POINTWISE-IN-TIME A-PRIORI AND A-POSTERIORI ERROR CONTROL FOR TIME-FRACTIONAL SEMILINEAR PARABOLIC EQUATIONS

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- Consider a fractional-order **semilinear** parabolic problem with $\alpha \in (0,1)$:

$$D_t^\alpha u + \mathcal{L}u + f(x,t,u) = 0 \quad \text{for } (x,t) \in \Omega \times (0,T]$$

where $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, subject to $u(x,0) = u_0(x)$ and $u = 0$ on $\partial\Omega$

$D_t^\alpha u(\cdot,t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha}\, \partial_s u(\cdot,s)\, ds$ =**Caputo fractional derivative**

$\mathcal{L}u := \sum_{k=1}^d \Big\{ -\partial_{x_k}(a_k(x,t)\, \partial_{x_k} u) + b_k(x,t)\, \partial_{x_k} u \Big\} + c(x,t)\, u$ =2nd order, elliptic

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$$D_t^\alpha u(\cdot,t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha}\, \partial_s u(\cdot,s)\, ds \qquad = \textbf{Caputo fractional derivative}$$

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. . . .

- For the a priori error analysis, we assume: there exists a unique solution of this problem in $C(\bar\Omega \times [0,T])$:

$$\boxed{|\partial_t^l u(\cdot,t)| \lesssim 1 + t^{\alpha - l}} \quad \text{for } l = 0,1,2$$

NOTE: This is a realistic assumption, in contrast to $|\partial^l u(\cdot,t)| \lesssim 1$...

Also, our framework applies to less singular solutions...

PART #1 (most of the talk)

Pointwise-in-time **a priori error analysis** on quasi-graded temporal meshes

N. Kopteva, *Error analysis for time-fractional semilinear parabolic equations using upper and lower solutions*, SIAM J. Numer. Anal., 58 (2020), 2212–2234.

MESSAGES:

+ works for the reaction coefficient of arbitrary sign (in the linear case) + Allen-Cahn case, etc.

+ works on quasi-graded meshes of arbitrary degree of grading

+ the above mesh may be ”arbitrarily” refined (any new nodes may be added)

+ predicts that milder (compared to the optimal) grading yields optimal convergence rates in positive time + ”optimal” grading yields global accuracy

+ prove that computed solutions lie within a certain range (similarly to u)

- Our AIM: estimate, **a priori**, the **pointwise-in-time errors** in $L_\infty(\Omega)$ and $L_2(\Omega)$ norms on **reasonably general temporal meshes**: quasi-graded meshes with arbitrary degree of grading that are allowed to be "arbitrarily" refined...

. . . .

- **Discrete Laplace transform approach**: low regularity assumptions on the exact solution, BUT **uniform meshes** (frequently convergence in positive time)
  [B. Jin, R. Lazarov, Z. Zhou, IMA J. Numer. Anal., 2016], ...
  [B. Jin, R. Lazarov, Z. Zhou, CMAME, 2019 – review]
- **Graded temporal meshes** $\Rightarrow$ global in time convergence:
  [H. Brunner, Math. Comp., 1985] – collocation for Volterra integral equations
  [W. McLean, K. Mustapha, Numer. Math., 2007] – fractional wave equation
  [K. Mustapha, B. Abdallah, K. M. Furati, 2014] — high-order Petrov-Galerkin in time
  [M. Stynes, E. O'Riordan, J. L. Gracia, SINUM, 2017] — L1 method
- **Discrete Grönwall inequality** on general temporal meshes
  [H.-L. Liao, D. Li, J. Zhang, SINUM, 2018],
  [H.-L. Liao, W. McLean, J. Zhang, SINUM, 2019],...
- **Barrier functions on quasi-graded temporal meshes** $\Rightarrow$ sharp pointwise-in-time bounds
  [N. Kopteva, X. Meng, SINUM, 2020]: L1 and Alikhanov,
  [N. Kopteva, SINUM, 2021]: L2 method

- Some earlier work: [Q. Du, J. Yang, Z. Zhou, J. Sci. Comput., 2020], [B. Jin, B. Li, Z. Zhou, SINUM, 2018], [B. Ji, H.-L. Liao, L. Zhang, Adv. Comput. Math, 2020], [H.-L. Liao, T. Tang, T. Zhou, , J. Sci. Comput., 2020], ... energy stable methods...

. . . .

- We employ the **method of discrete upper and lower solutions**
  - They work for arbitrarily large times
  - Under conditions A1 and A2, whenever the exact solution lies within a certain range (e.g., $[\sigma_1, \sigma_2]$, or it is positive), the method of discrete upper and lower solutions easily yields a similar property for the computed solutions.

- The **pointwise-in-time error estimates**: from the linear to the semilinear case
  - The main stability property is extended to the case of reaction coefficient of arbitrary sign

    (a version for arbitrarily large T is also discussed)

    A1 $\Rightarrow$ same pointwise-in-time error bounds as in the linear case....
  - Generalizations of the above results for other types of boundary conditions:

    nonhomogeneous Dirichlet + periodic + Neumann/Robin/mixed

§**1** Assumptions A1 + A2 on the **nonlinearity** f (and where they are used):

A1 is the only assumption on f required for the convergence analysis!

