Numerical methods for nonlocal and nonlinear parabolic equations with applications in hydrology and climatology

Łukasz Płociniczak

Hugo Steinhaus Center, Faculty of Pure and Applied Mathematics,
Wroclaw University of Science and Technology

10 November 2021
IMDETA

Support: National Science Centre, Poland (NCN)
Grant: NCN 2020/38/E/ST1/00153

Nonlocality is ubiquitous.

- Physics (plasma, turbulent flow, complex fluids, viscoelasticity, electronics, complex materials)
- Hydrology (porous media, flow in concrete, bed-load transport)
- Signal and image processing
- Biology (cell biochemistry, MRI, fractional neuron models, modelling bone tumours)
- Finance (heavy-tailed distributions, option pricing)
- Many more...[1]

[1] Sun, HongGuang, et al. "A new collection of real world applications of fractional calculus in science and engineering." Communications in Nonlinear Science and Numerical Simulation 64 (2018): 213-231.

Introduction

Usually nonlocality is **temporal** or **spatial**. Mathematical modelling is done with **integro-differential** operators such as:

- fractional integrals and derivatives (Riemann-Liouville, Caputo, Weyl, ...),
- singular integral operators (Riesz derivatives, fractional Laplacian, fractional gradient, ...),
- other operators with memory kernels.

Interesting theory of PDEs and numerical methods for solving them!

Introduction

Usually nonlocality is **temporal** or **spatial**. Mathematical modelling is done with **integro-differential** operators such as:

- fractional integrals and derivatives (Riemann-Liouville, Caputo, Weyl, ...),
- singular integral operators (Riesz derivatives, fractional Laplacian, fractional gradient, ...),
- other operators with memory kernels.

Interesting theory of PDEs and numerical methods for solving them!
Especially for <u>nonlinear</u> equations.

Time-fractional porous medium

- Let $u(x, t)$ be the moisture concentration in porous medium at point $x \geq 0$ and time t.
- Initial-boundary conditions (nondimensional form)

$$u(0, t) = 1, \quad u(x, 0) = 0.$$

- **Self-similarity** - a characteristic feature of diffusion in our experiment. Moisture concentration $u(x, t)$ can be drawn on a single curve[2,3]:

$$u(x, t) = U(\eta), \quad \eta = x\, t^{-\frac{\alpha}{2}},$$

for $U(0) = 1$, $U(\infty) = 0$ and $0 < \alpha < 1$.

- Transport in porous media is **substantially nonlinear** (diffusivity depends on concentration).

[2] L. Pel et al., J. Phys. D.: Appl. Phys. 28 (1995) 675–680.
[3] Abd El-Ghany et al., J. Phys. D.: Appl. Phys. 37 (2004) 2305–2313.

Time-fractional porous medium

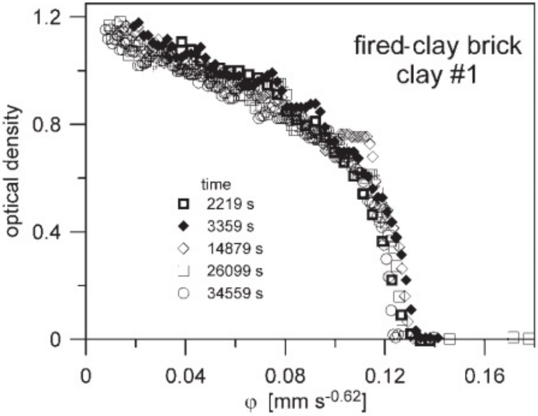

Figure: An exemplary shape of the self-similar moisture curve.

