikhonov regularizations is used to solve this equation
- [Wei et al., 2016]:
  - $Lu = -\Delta u, \nabla u \cdot \boldsymbol{\nu} = 0$ on $\partial\Omega$
  - Additional data: $u(\mathbf{x}, t) = g(\mathbf{x}, t)$ with $\mathbf{x} \in \partial\Omega' \subset \partial\Omega$ for $t \in (0, T]$
  - Uniqueness and stability estimate is provided
  - Tikhonov regularization method for solving ISP
  - Conjugate gradient method combined with Morozov's discrepancy principle

Literature overview: fractional diffusion equation II

- [Šišková and Slodička, 2017]:
  - Same problem setting
  - Existence and uniqueness of a weak solution for exact data was proved
  - Numerical algorithm based on Rothe's method was established
  - Convergence of approximations towards the exact solution was demonstrated
  - However, the analysis in this paper gives that the solution is continuously differentiable on the closed time interval
  - An essential feature of the time Caputo fractional subdiffusion problem is that the solution lacks the smoothness near the initial time although it would be smooth away from $t = 0$
    - See e.g. [Brunner et al., , MCLEAN, 2010, Jin et al., 2016, Sakamoto and Yamamoto, 2011, Luchko, 2012]
    - [Stynes et al., 2017] showed that under proper regularity and compatibility assumptions, the one-dimensional subdiffusion problem $\partial_t^\beta u - pu_{xx} + c(x)u = f(x,t)$ with homogeneous DBC has a unique classical solution, and there exists a constant C_u such that

$$|u''(t)| \leqslant C_u(1 + t^{\beta-2}), \quad 0 < t \leqslant T$$

    - [Kopteva, 2019, Section 6.1] generalized this result to the case $\Omega \subset \mathbb{R}^d$ for $d \in \{2,3\}$ and more general autonomous operator L

Main results

- We will design two numerical algorithms based on Rothe's method over uniform and graded grids (using graded $L1$-approximation)
- We will derive a priori estimates and prove convergence of iterates towards the exact solution
- Rothe's method on a uniform grid will address the existence of a unique solution for exact data under low regularity assumptions
  - It will include non-smooth solution with t^{γ} term where $1 > \gamma > \beta$
- Rothe's method over graded grids will have the advantage to cope better with the behaviour at $t = 0$ ($\partial_t u$ possibly blows up as $t \to 0^+$)
  - Here t^{β} will be included in the class of admissible solutions
- The theoretical obtained results will be supported by numerical experiments

Properties convolution kernel

- We rewrite the Caputo fractional derivative as follows

$$\left(\partial_t^{\beta} u\right)(\mathbf{x}, t) = \partial_t \left(k * (u - \tilde{u}_0)\right)(\mathbf{x}, t), \qquad (\mathbf{x}, t) \in Q_T,$$

with

$$k(t) = \frac{t^{-\beta}}{\Gamma(1-\beta)}, \qquad t > 0$$

- The symbol '$*$' stands for the convolution product defined by

$$(k * z)(t) = \int_0^t k(t-s) z(s) \, \mathrm{d}s$$

- The singular kernel $k \in \mathrm{L}^1(0, T)$ satisfies $k(t) \geqslant 0$ for $t > 0$
- $\partial_t k \in \mathrm{L}^1_{\mathrm{loc}}(0, T)$ with $\partial_t k(t) \leqslant 0$ for all $t > 0$
- k is strongly positive definite as also $\partial_{tt} k(t) \geqslant 0$ for all $t > 0$, see [Nohel and Shea, 1976, Corollary 2.2] or [Cannarsa and Sforza, 2011]

Reformulation as coupled direct problem

- Integrate the PDE over the domain Ω and apply the Divergence Theorem to obtain that

$$h(t) = \frac{(k * m')(t) + \int_\Gamma g(\mathbf{x},t)\ \mathrm{d}\mathbf{x} + c(t)m(t) - \int_\Omega \left(\int_0^t F(\mathbf{x}, s, u(\mathbf{x}, s))\ \mathrm{d}s \right) \mathrm{d}\mathbf{x}}{\int_\Omega f(\mathbf{x})\ \mathrm{d}\mathbf{x}}, \qquad \text{(MP)}$$

  where we have assumed that

$$\int_\Omega f(\mathbf{x})\ \mathrm{d}\mathbf{x} \neq 0$$

  and that the measurement m is absolutely continuous

- Variational formulation:

  search $\{h, u\} \in \mathrm{L}^2(0,T) \times \mathrm{L}^2\left((0,T), \mathrm{H}^1(\Omega)\right)$ with $\partial_t(k * (u - \tilde{u}_0)) \in \mathrm{L}^2\left((0,T), \mathrm{H}^1_0(\Omega)^*\right)$ such that for a.a. $t \in (0,T)$ it holds that

$$\langle \partial_t (k * (u - \tilde{u}_0))(t), \varphi \rangle_{\mathrm{H}^1(\Omega)^* \times \mathrm{H}^1(\Omega)} + \mathcal{L}(t)\,(u(t), \varphi) = h(t)\,(f, \varphi) + \left(\int_0^t F(s, u(s))\ \mathrm{d}s, \varphi \right) - (g(t), \varphi)_\Gamma, \quad \forall \varphi \in \mathrm{H}^1(\Omega), \qquad \text{(P)}$$

  with $h(t)$ given by (MP)