Examples: reaction coefficient of arbitrary sign, Allen-Cahn, Fisher, etc.

§**2** **Assumptions on temporal meshes**: quasi-graded, of arbitrary degree of grading, may be "arbitrarily" refined (any new nodes may be added)

§**3** **Stability result for the nonlinear case** for the **L1 method**

sharp + general + relatively simple proof + useful

of type: [N. Kopteva and X. Meng, *Error analysis for a fractional-derivative parabolic problem on quasi-graded meshes using barrier functions*, SIAM J. Numer. Anal., 58 (2020), 1217–1238]

§**4** **Main convergence result** + discussion + numerical results:

+ optimal grading $r = (2 - \alpha)/\alpha$ yields optimal convergence globally
+ milder grading $r > 2 - \alpha$ yields optimal convergence rates in positive time, etc.

L1 semi-discretizations in time + finite differences + finite elements + various BC

- Consider a semilinear fractional-order parabolic problem with $\alpha \in (0,1)$:

$$D_t^\alpha u + \mathcal{L}u + f(x,t,u) = 0 \quad \text{for } (x,t) \in \Omega \times (0,T]$$

A1. Let f be continuous in s and satisfy $f(\cdot,t,s) \in L_\infty(\Omega)$ for all $t > 0$ and $s \in \mathbb{R}$, and the one-sided Lipschitz condition with some constant $\boxed{\lambda \geqslant 0}$:

$$f(x,t,s_1) - f(x,t,s_2) \geqslant -\lambda(s_1 - s_2) \qquad \forall s_1 \geqslant s_2, \quad x \in \Omega, \quad t > 0$$

equivalent to $(s_1 - s_2)\left(f(x,t,s_1) - f(x,t,s_2)\right) \geqslant -\lambda(s_1 - s_2)^2 \ \forall s_1, s_2 \in \mathbb{R}$

also equivalent to $\partial_u f \geqslant -\lambda$ if f is smooth

. . . .

IMPORTANT MESSAGE:

A1 is the only assumption on f required for the convergence analysis!

- Consider a semilinear fractional-order parabolic problem with $\alpha \in (0,1)$:

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A2. There exist constants $\sigma_1 \leqslant 0 \leqslant \sigma_2$: $f(\cdot,\cdot,\sigma_1) \leqslant 0$ and $f(\cdot,\cdot,\sigma_2) \geqslant 0$.

. . . .

- Consider a semilinear fractional-order parabolic problem with $\alpha \in (0,1)$:

$$D_t^\alpha u + \mathcal{L}u + f(x,t,u) = 0 \quad \text{for } (x,t) \in \Omega \times (0,T]$$

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. . . .

- Example 1 (Negative reaction coefficient). The linear $f = c^*(x,t)\,u - F(x,t)$, with a possibly negative diffusion coefficient $c^* \geqslant -\lambda$, clearly satisfies **A1**; e.g. $D_t^\alpha u + \mathcal{L}u - u = F(x,t)$...

  Example 2 (Allen-Cahn equation). The cubic $f = u^3 - u$ satisfies both **A1** and A2 with, e.g., $-\sigma_1 = \sigma_2 = 1$. Note that if $|u_0| \leqslant 1$, then $|u| \leqslant 1\ \forall\, t$, while our results below imply a similar property for the computed solutions.

  Example 3 (Fisher equation). The quadratic $f = u^2 - u$ satisfies A2 with, e.g., $\sigma_1 = 0$ and $\sigma_2 = 1$, but **not A1** (which is easily addressed below...)

- Consider a semilinear fractional-order parabolic problem with $\alpha \in (0,1)$:

$$D_t^\alpha u + \mathcal{L}u + f(x,t,u) = 0 \quad \text{for } (x,t) \in \Omega \times (0,T]$$

- Approach I (well known for classical semilinear equations...)

Suppose that $\sigma_1 \leqslant u \leqslant \sigma_2$ $\forall (x,t) \in \Omega \times [0,T]$ (equivalent to u bounded)

i. Suppose $\tilde{f}(x,t,u) := \begin{cases} f(x,t,\sigma_1^*) & \text{for } u < \sigma_1^* < \sigma_1 \\ f(x,t,u) & \text{for } \sigma_1^* \leqslant u \leqslant \sigma_2^* \\ f(x,t,\sigma_2^*) & \text{for } u > \sigma_2^* > \sigma_2 \end{cases}$ satisfies **A1**.

ii. Let $\tilde{u}_h$ be the computed solution using $\tilde{f}$

$$\Rightarrow \quad \tilde{u}_h = u + O(M^{-q}) \quad \text{(under assumption A1; see §3+§4 below)}$$

iii. If M is sufficiently large $\Rightarrow$ $|\tilde{u}_h - u| \leqslant \max\{|\sigma_1^* - \sigma_1|, |\sigma_2^* - \sigma_2|\}$

$$\Rightarrow \sigma_1^* \leqslant \tilde{u}_h \leqslant \sigma_2^* \quad \Rightarrow \tilde{f}(x,t,\tilde{u}_h) = f(x,t,\tilde{u}_h)$$

Hence, $\tilde{u}_h = u_h$, computed solution using f.

$$\Rightarrow \boxed{u_h = u + O(M^{-q})} \qquad \square$$

- Consider a semilinear fractional-order parabolic problem with $\alpha \in (0,1)$:

$$D_t^\alpha u + \mathcal{L}u + f(x,t,u) = 0 \quad \text{for } (x,t) \in \Omega \times (0,T]$$

A2. There exist constants $\sigma_1 \leqslant 0 \leqslant \sigma_2$: $f(\cdot,\cdot,\sigma_1) \leqslant 0$ and $f(\cdot,\cdot,\sigma_2) \geqslant 0$.