Time-fractional porous medium

- The model is a **nonlocal and nonlinearly degenerate** parabolic PDE

$$\frac{\partial^\alpha u}{\partial t^\alpha} = \frac{\partial}{\partial x}\left(u^m \frac{\partial u}{\partial x}\right), \quad 0 < \alpha < 1, \quad m \geq 1,$$

  with initial-boundary conditions $u(0,t) = 1$, $u(x,0) = 0$.
- We seek for a self-similar slution $u(x,t) = U(\eta)$, where $\eta = x/t^{\alpha/2}$ and obtain an ordinary integro-differential equation

$$\boxed{\frac{\partial}{\partial \eta}\left(U^m \frac{\partial U}{\partial \eta}\right) = \left[(1-\alpha) - \frac{\alpha}{2}\eta \frac{d}{d\eta}\right] F_\alpha U, \quad F_\alpha := I_{-\frac{2}{\alpha}}^{0,1-\alpha}, \quad m \geq 1,}$$

  with $U(0) = 1$ and $U(\infty) = 0$, where the integral operator is of the **Erdélyi-Kober** type

$$I_c^{a,b} U(\eta) := \frac{1}{\Gamma(b)} \int_0^1 (1-z)^{b-1} z^a U(\eta z^{\frac{1}{c}}) dz.$$

- This is a **free-boundary** problem.

Time-fractional porous medium

- The existence and uniqueness of the solution can be proved by several transformations. This gives us an **idea** for an efficient numerical method
  1. Transform the governing equation into the self-similar form.
  2. Conduct the second transformation into the initial-value problem.
  3. Integrate to obtain the integral equation.
  4. Discretize the integral equation.
  5. Solve!
- **Partial** nonlocal nonlinear equation with a free boundary $\longrightarrow$ **Ordinary** nonlinear integral equation $\longrightarrow$ **Much faster method**!
- Relevant papers:

  Ł.P., *Numerical method for a time-fractional porous medium equation*, SIAM Journal on Numerical Analysis, 57(2) (2019), 638–656

  Ł.P., M. Świtała, *Existence and uniqueness results for a time-fractional nonlinear diffusion equation*, JMAA 462(2) (2018), 1425-1434.

Time-fractional porous medium equation

- There exists a transformation that takes self-similar form of u into a nonlinear Volterra equation

$$y(z)^{m+1} = \int_0^z K(z,s)y(s)ds, \quad 0 \le z \le 1,$$

where $K_-(z-s)^\gamma \le K(z,s) \le K_+(z-s)^\gamma$ with $\gamma \ge 0$.
- Even better is to substitute $y(z) = z^{\frac{\gamma+1}{m}} v(z)$ because then, according to general theory, we have $0 < C_- \le v(z) \le C_+$.
- The numerical method is based on a quadrature for the integral

$$v_n^{m+1} = z_n^{-\frac{(m+1)(\gamma+1)}{m}} \sum_{i=0}^{n-1} w_{n,i}(h) v_i,$$

where $w_{n,i}(h)$ are specific weights.
- Higher order methods are **difficult** to construct.
- Equation has a trivial solution and thus we have to impose an appropriate **initialization** of the scheme.

Time-fractional porous medium equation

- We have constructed an explicit **second-order scheme** by linear reconstruction. The quadrature **must not involve** the terminal point.
- In each **three node interval** we approximate the solution by a linear function based on **two first nodes**.
- For example, if total number of nodes is even we have

$$\boxed{w_{n,i}(h) = \int_{z_i}^{z_{i+2}} K(z_n, s) s^{\frac{\gamma+1}{m}} \left(\begin{cases} 1 - \frac{s-z_i}{h}, & i \text{ even} \\ \frac{s-z_i}{h}, & i \text{ odd} \end{cases} \right) ds.}$$

- We have to prescribe **two initial steps**. The zeroth one is exact

$$v_0 = v(0) = \lim_{h \to 0^+} \left(h^{-\gamma} \int_0^1 K(h, h\sigma) \sigma^{\frac{\gamma+1}{m}} ds \right)^{\frac{1}{m}}.$$

  The first one is **implicitly** given by rectangle method: approximate the solution by a linear function between z_0 and z_1.
- Relevant paper with **convergence proofs**: **H.Okrasińska-Płociniczak, Ł.P.**, *Second order scheme for self-similar solutions of a time-fractional porous medium equation on the half-line*, arXiv:2106.05138.

