

RECENT RESULTS ON POINTWISE-IN-TIME
A POSTERIORI ERROR CONTROL FOR
TIME-FRACTIONAL PARABOLIC EQUATIONS

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Joint work with *Martin Stynes, Beijing CSRC, and Sebastian Franz, TU Dresden.*

Some insights from the a-priori analysis jointly with *Xiangyun Meng, Beijing Jiaotong University*

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Beijing Computational Science Research Center, July 2023*

I will start with a review of [1], which was presented at the 2021 edition of this workshop. For time-fractional parabolic equations with a Caputo time derivative of order $\alpha \in (0, 1)$, we give [pointwise-in-time a posteriori error bounds in the spatial \$L_2\$ and \$L_\infty\$ norms](#). Hence, an [adaptive time stepping algorithm](#) is applied for the L1 method, which yields optimal convergence rates $2 - \alpha$ in the presence of solution singularities. Interestingly, the proposed time stepping algorithm yields the grids similar to a-priori-constructed optimal grids in [2, 3].

In the main part of the talk, we shall discuss [recent extensions](#) of the proposed methodology to [variable-coefficient multiterm time-fractional subdiffusion equations](#) [4], and to the case of [higher-order discretizations](#) [5]. The [stable implementation](#) of the proposed algorithm will also be addressed [5].

1. N. Kopteva, Pointwise-in-time a posteriori error control for time-fractional parabolic equations, *Appl. Math. Lett.*, 123 (2022), 107515.
2. 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.
3. N. Kopteva, *Error analysis for time-fractional semilinear parabolic equations using upper and lower solutions*, *SIAM J. Numer. Anal.*, 58 (2020), 2212–2234.
4. N. Kopteva and M. Stynes, A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations, *J. Sci. Comput.*, (2022).
5. S. Franz and N. Kopteva, Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations, *J. Comput. Appl. Math.*, volume 427 (2023), 115122.

- Consider a 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 $\partial\Omega$

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

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

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.....

- In the a priori error analysis, an initial singularity of the exact solution is typically addressed, such as

$$\boxed{|\partial_t^l u(\cdot, t)| \lesssim 1 + t^{\alpha-l}} \quad \text{or similar...}$$

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

- AIM: an **adaptive framework (a posteriori error estimates + an adaptive time stepping algorithm)** capable of identifying various solution singularities...

1. A-priori pointwise-in-time error bounds

- + give lots of insight in what can be expected of the error;
- + a-priori chosen temporal meshes are our main competition, so to speak :)

2. Review of N. Kopteva, Pointwise-in-time a posteriori error control for time-fractional parabolic equations, Appl. Math. Lett., 123 (2022), 107515.

3. RECENT EXTENSIONS:

- + N. Kopteva and M. Stynes, A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations, J. Sci. Comput., (2022).

- + S. Franz and N. Kopteva, Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations, J. Comput. Appl. Math., volume 427 (2023), 115122.

- + Stable implementation is also addressed in the latter

- **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], ...

[Y. Yan, M. Khan, N.J. Ford, SINUM, 2018], ...

[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 graded (general) meshes – quite intricate...

[H.-L. Liao, D. Li, J. Zhang, SINUM, 2018],

[H.-L. Liao, W. McLean, J. Zhang, SINUM, 2019],...

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- In this talk, I rely on **insights from sharp a-priori pointwise-in-time bounds using barrier functions on quasi-graded grids** with arbitrary degree of grading: [N. Kopteva, X. Meng, SINUM, 2020], also [N. Kopteva, Math. Comp., 2019]...

- **THEOREM [Kopteva+Meng]:** Using **(quasi-)graded mesh** $\{t_j = T(j/M)^r\}_{j=0}^M$ with $r \geq 1$, if $\|\partial_t^l u(t)\| \lesssim 1 + t^{\alpha-l}$ for $l = 1, 2$ and $t \in (0, T]$, then

$$\|u(t_m) - U^m\| \lesssim \begin{cases} M^{-r} t_m^{\alpha-1} & \text{if } 1 \leq r < 2 - \alpha, \\ M^{\alpha-2} t_m^{\alpha-1} [1 + \ln(t_m/t_1)] & \text{if } r = 2 - \alpha, \\ M^{\alpha-2} t_m^{\alpha-(2-\alpha)/r} & \text{if } r > 2 - \alpha. \end{cases}$$

Particular cases:

- When the optimal grading parameter $r_{opt} = (2 - \alpha)/\alpha$ is used, then the error is bounded by $M^{\alpha-2} \cdot 1$, i.e. we recover the **optimal global convergence rates** of $2 - \alpha$, as particular cases of our more general error bounds.
- Another straightforward particular case of our error bounds indicates that the **optimal convergence rates** of $2 - \alpha$ in positive time $t \gtrsim 1$ are attained using

much milder grading with $r > 2 - \alpha$.

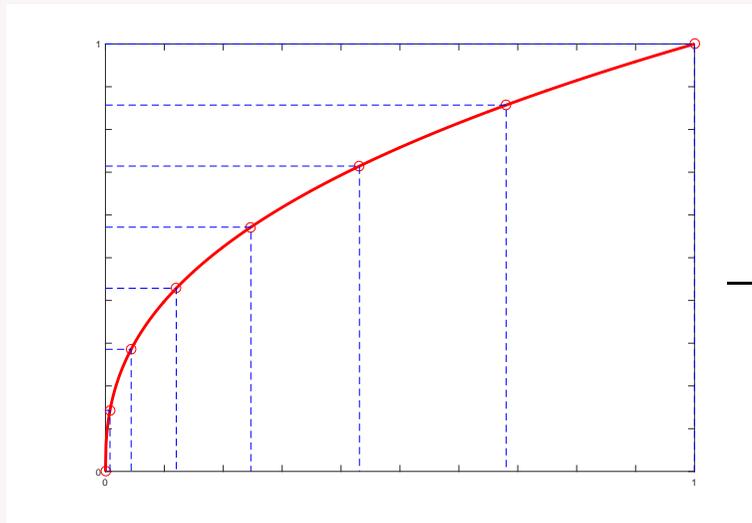
- Frequently assumed: there exists a unique solution of this problem in $C(\bar{\Omega} \times [0, T])$:

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

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

- **Graded meshes** in time:

$$\{t_j = T(j/M)^r\}_{j=0}^M \quad \text{with some } r > 1$$



—yield **global accuracy**...

- **Uniform meshes** in time: i.e. $r = 1$ — yield **convergence in positive time**...