. . . .

- Example 3 (Fisher equation). The quadratic $f = u^2 - u$ satisfies A2 with, e.g., $\sigma_1 = 0$ and $\sigma_2 = 1$, but **not A1** (which is easily addressed below...)

. . . .

- Approach II —using **A2**

  see [§8.1 in N. Kopteva, *Error analysis for time-fractional semilinear parabolic equations using upper and lower solutions*, SIAM J. Numer. Anal., 58 (2020), 2212–2234]

Steps i+ii: as before, only with $\sigma_1^* = \sigma_1$ and $\sigma_2^* := \sigma_2$. Now $\tilde{f}(x,t,u)$ satisfies **A1** + **A2**.

iii. By **A2**, the unique computed solution $\boxed{\sigma_1 \leqslant \tilde{u}_h \leqslant \sigma_2}$

see [§2–*Discrete upper and lower solutions* in the above paper]

Hence, again $\tilde{u}_h = u_h$, computed solution using $f \;\Rightarrow\; \boxed{u_h = u + O(M^{-q})}$ $\square$

- Our ASSUMPTION on the temporal mesh $\{t_j\}_{j=0}^{M}$ on $[0,T]$:

$$\boxed{\tau := t_1 \simeq M^{-r}, \qquad \tau_j := t_j - t_{j-1} \lesssim \tau^{1/r}\, t_j^{1-1/r}}$$

with some $r \geqslant 1$

see [§2.4 in Kopteva+Meng, SINUM, 2020]

- **Graded** temporal mesh $\boxed{\{t_j = T(j/M)^r\}_{j=0}^{M}}$ satisfies $\tau_j \simeq \tau^{1/r}\, t_j^{1-1/r}$

- Given a **(quasi-)graded** temporal mesh $\boxed{\tau_j \simeq \tau^{1/r}\, t_j^{1-1/r}}$, we are allowed to **add new nodes** in an arbitrary manner, but with the first mesh interval unchanged...

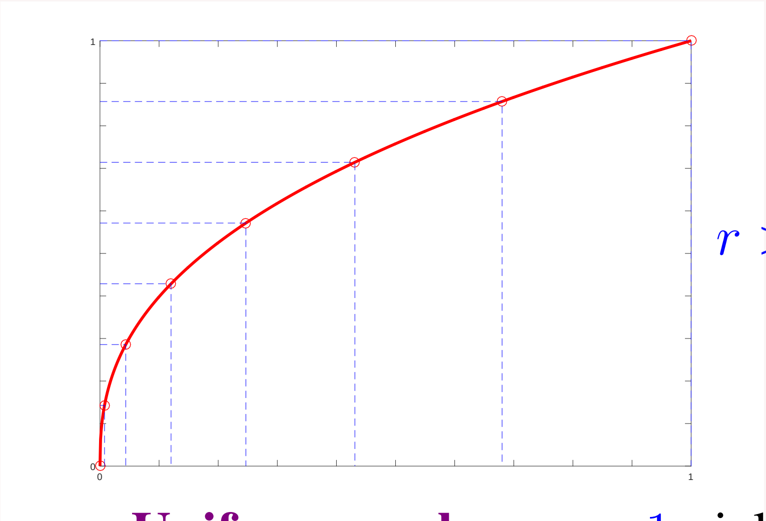
- Note the case $\boxed{r = 1}$: we are allowed **add new nodes** in an arbitrary manner to a **quasi-uniform** mesh, but the first mesh interval unchanged

- We assume: there exists a unique solution of this problem in $C(\bar\Omega \times [0,T])$:

$$\boxed{|\partial_t^l u(\cdot,t)| \lesssim 1 + t^{\alpha-l}} \quad \text{for } l = 0,1,2$$

NOTE: This is a realistic assumption, in contrast to $|\partial^l u(\cdot,t)| \lesssim 1$;

- **Graded meshes** in time: $\boxed{\{t_j = T(j/M)^r\}_{j=0}^{M} \text{ with some } r > 1}$



$r = (2-\alpha)/\alpha$ yields **optimal global accuracy**

$r > 2-\alpha$ yields **optimal accuracy in positive time**

- **Uniform meshes**: $r = 1$ yields **sub-optimal convergence in positive time**...