Time-fractional porous medium equation

- Numerically calculated order of convergence for fractional diffusion.

m \ α	0.01	0.1	0.3	0.5	0.7	0.9	0.99
1	1.84	1.98	2.01	2.00	2.09	2.10	2.13
3	1.80	1.98	1.99	1.98	1.97	1.96	1.96
5	1.74	1.92	1.92	1.92	1.91	1.89	1.89
7	1.71	1.88	1.88	1.87	1.87	1.91	1.86
10	1.70	1.85	1.85	1.84	1.84	1.86	1.83
20	1.73	1.85	1.84	1.83	1.83	1.85	1.82

- Wetting front calculation for $\alpha = 1$ and $m = 2$. Here, $U(\eta) = 0$ for $\eta \geq \eta^*$. Falls to zero like N^{-2}.

N	10	20	50	100	200
$\lvert\eta^* - \eta^*_{exact}\rvert$	1.1×10^{-4}	2.9×10^{-5}	4.6×10^{-6}	1.1×10^{-6}	2.8×10^{-7}

Quasilinear subdiffusion equation

- Now, we focus on the **general** Quasilinear subdiffusion equation

$$\begin{cases} \partial_t^\alpha u = (D(u)u_x)_x + f(x,t,u), \quad x \in (0,1), \quad t \in (0,T), \quad \alpha \in (0,1), \\ u(x,0) = \varphi(x), \\ u(0,t) = 0, \ u(1,t) = 0, \end{cases}$$

with Caputo derivative

$$\partial_t^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} u_t(x,s) ds.$$

- We assume nondegeneracy (coercivity) and some regularity

$$0 < D_- \leq D(u) \leq D_+, \quad |f(x,t,u)| \leq F, \quad |D'(u)| + |f_u(x,t,u)| \leq L.$$

- We have constructed a **Galerkin spectral method** however, all the proofs can be easily translated into FEM framework.
- Relevant paper with **convergence proofs**:
  Ł.P., *A linear Galerkin numerical method for a strongly nonlinear subdiffusion equation*, arXiv:2107.10057.

Quasilinear subdiffusion equation

- The problem in the weak setting is

$$(\partial_t^\alpha u, v) + a(D(u); u, v) = (f(t, u), v), \quad v \in H_0^1(0,1),$$

  where $a(D(w); u, v) = \int_0^1 D(w(x)) u_x(x) v_x(x) dx$.
- We choose a N-th dimensional subspace of trigonometric or algebraic polynomials, i.e. $V_N \subset H_0^1(0,1)$.
- Let P_N be the **orthogonal projection** onto V_N. For sufficiently regular functions we have

$$\|u - P_n u\| \le C N^{-m} \|u\|_m, \quad \|u - P_n u\|_l \le C N^{2l - \frac{1}{2} - m} \|u\|_m, \quad u \in H_0^m.$$

- We also define the **Ritz elliptic projection** (it has similar regularity estimates as P_N but is much more useful)

$$a(D(u); R_N u - u, v) = 0, \quad v \in V_N.$$

- Since we want a **completely linear scheme** we introduce the $O(h^2)$ extrapolation

$$\widehat{y}(t_n) := 2y(t_{n-1}) - y(t_{n-2}).$$

Quasilinear subdiffusion equation

- Introduce the time grid $t_n = nh$ with $h > 0$ being the time step.
- The **fully discrete** numerical method can be formulated as

$$\boxed{(\delta^\alpha U^n, v) + a(D(\widehat{U}^n); U^n, v) = (f(t_n, \widehat{U}^n), v), \quad v \in V_N, \quad n \geq 2,}$$

where the Caputo derivative is discretized via the **L1 scheme**

$$\delta^\alpha U^n = \frac{h^{-\alpha}}{\Gamma(2-\alpha)} \sum_{i=0}^{n-1} b_{n-i}(1-\alpha)(U^{i+1} - U^i),$$

with $b_j(\beta) = j^\beta - (j-1)^\beta$.

Convergence

Let $u \in C^2((0,T); H^m)$ be a solution of the PDE and U^n a solution of the numerical scheme. For sufficiently large m and small $h > 0$ we have

$$\|u(t_n) - U^n\| \leq C\left(N^{-m} + h^{2-\alpha}\right),$$

where the constant C depends on α and derivatives of u.

