Structure preserving methods for time-fractional reaction-diffusion problems

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Fractional differential equations

ODEs

$$\begin{cases} \frac{d^n y}{dt^n} = f(t, y), & t \in [0, T] \\ y^{(k)}(0) = y_0^{(k)}, & k = 0, \dots, n-1 \end{cases}$$

FDEs

$$\begin{cases} \frac{d^{\alpha} y}{dt^{\alpha}} = f(t, y), & t \in [0, T] \\ \text{initial conditions} \end{cases}$$

$$n - 1 < \alpha < n, n \in \mathbb{N}$$

Fractional differential operators are intermediate operators which model the behaviour of processes which cannot be successfully described by integer order differential operators

Examples

- viscoelastic materials
- transport in porous media
- vegetation spread

Some modeling aspects

- *Several* definitions of fractional derivative. Most popular ones: Grunwald-Leitnikov, Riemann-Liouville, Caputo.
- In any case, $D^\alpha y(t)$ depends on the past history of $y(t)$, thus:

FDEs are naturally suitable to describe phenomena with memory

Caputo's definition

$$D_t^\alpha y(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-s)^{n-\alpha-1} y^{(n)}(s) ds, \quad n-1 < \alpha < n, n \in \mathbb{N}$$

widely used in the applications. It needs for initial conditions in terms of integer order derivatives $\rightarrow$ *physical meaning*. Moreover $D^\alpha const = 0$.

$$\begin{cases} D^\alpha y(t) = f(t, y(t)), & t \in [0, T] \\ y^{(k)}(0) = y_0^{(k)}, & k = 0, \dots, n \end{cases}$$

Numerical solution

- analytical solution usually *not smooth*
  $\rightarrow$ *low order* of convergence of standard numerical methods
- *history term* discretization
  $\longrightarrow$ *expensive*, especially for long time integration
- *real problems* simulation
  $\longrightarrow$ reproduce *qualitative behaviour* of the analytical solution

specially tuned numerical solvers must be adopted

Time-fractional reaction-advection-diffusion system

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = A\,\nabla\cdot u(x,t) + B\,\nabla^2 u(x,t) + f(x,t,u(x,t)), \quad (t,x) \in [0,T]\times\Omega$$

subject to some boundary conditions and suitable initial conditions.

Perspective

Advanced numerical methods should be able to preserve the properties of the dynamical system.

Conservation laws of fractional PDEs (FPDEs)

$$\text{FPDE:} \quad \mathcal{A}(x, t, [u]_\alpha) = 0.$$

- A conservation law is of the form

$$\text{Div}\,\mathbf{F} \equiv D_x\{F(x,t,[u]_\alpha)\} + D_t\{G(x,t,[u]_\alpha)\} = 0, \quad \text{when } \mathcal{A} = 0,$$

- A discrete conservation law is an expression of the form

$$D_{\Delta x}\tilde{F}(x_i, t_j, u_{i,j}) + D_{\Delta t}\tilde{G}(x_i, t_j, u_{i,j}) = 0, \ \text{when } \widetilde{\mathcal{A}} = \mathbf{0}.$$

$[u]_\alpha$ denotes u, its fractional and integer derivatives, its fractional integrals.

A mixed finite-difference method in space and a spectral method in time for time-fractional reaction-diffusion pbs

- space discretization: easy, coefficients *specially tuned* on the problem
- spectral method along time: strong reduction of the comp. cost, by avoiding the history term discretization; exponential convergence
- preservation of the discrete conservation laws for FPDEs ${}^{RL}D_t^{\alpha} u = K(u)_{xx}$
- parallel implementation
- suitable extension for stochastic FDEs

K. Burrage, A. Cardone, R. D'Ambrosio, B. Paternoster, *Numerical solution of time fractional diffusion systems*, Appl. Numer. Math. **116**, 82-94 (2017).

A. Cardone, G. Frasca Caccia, *Numerical conservation laws of time fractional diffusion PDEs*, Fract. Calc. Appl. Anal. **25**, 1459–1483 (2022).