- 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. **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. **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. **L2 scheme**
- 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**

- B. Jin, R. Lazarov and Z. Zhou, *Numerical methods for time-fractional evolution equations with nonsmooth data: a concise overview*, *Comput. Methods Appl. Mech. Engrg.*, 346 (2019), 332–358.
- B. Jin, R. Lazarov and Z. Zhou, *An analysis of the L1 scheme for the subdiffusion equation with nonsmooth data*, *IMA J. Numer. Anal.* 36 (2016), 197–221. uniform mesh
- H. Brunner, *The numerical solution of weak singular Volterra integral equations by collocation on graded meshes*, *Math. Comp.*, 45 (1985), 417–437.
- W. McLean and K. Mustapha, *A second-order accurate numerical method for a fractional wave equation*, *Numer. Math.*, 105 (2007), 481–510. graded mesh
- K. Mustapha, B. Abdallah and K. M. Furati, *A discontinuous Petrov-Galerkin method for time-fractional diffusion equations*, *SIAM J. Numer. Anal.*, 52 (2014), 2512–2529. graded mesh
- M. Stynes, E. O’Riordan and J. L. Gracia, *Error analysis of a finite difference method on graded meshes for a time-fractional diffusion equation*, *SINUM*, 55 (2017), 1057–1079. L_1 + graded
- H.-L. Liao, W. McLean and J. Zhang, *A discrete Grönwall inequality with application to numerical schemes for fractional reaction-subdiffusion problems*, *SIAM J. Numer. Anal.*, 57 (2019), 218–237.
- H.-L. Liao, D. Li and J. Zhang, *Sharp error estimate of the nonuniform L1 formula for linear reaction-subdiffusion equations*, *SIAM J. Numer. Anal.*, 56 (2018), 1112–1133.
- H.-L. Liao, W. McLean and J. Zhang, *A second-order scheme with nonuniform time steps for a linear reaction-subdiffusion problem*, arXiv:1803.09873v4, (2018). discrete Grönwall inequalities
- A. A. Alikhanov, *A new difference scheme for the time fract...*, *J. Comput. Phys.*, 280 (2015), 424–438.
- H. Chen and M. Stynes, *Error analysis of a second-order method on fitted meshes for a time-fractional diffusion problem*, *J. Sci. Comput.*, 79 (2019), 624–647. Alihanov + graded mesh
- C. Lv and C. Xu, *Error analysis of a high order method for time-fractional diffusion equations*, *SIAM J. Sci. Comput.* 38 (2016), A2699–A2724. L_2 scheme + uniform mesh

OUR MAIN FOCUS IN THIS TALK:

Pointwise-in-time a posteriori error control for time-fractional 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

1. A-priori pointwise-in-time error bounds

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- + S. Franz and N. Kopteva, Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations, *J. Comput. Appl. Math.*, volume 427 (2023), 115122.

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

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-
- 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**

Main REF for this part: NK, Pointwise-in-time a posteriori error control for time-fractional parabolic equations, Applied Mathematics Letters, 123 (2022), 107515

NOTE also: Lehel Banjai and Charalambos G. Makridakis, A posteriori error analysis for approximations of time-fractional subdiffusion problems. Math. Comp., 2022. (no algorithm)

- 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**

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

Crucial LEMMA:

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

THEOREM: error estimate via the residual R_h

$$\|(u_h - u)(\cdot, t)\|_{L_2(\Omega)} \leq (D_t^\alpha + \lambda)^{-1} \|R_h(\cdot, t)\|_{L_2(\Omega)}$$

Residual BARRIERS to guarantee a desirable error profile...

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

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

Adaptive time stepping algorithm + Numerics

Optimal orders of convergence: globally / in positive time

Competitive in comparison with a-priori-chosen graded meshes

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

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

- We look for *a posteriori error estimates*

$$\|\text{error}(t)\|_{L_p(\Omega)} \leq \text{function}(\text{mesh}, \text{comp.sol-n})$$

with **all constants explicit** in the RHS

- Substantial literature for classical parabolic and elliptic PDEs
- We shall only consider discretizations in time (i.e. in space we keep \mathcal{L} undiscretized)
- We shall first consider the popular **L1 method** = an analogue of the backward Euler method extended to fractional-parabolic equations (works for **wide classes of methods...**)
- **residual** of the computed solution $R_h(\cdot, t) := (D_t^\alpha + \mathcal{L})u_h(\cdot, t) - f(\cdot, t)$ (sometimes, $\partial_t u_h$ may be a distribution...)
- to compute the residual, one needs to (appropriately) **interpolate the computed solution** in time between time layers

- **LEMMA:** Let $v(\cdot, 0) = 0$ and $v \in L_\infty(0, t; L_2(\Omega)) \cap W^{1,\infty}(\epsilon, t; L_2(\Omega))$ for any $0 < \epsilon < t \leq T$. Then

$$\langle D_t^\alpha v(\cdot, t), v(\cdot, t) \rangle \geq (D_t^\alpha \|v(\cdot, t)\|) \|v(\cdot, t)\| \quad \text{for } t > 0$$

- Discrete version for the L1 discretization is quite obvious:

$$D_t^\alpha v(\cdot, t_m) \approx \delta_t^\alpha v^m = \underbrace{\kappa_{m,m}}_{>0} v^m - \sum_{j=1}^m \underbrace{(\kappa_{m,j} - \kappa_{m,j-1})}_{>0} v^{j-1}$$

where $\kappa_{m,j} := \frac{\tau_j^{-1}}{\Gamma(1-\alpha)} \int_{t_{j-1}}^{t_j} (t_m - s)^{-\alpha}$, so

$$\langle \delta_t^\alpha v^m, v^m \rangle \geq \underbrace{\kappa_{m,m}}_{>0} \|v^m\|^2 - \sum_{j=1}^m \underbrace{(\kappa_{m,j} - \kappa_{m,j-1})}_{>0} \|v^{j-1}\| \|v^m\| = (\delta_t^\alpha \|v^m\|) \|v^m\|$$

see, e.g., [NK, *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)]

- **LEMMA:** Let $v(\cdot, 0) = 0$ and $v \in L_\infty(0, t; L_2(\Omega)) \cap W^{1,\infty}(\epsilon, t; L_2(\Omega))$ for any $0 < \epsilon < t \leq T$. Then

$$\langle D_t^\alpha v(\cdot, t), v(\cdot, t) \rangle \geq (D_t^\alpha \|v(\cdot, t)\|) \|v(\cdot, t)\| \quad \text{for } t > 0$$

- PROOF of the continuous version relies on the **alternative (equivalent) definition** of D_t^α (for the case $v(\cdot, 0) = 0$):

$$\Gamma(1 - \alpha) D_t^\alpha v(\cdot, t) = t^{-\alpha} v(\cdot, t) + \int_0^t \alpha(t - s)^{-\alpha-1} \{v(\cdot, t) - v(\cdot, s)\} ds$$