Quasilinear subdiffusion equation

- The proof is based on the decomposition

$$u(t_n) - U^n = u(t_n) - R_N u(t_n) + R_N u(t_n) - U^n = r^n + e^n.$$

- The projection error r^n is estimated from the approximation theory so we can focus on e^n which is calculated in **finite dimensions**.
- By the fact that $(\delta^\alpha y^n, y^n) \geq \frac{1}{2}\delta^\alpha \|y^n\|^2$ we obtain the **error inequality**

$$\frac{1}{2}\delta^\alpha \|e^n\|^2 + D_0 \|e^n\|_1 \leq \rho_{Caputo} + \rho_{diffusivity} + \rho_{source}.$$

- By careful estimates for each remainder we obtain

$$\delta^\alpha \|e^n\|^2 \leq C\left(\|e^{n-1}\|^2 + \|e^{n-2}\|^2 + \left(N^{-m} + h^{2-\alpha}\right)^2\right).$$

- The fractional discrete Grönwall lemma[4] then yields

$$\|e^n\|^2 \leq C\left(\|e^0\|^2 + \left(N^{-m} + h^{2-\alpha}\right)^2\right).$$

[4] Liao, Hong-lin, Dongfang Li, and Jiwei Zhang. SIAM Journal on Numerical Analysis 56.2 (2018): 1112-1133.

Quasilinear subdiffusion equation

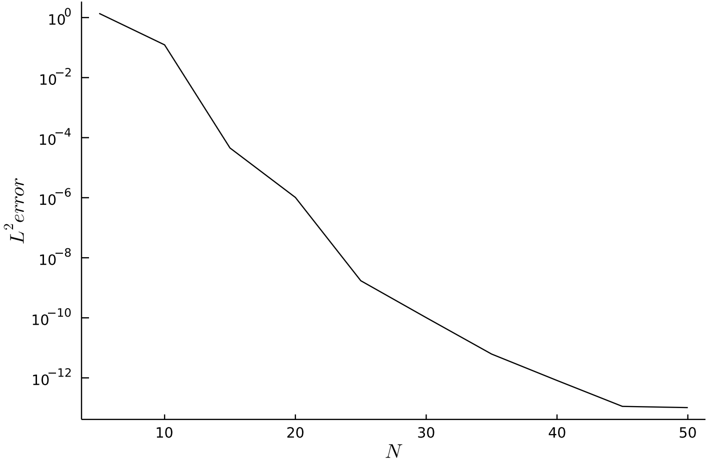

Figure: A semi-log plot of the L^2 error $\alpha = 0.5$ as a function of N with fixed $h = 10^{-3}$.

Quasilinear subdiffusion equation

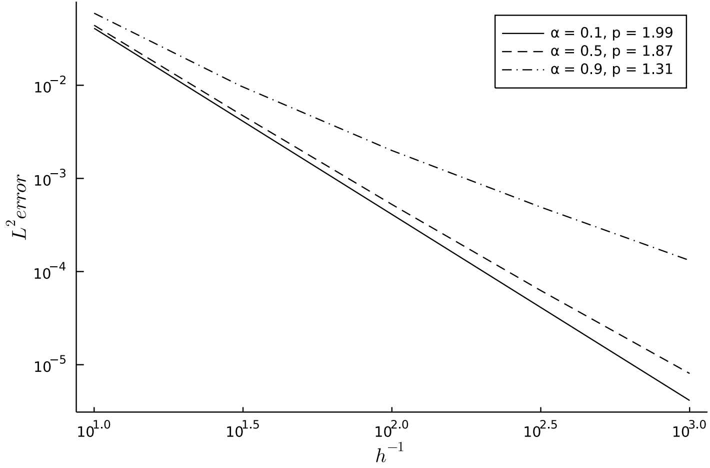

Figure: A log-log plot of the L^2 error for with $N = 30$. Calculated order of convergence p is given in the legend for different α.

Nonlocal equation arising in climatology

- In climate dynamics one frequently uses **Energy Balance Models** (EBMs). One of them is described by the following **degenerate** parabolic problem[5]

$$\begin{cases} u_t + u = (D(u)(1-x^2)u_x)_x + f(x,t,u,Ju), \quad x \in (0,1), \quad t \in (0,t_0), \\ u_x(0,t) = 0, \quad u_x(1,t) < \infty, \\ u(x,s) = \psi(x,s), \quad -\tau \le s \le 0, \end{cases}$$

  where the nonlocal operator is usually in the form

$$Ju(x,t) = \int_0^\tau K(s)u(x,t-s)ds.$$

- We assume: $0 < D_- \le D(u) \le D_+ < \infty, \quad |D_u| + |f_u| + |f_w| \le C.$
- Relevant paper: **Ł.P.**, *Linear Galerkin-Legendre spectral scheme for a degenerate nonlinear and nonlocal parabolic equation arising in climatology*, arXiv:2106.05140.