- **STABILITY result** [Kopteva+Meng]: Given an **inverse-monotone** discrete fractional-derivative operator δ_t^α, associated with a temporal mesh $\{t_j\}_{j=0}^M$ on $[0,T]$ with $\boxed{\tau := t_1}$, and $\gamma \in \mathbb{R}$, under the above condition on the mesh:

$$\boxed{\left.\begin{array}{l} |\delta_t^\alpha V^j| \lesssim (\tau/t_j)^{\gamma+1} \\ \forall j \geqslant 1, \quad V^0 = 0 \end{array}\right\} \;\Rightarrow\; |V^j| \lesssim \mathcal{V}^j := \tau t_j^{\alpha-1} \begin{cases} 1 & \text{if } \gamma > 0 \\ 1 + \ln(t_j/\tau) & \text{if } \gamma = 0 \\ (\tau/t_j)^\gamma & \text{if } \gamma < 0 \end{cases}}$$

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- SHARP consistent with the analogous property for the continuous D_t^α...
- USEFUL as truncation errors in time are bounded by negative powers of t_j

  $\Rightarrow$ **sharp pointwise-in-time error bounds**
- Relatively SIMPLE proof using clever **BARRIER functions** + **DMP**...
- GENERAL this approach was applied to
  - **3 discrete fractional-derivative operators**: L1 + Alikhanov + L2...
  - **Quasi-graded temporal meshes** with arbitrary degree of grading...

- **STABILITY result** [Kopteva+Meng]: Given an **inverse-monotone** discrete fractional-derivative operator δ_t^α, associated with a temporal mesh $\{t_j\}_{j=0}^M$ on $[0,T]$ with $\boxed{\tau := t_1}$, and $\gamma \in \mathbb{R}$, under the above condition on the mesh:

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- $\boxed{\text{SHARP}}$ consistent with the analogous property for the continuous D_t^α:

$$\left.\begin{array}{c} D_t^\alpha v(t) = F(t) := \min\{1, (\tau/t)^{\gamma+1}\} \\ \forall t > 0, \qquad v(0) = 0 \end{array}\right\} \Rightarrow v(t) \simeq \mathcal{V}(t) \quad \text{for } t \geqslant \tau$$

— using $v(t) = J_t^\alpha F(t) = \{\Gamma(\alpha)\}^{-1} \int_0^t (t-s)^{\alpha-1} F(s)\, ds$

- NOTE: the explicit inverse of D_t^α is J_t^α — readily available;

- HOWEVER, for any discrete δ_t^α, the above result is **NON-TRIVIAL**

- **STABILITY result** [Kopteva+Meng]: Given an **inverse-monotone** discrete fractional-derivative operator δ_t^α, associated with a temporal mesh $\{t_j\}_{j=0}^M$ on $[0,T]$ with $\boxed{\tau := t_1}$, and $\gamma \in \mathbb{R}$, under the above condition on the mesh:

$$\left.\begin{array}{c} |\delta_t^\alpha V^j| \lesssim (\tau/t_j)^{\gamma+1} \\ \forall j \geqslant 1, \quad V^0 = 0 \end{array}\right\} \Rightarrow \quad |V^j| \lesssim \mathcal{V}^j := \tau t_j^{\alpha-1} \begin{cases} 1 & \text{if } \gamma > 0 \\ 1 + \ln(t_j/\tau) & \text{if } \gamma = 0 \\ (\tau/t_j)^\gamma & \text{if } \gamma < 0 \end{cases}$$

. . . .

- **New STABILITY result:** Given an **L1-type** discrete fractional-derivative operator δ_t^α, associated with a temporal mesh $\{t_j\}_{j=0}^M$ on $[0,T]$ with $\boxed{\tau := t_1}$, and $\gamma \in \mathbb{R}$, under the above condition on the mesh and $\lambda \tau_j^\alpha \leqslant \{\Gamma(2-\alpha)\}^{-1}$:

$$\left.\begin{array}{c} |(\delta_t^\alpha - \lambda) V^j| \lesssim (\tau/t_j)^{\gamma+1} \\ \forall j \geqslant 1, \quad V^0 = 0 \end{array}\right\} \Rightarrow \quad |V^j| \lesssim \mathcal{V}^j := \tau t_j^{\alpha-1} \begin{cases} 1 & \text{if } \gamma > 0 \\ (\tau/t_j)^\gamma & \text{if } \gamma < 0 \end{cases}$$

Does NOT follow from [Kopteva+Meng] (as $\lambda > 0$)

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$$\left.\begin{array}{c} |(\delta_t^\alpha - \lambda)V^j| \lesssim (\tau/t_j)^{\gamma+1} \\ \forall j \geqslant 1, \quad V^0 = 0 \end{array}\right\} \Rightarrow \quad |V^j| \lesssim \mathcal{V}^j := \tau t_j^{\alpha-1} \begin{cases} 1 & \text{if } \gamma > 0 \\ (\tau/t_j)^\gamma & \text{if } \gamma < 0 \end{cases}$$

Does NOT follow from [Kopteva+Meng] (as $\lambda > 0$)

- **PROOF:**

Step 1 [Comparision principle for $\delta_t^\alpha - \lambda$] Let $\lambda\tau_j^\alpha < \{\Gamma(2-\alpha)\}^{-1}\ \forall\, j \geqslant 1$. Then $V^0 \leqslant B^0$ and $(\delta_t^\alpha - \lambda)V^m \leqslant (\delta_t^\alpha - \lambda)B^m\ \forall\, m$ imply $V^m \leqslant B^m\ \forall\, m$.

(The proof is elementary. $\{B^m\}$ is called an upper barrier or an upper solution.)

Step 2 **Construction of a suitable barrier $\{B^m\}$ — the non-trivial part!**

so that $-B^m \leqslant V^m \leqslant B^m$...

HINT: we use a certain **linear combination of certain barriers from [Kopteva+Meng]**...