- Note: $\mathcal{L}(t)\,(u(t), \varphi) := (Lu, \varphi) = (\boldsymbol{A}(t)\nabla u(t), \nabla \varphi) + c(t)\,(u(t), \varphi)$

Uniqueness if $\partial_t (k * (u - \tilde{u}_0)) \in \mathrm{L}^2\left((0,T), \mathrm{H}^1(\Omega)^*\right)$: sketch of proof I

- Consider $L = -\Delta u + u$
- Assume that F is linear in u, i.e. $F(\mathbf{x}, t, u) = \mathcal{G}(\mathbf{x}, t) u$ with $\partial_t \mathcal{G} \in \mathrm{L}^\infty(Q_T)$
- Suppose that two solutions $\{h_1, u_1\}$ and $\{h_2, u_2\}$ exist
- Then, the differences $h := h_1 - h_2$ and $u := u_1 - u_2$ are satisfying

$$\langle \partial_t (k * u)(t), \varphi \rangle_{\mathrm{H}^1(\Omega)^* \times \mathrm{H}^1(\Omega)} + (\nabla u(t), \nabla \varphi) + (u(t), \varphi) = h(t)(f, \varphi) + \left(\int_0^t \mathcal{G}(s) u(s) \, \mathrm{d}s, \varphi \right), \quad \forall \varphi \in \mathrm{H}^1(\Omega),$$

and

$$h(t) = \frac{\left(\int_0^t \mathcal{G}(s) u(s) \, \mathrm{d}s, 1 \right)}{(f, 1)}$$

as $u(0) = 0$, $m = 0$ and $g = 0$

Uniqueness if $\partial_t\left(k*(u-\tilde{u}_0)\right) \in \mathrm{L}^2\left((0,T),\mathrm{H}^1(\Omega)^*\right)$: sketch of proof II

- Integrate the variational formulation with respect to time over $t \in (0,\eta) \subset (0,T)$, taking $\varphi = u(\eta)$ and integrate again over $t \in (0,\xi) \subset (0,T)$

$$\int_0^{\xi} ((k*u)(\eta),u(\eta))\,\mathrm{d}\eta + \frac{1}{2}\left\|\int_0^{\xi}\nabla u(t)\,\mathrm{d}t\right\|^2 + \frac{1}{2}\left\|\int_0^{\xi} u(t)\,\mathrm{d}t\right\|^2$$
$$= \int_0^{\xi}\left(\int_0^{\eta} h(t)\,\mathrm{d}t\right)(f,u(\eta))\,\mathrm{d}\eta + \int_0^{\xi}\left(\int_0^{\eta}\int_0^{t}\mathcal{G}(s)u(s)\ \mathrm{d}s\,\mathrm{d}t, u(\eta)\right)\mathrm{d}\eta$$

- k is strongly positive definite: $\int_0^{\xi}((k*u)(\eta),u(\eta))\,\mathrm{d}\eta \geqslant 0$
- Using partial integration, it follows that

$$|h(t)| = \left|\frac{1}{(f,1)}\left[\left(-\int_0^t \partial_s\mathcal{G}(s)\left(\int_0^s u(t)\,\mathrm{d}t\right)\,\mathrm{d}s + \mathcal{G}(t)\int_0^t u(s)\ \mathrm{d}s, 1\right)\right]\right|$$
$$\leqslant C\left\|\int_0^t u(s)\ \mathrm{d}s\right\|, \quad \text{for } t \in [0,T]$$

Uniqueness if $\partial_t (k * (u - \tilde{u}_0)) \in L^2\left((0,T), H^1(\Omega)^*\right)$: sketch of proof III

- Again using partial integration, we have that

$$\left|\int_0^\xi \left(\int_0^\eta h(t)\,dt\right)(f, u(\eta))\,d\eta\right| \leqslant C_\varepsilon \int_0^\xi \left\|\int_0^t u(s)\ ds\right\|^2 dt + \varepsilon \left\|\int_0^\xi u(t)\,dt\right\|^2$$

- Similarly

$$\left|\int_0^\xi \left(\int_0^\eta \int_0^t \mathcal{G}(s)u(s)\ ds\,dt, u(\eta)\right)d\eta\right| \leqslant C_\varepsilon \int_0^\xi \left\|\int_0^t u(s)\ ds\right\|^2 dt + \varepsilon \left\|\int_0^\xi u(t)\,dt\right\|^2$$

- Therefore

$$\left(\frac{1}{2} - \varepsilon\right)\left\|\int_0^\xi u(t)\,dt\right\|^2 + \frac{1}{2}\left\|\int_0^\xi \nabla u(t)\,dt\right\|^2 \leqslant C_\varepsilon \int_0^\xi \left\|\int_0^t u(s)\ ds\right\|^2 dt$$

- Grönwall lemma: $\int_0^\xi u(t)\,dt = 0$ a.e. in Ω for all $\xi \in (0,T)$
- Differentiating with respect to ξ gives that $u = 0$ a.e. in Q_T
- It follows that $h = 0$ in $(0,T)$