[5] Bhattacharya, K and Ghil, M and Vulis, IL, Journal of Atmospheric Sciences 39(8) (1982), 1747–1773

Nonlocal equation arising in climatology

- The Earth is idealized as sphere on which the heat is averaged zonally. This means that the temperature depends on $x = \sin\theta$ with θ - the latitude.
- EBMs are simple conservation models that started with Budyko and Sellers works

$$cT_t = R_i - R_o + H,$$

  where T is the temperature, R_i incoming radiation, R_o outgoing infrared radiation, and H horizontal transport.
- R_i depends on the solar constant Q, the spatial distribution of the radiation $S(x,t)$, and the *albedo* (ice-albedo feedback: lower temperatures $\to$ more ice $\to$ higher reflectivity $\to$ lower temperatures)

$$R_i = QS(x,t)(1 - \alpha(x, T, JT)).$$

- The **nonlocality in time** enters through the albedo.
- R_o is given by the Stefan-Boltzmann's Law, i.e. $R_o = \sigma T^4$.
- The horizontal flux is diffusive

$$H = \nabla \cdot (d(u)\nabla T) = \left(d(u)(1-x^2)T_x\right)_x.$$

Nonlocal equation arising in climatology

- The weak form of the problem

$$\begin{cases} (u_t, v) + a(D(u); u, v) = (f(t, u, Ju), v), \quad v \in V, \\ u(s) = \psi(s), \quad -\tau \le s \le 0, \end{cases}$$

with the form

$$a(D(w); u, v) = \int_0^1 D(w)(1 - x^2) u_x v_x dx + \int_0^1 uv\, dx.$$

- A choice of the appropriate space V helps to deal with the degeneracy

$$V = \left\{ v \in H^1(0,1) : \sqrt{1 - x^2}\, v_x \in L^2(0,1) \right\},$$

$$\|v\|_V = \int_0^1 (1 - x^2) v_x^2\, dx + \int_0^1 v^2 dx.$$

- There has been an vigorous research done for the various variants of the above problem[6].

[6] Díaz, Jesús Ildefonso. The mathematics of models for climatology and environment. Springer, Berlin, Heidelberg, 1997. 217-251.

Nonlocal equation arising in climatology

- We choose the finite dimensional subspace $V_N \subset V$ of polynomials (in our case Legendre) and look for solutions to a **fully linear scheme**

$$\boxed{(\delta U^n, v) + a(D(\widehat{U}^{n-\theta}); \overline{U}^{n-\theta}, v) = (f_h(\widehat{U}^{n-\theta}), v), \quad v \in V_N,}$$

where $\delta U^n = h^{-1}(U^n - U^{n-1})$, the $O(h^2)$ extrapolation is

$$\widehat{U}^{n-\theta} := (2-\theta)U^{n-1} - (1-\theta)U^{n-2}, \quad 0 \leq \theta \leq 1$$

and the θ-average

$$\overline{U}^{n-\theta} := \theta U^{n-1} + (1-\theta)U^n, \quad 0 \leq \theta \leq 1.$$

- The initialization is done via the Predictor-Corrector method.
- Since Legendre polynomials are **eigenfunctions** of the diffusion operator, we obtain an optimal scheme and estimates.