- **New STABILITY result:** Given an **L1-type** discrete fractional-derivative operator δ_t^α, associated with a temporal mesh $\{t_j\}_{j=0}^M$ on $[0,T]$ with $\boxed{\tau := t_1}$, and $\gamma \in \mathbb{R}$, under the above condition on the mesh and $\lambda\tau_j^\alpha \leqslant \{\Gamma(2-\alpha)\}^{-1}$:

$$\boxed{\left.\begin{array}{c} |(\delta_t^\alpha - \lambda)V^j| \lesssim (\tau/t_j)^{\gamma+1} \\ \forall j \geqslant 1, \quad V^0 = 0 \end{array}\right\} \Rightarrow \; |V^j| \lesssim \mathcal{V}^j := \tau t_j^{\alpha-1} \begin{cases} 1 & \text{if } \gamma > 0 \\ (\tau/t_j)^\gamma & \text{if } \gamma < 0 \end{cases}}$$

- Note a **straightforward EQUIVALENT version:**

$$\boxed{\left.\begin{array}{c} (\delta_t^\alpha - \lambda)W^j \lesssim (\tau/t_j)^{\gamma+1} \\ \forall j \geqslant 1, \quad W^0 = 0 \end{array}\right\} \Rightarrow \; W^j \lesssim \mathcal{V}^j := \tau t_j^{\alpha-1} \begin{cases} 1 & \text{if } \gamma > 0 \\ (\tau/t_j)^\gamma & \text{if } \gamma < 0 \end{cases}}$$

PROOF (standard in the context of finite differences; rely on $|a| \leqslant b \Leftrightarrow -b \leqslant a \leqslant b$)

$\boxed{\Leftarrow}$ Apply the above for $W^j = \pm V^j$... $\boxed{\Rightarrow}$ Either use the same barrier directly for $\{W^j\}$;

OR employ $(\delta_t^\alpha - \lambda)V^j = (\tau/t_j)^{\gamma+1}$ subject to $V^0 = 0 \Rightarrow W^j \leqslant V^j \lesssim \cdots$

NOTE: **in the above, one may, of course, replace W^j by $|W^j|$ and get another useful version...**

- **New STABILITY result:** Given an **L1-type** discrete fractional-derivative operator δ_t^α, associated with a temporal mesh $\{t_j\}_{j=0}^M$ on $[0,T]$ with $\boxed{\tau := t_1}$, and $\gamma \in \mathbb{R}$, under the above condition on the mesh and $\lambda\tau_j^\alpha \leqslant \{\Gamma(2-\alpha)\}^{-1}$:

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- **Another possible version**

$$\boxed{\left.\begin{array}{c} |(\delta_t^\alpha - \lambda)V^j - \lambda^* V^{j-1}| \lesssim (\tau/t_j)^{\gamma+1} \\ \forall j \geqslant 1, \quad V^0 = 0 \end{array}\right\} \Rightarrow |V^j| \lesssim \mathcal{V}^j := \tau t_j^{\alpha-1} \begin{cases} 1 & \text{if } \gamma > 0 \\ (\tau/t_j)^\gamma & \text{if } \gamma < 0 \end{cases}}$$

- **PROOF requires very minor changes**

  Step 1 [Comparision principle for $(\delta_t^\alpha - \lambda)V^j - \lambda^* V^{j-1}$] is as straightforward...

  Step 2 **Similar barrier $\{B^m\}$ works...**

The convergence results in [Kopteva, SINUM, 2020] are presented as follows:

- Section 4 Paradigm for temporal-discretization error analysis:
  simplest example $D_t^\alpha u + f(t, u) = 0$

- Section 5 + 6 + 7 **Semi-linear parabolic case**
  - Semidiscretization in time: $L_2(\Omega)$ and $L_\infty(\Omega)$

    Extends the above, in a simple way, to the equation with spatial derivatives

  - Finite differences: $L_\infty(\Omega)$

    Employ the discrete maximum principle of the spatial discrete operator...

  - Finite elements: $L_2(\Omega)$ and $L_\infty(\Omega)$ norms

    Ritz projection is employed in the analysis...

- Section 8 Nonhom. Dirichlet + Periodic + Neumann + mixed bound. conditions

- **L1 semidiscretization in time:**

$$\boxed{\delta_t^\alpha U^j + \mathcal{L}U^j + f(\cdot, t_j, U^j) = 0 \text{ in } \Omega, \quad U^j = 0 \text{ on } \partial\Omega \quad \text{for } j \geqslant 1; \quad U^0 = u_0}$$

- THEOREM: (i) Assuming **A1**, there exists a unique solution $\{U^m\}$ and

$$\|u(\cdot, t_m) - U^m\|_{L_p(\Omega)} \lesssim \begin{cases} M^{-r}\, t_m^{\alpha-1} & \text{if } 1 \leqslant r < 2-\alpha, \\ M^{-r(1-\epsilon)}\, t_m^{\alpha-(1-\epsilon)} & \text{if } r = 2-\alpha, \\ M^{\alpha-2}\, t_m^{\alpha-(2-\alpha)/r} & \text{if } r > 2-\alpha, \end{cases} \qquad \text{for } p \in \{2, \infty\}$$

(ii) If, additionally, f satisfies **A2**, and $\sigma_1 \leqslant u_0 \leqslant \sigma_2$, then $\sigma_1 \leqslant U^m \leqslant \sigma_2 \; \forall\, m$.