A. Cardone, P. De Luca, A. Galletti, L. Marcellino, *Solving time-fractional reaction–diffusion systems through a tensor-based parallel algorithm*, Phys. A: Stat. Mech. Appl. **611**, 2023, 128472.

A. Cardone, R. D'Ambrosio, B. Paternoster, *A spectral method for stochastic fractional differential equations*, Appl. Numer. Math. **139** (2019), 115-119.

Contents

Time-fractional reaction-advection-diffusion (RAD) equation with positive solution

$$D_t^\alpha u + Au_x - Du_{xx} + Ru = 0, \qquad (x,t) \in [a,b] \times [0,T],$$
$$u(x,0) = u_0(x), \quad x \in [a,b]$$

Dirichlet or periodic BC

$A, D, R > 0$, $0 < \alpha < 1$.

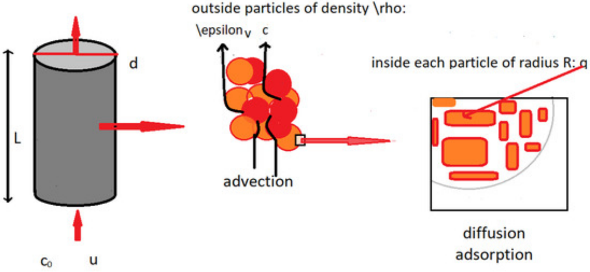
We assume that: $u_0 \geq 0 \Longrightarrow$ **the solution u is positive**.

Applications:

- dispersion in porous media
- anomalous diffusion

Anomalous diffusion model in a packed bed reactor

within an interstitial void space ϵ of the adsorption packed bed, with advection in the pores of spherical adsorbent particles, dispersion effects and reactions describing mass transfer in the adsorption process. At the inlet of the reactor, there is u_{in} concentration of the species; at the outlet there is no diffusion.



A. Jannelli, *Numerical solutions of fractional differential equations arising in engineering sciences*, Mathematics, 8(2):215, 2020.

Anomalous diffusion model in a packed bed reactor

Mathematical model

$$\begin{cases} \partial_t^\alpha u + A u_x - D u_{xx} + \frac{1-\epsilon}{\epsilon} k_u a_v (u - u^*) = 0, & (x,t) \in [0,L] \times [0,T] \\ u(0,0) = u_0, \quad u(x,0) = 0,\ 0 < x \leq L, & \\ u(0,t) = u_{in}, \quad \frac{\partial u}{\partial x}(L,t) = 0, & t \in [0,T]. \end{cases}$$

$u =$ liquid phase concentration of a given substance

IC: an aqueous solution at $x = 0$ of the packed bed, with concentration u_0.
BC: At the inlet of the reactor, there is u_{in} concentration of the species; at the outlet there is no diffusion.
$A =$ interstitial velocity, $D =$ dispersion coeff., $k_u =$ mass transfer coeff., $a_v =$ volumetric surface area of the packed bed, $u^* =$ solubility value.

A 2D time-fractional nonlinear drift reaction–diffusion equation in electrical engineering

It is model for charge carriers, applicable in batteries based on disordered semiconductors, such as P3HT used in lithium batteries. Since carriers move in a disordered material, **anomalous diffusion** arises.

$$\frac{\partial^\alpha}{\partial t^\alpha}u(x,y,t) = \Delta u(x,y,t) - \nu_1 \frac{\partial}{\partial x}u(x,y,t) - \nu_2 \frac{\partial}{\partial y}u(x,y,t)$$
$$- \eta u(x,y,t)(1-u(x,y,t)) + f(x,t,u(x,t))$$

$u(x,y,t)$= charge carriers concentration
ν_i convection coeff.$= \mu_i F_0$, with μ_i mobility and F_0 uniform electric field

Anjuman, Leung, Das, Two-Dimensional Time-Fractional Nonlinear Drift Reaction–Diffusion Equation Arising in Electrical Field. Fractal Fract. 2024, 8, 456.