This representation was also used by:

[Y. Luchko, *Maximum principle for the generalized time-fractional diffusion equation*, J. Math. Anal. Appl., 351 (2009), 218–223],

[H. Brunner, H. Han and D. Yin, *The maximum principle for time-fractional diffusion equations and its application*, Numer. Funct. Anal. Optim., 36 (2015), 1307–1321]

- **THEOREM:** Let \mathcal{L} , for some $\lambda \in \mathbb{R}$, satisfy $\langle \mathcal{L}v, v \rangle \geq \lambda \|v\|^2 \forall v \in H_0^1(\Omega)$. Suppose the exact solution u and its approximation u_h are in $L_\infty(0, t; L_2(\Omega)) \cap W^{1,\infty}(\epsilon, t; L_2(\Omega))$ for any $0 < \epsilon < t \leq T$, and also in $H_0^1(\Omega)$ for any $t > 0$, while $u_h(\cdot, 0) = u_0$ and $R_h(\cdot, t) := (D_t^\alpha + \mathcal{L})u_h(\cdot, t) - f(\cdot, t)$. Then

$$\|(u_h - u)(\cdot, t)\|_{L_2(\Omega)} \leq (D_t^\alpha + \lambda)^{-1} \|R_h(\cdot, t)\|_{L_2(\Omega)} \quad \text{for } t > 0$$

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- **NOTATION:** $(D_t^\alpha + \lambda)^{-1}v(t) := \int_0^t (t - s)^{\alpha-1} E_{\alpha,\alpha}(-\lambda[t - s]^\alpha) v(s) ds$

Here $E_{\alpha,\beta}(s) = \sum_{k=0}^\infty \{\Gamma(\alpha k + \beta)\}^{-1} s^k$ is a generalized Mittag-Leffler function, while $(D_t^\alpha + 0)^{-1}v := J_t^\alpha v = \int_0^t (t - s)^{\alpha-1} v(s) ds$.

- Also, $w(t) = (D_t^\alpha + \lambda)^{-1}v(t)$ is a solution of the equation $(D_t^\alpha + \lambda)w(t) = v(t)$ for $t > 0$ subject to $w(0) = 0$.

As $E_{\alpha,\alpha} > 0$, so $v \geq 0$ implies $w \geq 0$ — **comparison principle!**

- **THEOREM:** Let \mathcal{L} , for some $\lambda \in \mathbb{R}$, satisfy $\langle \mathcal{L}v, v \rangle \geq \lambda \|v\|^2 \forall v \in H_0^1(\Omega)$. Suppose the exact solution u and its approximation u_h are in $L_\infty(0, t; L_2(\Omega)) \cap W^{1,\infty}(\epsilon, t; L_2(\Omega))$ for any $0 < \epsilon < t \leq T$, and also in $H_0^1(\Omega)$ for any $t > 0$, while $u_h(\cdot, 0) = u_0$ and $R_h(\cdot, t) := (D_t^\alpha + \mathcal{L})u_h(\cdot, t) - f(\cdot, t)$. Then

$$\|(u_h - u)(\cdot, t)\|_{L_2(\Omega)} \leq (D_t^\alpha + \lambda)^{-1} \|R_h(\cdot, t)\|_{L_2(\Omega)} \quad \text{for } t > 0$$

.....

- **PROOF:** Set $e := u_h - u$. Then $e(\cdot, 0) = 0$ and $(D_t^\alpha + \mathcal{L})e(\cdot, t) = R_h(\cdot, t)$ for $t > 0$ subject to $e = 0$ on $\partial\Omega$.

Taking the inner product of this equation with $e(\cdot, t)$, then applying the obvious

$$\langle \mathcal{L}e, e \rangle \geq \lambda \|e\|^2 \quad \text{and (crucially!) } \langle D_t^\alpha e(\cdot, t), e(\cdot, t) \rangle \geq (D_t^\alpha \|e(\cdot, t)\|) \|e(\cdot, t)\|$$

(by our crucial **LEMMA**), one arrives at $(D_t^\alpha + \lambda)\|e(\cdot, t)\| \leq \|R_h(\cdot, t)\|$ for $t > 0$.

Then $(D_t^\alpha + \lambda)\{(D_t^\alpha + \lambda)^{-1}\|R_h(\cdot, t)\| - \|e(\cdot, t)\|\} \geq 0$, so the comparison principle yields the desired bound. □

Using the comparison principle, one can derive **residual barriers** that guarantee certain desirable **pointwise-in-time error profiles**.

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

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

NOTE: The above corollary may seem to imply that one can get any **desirable pointwise-in-time error profile** $\mathcal{E}(t)$ on demand. The tricky part is to ensure that $(D_t^\alpha + \lambda)\mathcal{E}(t) > 0$ for $t > 0$, which is not true for a general positive \mathcal{E} . Two possible error profiles will be described by the following result.

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

- **COROLLARY:** If $\|R_h(\cdot, t)\|_{L_p(\Omega)} \leq (D_t^\alpha + \lambda)\mathcal{E}(t) \forall t > 0$ for some barrier function $\mathcal{E}(t) \geq 0 \forall t \geq 0$, then $\|(u_h - u)(\cdot, t)\|_{L_p(\Omega)} \leq \mathcal{E}(t) \forall t \geq 0$.
- **COROLLARY:** Suppose that $\lambda \geq 0$. Then for the error $e = u_h - u$ one has

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

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

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

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

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

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...**

```

 $u_h^0 := u_0; t_0 := 0; t_1 := \min\{\tau_*, T\}; m := 0;$ 
while  $t_m < T$ 
   $m := m + 1; flag := 0;$ 
  while  $t_m - t_{m-1} > \tau_{**}$ 
    compute  $u_h^m$  using the L1 method
    if  $\|R_h(\cdot, t)\| \leq TOL \cdot \mathcal{R}_p(t) \forall t \in (t_{m-1}, t_m)$ 
      if  $t_m = T$ 
         $M := m; break$ 
      elseif  $t_m < T$ 
         $\tilde{u}_h^m := u_h^m; \tilde{t}_m := t_m;$ 
         $t_m := \min\{t_{m-1} + Q(t_m - t_{m-1}), T\}; flag := 1;$ 
      end
    else
      if  $flag = 0$ 
         $t_m := t_{m-1} + (t_m - t_{m-1})/Q;$ 
      else
         $u_h^m := \tilde{u}_h^m; t_m := \tilde{t}_m;$ 
         $t_{m+1} := \min\{t_m + (t_m - t_{m-1}), T\}; break$ 
      end
    end
  end
end
end
end

```

Parameters: $Q := 1.1$,
 $\tau_* := 5 TOL^{1/\alpha}$ for
 \mathcal{R}_0 and $\tau_* := TOL$ for
 $\mathcal{R}_1, \tau_{**} := 0$.