Uniqueness if $\partial_t (k * (u - \tilde{u}_0)) \in L^2\left((0,T), H^1(\Omega)^*\right)$: sketch of proof IV

- For the general operator L, we need to assume that
  - $\boldsymbol{A} \in \mathbf{L}^\infty(\overline{Q_T}) := \left(L^\infty(\overline{Q_T})\right)^{d\times d}$ is symmetric ($\boldsymbol{A}^\top = \boldsymbol{A}$) and uniformly elliptic, i.e. there exists a constant $\alpha > 0$ such that
    $$\sum_{i,j=1}^{d} a_{ij}(\mathbf{x},t)\xi_i\xi_j \geqslant \alpha\,|\xi|^2, \quad \text{for a.a. } (\mathbf{x},t) \in \overline{Q_T} \text{ and for all } \xi \in \mathbb{R}^d$$
  - $c \in L^\infty([0,T])$ such that
    $$c(t) \geqslant c_0 > 0, \qquad t \in [0,T]$$
  - $\partial_t \boldsymbol{A} \in (L^\infty(Q_T))^{d\times d}$, $\partial_t c \in L^\infty(0,T)$
- The proof seems not valid if c is also space-dependent

Uniqueness if $\partial_t (k * (u - \tilde{u}_0)) \in \mathrm{L}^2\left((0,T), \mathrm{L}^2(\Omega)\right)$: sketch of proof I

- Consider $L = -\Delta u$
- F be globally Lipschitz continuous it all its variables
- The differences $h := h_1 - h_2$ and $u := u_1 - u_2$ are satisfying

$$
\begin{aligned}
&((k * \partial_t u)(t), \varphi) + (\nabla u(t), \nabla\varphi) \\
&\qquad = h(t)\,(f,\varphi) + \left(\int_0^t [F(s,u_1(s)) - F(s,u_2(s))]\ \mathrm{d}s, \varphi\right), \quad \forall \varphi \in \mathrm{H}^1(\Omega),
\end{aligned}
$$

and

$$
h(t) = \frac{\left(\int_0^t [F(s,u_2(s)) - F(s,u_1(s))]\ \mathrm{d}s, 1\right)}{(f,1)}
$$

- We have that

$$
|h(t)| \leqslant C \int_0^t \|u(s)\|\ \mathrm{d}s, \quad \text{for } t \in [0,T]
$$

Uniqueness if $\partial_t\left(k * (u - \tilde{u}_0)\right) \in \mathrm{L}^2\left((0,T), \mathrm{L}^2(\Omega)\right)$: sketch of proof II

- Take $\varphi = u(t)$ in and integrate with respect to time over $(0,\eta) \subset (0,T)$

$$\int_0^\eta \left(\partial_t\left(k * u\right)(t), u(t)\right) \mathrm{d}t + \int_0^\eta \|\nabla u(t)\|^2 \, \mathrm{d}t$$
$$= \int_0^\eta h(t)\left(f, u(t)\right) \mathrm{d}t + \int_0^\eta \left(\int_0^t \left[F(s, u_1(s)) - F(s, u_2(s))\right] \, \mathrm{d}s, u(t)\right) \mathrm{d}t,$$

where we used Leibniz's rule for differentiation under the integral sign, i.e.

$$\partial_t\left(k * u\right) = k * \partial_t u + k\tilde{u}_0 = k * \partial_t u, \qquad \text{a.e. in } Q_T$$

- [Kubica and Yamamoto, 2018, Corollary 2] gives that

$$\int_0^\eta \left(\partial_t\left(k * u\right)(t), u(t)\right) \mathrm{d}t \geqslant \frac{k(T)}{2} \int_0^\eta \|u(t)\|^2 \, \mathrm{d}t$$

Uniqueness if $\partial_t\left(k * (u - \tilde{u}_0)\right) \in L^2\left((0,T), L^2(\Omega)\right)$: sketch of proof III

- We have that

$$\left|\int_0^\eta h(t)\,(f, u(t))\,\mathrm{d}t\right| \leqslant C_\varepsilon \int_0^\eta |h(t)|^2\,\mathrm{d}t + \varepsilon \int_0^\eta \|u(t)\|^2\,\mathrm{d}t$$
$$\leqslant C_\varepsilon \int_0^\eta \left(\int_0^t \|u(s)\|^2\,\mathrm{d}s\right)\mathrm{d}t + \varepsilon \int_0^\eta \|u(t)\|^2\,\mathrm{d}t$$

$$\int_0^\eta \left(\int_0^t [F(s, u_1(s)) - F(s, u_2(s))]\,\mathrm{d}s, u(t)\right)\mathrm{d}t$$
$$\leqslant C_\varepsilon \int_0^\eta \left(\int_0^t \|u(s)\|^2\,\mathrm{d}s\right)\mathrm{d}t + \varepsilon \int_0^\eta \|u(t)\|^2\,\mathrm{d}t$$

