Fractional Calculus in the Mathematical Modelling

Emilia Bazhlekova

Institute of Mathematics and Informatics
Bulgarian Academy of Sciences
e.bazhlekova@math.bas.bg

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Outline

- Motivation: linear viscoelasticity
- Introduction to Fractional Calculus
- Ordinary differential equations of fractional order
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    - Damped oscillations
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- Fractional models in the linear viscoelasticity
- Other fractional derivative models

Motivation: linear viscoelasticity

The use of fractional derivatives for the mathematical modelling of viscoelastic materials is quite natural:

$\sigma(t)$ - stress, $\varepsilon(t)$ - strain (at time t)

Constitutive equations give the relation between σ and ε.

Mathematical models for an ideal solid material and for an ideal fluid:

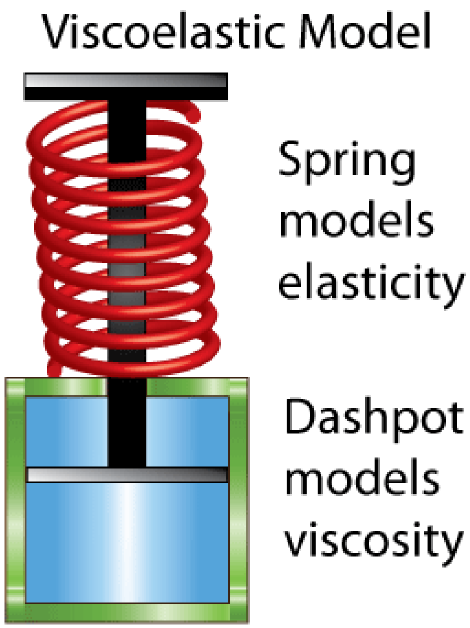
Solids (Hooke's law): $\sigma(t) = E\varepsilon(t)$;   **Newtonian fluids**: $\sigma(t) = \eta \dfrac{d\varepsilon(t)}{dt}$.

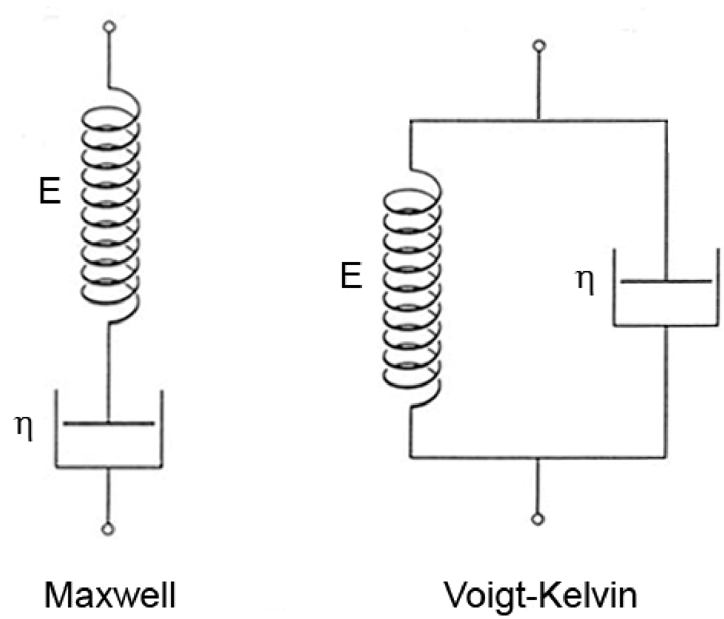
E - elastic modulus, η - viscosity (material parameters)

Real materials combine properties of those two limit cases and lie somewhere between ideal solids and ideal fluids.

Intrger-order models for viscoelastic materials

Solids (Hooke's law): $\sigma(t) = E\varepsilon(t)$; Newtonian fluids: $\sigma(t) = \eta \dfrac{d\varepsilon(t)}{dt}$.