Here we used the standard mathematical notation combined with the MatLab while loop syntax (where, to be precise, break denotes an exit from the interior while loop).

Given an arbitrary temporal mesh $\{t_j\}_{j=0}^M$ on $[0, T]$, let $\{u_h^j\}_{j=0}^M$ be the semi-discrete approximation obtained using the popular L1 method.

Then its standard Lagrange **piecewise-linear-in-time interpolant** u_h , defined on $\bar{\Omega} \times [0, T]$, satisfies

$$(D_t^\alpha + \mathcal{L})u_h(x, t_j) = f(x, t_j) \quad \text{for } x \in \Omega, \quad j = 1 \dots, M,$$

subject to $u_h^0 := u_0$ and $u_h = 0$ on $\partial\Omega$.

So for the residual of u_h one immediately gets $R_h(\cdot, t_j) = 0$ for $j \geq 1$, i.e. on each (t_{j-1}, t_j) for $j > 1$, the **residual is a non-symmetric bubble**.

Hence, for the piecewise-linear interpolant R_h^I of R_h one has $R_h^I = 0$ for $t \geq t_1$,

and, more generally, $R_h^I = [\mathcal{L}u_0 - f(\cdot, 0)](1 - t/t_1)^+$ for $t > 0$.

Finally, note that $R_h - R_h^I = (D_t^\alpha u_h - f) - (D_t^\alpha u_h - f)^I$ (as $(\mathcal{L}u_h)^I = \mathcal{L}u_h$).

NOTE: one can compute R_h by sampling, using parallel/vector evaluations, without a direct application of \mathcal{L} to $\{u_h^j\}$.

Test problem A. $(D_t^\alpha + 3)u = f(t)$ with the exact solution $u = u(t) = t^\alpha - t^2$ (which exhibits a typical singularity at $t = 0$) for $t \in (0, 1]$.

The adaptive algorithm constructed a temporal mesh: $\|R_h(\cdot, t)\| \leq TOL \cdot \mathcal{R}_p(t)$, $p = 0, 1$ (with $\tau := t_1$ in \mathcal{R}_1 on next page).

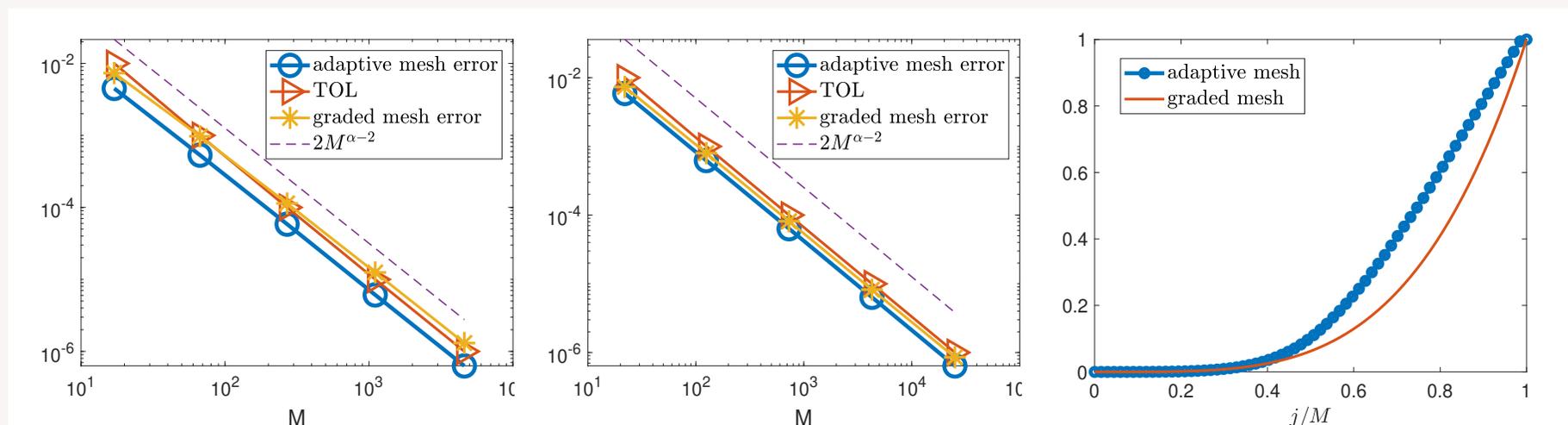


Figure 1: Adaptive algorithm with $\mathcal{R}_0(t)$: $\max_{[0, T]} |e(t)|$ on the adaptive mesh, the corresponding TOL and error on the graded mesh, $\alpha = 0.4$ (left) and $\alpha = 0.7$ (centre). Right: graphs of $\{t_j\}_{j=0}^M$ as a function of j/M for the adaptive mesh v graded mesh with $r = (2 - \alpha)/\alpha$, $\alpha = 0.7$, $TOL = 10^{-3}$, $M = 67$.

- For \mathcal{R}_0 , the errors on the adaptive meshes were compared with the errors on the **optimal graded meshes** $\{t_j = T(j/M)^r\}_{j=0}^M$ with $r = (2 - \alpha)/\alpha$.
- We observe that the **optimal global rates of convergence** $2 - \alpha$ are attained.