- Therefore

$$\left(\frac{k(T)}{2} - \varepsilon\right)\int_0^\eta \|u(t)\|^2\,\mathrm{d}t + \int_0^\eta \|\nabla u(t)\|^2\,\mathrm{d}t \leqslant C_\varepsilon \int_0^\eta \left(\int_0^t \|u(s)\|^2\,\mathrm{d}s\right)\mathrm{d}t$$

- Grönwall argument: $u = 0$ a.e. in Q_T and thus $h = 0$ a.e. in $(0, T)$

Uniqueness if $\partial_t (k * (u - \tilde{u}_0)) \in \mathrm{L}^2\left((0,T), \mathrm{L}^2(\Omega)\right)$: sketch of proof IV

- For the general operator L, we need to assume that
  - $\boldsymbol{A} \in \mathbf{L}^\infty(\overline{Q_T}) := \left(\mathrm{L}^\infty(\overline{Q_T})\right)^{d\times d}$ is symmetric ($\boldsymbol{A}^\top = \boldsymbol{A}$) and uniformly elliptic, i.e. there exists a constant $\alpha > 0$ such that

$$\sum_{i,j=1}^{d} a_{ij}(\mathbf{x},t)\xi_i\xi_j \geqslant \alpha\,|\xi|^2\,, \quad \text{for a.a. } (\mathbf{x},t) \in \overline{Q_T} \text{ and for all } \xi \in \mathbb{R}^d$$

  - $c \in \mathrm{L}^\infty([0,T])$ such that

$$c(t) \geqslant 0, \qquad t \in [0,T]$$

Existence of a solution for exact data: uniform mesh

- Rothe's method [Kačur, 1985]: divide $[0, T]$ into $n \in \mathbb{N}$ equidistant subintervals $(t_{i-1}, t_i]$ for $t_i = i\tau$, where $\tau = T/n < 1$ and for any function z

$$z_i \approx z(t_i), \qquad \partial_t z(t_i) \approx \delta z_i := \frac{z_i - z_{i-1}}{\tau}$$

- The time discrete convolution is defined as follows

$$(k * z)(t_i) \approx (k * z)_i := \sum_{l=1}^{i} k_{i+1-l} z_l \tau,$$

where we define

$$(k * z)_0 := 0$$

Time-discrete problem: uniform mesh

- Based on (P) and (MP), the following decoupled system for approximating the unknowns (h, u) at time t_i, $1 \leqslant i \leqslant n$, is proposed: Find $u_i \in \mathrm{H}^1(\Omega)$ and $h_i \in \mathbb{R}$ such that for all $\varphi \in \mathrm{H}^1(\Omega)$ it holds that

$$\langle (k * \delta u)_i, \varphi \rangle_{\mathrm{H}^1(\Omega)^* \times \mathrm{H}^1(\Omega)} + \mathcal{L}_i(u_i, \varphi) = h_i\,(f, \varphi) + \left(\sum_{l=1}^{i} F(t_l, u_{l-1})\tau, \varphi \right) - (g_i, \varphi)_\Gamma\,, \quad \text{(DPu}i\text{)}$$

with

$$h_i = \frac{(k * m')_i + \int_\Gamma g_i(\mathbf{x})\ \mathrm{d}\mathbf{x} + c_i m_i - \int_\Omega \left(\sum_{l=1}^{i} F(\mathbf{x}, t_l, u_{l-1}(\mathbf{x}))\tau \right) \mathrm{d}\mathbf{x}}{\int_\Omega f(\mathbf{x})\ \mathrm{d}\mathbf{x}} \qquad \text{(DMPu}i\text{)}$$

- For given $i \in \{1, \ldots, n\}$, first (DMPui) is solved and then (DPui)

- In the next lemmas, we put conditions on m such that $(k * m')_i$ is uniformly bounded and $(k * m')(0) = 0$
- Note that $(k * m')(0)$ is not necessarily equal to zero or well-defined for $m \in \mathrm{C}^1((0, T])$ as the following example shows:
  $m(t) = t^\gamma$ with $\gamma \in (0, \infty)$, then

$$(k * m)(t) = \begin{cases} \frac{t^{1-\beta+\gamma}\Gamma(1+\gamma)}{\Gamma(2-\beta+\gamma)} & \gamma \neq \beta, \\ t\Gamma(\beta+1) & \gamma = \beta, \end{cases}$$

$$(k * m')(t) = \begin{cases} \frac{t^{-\beta+\gamma}\Gamma(\gamma+1)}{\Gamma(-\beta+\gamma+1)} & \gamma \neq \beta, \\ \Gamma(\beta+1) & \gamma = \beta, \end{cases}$$

  and

$$(k * m')(0) = \lim_{t \searrow 0} (k * m')(t) = \begin{cases} 0 & \gamma > \beta, \\ \Gamma(\beta+1) & \gamma = \beta, \\ \infty & \gamma < \beta \end{cases}$$

- See also [Stynes, 2016]

- Existence of a unique solution on every time step follows from the Lax-Milgram lemma and it is stated in the following lemma