Maxwell model: $\dfrac{\sigma(t)}{\eta} + \dfrac{1}{E}\dfrac{d\sigma(t)}{dt} = \dfrac{d\varepsilon(t)}{dt}$ $\quad \left(\sigma = const \Rightarrow \dfrac{d\varepsilon(t)}{dt} = const\right)$

Voigt-Kelvin model: $\sigma(t) = E\varepsilon(t) + \eta \dfrac{d\varepsilon(t)}{dt}$ $\quad (\varepsilon = const \Rightarrow \sigma = const$

$\Rightarrow$ does not reflect the experimentally observed stress relaxation)

Fractional-order models for viscoelastic materials

Hooke element: $\sigma(t) = E\varepsilon(t)$; Newton element: $\sigma(t) = \eta \frac{d\varepsilon(t)}{dt}$

Idea: viscoelastic materials are "intermediate" $\Rightarrow$

stress may be proportional to the "intermediate" (non-integer) derivative of strain (Scott-Blair element):

$$\sigma(t) = aD_t^{\alpha}\varepsilon(t), \quad 0 < \alpha < 1.$$

Fractional generalizations of the classical models:

Generalized Maxwell model: $\sigma(t) + a_1 D_t^{\alpha}\sigma(t) = b_0\varepsilon(t)$.

Generalized Voigt model: $\sigma(t) = b_0\varepsilon(t) + b_1 D_t^{\alpha}\varepsilon(t)$.

Fractional derivative models:

provide a higher level of adequacy, preserving linearity.

Introduction to Fractional Calculus

$$D_t^1 = \frac{d}{dt}, \qquad D_t^n = \frac{d^n}{dt^n}, \qquad n = 1, 2, 3, ...$$

In a letter to L'Hôpital in 1695 Leibniz raised the question:
"Can the meaning of derivatives with integer order be generalized to derivatives with noninteger orders?"

L'Hôpital was somewhat curious and replied with another question to Leibniz:
"What if the order will be 1/2?"

Leibniz, in a letter dated September 30, 1695 - the exact birthday of the Fractional Calculus - replied:

"It will lead to a paradox, from which one day useful consequences will be drawn."

In the last years: a vast amount of research publications in the area of Fractional Calculus (exponential growth is observed of the number of publications).

Journal:

Fractional Calculus and Applied Analysis

Founding Publisher (1998 - 2010) and Supporting Organization (1998 - now): Institute of Mathematics and Informatics, Bulgarian Academy of Sciences

Managing Editor: Prof. Virginia Kiryakova

Thomson Reuters announced in 2013 JCR Sci. Ed. the first Impact Factor of FCAA - it is IF (2013) = 2.974, and places the journal at 4th place in category "Mathematics, Interdisciplinary" (among 95) and at 5th place in category "Mathematics, Applied" (among 250).

Fractional integration

$$J_t f(t) = \int_0^t f(\tau)\, d\tau,$$

$$\begin{aligned} J_t^2 f(t) &= \int_0^t \left(\int_0^{t_1} f(t_2)\, dt_2 \right) dt_1 \\ &= \int_0^t \left(\int_{t_2}^t dt_1 \right) f(t_2)\, dt_2 = \int_0^t (t - t_2) f(t_2)\, dt_2 \end{aligned}$$

$$J_t^n f(t) = \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} f(t_n)\, dt_n, \quad n \in \mathbb{N}.$$

By induction:

$$\Rightarrow J_t^n f(t) = \frac{1}{(n-1)!} \int_0^t (t-\tau)^{n-1} f(\tau)\, d\tau, \quad n \in \mathbb{N}.$$

Riemann-Liouville fractional integral

$$J_t^n f(t) = \frac{1}{(n-1)!}\int_0^t (t-\tau)^{n-1} f(\tau)\,d\tau, \quad n \in \mathbb{N}.$$

What if $n = \alpha > 0$ - noninteger?