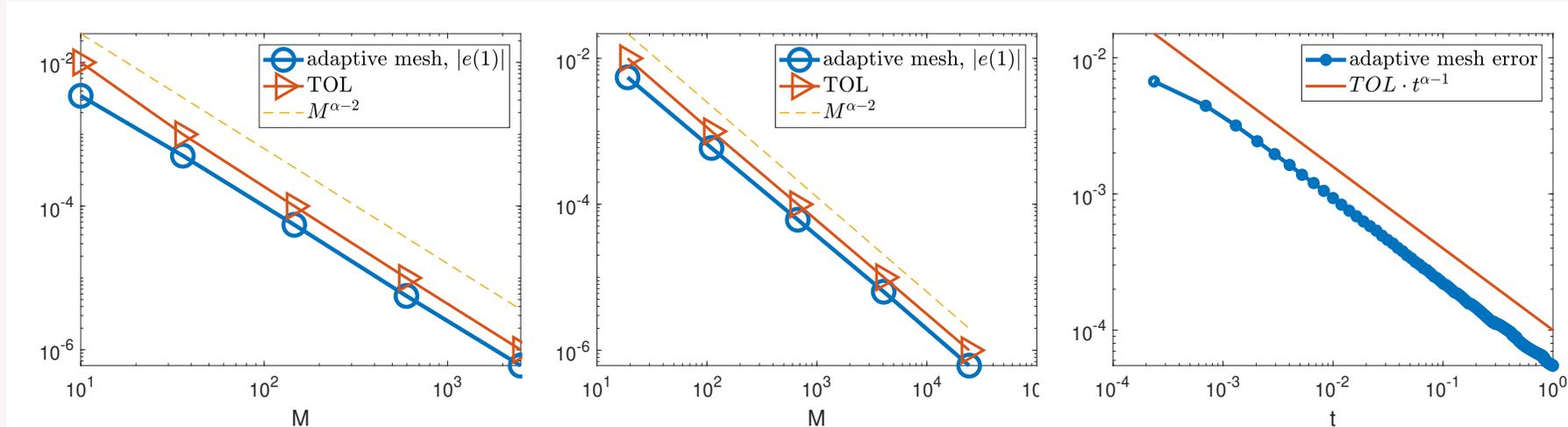


Figure 2: Adaptive algorithm with $\mathcal{R}_1(t)$ for test problem A: $|e(1)|$ on the adaptive mesh and the corresponding TOL, $\alpha = 0.4$ (left) and $\alpha = 0.7$ (centre). Right: log-log graph of the pointwise error $|e(t_j)|$ on the adaptive mesh v $TOL \cdot t^{\alpha-1}$, $\alpha = 0.4$, $TOL = 10^{-4}$, $M = 146$.

- For \mathcal{R}_1 , we observe the **optimal rates of convergence $2 - \alpha$ at terminal time $t = 1$** .
- This is **consistent with the a priori error bound** [NK, X. Meng, SINUM (2020)] for a **mildly graded mesh** $\{t_j = T(j/M)^r\}_{j=0}^M$ with $r = 2 - \alpha$:

the error behaves as $M^{-r}t^{\alpha-1}$ for $1 \leq r \leq 2 - \alpha$ (with a logarithmic factor for $r = 2 - \alpha$), while the **optimal convergence rate $2 - \alpha$ in positive time** is attained if $r \approx 2 - \alpha$.

Test problem B. Consider $(x, t) \in (0, \pi) \times (0, 1]$ with $\mathcal{L} = -\partial_x^2$ and the exact solution $u := (t^\alpha - t^2) \sin(x^2/\pi)$, so we set $\lambda := 1$.

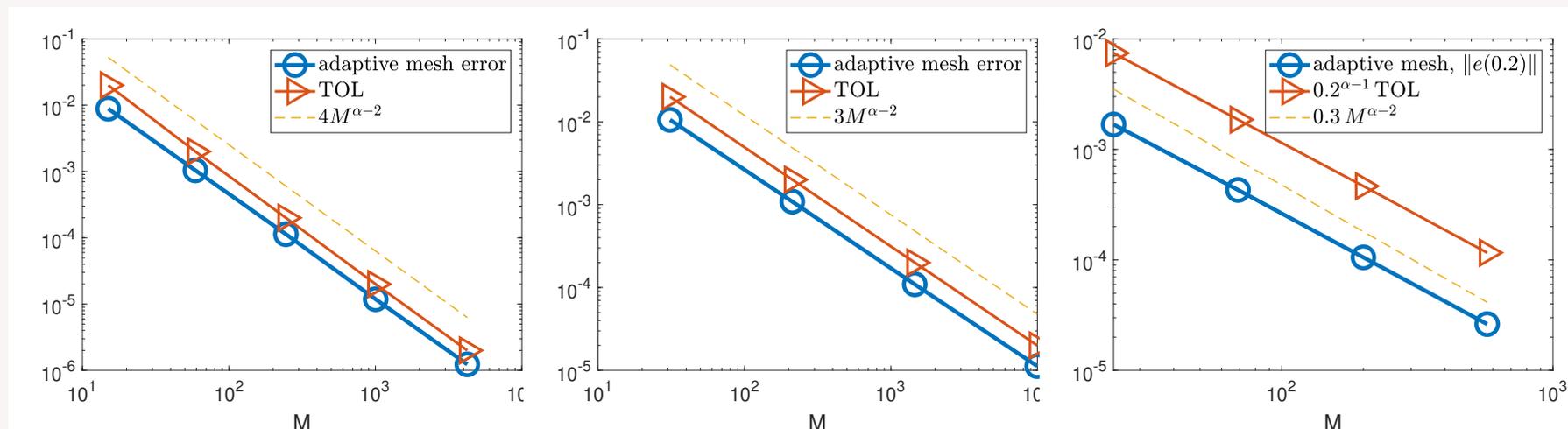


Figure 3: Adaptive algorithm with $\mathcal{R}_0(t)$ for parabolic test problem B: $\max_{t_j \in (0, T]} \|e(t_j)\|$ on the adaptive mesh and the corresponding TOL, $\alpha = 0.4$ (left) and $\alpha = 0.8$ (centre). Adaptive algorithm with $\mathcal{R}_1(t)$ for parabolic test problem C: $\|e(0.2)\|$ and TOL, $\alpha = 0.6$ (right).

Test problem C. Consider $(x, t) \in (0, \pi) \times (0, 0.2]$ with $\mathcal{L} = -\partial_x^2$, so $\lambda := 1$. Now $u_0 := x$ for $x \leq 1$ and $u_0 := 1 - (x - 1)/(\pi - 1)$ for $x \geq 1$, while $f := 0$.

As $\mathcal{L}u_0 \notin L_2(\Omega)$, to be able to compute $\|R_h\|$ on $(0, t_1)$, we **change the interpolation of the computed solution** $\{u_h^j\}_{j=0}^M$ on $(0, t_1]$ to **piecewise-constant**...

NOTE: all changes in u_h are reflected when computing its residual R_h !

- **THEOREM:** Let $\mathcal{L}u := \sum_{k=1}^d \left\{ -a_k(x) \partial_{x_k}^2 u + b_k(x) \partial_{x_k} u \right\} + c(x) u$, with sufficiently smooth coefficients $\{a_k\}$, $\{b_k\}$ and c in $C(\bar{\Omega})$, for which we assume that $a_k > 0$ in $\bar{\Omega}$, and also $c \geq \lambda \in \mathbb{R}$ (while $\langle \mathcal{L}v, v \rangle \geq \lambda \|v\|^2$ is no longer required).

Let the exact solution u and its approximation u_h be in $C(\bar{\Omega} \times [0, t]) \cap W^{1,\infty}(\epsilon, t; L_\infty(\Omega))$ for any $0 < \epsilon < t \leq T$, and also in $C^2(\Omega)$ for any $t > 0$.

Then the error bounds of the **above THEOREM and both COROLLARIES remain true** with $\|\cdot\|_{L_2(\Omega)}$ replaced by $\|\cdot\|_{L_\infty(\Omega)}$.