- COROLLARY: If $\|\partial_t^l u(\cdot, t)\|_{L_p(\Omega)} \lesssim 1 + t^{\alpha-l}$ for $l = 1, 2$ and $t \in (0, T]$, then

$$\boxed{\max_{t_m} \|u(\cdot, t_m) - U^m\|_{L_p(\Omega)} \lesssim M^{-\min\{\alpha r,\, 2-\alpha\}}} \Rightarrow r_{optimal} = (2-\alpha)/\alpha$$

$$\boxed{\|u(\cdot, t_m) - U^m\|_{L_p(\Omega)} \lesssim M^{-\min\{r,\, 2-\alpha\}} \quad \text{for } t_m \simeq 1 \text{ and } r \neq 2-\alpha} \Rightarrow r > 2-\alpha$$

2d Test Problem: $\mathcal{L} = -(\partial^2_{x_1} + \partial^2_{x_2})$, Allen-Cahn type nonlinearity $f = (u^3 - u)/\alpha$, $\Omega = (0, \pi)^2$ for $t \in [0, 1]$, subject to $u(0, t) = u_0 = \frac{2}{5}(2y - x^2)\,\sin x\,\sin y$, graded temporal mesh, finite differences in space.

Maximum nodal errors at $t = 1$ and **Computational Rates** q in M^{-q} or N^{-q}

	errors and convergence rates in time $N = 2M$				errors and convergence rates in space $M = N^2$			
	$M = 2^5$	$M = 2^6$	$M = 2^7$	$M = 2^8$	$N = 2^3$	$N = 2^4$	$N = 2^5$	$N = 2^6$
				$r = 1$				
$\alpha = 0.3$	1.88e-3	8.98e-4	4.37e-4	2.15e-4	1.23e-2	2.99e-3	7.49e-4	1.87e-4
	1.07	**1.04**	**1.02**		**2.05**	2.00	2.00	
$\alpha = 0.5$	7.41e-4	3.35e-4	1.58e-4	7.65e-5	8.09e-3	2.07e-3	5.13e-4	1.28e-4
	1.15	**1.08**	**1.05**		1.97	2.01	2.00	
$\alpha = 0.7$	1.06e-3	4.83e-4	2.27e-4	1.08e-4	5.87e-3	1.48e-3	3.67e-4	9.14e-5
	1.13	**1.09**	**1.06**		1.98	2.02	2.01	
				$r = \frac{2-\alpha}{.9}$				
$\alpha = 0.3$	5.87e-4	1.79e-4	5.49e-5	1.69e-5	1.15e-2	2.81e-3	7.04e-4	1.75e-4
	1.71	**1.71**	**1.70**		2.04	2.00	2.00	
$\alpha = 0.5$	3.30e-4	1.09e-4	3.70e-5	1.29e-5	7.88e-3	2.01e-3	4.98e-4	1.24e-4
	1.60	**1.56**	**1.53**		1.97	2.01	2.00	
$\alpha = 0.7$	7.14e-4	2.83e-4	1.15e-4	4.75e-5	5.66e-3	1.42e-3	3.49e-4	8.66e-5
	1.33	**1.30**	**1.28**		1.99	2.02	2.01	

2d Test Problem: $\mathcal{L} = -(\partial^2_{x_1} + \partial^2_{x_2})$, Allen-Cahn type nonlinearity $f = (u^3 - u)/\alpha$, $\Omega = (0,\pi)^2$ for $t \in [0,1]$, subject to $u(0,t) = u_0 = \frac{2}{5}(2y - x^2)\sin x \sin y$, graded temporal mesh, finite differences in space.

Maximum nodal errors at and **Computational Rates** q in M^{-q} or N^{-q}

	errors and convergence rates in time $r = \frac{2-\alpha}{\alpha}$, $N = \frac{1}{2}M$				errors and convergence rates in space $r = \frac{2-\alpha}{\alpha}$, $M = N^2$			
	$M = 2^8$	$M = 2^9$	$M = 2^{10}$	$M = 2^{11}$	$N = 2^3$	$N = 2^4$	$N = 2^5$	$N = 2^6$
$\alpha = 0.3$	1.49e-4	4.79e-5	1.55e-5	4.97e-6	1.96e-2	4.82e-3	1.20e-3	3.01e-4
	1.64	**1.63**	**1.64**		**2.02**	**2.00**	**2.00**	
$\alpha = 0.5$	3.91e-4	1.43e-4	5.20e-5	1.88e-5	1.24e-2	3.18e-3	7.95e-4	1.98e-4
	1.45	**1.46**	**1.47**		**1.97**	**2.00**	**2.01**	
$\alpha = 0.7$	8.90e-4	3.83e-4	1.63e-4	6.83e-5	1.43e-2	3.63e-3	8.76e-4	2.12e-4
	1.22	**1.24**	**1.25**		**1.98**	**2.05**	**2.05**	