$\Gamma(\cdot)$ - **Gamma function**: $\Gamma(\alpha) = \int_0^\infty e^{-t} t^{\alpha-1}\,dt, \quad \Re\alpha > 0.$

Properties: $\Gamma(1) = 1,\ \Gamma(\alpha+1) = \alpha\Gamma(\alpha).$

$$\text{Proof: } \Gamma(\alpha+1) = \int_0^\infty e^{-t} t^{\alpha}\,dt = \left[-e^{-t}t^{\alpha}\right]_{t=0}^{t=\infty} + \alpha\int_0^\infty e^{-t} t^{\alpha-1}\,dt = \alpha\Gamma(\alpha).$$

$$\Rightarrow \Gamma(n) = (n-1)!$$

J_t^α - **fractional Riemann-Liouville integral** of order $\alpha > 0$:

$$J_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)}\int_0^t (t-\tau)^{\alpha-1} f(\tau)\,d\tau.$$

Fractional differentiation

Riemann-Liouville fractional integral of order $\alpha > 0$:

$$J_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau)\, d\tau.$$

Riemann-Liouville fractional derivative D_t^α of order $\alpha > 0$:

$$D_t^\alpha = D_t^n J_t^{n-\alpha}, \quad \text{where } n = \lceil \alpha \rceil; \quad (\lceil \alpha \rceil = [\alpha] + 1).$$

For example if $\alpha \in (0,1) \Rightarrow D_t^\alpha = D_t^1 J_t^{1-\alpha}$

In particular: $D_t^{1/2} f(t) = D_t^1 J_t^{1/2} f(t) = \dfrac{1}{\sqrt{\pi}} \cdot \dfrac{d}{dt} \displaystyle\int_0^t \frac{f(\tau)}{(t-\tau)^{1/2}}\, d\tau.$

Caputo fractional derivative $\mathbf{D}_t^\alpha$ of order $\alpha > 0$:

$$\mathbf{D}_t^\alpha = J_t^{n-\alpha} D_t^n, \quad n = \lceil \alpha \rceil.$$

Fractional differentiation

Riemann-Liouville fractional derivative D_t^α of order $\alpha > 0$:

$$D_t^\alpha = D_t^n J_t^{n-\alpha}, \quad n = \lceil \alpha \rceil .$$

Caputo fractional derivative $\mathbf{D}_t^\alpha$ of order $\alpha > 0$:

$$\mathbf{D}_t^\alpha = J_t^{n-\alpha} D_t^n, \quad n = \lceil \alpha \rceil .$$

Introduced in the framework of the theory of elasticity and seismic waves:
Michele Caputo, *Elasticitá e Dissipazione*, Zanichelli, Bologna, 1969.

Integer-order differentiation: **local** character.

Fractional differentiation: **nonlocal** character $\rightarrow$ appropriate for modelling of **materials and processes with memory**.

Basic properties of the operators of Fractional Calculus

$$J_t^\alpha J_t^\beta = J_t^{\alpha+\beta}, \quad \alpha,\beta > 0, \ - \text{ semigroup property,}$$

$$J_t^\alpha\{t^\gamma\} = \frac{\Gamma(\gamma+1)}{\Gamma(\alpha+\gamma+1)} t^{\gamma+\alpha}, \quad \gamma > -1,$$

$$\mathbf{D}_t^\alpha\{t^\gamma\} = D_t^\alpha\{t^\gamma\} = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma-\alpha+1)} t^{\gamma-\alpha}, \quad \gamma > 0.$$

$$\mathbf{D}_t^\alpha\{c\} \equiv 0,\ \forall\alpha > 0, \qquad D_t^\alpha\{c\} = \frac{ct^{-\alpha}}{\Gamma(1-\alpha)} \neq 0,\ \alpha > 0, \alpha \notin \mathbb{N}.$$

In general: $\mathbf{D}_t^\alpha \mathbf{D}_t^\beta \neq \mathbf{D}_t^{\alpha+\beta}$