.....

- **PROOF:** relies on the **maximum principle** from [Y. Luchko, *Maximum principle for the generalized time-fractional diffusion equation*, J. Math. Anal. Appl., 351 (2009), 218–223] ($\lambda \geq 0$) and [NK, *Maximum principle for time-fractional parabolic equations with a reaction coefficient of arbitrary sign*, Appl. Math. Lett., (2022)] ($\lambda \in \mathbb{R}$).

Maximum/Comparison principle: Suppose that $v(x, t) \geq 0$ for $t = 0$ and $x \in \partial\Omega$, and v is in $C(\bar{\Omega} \times [0, t]) \cap W^{1,\infty}(\epsilon, t; L_\infty(\Omega))$ for any $0 < \epsilon < t \leq T$ and also in $C^2(\Omega)$ for any $t > 0$. Then $(D_t^\alpha + \mathcal{L})v \geq 0$ in $(0, T] \times \Omega$ implies $v \geq 0$ in $[0, T] \times \bar{\Omega}$.

- 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**

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

Crucial LEMMA:

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

THEOREM: error estimate via the residual R_h

$$\|(u_h - u)(\cdot, t)\|_{L_2(\Omega)} \leq (D_t^\alpha + \lambda)^{-1} \|R_h(\cdot, t)\|_{L_2(\Omega)}$$

Residual BARRIERS to guarantee a desirable error profile...

⇒ no need to store past values of the sampled residual...

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

Adaptive time stepping algorithm + Numerics

Optimal orders of convergence: globally / in positive time

Competitive in comparison with a-priori-chosen graded meshes

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

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

1. A-priori pointwise-in-time error bounds

- + give lots of insight in what can be expected of the error;
- + a-priori chosen temporal meshes are our main competition, so to speak :)

2. Review of N. Kopteva, Pointwise-in-time a posteriori error control for time-fractional parabolic equations, Appl. Math. Lett., 123 (2022), 107515.

3. **RECENT EXTENSIONS:**

+ N. Kopteva and M. Stynes, A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations, J. Sci. Comput., (2022).

+ S. Franz and N. Kopteva, Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations, J. Comput. Appl. Math., volume 427 (2023), 115122.

+ Stable implementation is also addressed in the latter

- The above framework was extended to a **variable-coefficient multiterm time-fractional case** (joint work with **M. Stynes**, JSC, 2022)

$$\sum_{i=1}^{\ell} [q_i(t) D_t^{\alpha_i} u(x, t)] + \mathcal{L}u = f(x, t) \quad \text{for } (x, t) \in \Omega \times (0, T]$$

$0 < \alpha_{\ell} < \dots < \alpha_2 < \alpha_1 \leq 1$, while each $q_i \in C[0, T]$ with

$$\sum_{i=1}^{\ell} q_i(t) > 0 \quad \text{and} \quad q_i(t) \geq 0 \quad \forall i,$$

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

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

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

Using the comparison principle, one can derive **residual barriers** that guarantee certain desirable **pointwise-in-time error profiles**.

- **THEOREM:** If $\|R_h(\cdot, t)\| \leq (\sum_{i=1}^{\ell} [q_i(t) D_t^{\alpha_i} u(x, t)] + \lambda)\mathcal{E}(t) \forall t > 0$ for some barrier function $\mathcal{E}(t) \geq 0 \forall t \geq 0$, then $\|(u_h - u)(\cdot, t)\| \leq \mathcal{E}(t) \forall t \geq 0$.

As in the single-term case:

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

NOTE: The above corollary may seem to imply that one can get any **desirable pointwise-in-time error profile** $\mathcal{E}(t)$ on demand. The tricky part is to ensure that $(D_t^{\alpha} + \lambda)\mathcal{E}(t) > 0$ for $t > 0$, which is not true for a general positive \mathcal{E} . Two possible error profiles will be described by the following result.

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

- **THEOREM:** If $\|R_h(\cdot, t)\| \leq (\sum_{i=1}^{\ell} [q_i(t) D_t^{\alpha_i} u(x, t)] + \lambda) \mathcal{E}(t) \forall t > 0$ for some barrier function $\mathcal{E}(t) \geq 0 \forall t \geq 0$, then $\|(u_h - u)(\cdot, t)\| \leq \mathcal{E}(t) \forall t \geq 0$.
- **COROLLARY:** Suppose that $\lambda \geq 0$. Then for the error $e = u_h - u$ one has

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

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

$$\mathcal{R}_0(t) := \sum_{i=1}^{\ell} [q_i(t) \{\Gamma(1 - \alpha_i)\}^{-1} t^{-\alpha_i} + \lambda, \quad \mathcal{R}_1(t) := \sum_{i=1}^{\ell} [\dots] + \lambda \mathcal{E}_1(t),$$

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

$\mathcal{R}_1(t)$ is explicit (but more intricate),

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...**

- **COROLLARY:** Let \mathcal{L} , for some $\lambda \in \mathbb{R}$, satisfy $\langle \mathcal{L}v, v \rangle \geq \lambda \|v\|^2 \forall v \in H_0^1(\Omega)$. Suppose the exact solution u and its approximation u_h are in $L_\infty(0, t; L_2(\Omega)) \cap W^{1,\infty}(\epsilon, t; L_2(\Omega))$ for any $0 < \epsilon < t \leq T$, and also in $H_0^1(\Omega)$ for any $t > 0$, while $u_h(\cdot, 0) = u_0$ and $R_h(\cdot, t) := (\sum_{i=1}^\ell [q_i(t) D_t^{\alpha_i} u(x, t)] + \mathcal{L})u_h(\cdot, t) - f(\cdot, t)$. Then

$$\|(u_h - u)(\cdot, t)\|_{L_2(\Omega)} \leq \left(\sum_{i=1}^\ell [q_i(t) D_t^{\alpha_i} u(x, t)] + \lambda \right)^{-1} \|R_h(\cdot, t)\|_{L_2(\Omega)}$$

for $t > 0$, assuming that the RHS exists.

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- Extensions to the spatial $L_\infty(\Omega)$ norm are also given.
- We also performed extensive numerical experiments (5 pages):
with various configurations of $\{q_i(t)\}$ including $q_1(t)$ being initially 0;
in all considered cases, the time stepping algorithm produced desired error profiles and captured solution singularities.