Lemma

Assume that $\tilde{u}_0 \in \mathrm{L}^2(\Omega)$, $f \in \mathrm{L}^2(\Omega)$ *with* $\int_\Omega f(\mathbf{x})\ \mathrm{d}\mathbf{x} \neq 0$, F *be globally Lipschitz continuous in all variables and* $g \in \mathrm{L}^2\left((0,T), \mathrm{L}^2(\Gamma)\right)$. *Moreover, assume* $m \in \mathrm{C}^1((0,T])$ *satisfying*

$$\left|\frac{\partial^l m}{\partial t^l}(t)\right| \leqslant C(1 + t^{\gamma - l}) \quad \text{for } l = 0,1, \quad \text{and for } 0 < t \leqslant T;$$

with $\gamma \in (\beta, 1)$ *fixed. Then, for any* $i = 1, 2, \ldots, n$, *there exists a unique couple* $\{u_i, h_i\} \in \mathrm{H}^1(\Omega) \times \mathbb{R}$ *solving* (DPui)-(DMPui)

- Next: derivation a priori estimates

Lemma (See Lemma 3.3 in [Šišková and Slodička, 2017])

Positive constants C *and* τ_0 *exist such that for and* $\tau < \tau_0$ *and every* $j = 1, 2, \ldots, n$, *the following relations hold*

$$\left(k * \|u\|^2\right)_j + \sum_{i=1}^{j} k_i \|u_i\|^2 \tau + \sum_{i=1}^{j} \|u_i\|^2_{\mathrm{H}^1(\Omega)} \tau \leqslant C, \qquad \left|h_j\right| \leqslant C$$

Lemma

Assume additionally that $\tilde{u}_0 \in \mathrm{H}^1(\Omega)$. *Moreover, assume that* (MP) *is well-defined at* $t = 0$ *with* $(k * m')(0) = 0$, *i.e.* $m \in \mathrm{C}^1((0,T])$ *and* $g \in \mathrm{C}^1\left((0,T], \mathrm{L}^2(\Gamma)\right)$ *satisfying*

$$\left|\frac{\partial^l m}{\partial t^l}(t)\right| \leqslant C(1 + t^{\gamma - l}) \qquad \text{for } l = 0,1 \quad \text{and for } 0 < t \leqslant T;$$

$$\left|(k * m')'(t)\right| \leqslant C(1 + t^{\gamma - \beta - 1}) \qquad \text{for } 0 < t \leqslant T;$$

$$\left\|\frac{\partial^l g}{\partial t^l}(t)\right\|_{\mathrm{L}^2(\Gamma)} \leqslant C(1 + t^{\gamma - l}) \qquad \text{for } l = 0,1 \quad \text{and for } 0 < t \leqslant T;$$

with $\gamma \in (\beta, 1)$ *fixed. Then, there exist positive constants* C *and* τ_0 *such that for every* $j = 1, 2, \ldots, n$ *and* $\tau < \tau_0$, *the followings relations hold true*

$$\|u_j\|^2_{\mathrm{H}^1(\Omega)} + \sum_{i=1}^{j} \|u_i - u_{i-1}\|^2_{\mathrm{H}^1(\Omega)} \leqslant C \quad \text{and} \quad \sum_{i=1}^{j} \left|\delta h_i\right| \tau \leqslant C$$

Corollary

There exist positive constants C *and* τ_0 *such that for every* $j = 1, 2, \ldots, n$ *and* $\tau < \tau_0$, *the following relation hold*

$$\left\|(k * \delta u)_j\right\|_{\mathrm{H}^1(\Omega)^*} \leqslant C$$

Rothe functions

- Piecewise constant and linear in time spline of the solutions $u_i, i = 1, \ldots, n$

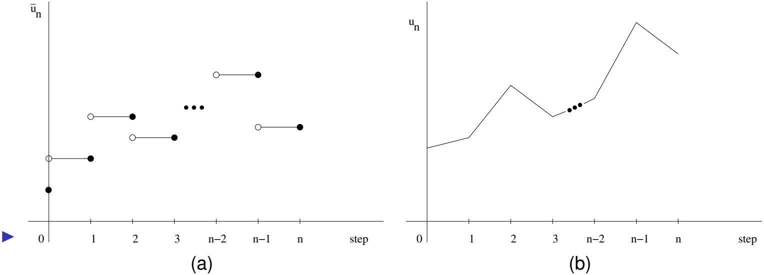


Figure: Rothe's piecewise constant function $\overline{u}_n$ (a) and Rothe's piecewise linear in time function u_n (b).

- Similarly, we define $\overline{k}_n$, $\overline{\mathcal{L}}_n$, $\overline{F}_n$, $\overline{g}_n$, $\overline{m}_n$, $\overline{m'}_n$ and $\overline{h}_n$
- Moreover, we define [Van Bockstal, 2020]

$$(k * u)_n : [0, T] \to \mathrm{L}^2(\Omega) : t \mapsto \begin{cases} 0 & t = 0 \\ (k * u)_{i-1} + (t - t_{i-1})\delta(k * u)_i & t \in (t_{i-1}, t_i] \end{cases}$$

- Using the a priori estimates and the Riesz-Frechét-Kolmogorov theorem [Kufner et al., 1977, Theorem 2.13.1], we obtain the following result

Theorem (Existence)