Example: if $0 < \alpha < 1/2$ then $\mathbf{D}_t^\alpha t^\alpha = \Gamma(\alpha+1)$ and thus $\mathbf{D}_t^\alpha(\mathbf{D}_t^\alpha t^\alpha) = 0$, but

$$\mathbf{D}_t^{2\alpha} t^\alpha = \frac{\Gamma(1+\alpha)}{\Gamma(1-\alpha)} t^{-\alpha} \quad \Rightarrow \quad \mathbf{D}_t^\alpha(\mathbf{D}_t^\alpha t^\alpha) \neq \mathbf{D}_t^{2\alpha} t^\alpha.$$

Also: $\mathbf{D}_t^\alpha(fg) \neq (\mathbf{D}_t^\alpha f)g + f(\mathbf{D}_t^\alpha g)$ (there is no useful formula of this type!)

Let $\alpha > 0$, $n = \lceil \alpha \rceil$. Fractional integration and differentiation are related by:

$$\mathbf{D}_t^\alpha J_t^\alpha f(t) = D_t^\alpha J_t^\alpha f(t) = f(t)$$

$$J_t^\alpha \mathbf{D}_t^\alpha f(t) = f(t) - \sum_{k=0}^{n-1} f^{(k)}(0) \cdot \frac{t^k}{k!}$$

$$J_t^\alpha D_t^\alpha f(t) = f(t) - \sum_{k=0}^{n-1} \left(J_t^{n-\alpha} f\right)^{(k)}(0) \cdot \frac{t^{\alpha+k-n}}{\Gamma(\alpha+k-n+1)}.$$

The Caputo and R-L derivatives are related by the identity:

$$\mathbf{D}_t^\alpha f(t) = D_t^\alpha \left(f(t) - \sum_{k=0}^{n-1} f^{(k)}(0) \cdot \frac{t^k}{k!} \right)$$

$$= D_t^\alpha f(t) - \sum_{k=0}^{n-1} f^{(k)}(0) \cdot \frac{t^{k-\alpha}}{\Gamma(k-\alpha+1)}.$$

Laplace transform and fractional operators

Laplace transform:

$$\mathcal{L}\{f(t)\}(s) = \widehat{f}(s) = \int_0^\infty e^{-st} f(t)\,dt$$

If $\alpha > 0$, $n = \lceil \alpha \rceil$, then:

$$\mathcal{L}\{J_t^\alpha f\}(s) = s^{-\alpha}\mathcal{L}\{f\}(s),$$

$$\mathcal{L}\{\mathbf{D}_t^\alpha f\}(s) = s^\alpha \mathcal{L}\{f\}(s) - \sum_{k=0}^{n-1} f^{(k)}(0)\cdot s^{\alpha-1-k},$$

$$\mathcal{L}\{D_t^\alpha f\}(s) = s^\alpha \mathcal{L}\{f\}(s) - \sum_{k=0}^{n-1} \left(J_t^{n-\alpha} f\right)^{(k)}(0)\cdot s^{n-1-k}.$$

Ordinary fractional differential equations: slow relaxation

The simplest case: Fractional relaxation equation

$$\mathbf{D}_t^\alpha u(t) + \lambda u(t) = 0, \quad 0 < \alpha \leq 1, \ \lambda > 0, \ t > 0;$$
$$u(0) = 1.$$

Solution:
$\alpha = 1$: $u(t) = \exp(-\lambda t)$ - ordinary (exponential) relaxation,