Choo, Muniandy, Woon, Gan, Ong, Modeling anomalous charge carrier transport in disordered organic semiconductors using the fractional drift-diffusion equation, Org. Electron., **41**, 2017, pp 157-165.

Research aim

Time-fractional RAD problem with non-negative solution

$$D_t^\alpha u + Au_x - Du_{xx} + Ru = 0, \qquad (x,t) \in [a,b] \times [0,T],$$
$$u(x,0) = u_0(x),\ x \in [a,b], \qquad \text{Dirichlet or periodic BC}$$

Classical schemes

- numerical instability for explicit schemes
- preserve positivity only for small stepsizes

Our goal

To develop reliable and stable numerical schemes

which preserve the positivity of the analytical solution

Nonstandard finite difference (NSFD) methods for ODEs

$$y' = f(t, y)$$

Standard approach: $$\frac{y_{k+1} - y_k}{h} = f(t_k, y_k)$$

NSFD if at least one of the following settings are imposed

- **nonlocal representation** of the rhs, for example

$$f(t, y) = y^2 \to f(t_k, y_k) = y_k y_{k+1}$$

- denominator function

$$\frac{y_{k+1} - y_k}{\phi(h, \theta)} = f(t_k, y_k)$$

with $\phi(h, \theta) = h + O(h^2)$, $\theta =$ parameter of the problem.

R. Mickens, *Nonstandard finite difference models of differential equations*, World Scientific Publishing, 1994.

Some references on positive preserving schemes for time fractional differential problems

A few numerical approaches considered this aspect. Among them, Moaddy *et al.* and Verma *et al.* proposed nonstandard schemes.

- B. Jin, R. Lazarov, R., V. Thomée, Z. Zhou, *On nonnegativity preservation in finite element methods for subdiffusion equations*, Math. Comput. 86, 2239–2260 (2017)
- K. Moaddy, S. Momani, I. Hashim, *The non-standard finite difference scheme for linear fractional PDEs in fluid mechanics*, Comput. Math. Appl. **61**(4), 2011, 1209–1216.
- A. Verma, M.K. Rawani, R.P. Agarwal, *A novel approach to compute the numerical solution of variable coefficient fractional Burgers' equation with delay*. J. Appl. Comput. Mech., 2021; 7(3): 1550-1564.
- B. Yu, Y. Li, J. Liu, *A Positivity-Preserving and Robust Fast Solver for Time-Fractional Convection–Diffusion Problems*, J. Sci. Comput. 98, 59 (2024).

Our proposal

A nonstandard finite-difference scheme along space combined with a L1 or Grünwald-Letnikov method along time

- easy to implement
- enough accurate for most applications

main goals

- unconditional stability
- unconditional positivity

REMARK: Due to the high computational cost of the time-discretization, the most serious issue concerns the **limitations on the time-step**.

Approximation of the fractional derivative

$$D_t^\alpha y(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} y(s) ds, \quad 0 < \alpha < 1$$

L1 or Grünwald-Letnikov (GL) formulae

$$\partial_{\Delta t}^\alpha u_{m,n} = \frac{1}{\Delta t^\alpha} \sum_{j=0}^{n} w_j u_{m,n-j}, \tag{1}$$

where $u_{m,n} \approx u(x_m, t_n)$, $w_0 = 1$ and

- **L1** (order $2-\alpha$): $w_n = \left((n-1)^{1-\alpha} - n^{1-\alpha}\right) / \Gamma(2-\alpha)$

  $$w_j = \left((j+1)^{1-\alpha} - 2j^{1-\alpha} + (j-1)^{1-\alpha}\right) / \Gamma(2-\alpha), j = 1, \ldots, n-1,$$

- **GL** (order 1): $w_j = (-1)^j \binom{\alpha}{j} = (-1)^j \dfrac{\Gamma(\alpha+1)}{j!\Gamma(\alpha-j+1)}$

Properties of the time discretization schemes

Lemma (Dimitrov; Scherer *et al.*)