Let F be linear in u. There exists a unique couple $\{u, h\}$ *to the problem* (MP)-(P) *with*

$$u \in \mathrm{C}\left([0,T], \mathrm{H}^1(\Omega)^*\right) \cap \mathrm{L}^\infty\left((0,T), \mathrm{H}^1(\Omega)\right), \ h \in \mathrm{L}^\infty(0,T)$$

and

$$\partial_t (k * (u - \tilde{u}_0)) \in \mathrm{L}^\infty\left((0,T), \mathrm{H}^1(\Omega)^*\right)$$

Existence of a solution for exact data: graded mesh

- Now, we consider a graded time-partitioning of the time frame $[0, T]$
- Set $t_j = T(j/n)^r$ for $j = 0, 1, \dots, n$, where the constant mesh grading $r \geqslant 1$ is chosen by the user
- If $r = 1$, then the mesh is uniform
- We put $\tau_j := t_j - t_{j-1}$ for $j = 1, \dots, n$
- The $L1$-approximation on the graded meshes to the Caputo fractional derivative of order $\beta \in (0, 1)$ at the node t_i is given by [Brunner, 1985]

$$\left.\frac{\partial^\beta u}{\partial t^\beta}\right|_{t=t_i} = \int_0^{t_i} \frac{\partial u(s)}{\partial s} g_{1-\beta}(t_i - s)\ \mathrm{d}s \approx \sum_{l=1}^{i} \frac{u_l - u_{l-1}}{\tau_l} \int_{t_{l-1}}^{t_l} g_{1-\beta}(t_i - s)\ \mathrm{d}s + Q^i$$
$$= \sum_{l=1}^{i} \tilde{a}_{i,l}\,(u_l - u_{l-1}) + Q^i =: D_n^\beta u_i + Q^i,$$

where Q^i is the truncation error, the kernel $g_\beta(t) = \frac{t^{\beta-1}}{\Gamma(\beta)}$, and the coefficients $\tilde{a}_{i,l}$ can be evaluated by

$$\tilde{a}_{i,l} = \frac{g_{2-\beta}(t_i - t_{l-1}) - g_{2-\beta}(t_i - t_l)}{\tau_l}, \quad 1 \leqslant l \leqslant i$$

- A bound on the truncation error Q^j for the graded mesh can be found in the lemma below [Stynes et al., 2017, Lemma 5.1]

Lemma

Assume that $u \in C^2((0,T])$ *and there exists positive constants* C *such that*

$$\left|\frac{\partial^l u}{\partial t^l}(t)\right| \leqslant C(1 + t^{\beta - l}) \quad \text{for } l = 0,1,2, \quad \text{and for } 0 < t \leqslant T.$$

If the nonuniform grid fulfills

$$\tau_{j-1} \leqslant \tau_j, \quad 2 \leqslant j \leqslant n,$$

then the following inequality is achieved for $j \geqslant 1$,

$$\left|Q^j\right| = \left|\frac{\partial^\beta}{\partial t^\beta} u(t_j) - D_n^\beta u(t_j)\right| \leqslant C j^{-\min\{r\beta, 2-\beta\}}$$

- The optimal graded mesh is obtained when $r_{\text{opt}} := (2-\beta)/\beta$, and this gives the most possible high rate of convergence $\mathcal{O}\left(n^{-\{2-\beta\}}\right)$
- Additionally, if we choose $r > r_{\text{opt}}$, this will increase the temporal mesh near $t = T$ and so the constant multiplier C will be increased

Time-discrete problem: graded mesh

Using the graded mesh, we approximate problem (MP)-(P) at time $t = t_i$ as follows: Find $u_i \in \mathrm{H}^1(\Omega)$ and $h_i \in \mathbb{R}$ such that for all $\varphi \in \mathrm{H}^1(\Omega)$ it holds that

$$\left(D_n^{\beta} u_i, \varphi\right)_{\mathrm{H}^1(\Omega)^* \times \mathrm{H}^1(\Omega)} + \mathcal{L}_i(u_i, \varphi) = h_i (f, \varphi) + \left(\sum_{l=1}^{i} F(t_l, u_{l-1})\tau_l, \varphi\right) - (g_i, \varphi)_{\Gamma}, \quad \text{(DMPg}i\text{)}$$

and

$$h_i = \frac{D_n^{\beta} m_i + (g_i, 1)_{\Gamma} + c_i m_i - \left(\sum_{l=1}^{i} F(t_l, u_{l-1})\tau_l, 1\right)}{(f, 1)} \quad \text{(DPg}i\text{)}$$

- Following fractional Grönwall lemma [Liao et al., 2018, Lemma 2.2] related to graded meshes is used when establishing a priori estimates for u_j and h_j

Lemma (Nonuniform discrete fractional Grönwall inequality)

For any finite time $t_n = T > 0$, and a given nonnegative sequence $(\lambda_l)_{l=0}^{n-1}$, assume that there exists a constant λ, independent of time-steps, such that $\lambda \geqslant \sum_{l=0}^{n-1} \lambda_l$ and let $\{u_i\}_{i=1}^{n}$ and $\{\zeta_i, g_i\}_{i=1}^{n}$ be sequences of non-negative numbers that satisfy

$$D_n^{\beta}(u_i)^2 \leqslant \sum_{l=1}^{i} \lambda_{i-l}(u_l)^2 + u_i(\zeta_i + g_i), \quad \text{or} \quad D_n^{\beta}(u_i)^2 \leqslant \sum_{l=1}^{i} \lambda_{i-l}(u_l)^2 + \zeta_i + g_i, \quad \forall\, i = 1, \dots, n.$$