	errors and convergence rates in time $r = 1$, $N = \frac{1}{128}M$				$r = 2-\alpha$, $N = \frac{1}{4}M$			
	$M = 2^{15}$	$M = 2^{16}$	$M = 2^{17}$	$M = 2^{18}$	$M = 2^{10}$	$M = 2^{11}$	$M = 2^{12}$	$M = 2^{13}$
$\alpha = 0.3$	1.30e-2	1.13e-2	9.77e-3	8.37e-3	9.77e-3	7.47e-3	5.59e-3	4.11e-3
	0.20	**0.21**	**0.22**		**0.39**	**0.42**	**0.45**	
$\alpha = 0.5$	2.73e-3	1.95e-3	1.39e-3	9.88e-4	2.73e-3	1.64e-3	9.88e-4	5.94e-4
	0.49	**0.49**	**0.49**		**0.73**	**0.73**	**0.73**	
$\alpha = 0.7$	3.15e-4	1.93e-4	1.19e-4	7.33e-5	9.84e-4	5.27e-4	2.82e-4	1.51e-4
	0.70	**0.70**	**0.70**		**0.90**	**0.90**	**0.90**	

§**1** Assumptions A1 + A2 on the **nonlinearity** f (and where they are used):

$\boxed{\text{A1 is the only assumption on } f \text{ required for the convergence analysis!}}$

Examples: reaction coefficient of arbitrary sign, Allen-Cahn, Fisher, etc.

§**2** **Assumptions on temporal meshes**: quasi-graded, of arbitrary degree of grading,

may be ”arbitrarily” refined (any new nodes may be added)

§**3** **Stability result for the nonlinear case**

$\boxed{\text{sharp + general + relatively simple proof + useful}}$

of type: [N. Kopteva and X. Meng, *Error analysis for a fractional-derivative parabolic problem on quasi-graded meshes using barrier functions*, SIAM J. Numer. Anal., 58 (2020), 1217–1238]

§**4** **Main convergence result** + discussion + numerical results:

+ optimal grading $r = (2 - \alpha)/\alpha$ yields optimal convergence globally
+ milder grading $r > 2 - \alpha$ yields optimal convergence rates in positive time, etc.

L1 semi-discretizations in time + finite differences + finite elements + various BC

PART #2 (very brief)

Pointwise-in-time a posteriori error control for time-fractional semilinear parabolic equations

MESSAGES:

+ pointwise-in-time a posteriori error bounds in the $L_2(\Omega)$ and $L_\infty(\Omega)$ norms
+ explicit upper barriers on the residual are given that guarantee that the error remains within a prescribed tolerance and within certain desirable pointwise-in-time error profiles
+ applicability to wide classes of time discretizations and arbitrarily large times

AIM TO GENERALIZE TO THE SEMILINEAR CASE:

N. Kopteva, *Pointwise-in-time a posteriori error control for time-fractional parabolic equations*, Applied Mathematics Letters, 123 (2022), 107515.

- Our AIM: **pointwise-in-time a posteriori error estimates** in $L_2(\Omega)$ and $L_\infty(\Omega)$ norms on **general temporal meshes** for reasonably **general discretizations**

. . . .

- First, recall

  [NK, *Pointwise-in-time a posteriori error control for time-fractional parabolic equations*, Applied Mathematics Letters, 123 (2022), 107515]

  for a **linear** fractional-order parabolic problem with $\alpha \in (0,1)$:

$$D_t^\alpha u + \mathcal{L}u = f(x,t) \quad \text{for } (x,t) \in \Omega \times (0,T]$$

where $\Omega \subset \mathbb{R}^d$, $d \in \{1,2,3\}$, subject to $u(x,0) = u_0(x)$ and $u = 0$ on $\partial\Omega$

$D_t^\alpha u(\cdot,t) := \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha}\, \partial_s u(\cdot,s)\, ds = J_t^{1-\alpha} \partial_t u$ =**Caputo fractional derivative**

$\mathcal{L}$ is a second-order elliptic operator

- **A posteriori error estimates in the $L_2(\Omega)$ norm**:

  Crucial LEMMA:

  $$\langle D_t^\alpha v(\cdot,t),\, v(\cdot,t)\rangle \geqslant \big(D_t^\alpha \|v(\cdot,t)\|\big)\|v(\cdot,t)\|$$

  THEOREM: error estimate via the residual R_h

  $$\lambda \in \mathbb{R} : \langle \mathcal{L}v, v\rangle \geqslant \lambda\|v\|^2 \;\Rightarrow\; \|(u_h - u)(\cdot,t)\|_{L_2(\Omega)} \leqslant (D_t^\alpha + \lambda)^{-1}\|R_h(\cdot,t)\|_{L_2(\Omega)}$$

  Residual BARRIERS to guarantee a desirable error profile...

  $\Rightarrow$ no need to store past values of the sampled residual...

- **A posteriori error estimates in the $L_\infty(\Omega)$ norm** (using max principle)

  $$\text{react.coefficient} \geqslant \lambda \in \mathbb{R} \;\Rightarrow\; \|(u_h - u)(\cdot,t)\|_{L_\infty(\Omega)} \leqslant (D_t^\alpha + \lambda)^{-1}\|R_h(\cdot,t)\|_{L_\infty(\Omega)}$$

. . . .

- **Application for the L1 method:** (for other methods, see [NK + S.Franz, Sep-2022?])