Let $\{w_j\}_{j\geq 0}$ *be the coefficients of the L1 or the GL scheme. Then*

$$w_0 = 1, \qquad w_j < 0,\ j = 1, \ldots, n;$$
$$\sum_{j=0}^{n} w_j = 0 \text{ for L1}, \qquad \lim_{n\to\infty} \sum_{j=0}^{n} w_j = 0 \text{ for GL}.$$

Lemma

Let $\{w_j\}_{j\geq 0}$ *be the coefficients of the L1 or the GL method. If* $\rho \in \mathbb{C}$, *with* $|\rho| > 1$, *then*

$$\left| \sum_{j=1}^{n-1} w_j \rho^{1-j} \right| < 1.$$

Explicit nonstandard (NS) time-stepping methods

$$D_t^\alpha u + Au_x - Du_{xx} + Ru = 0, \qquad (x,t) \in [a,b] \times [0,T],$$

Explicit nonstandard methods with order 1 in space

$$\partial_{\Delta t}^\alpha u_{m,n} + A\frac{u_{m,n} - u_{m-1,n-1}}{\Delta x} - D\frac{u_{m+1,n-1} - 2u_{m,n} + u_{m-1,n-1}}{\Delta x^2} + Ru_{m,n} = 0,$$

In the standard explicit scheme $u_{m,n} \Longrightarrow u_{m,n-1}$

Reference for the explicit NS methods, for the integer order problems:

B.M. Chen-Charpentier, H.V. Kojouharov, *An unconditionally positivity preserving scheme for advection-diffusion reaction equations*, Math. Comput. Modelling, **57**(9-10), 2177–2185, 2013.

Implicit Nonstandard (NS) time-stepping methods

$$D_t^\alpha u + Au_x - Du_{xx} + Ru = 0, \qquad (x,t) \in [a,b] \times [0, T],$$

NS implicit methods with order 2 in space

$$\partial_{\Delta t}^\alpha u_{m,n} + A\frac{u_{m+1,n} - u_{m-1,n}}{2\Delta x} - D\frac{u_{m+1,n} - 2u_{m,n} + u_{m-1,n}}{\Delta x^2} + R\hat{u}_{m,n} = 0,$$

with $\hat{u}_{m,n} = \sigma(u_{m,n}) + (1-\sigma)(u_{m,n-1})$.

- $\sigma = 1 \Longrightarrow$ standard implicit L1- or GL-finite difference scheme

We will analyze how σ may affect stability, positivity and accuracy.

Preservation of positivity

Explicit NS methods

The methods are positivity preserving, for any $\Delta x > 0$ and $\Delta t > 0$.

Implicit NS methods

Let

$$\sigma \geq 1, \qquad \Delta x \leq \frac{2D}{A},$$

then the methods are positivity preserving, for any $\Delta t > 0$.

These theorems hold both for L1 and GL time discretizations.

Stability

By the standard von Neumann stability analysis we proved

Explicit NS methods

The methods are stable, for any $\Delta x > 0$ and $\Delta t > 0$.

Implicit NS methods

Let

$$\sigma \geq \frac{1}{2},$$

then the methods are stable, for any $\Delta t > 0$ and $\Delta x > 0$.

These theorems hold both for L1 and GL time discretizations.

Error analysis

$T_{m,n}$=truncation error

Explicit NS methods

$$T_{m,n} = \mathcal{O}(\Delta x) + \mathcal{O}(\Delta t) + \mathcal{O}\left(\frac{\Delta t}{\Delta x^2}\right),$$

both for GL and L1 time discretization.

Implicit NS methods

$$\text{GL:}\ T_{m,n} = \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta t)$$
$$\text{L1:}\ T_{m,n} = \mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta t^{2-\alpha}) + (1-\sigma)\mathcal{O}(\Delta t)$$

Thus, when L1 is applied:
if the timestep is small, $\sigma = 1$ (i.e. classical implicit) $\rightarrow$ best accuracy, otherwise $\sigma > 1$ (i.e. NS approach) may be preferable.