If the time grids satisfy $\tau_{j-1} \leqslant \tau_j, 2 \leqslant j \leqslant n$, with the maximum time grid $\tau_n \leqslant \tau^{\triangle} = \sqrt[\beta]{\frac{1}{2\Gamma(2-\beta)\lambda}}$, the following inequality holds

$$u_i \leqslant 2\left(u_0 + \mathrm{g}_{1+\beta}(t_i) \max_{1 \leqslant j \leqslant i}\left(\zeta_j + g_j\right)\right) E_{\beta}(2\lambda t_i^{\beta}), \quad 1 \leqslant i \leqslant n,$$

where E_β denotes the Mittag–Leffler function with parameter β

- A priori estimate

Lemma

Assume that $\tilde{u}_0 \in \mathrm{L}^2(\Omega)$, $f \in \mathrm{L}^2(\Omega)$ *with* $\int_\Omega f(\mathbf{x})\,\mathrm{d}\mathbf{x} \neq 0$, $c(t) \geqslant \tilde{c}_0 > 0$ *for* $t \in [0,T]$, F *be globally Lipschitz continuous in all variables and* $g \in \mathrm{L}^\infty\left((0,T),\mathrm{L}^2(\Gamma)\right)$. *Moreover, suppose that* $m \in \mathrm{C}^1((0,T])$ *is satisfying*

$$\left|\frac{\partial^l m}{\partial t^l}(t)\right| \leqslant C(1+t^{\beta-l}) \quad \text{for } l=0,1,2 \quad \text{and for } 0<t\leqslant T;$$

Then, for any $i=1,2,\dots,n$, *there exists a unique couple* $\{u_i,h_i\} \in \mathrm{H}^1(\Omega)\times\mathbb{R}$ *solving* (DMPgi)-(DPgi) *and there exist positive constants* C *such that*

$$\max_{1\leqslant i\leqslant n}\left\{D_n^\beta\|u_i\|^2 + \|u_i\|^2_{\mathrm{H}^1(\Omega)}\right\} \leqslant C, \quad \max_{1\leqslant i\leqslant n}|h_i| \leqslant C$$

Theorem (Existence and uniqueness: graded mesh)

Assume that $r\beta > 1$ *and that the solution* u *of* (MP)-(P) *and the measurement* m *satisfy the bounds*

$$\left|\frac{\partial^l u}{\partial t^l}(\mathbf{x},t)\right| \leqslant C(1+t^{\beta-l}) \quad \text{for } l=0,1,2, \quad \text{and for a.a. } \mathbf{x}\in\Omega \text{ and } 0<t\leqslant T;$$

$$\left|\frac{\partial^l m}{\partial t^l}(t)\right| \leqslant C(1+t^{\beta-l}) \quad \text{for } l=0,1,2, \quad \text{and for } 0<t\leqslant T.$$

Then there exists a unique couple $\{u,h\}$ *to the problem* (MP)-(P) *with*

$$u \in \mathrm{C}\left([0,T],\mathrm{L}^2(\Omega)\right)\cap\mathrm{L}^\infty\left((0,T),\mathrm{H}^1(\Omega)\right),\ h\in\mathrm{L}^\infty(0,T) \text{ and } k*\partial_t u \in \mathrm{L}^\infty\left((0,T),\mathrm{L}^2(\Omega)\right)$$

Numerical experiment: setting

- $T = 0.5$ and $\Omega = (0, 1)$
- $\boldsymbol{A} = \boldsymbol{I}$ and $c = 1$
- Number of time discretization intervals $n = 200$ and $r = r_{\text{opt}} = (2 - \beta)/\beta$ for the graded grid parameter
- $F(t, u) = -tu$
- We consider as exact solution the non-smooth function ($\partial_t u$ blows up as $t \to 0^+$) prescribed by

$$u_{\text{ex}}(x, t) = \left(t^3 + t^\gamma\right)\sin(x), \qquad \gamma \in (0, 1)$$

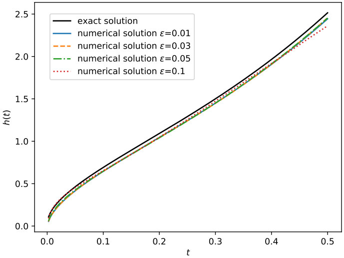
- Overview of experiments
  - Experiment 1: $\gamma = 0.9$ and $\beta = 0.5$;
  - Experiment 2: $\gamma = \beta = 0.5$;
  - Experiment 3: $\gamma = \beta = 0.2$;
  - Experiment 4: $\gamma = \beta = 0.8$
- For Experiments 2-4, only the conditions for the convergence of the graded $L1$-scheme are satisfied. However, we show also the results obtained via the convolution quadrature