  Adaptive algorithm + Numerics

  Optimal orders of convergence: globally / in positive time

  Competitive in comparison with a-priori-chosen graded meshes

- **Variable-coefficient multiterm time-fractional case** (jointly with M. Stynes, 2022)

Using the comparison principle, one can derive **residual barriers** that guarantee certain desirable **pointwise-in-time error profiles** for $\|e\|_{L_p(\Omega)}$ with $p \in \{2, \infty\}$.

- **COROLLARY:** If $\|R_h(\cdot,t)\|_{L_p(\Omega)} \leqslant (D_t^\alpha + \lambda)\mathcal{E}(t)\ \forall\, t > 0$ for some barrier function $\mathcal{E}(t) \geqslant 0\ \forall\, t \geqslant 0$, then $\|(u_h - u)(\cdot,t)\|_{L_p(\Omega)} \leqslant \mathcal{E}(t)\ \forall\, t \geqslant 0$.

- **COROLLARY:** Suppose that $\lambda \geqslant 0$. Then for the error $e = u_h - u$ one has

$$\|R_h(\cdot,s)\|_{L_p(\Omega)} \leqslant TOL \cdot \mathcal{R}_0(t) \quad \Rightarrow \quad \|e(\cdot,t)\|_{L_p(\Omega)} \leqslant TOL,$$

$$\|R_h(\cdot,s)\|_{L_p(\Omega)} \leqslant TOL \cdot \mathcal{R}_1(t) \quad \Rightarrow \quad \|e(\cdot,t)\|_{L_p(\Omega)} \leqslant TOL \cdot t^{\alpha-1},$$

$$\mathcal{R}_0(t) := \{\Gamma(1-\alpha)\}^{-1}\, t^{-\alpha} + \lambda, \qquad \mathcal{R}_1(t) := \{\Gamma(1-\alpha)\}^{-1}\, t^{-1} \varrho(\tau/t) + \lambda\, \mathcal{E}_1(t),$$

$$\mathcal{E}_1(t) := \max\{\tau, t\}^{\alpha-1},$$

$$\varrho(s) := s^{-\beta}[1 - ((1-s)^+)^\beta] \geqslant s^{-\beta} \min\{\beta s,\, 1\}, \quad \beta := 1-\alpha,$$

where $\tau > 0$ is an arbitrary parameter (and $t^{\alpha-1}$ can be replaced by $\mathcal{E}_1(t)$).

ADVANTAGE: **no need to store past values of the sampled residual...**

- Consider $D_t^\alpha u + \mathcal{L}u + g(x,t,u) = f(x,t)$ for $(x,t) \in \Omega \times (0,T]$, assuming that g is sufficiently smooth and, with some $\mu \in \mathbb{R}$, satisfies

$$\partial_v g(x,t,v) \geqslant \mu \qquad \forall (x,t,v) \in \Omega \times (0,T] \times \mathbb{R}.$$

Then, in view of the standard linearization

$$g(x,t,u_h) - g(x,t,u) = \hat{c}(x,t)\,(u_h - u), \quad \hat{c} := \int_0^1 \partial_v g(x,t,u+s(u_h-u))\,ds \geqslant \mu,$$

the error satisfies $(D_t^\alpha + \mathcal{L} + \hat{c})(u_h - u) = R_h$, with the updated definition of the residual $R_h := D_t^\alpha u_h + \mathcal{L}u_h + g(x,t,u_h) - f(x,t)$.

- **COROLLARY:** Assume that $\langle \mathcal{L}v, v\rangle \geqslant \lambda^* \|v\|^2$ for some $\lambda^* \in \mathbb{R}$ (instead of $\langle \mathcal{L}v, v\rangle \geqslant \lambda \|v\|^2$), or, similarly, $c \geqslant \lambda^*$ (instead of $c \geqslant \lambda$). Then one gets the above error bounds with $\boxed{\lambda := \lambda^* + \mu}$.

- **In PROGRESS:** A posteriori choice of $\lambda = \lambda_h(t)$, based on the a posteriori error control in the $L_\infty(\Omega)$ norm...

- N. Kopteva, *Error analysis for time-fractional semilinear parabolic equations using upper and lower solutions*, SIAM J. Numer. Anal., 58 (2020), 2212–2234. semilinear case
- N. Kopteva, *Error analysis of the L1 method on graded and uniform meshes for a fractional-derivative problem in two and three dimensions*, Math. Comp., 88 (2019), 2135–2155. linear: L1 + framework for spatial discretizations + bounds on the exact solutions
- N. Kopteva and X. Meng, *Error analysis for a fractional-derivative parabolic problem on quasi-graded meshes using barrier functions*, SIAM J. Numer. Anal., 58 (2020), 1217–1238. linear: L1 + Alikhanov
- N. Kopteva, *Error analysis of an L2-type method on graded meshes for a fractional-order parabolic problem*, Math. Comp., 90 (2021), 19-40. linear: L2 scheme

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- N. Kopteva, *Pointwise-in-time a posteriori error control for time-fractional parabolic equations*, Applied Mathematics Letters, 123 (2022), 107515.
- N. Kopteva and M. Stynes, *A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations*, J. Sci. Comput., (2022), doi: 10.1007/s10915-022-01936-2.
- N. Kopteva, Maximum principle for time-fractional parabolic equations with a reaction coefficient of arbitrary sign, Appl. Math. Lett., (2022), 108209.
- S. Franz and N. Kopteva, *Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations*, (Sep-2022) semilinear case

Final

Thank you!