Nonlocal equation arising in climatology

Convergence

Let $u(t) \in H^{2m}(0,1)$ for each $t \in [0, t_0]$ with $m \geq 1$. Further, assume that u_x, u_t, and u_{tt} are bounded. Then,

$$\|u(t_n) - U^n\| \leq C\left(N^{-2m} + \rho_0(h)\left(\theta - \frac{1}{2}\right)h + h^2\right), \quad (1)$$

where $\rho_0(h)$ is the local consistency error of the discretization of J

$$J_h U^n = \sum_{i=0}^{M} w_i(K) U^{n-i} + \rho_0(h).$$

- The proof utilizes a similar decomposition as in the subdiffusive case.
- It can also be proved that even in the degenerate case we have optimal bounds for the Ritz projection

$$\|u - R_N u\| + N^{-1}\|u - R_N u\|_V \leq C N^{-2m}\|u\|_{2m}.$$

Nonlocal equation arising in climatology

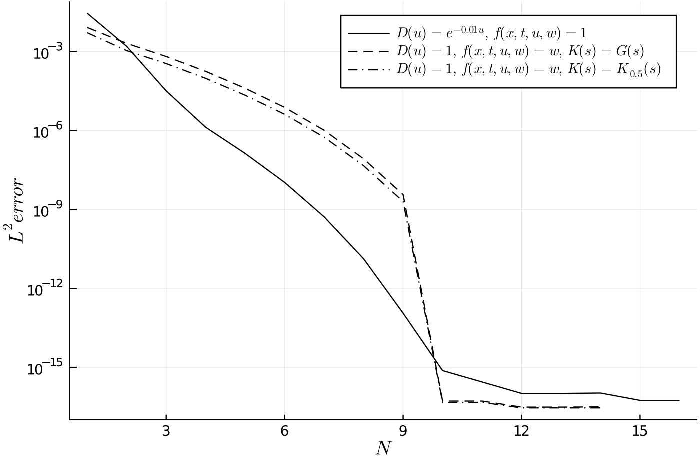

Figure: Numerically calculated L^2 error between solutions for different N and problems. The kernel G is Gaussian, while K_α is fractional integral.

Nonlocal equation arising in climatology

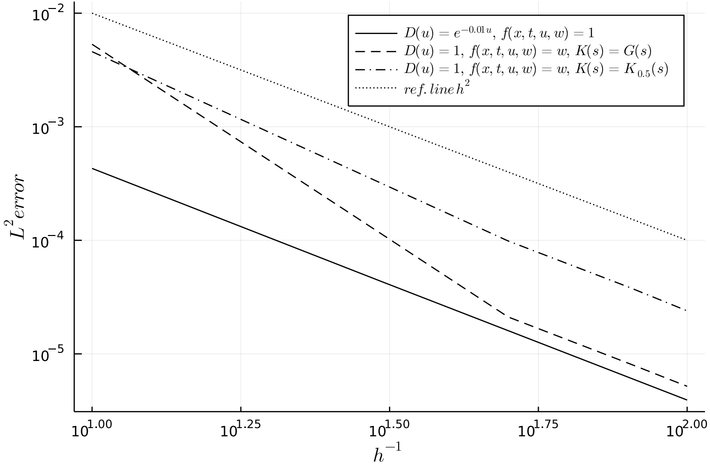

Figure: Numerically calculated L^2 error between solutions with for different h and problems. The kernel G is gaussian, while K_α is fractional integral.

Conclusion and future work

- Nonlocal equations pose an interesting and difficult subject for numerical analysis.
- Computational expense is **always higher** that in the classical case.
- The interplay between **nonlocality, nonlinearity, and degeneracy** has to be dealt with specific methods.
- **Future work**
  - Quasilinear subdiffusion with **degeneracy**.
  - Non-smooth data (usually time-fractional problems have singularity at $t \to 0^+$).
  - Higher dimensions (FEM).
  - **Parallel in time integration** (to utilize multi-threading for time-fractional derivatives).
  - **Spatial nonlocality**: fractional porous medium equation (fractional gradient and nonlinearity).

Conclusion and future work

- Nonlocal equations pose an interesting and difficult subject for numerical analysis.
- Computational expense is **always higher** that in the classical case.
- The interplay between **nonlocality, nonlinearity, and degeneracy** has to be dealt with specific methods.
- **Future work**
  - Quasilinear subdiffusion with **degeneracy**.
  - Non-smooth data (usually time-fractional problems have singularity at $t \to 0^+$).
  - Higher dimensions (FEM).
  - **Parallel in time integration** (to utilize multi-threading for time-fractional derivatives).
  - **Spatial nonlocality**: fractional porous medium equation (fractional gradient and nonlinearity).

Thank you!