Numerical experiment: setting

- At each time-step, the resulting elliptic forward problems are solved numerically by the finite element method (FEM) using first order (P1-FEM) Lagrange polynomials for the space discretization. A fixed uniform mesh consisting of 100 intervals is used
- A randomly generated uncorrelated noise is added to the additional condition in order to simulate the inherent errors present in real measurements (noise $\times \mathcal{N}(0,1)$)
- The noisy data is regularized by using the nonlinear least-squares method to obtain a function approximating the noisy datao the form

$$m_{\varepsilon,\mathrm{reg}}(t) = \alpha_5 t^{\alpha_4} + \alpha_3 t^3 + \alpha_2 t^2 + \alpha_1 t + \alpha_0, \quad \alpha_i \in \mathbb{R}$$

- FEniCS project — The finite element library DOLFIN [Logg and Wells, 2010, Logg et al., 2012b] from the FEniCS project [Logg et al., 2012a] is used



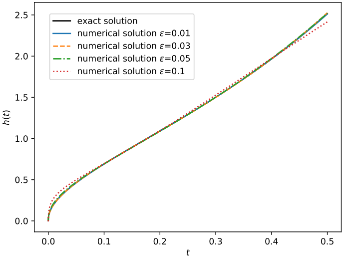


Figure: Experiment 1 ($\gamma = 0.9, \beta = 0.5$): The exact source and its numerical approximations using (a) uniform mesh and (b) graded mesh, obtained for various levels of noise.

- Both approximations are accurate but the absolute error is the smallest for the graded $L1$-scheme

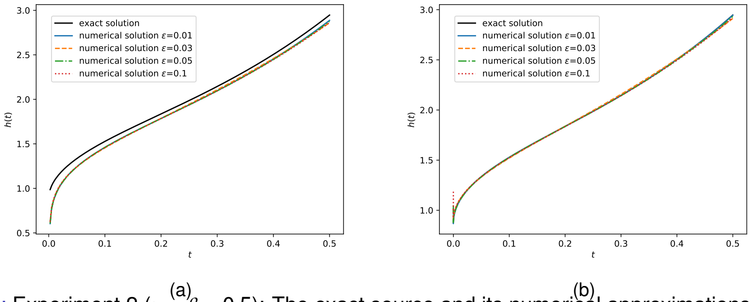


Figure: Experiment 2 ($\gamma = \beta = 0.5$): The exact source and its numerical approximations using (a) uniform mesh and (b) graded mesh, obtained for various levels of noise.

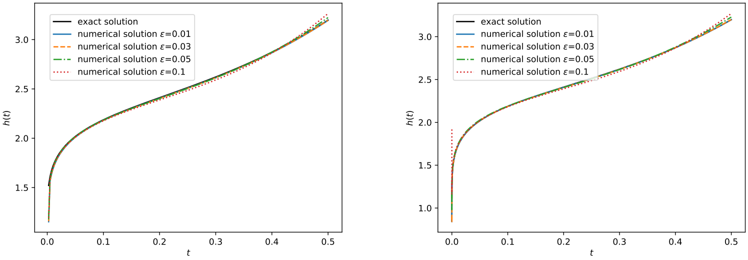
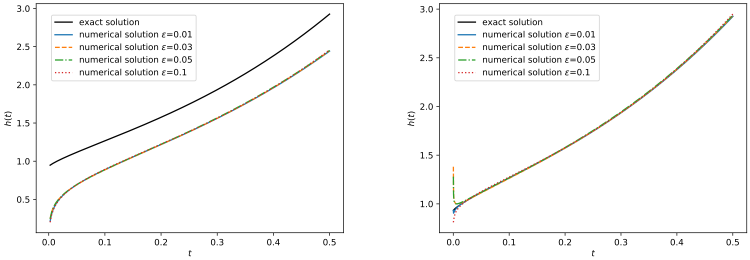


Figure: Experiment 3 ($\gamma = \beta = 0.2$): The exact source and its numerical approximations using (a) uniform mesh and (b) graded mesh, obtained for various levels of noise.



(a) (b)

Figure: Experiment 4 ($\gamma = \beta = 0.8$): The exact source and its numerical approximations using (a) uniform mesh and (b) graded mesh, obtained for various levels of noise.

- It is clear from these experiments that Rothe's method over graded meshes copes better with the behaviour at $t = 0$ of the solution
- In Experiment 4 the approximation obtained via the graded $L1$-scheme is less accurate than in the previous experiments as the graded grid parameter r_{opt} becomes closer to 1 for increasing β

Future research

- Results are submitted to *Journal of Scientific Computing*
- Performing the same experiments with $c = 0$ gives similar results, which suggests that the condition $c \geqslant c_0 > 0$ made in the analysis can be relaxed
- Consider $(k * m')(0) \in \mathbb{R}$ instead of $(k * m')(0) = 0$
- Improve the approximation of h_1
- Consider the measurement $\int_\Omega \omega(\mathbf{x}) u(\mathbf{x}, t) \, \mathrm{d}\mathbf{x}$, eventually with $\int_\Omega f(\mathbf{x}) \omega(\mathbf{x}) \, \mathrm{d}\mathbf{x} = 0$, i.e. when there is no access to the source
- Extend the results to multiterm fractional diffusion equations

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