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- + Stable implementation is also addressed in the latter

- Our **adaptive algorithm** is essentially independent of the method (or its order) and, additionally, does not require a preliminary a-priori error analysis either of the exact solution or its numerical approximation. The latter may be important **if the a-priori error analysis is lacking (such as for collocation methods)** or limited to, e.g., uniform meshes.
- We demonstrate that **high-order methods (incl. continuous collocation methods of order up to as high as 8)** exhibit a huge improvement in the accuracy when the time steps are chosen adaptively. In fact, our algorithm yields **optimal convergence rates of order $q - \alpha$** , where q denotes the order of the method, either globally in time or in positive time (depending on the desired error profile used by the algorithm). At the same time, the algorithm is capable of **capturing both initial singularities and local shocks/peaks in the solution**.
- We make **a few subtle improvements in the original version of the time stepping algorithm** that substantially reduce the computational time. In particular, we modify the choice and search for a suitable initial time step, and also numerically test the algorithm parameters.
- We provide clear and specific recommendations on the **stable and efficient implementation** of the resulting algorithm, which are essential, and not at all straightforward, in the context of higher-order methods. Hence, we obtain numerically stable and efficient implementations for all considered methods (including computations of their residuals) with α **at least within the range between 0.1 and 0.999** and for values of TOL as small as 10^{-8} .

Test problem. $D_t^\alpha u - \Delta u = f$ in $(0, 1) \times (0, 1)$ with the exact solution $u(x, t) = (t^\alpha - t^2 + 1) x (1 - x)$ (which exhibits a typical singularity at $t = 0$) for $t \in (0, 1]$.

Comparison of uniform v adaptive temporal grids:

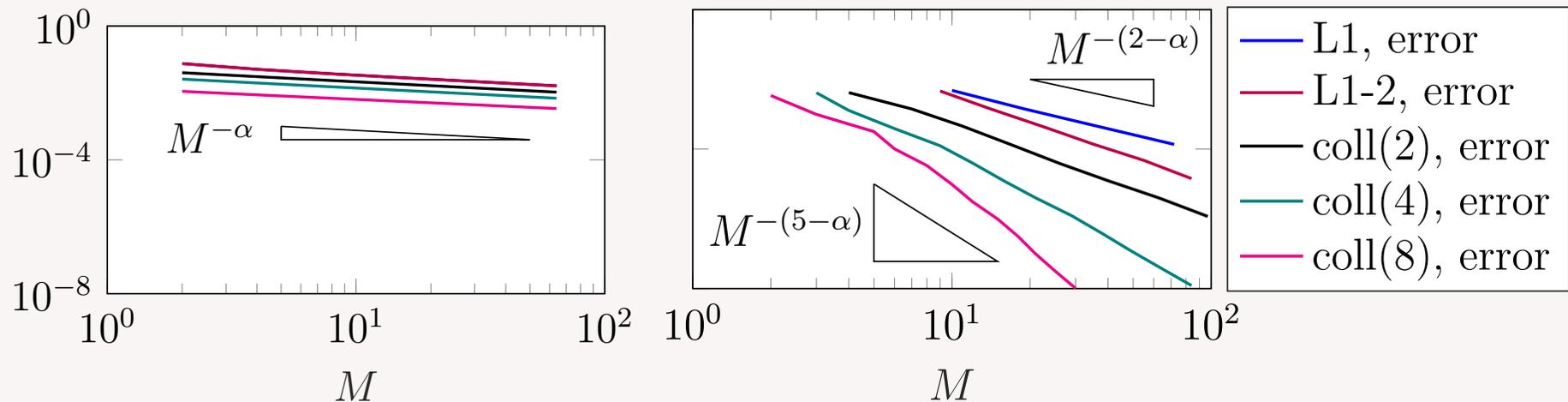


Figure 4: $L_\infty(0, T; L_\infty(\Omega))$ errors for various methods vs. number of time steps M for $\alpha = 0.4$ on uniform meshes (left), and adaptive meshes (right) with residual barrier \mathcal{R}_0 , $\lambda = \pi^2$, and $\omega = \lambda/8$

- We demonstrate that **high-order methods (incl. continuous collocation methods of order up to as high as 8)** exhibit a huge improvement in the accuracy when the time steps are chosen **adaptively**. In fact, our algorithm yields **optimal convergence rates of order $q - \alpha$** , where q denotes the order of the method, either globally in time or in positive time (depending on the desired error profile used by the algorithm).

Test problem. $D_t^\alpha u - \Delta u = f$ in $(0, 1) \times (0, 1)$ with the exact solution $u(x, t) = (t^\alpha - t^2 + 1) x (1 - x)$ (which exhibits a typical singularity at $t = 0$ for $t \in (0, 1]$).

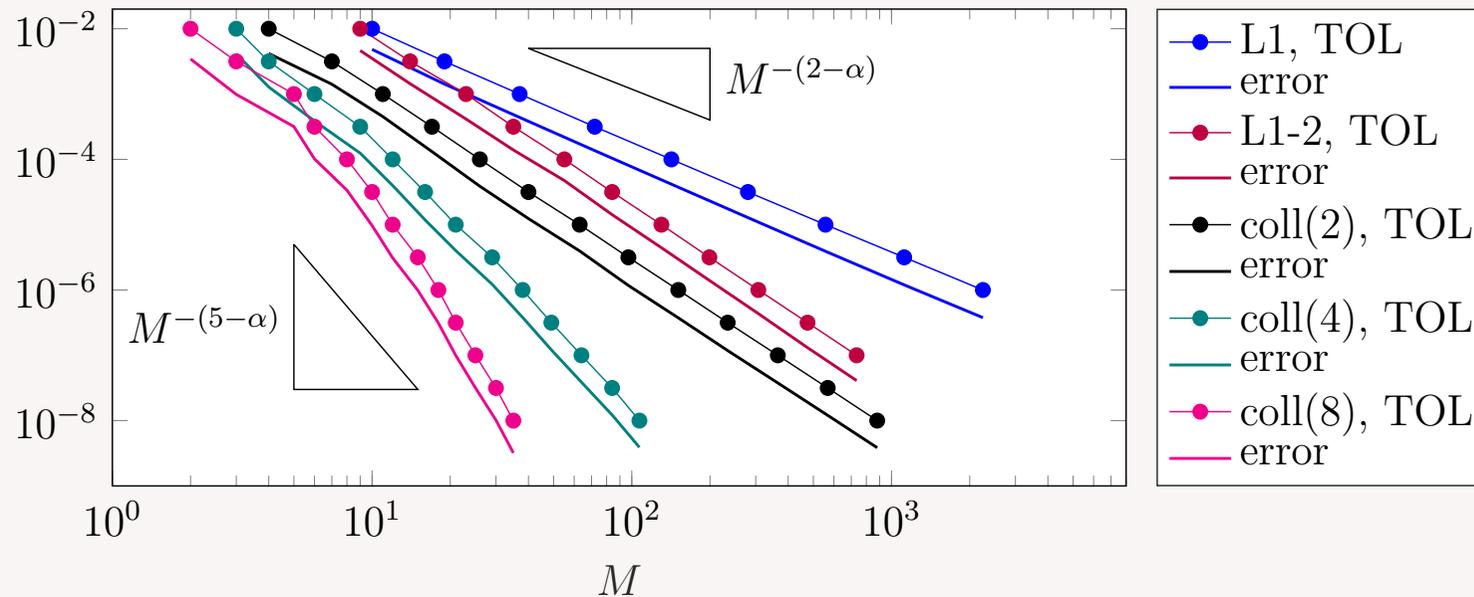


Figure 5: $L_\infty(0, T; L_\infty(\Omega))$ errors for various methods vs. number of time steps M for $\alpha = 0.4$, residual barrier \mathcal{R}_0 with $\lambda = \pi^2$ and $\omega = \lambda/8$