Summary

	positivity	stability	consistency	truncation error
Explicit NS	unconditionally		$\Delta t < \Delta x^2$	$O(\Delta x) + \mathcal{O}(\Delta t) + \mathcal{O}(\frac{\Delta t}{\Delta x^2})$
Implicit NS with $\sigma \geq 1$	$\Delta x < \frac{2D}{A}$	unconditionally		GL: $\mathcal{O}(\Delta x^2) + \mathcal{O}(\Delta t)$ L1: $\mathcal{O}(\Delta x^2)+$ $(1-\sigma)\mathcal{O}(\Delta t) + \mathcal{O}(\Delta t^{2-\alpha})$

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Numerical illustration

Problem 1

$$D_t^\alpha u + u_x - u_{xx} + u = 0, \qquad (x,t) \in [0,10] \times [0,0.85],$$
$$u(x,0) = \mathrm{e}^{-x},$$
$$u(0,t) = E_\alpha(t^\alpha), \qquad u(10,t) = \mathrm{e}^{-10} E_\alpha(t^\alpha).$$

The exact solution is

$$u_{\text{exact}}(x,t) = \mathrm{e}^{-x} E_\alpha(t^\alpha).$$

Exact and numerical solutions

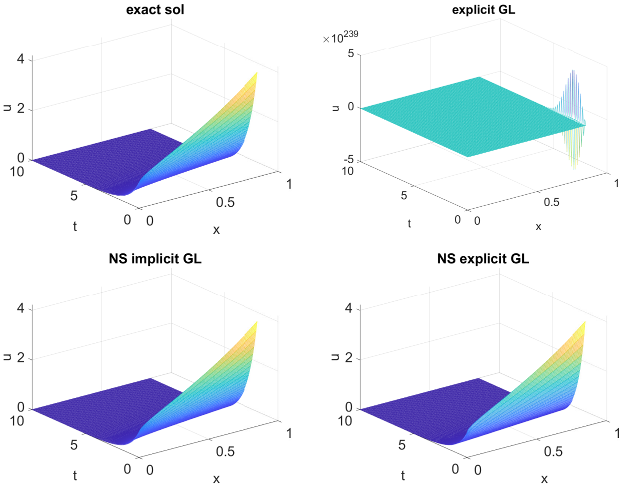
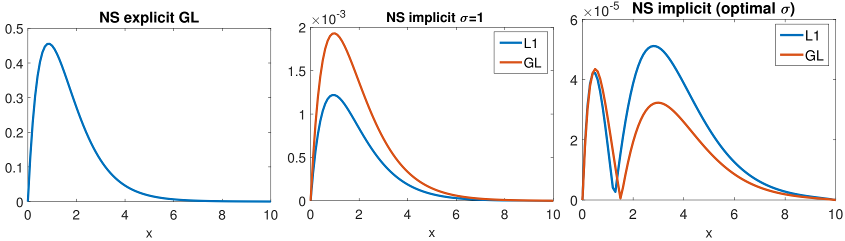


Figure: $\Delta x = 0.1$, $\Delta t = 0.005$.

Error plots

Absolute error at the final time, $\Delta x = 0.1$, $\Delta t = 0.005$

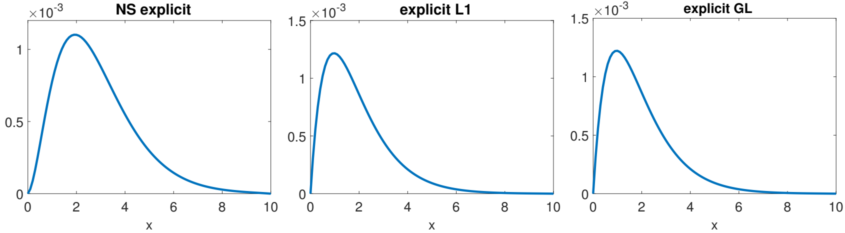


- left: NS explicit GL-method
- center: NS implicit with $\sigma = 1$ (= classical implicit)
- right: NS implicit with best σ wrt accuracy (by numerical search), i.e. $\sigma = 1.65$ for GL and $\sigma = 1.41$ for L1 .