- Our algorithm yields **optimal convergence rates of order $q - \alpha$** , where q denotes the order of the method, either globally in time or in positive time (depending on the desired error profile used by the algorithm). At the same time, the algorithm is capable of **capturing both initial singularities and local shocks/peaks in the solution** (see the paper...)

Fractional derivative in L1-method:

Evaluation for $D_t^\alpha u_h(\cdot, t)$ for any $t_{k-1} < t \leq t_k$:

$$D_t^\alpha u_h(\cdot, t) =$$

$$\frac{1}{\Gamma(2 - \alpha)} \left(- \sum_{j=1}^{k-1} \frac{U_j - U_{j-1}}{\tau_j} (t - s)^{1-\alpha} \Big|_{s=t_{j-1}}^{s=t_j} + \frac{U_k - U_{k-1}}{\tau_k} (t - t_{k-1})^{1-\alpha} \right)$$

Numerical ISSUES:

- singularity at $s = t$ in integral,
- **cancellation at $(t - s)^{1-\alpha} \Big|_{s=t_{j-1}}^{s=t_j}$** for $j \ll k$ and $t_{j-1} \approx t_j$

i.e. the **difference of two nearly equal numbers** (assuming that $(t - t_j) \approx (t - t_{j-1})$), which leads to noticeable **round-off errors!**

Stable implementation of L1-method:

- ISSUE: **cancellation at $(t - s)^{1-\alpha} \Big|_{s=t_{j-1}}^{s=t_j}$ for $j \ll k$ and $t_{j-1} \approx t_j$**
- Rewriting: Let $d_j(t) := t - t_j$

$$\begin{aligned} (t - s)^{1-\alpha} \Big|_{s=t_{j-1}}^{s=t_j} &= d_j(t)^{1-\alpha} - d_{j-1}(t)^{1-\alpha} = d_{j-1}(t)^{1-\alpha} \cdot \left(\left(\frac{d_j(t)}{d_{j-1}(t)} \right)^{1-\alpha} - 1 \right) \\ &= d_{j-1}(t)^{1-\alpha} \cdot \left(\exp \left((1 - \alpha) \ln \left(\frac{d_j(t)}{d_{j-1}(t)} \right) \right) - 1 \right) \end{aligned}$$

- **Taylor series**

$$\exp(x) - 1 = \sum_{n=0}^{\infty} \frac{x^n}{n!} - 1 = \sum_{n=1}^{\infty} \frac{x^n}{n!} = \text{expm1}(x) \quad (\text{MatLab})$$

$$\text{log1p}(y) := \ln(1 + y) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{y^n}{n}$$

Stable implementation of L1-method (continued):

- ISSUE: **cancellation at** $(t - s)^{1-\alpha} \Big|_{s=t_{j-1}}^{s=t_j}$ **for** $j \ll k$ **and** $t_{j-1} \approx t_j$
- Rewriting: Let $d_j(t) := t - t_j$

$$(t - s)^{1-\alpha} \Big|_{s=t_{j-1}}^{s=t_j} = d_{j-1}(t)^{1-\alpha} \cdot \left(\exp \left((1 - \alpha) \ln \left(\frac{d_j(t)}{d_{j-1}(t)} \right) \right) - 1 \right)$$

Let

$$\kappa_j(t) := \ln \left(\frac{d_j(t)}{d_{j-1}(t)} \right) = \ln \left(1 - \frac{\tau_j}{d_{j-1}(t)} \right) = \text{log1p} \left(-\frac{\tau_j}{d_{j-1}(t)} \right).$$

Then

$$(t - s)^{1-\alpha} \Big|_{s=t_{j-1}}^{s=t_j} = d_{j-1}(t)^{1-\alpha} \text{expm1} \left((1 - \alpha) \kappa_j(t) \right).$$

Stable implementation for high-order collocation methods + L2 method:

- Similar issue, but becomes even more problematic...
- See the paper for clear and specific recommendations on the **stable and efficient implementation** of the resulting algorithm for such methods (up to order 8). Hence, we obtain numerically stable and efficient implementations for all considered methods (including computations of their residuals) with α **at least within the range between 0.1 and 0.999** and for values of TOL as small as 10^{-8} .

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- + [Stable implementation](#) is also addressed in the latter

I will start with a review of [1], which was presented at the 2021 edition of this workshop. For time-fractional parabolic equations with a Caputo time derivative of order $\alpha \in (0, 1)$, we give [pointwise-in-time a posteriori error bounds in the spatial \$L_2\$ and \$L_\infty\$ norms](#). Hence, an [adaptive time stepping algorithm](#) is applied for the L1 method, which yields optimal convergence rates $2 - \alpha$ in the presence of solution singularities. Interestingly, the proposed time stepping algorithm yields the grids similar to a-priori-constructed optimal grids in [2, 3].

In the main part of the talk, we shall discuss [recent extensions](#) of the proposed methodology to [variable-coefficient multiterm time-fractional subdiffusion equations](#) [4], and to the case of [higher-order discretizations](#) [5]. The [stable implementation](#) of the proposed algorithm will also be addressed [5].

1. N. Kopteva, Pointwise-in-time a posteriori error control for time-fractional parabolic equations, *Appl. Math. Lett.*, 123 (2022), 107515.
2. 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.
3. N. Kopteva, *Error analysis for time-fractional semilinear parabolic equations using upper and lower solutions*, *SIAM J. Numer. Anal.*, 58 (2020), 2212–2234.
4. N. Kopteva and M. Stynes, A posteriori error analysis for variable-coefficient multiterm time-fractional subdiffusion equations, *J. Sci. Comput.*, (2022).
5. S. Franz and N. Kopteva, Pointwise-in-time a posteriori error control for higher-order discretizations of time-fractional parabolic equations, *J. Comput. Appl. Math.*, volume 427 (2023), 115122.

FINAL

Thank you!