Error of explicit methods

Standard implicit methods with $\Delta t = 5 \cdot 10^{-3}$ give maximum error$\approx 10^{-3}$.
To obtain the same accuracy with the explicit methods, these are the largest stepsizes to apply:

- NS explicit GL[1]: $\Delta t \approx 2 \cdot 10^{-4}$
- classical explicit L1: $\Delta t \approx 2 \cdot 10^{-5}$ (unstable for $\Delta t = 2 \cdot 10^{-4}$)
- classical explicit GL: $\Delta t \approx 10^{-5}$ (unstable for $\Delta t = 2 \cdot 10^{-4}$)



[1]similar results are obtained by NS explicit L1

Problem 2: chemical engineering

$$\begin{cases} \partial_t^\alpha u + Au_x - Du_{xx} + \frac{1-\epsilon}{\epsilon} k_u a_v (u - u^*) = 0, & (x,t) \in [0,L] \times [0,T] \\ u(0,0) = u_0, \quad u(x,0) = 0, \ 0 < x \leq L, & \\ u(0,t) = u_{in}, \quad \frac{\partial u}{\partial x}(L,t) = 0, & t \in [0,T]. \end{cases}$$

$L = 0.01$ (m), $T = 4$ (days), $\alpha = 0.5$,

$$\epsilon = 0.8, \quad A = 0.02(\mathrm{m/s}), \quad D = 1.63 \cdot 10^{-4}\mathrm{m}^2/\mathrm{s}, \quad k_u = 0.001(\mathrm{s}^{-1}),$$
$$a_v = 0.17(\mathrm{m}), \quad u^* = u_0 = u_{in} = 1.1(\mathrm{mM}).$$

Only a numerical reference solution is available.

A. Jannelli, *Numerical solutions of fractional differential equations arising in engineering sciences*, Mathematics, 8(2):215, 2020.

Problem 2: numerical solutions

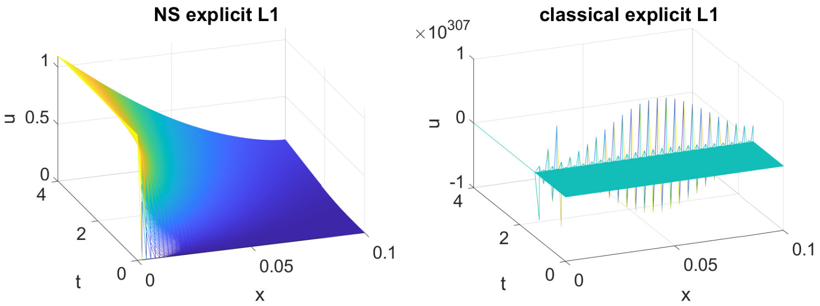


Figure: $\Delta x = 0.002$, $\Delta t = 0.004$.

Problem 2: 1D version of the battery model

$$\begin{cases} \partial_t^\alpha u + Au_x - Du_{xx} = Ru(1-u), & (x,t) \in [0,1] \times [0,13] \\ u(x,0) = u_0(x), & 0 \le x \le 1, \\ u(0,t) = u(1,t) = 0, & t \in [0,13], \end{cases}$$

with

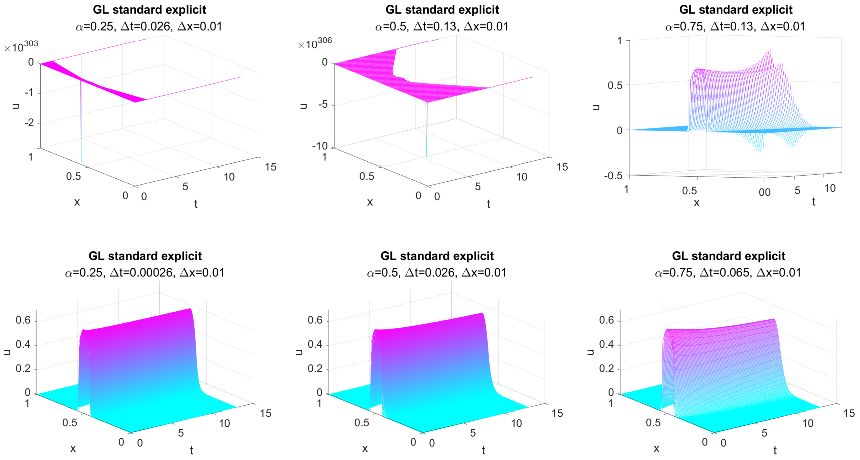
$$u_0(x) = \begin{cases} 0.7 \exp(-80(x - \frac{1}{2})^2), & |x - x_0| \le 0.06 \\ 0, & \text{otherwise} \end{cases}$$

$0 < \alpha < 1$, $A = 0$, $D = 0.0002$, $R = 0.05$.

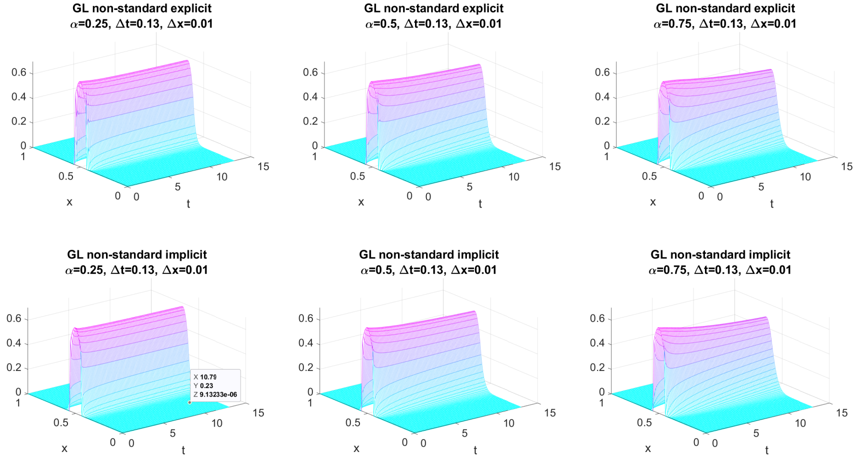
In the NS methods, the reaction term is discretized as follows:

$$Ru_{m,n-1}(1 - (1-\sigma)u_{m,n-1}) - R\sigma u_{m,n-1} u_{m,n}.$$

Problem 2: battery model, classical methods



Problem 3: battery model, non-standard methods



Problem 3: battery model, implicit and explicit nonstandard methods

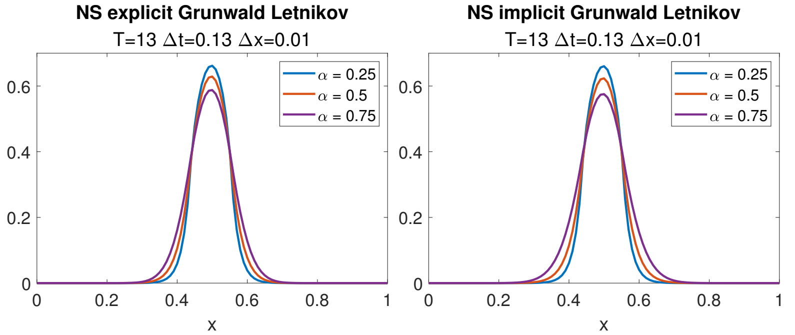


Figure: Solution at the end point of the time interval. For the NS implicit method, $\sigma = 2$.

Concluding remarks

- Structure preserving methods are required in applications, also when fractional differential models are considered
- We propose two classes of nonstandard numerical methods for time fractional RAD equations with positive solutions.
- We carried out error analysis, stability analysis and positivity preserving analysis.
- Numerical experiments confirm theoretical results and prove the advantage of nonstandard approach.

Future work

- Automatic procedure to find the best value of σ for the implicit NS methods
- Consider further classes of methods for the discretization of the fractional derivative

The end

THANK YOU!