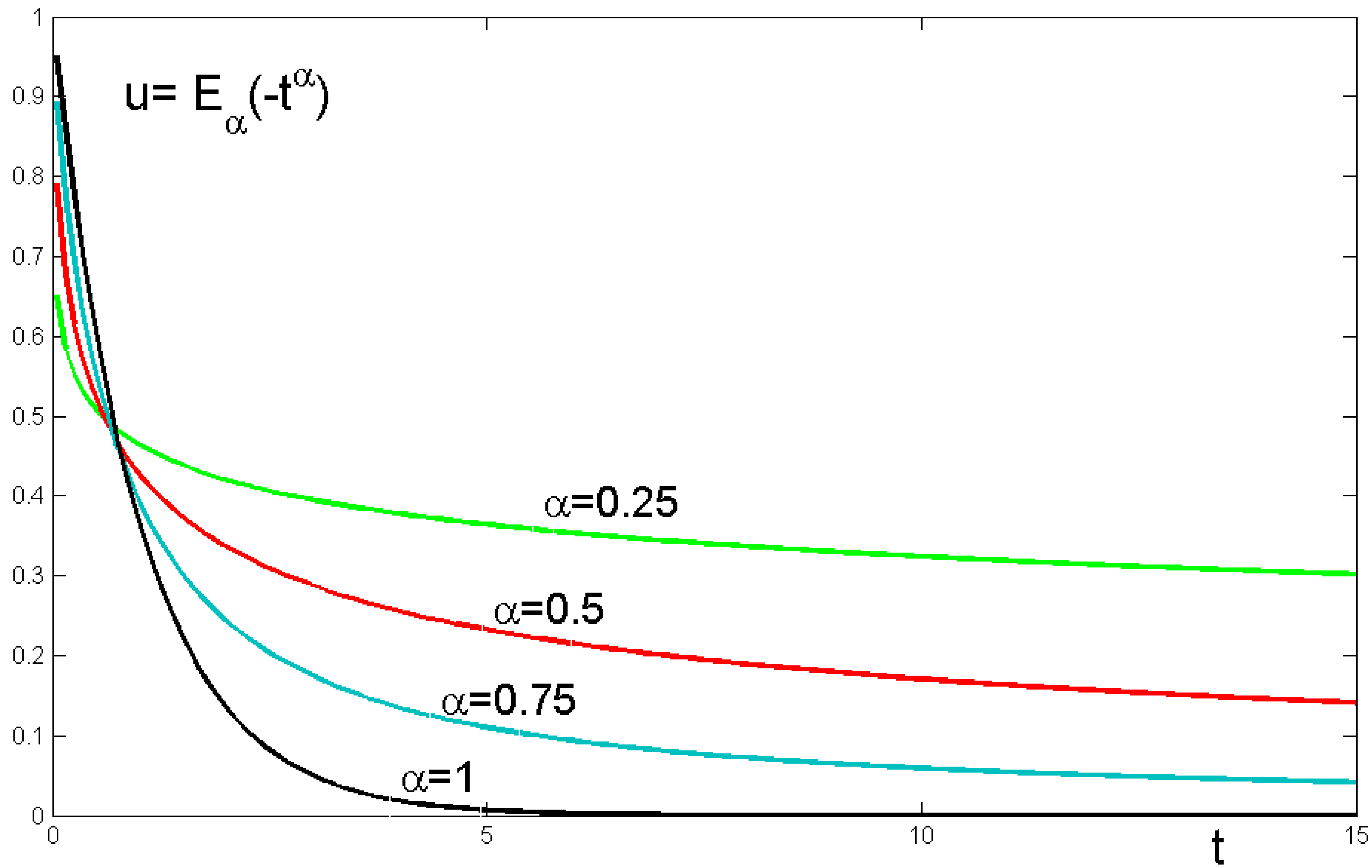
$0 < \alpha \leq 1$: $u(t) = E_\alpha(-\lambda t^\alpha)$, where

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}$$ – **Mittag-Leffler function**

It is a generalization of the exponential function:

$$E_1(z) = \sum_{k=0}^{\infty} \frac{z^k}{k!} = e^z$$

$\alpha \in (0, 1)$: Fractional (slow) relaxation



Plots of $E_\alpha(-t^\alpha)$ for different values of $\alpha \in (0, 1]$.
$\alpha = 1$ - exponential decay, $\alpha \in (0, 1)$ - algebraic decay $(t^{-\alpha})$.

Fractional relaxation-oscillation equation

$$\mathbf{D}_t^{\alpha} u(t) + \lambda u(t) = 0, \quad 1 < \alpha \leq 2,\ \lambda > 0,\ t > 0;$$
$$u(0) = 1, u'(0) = 0.$$

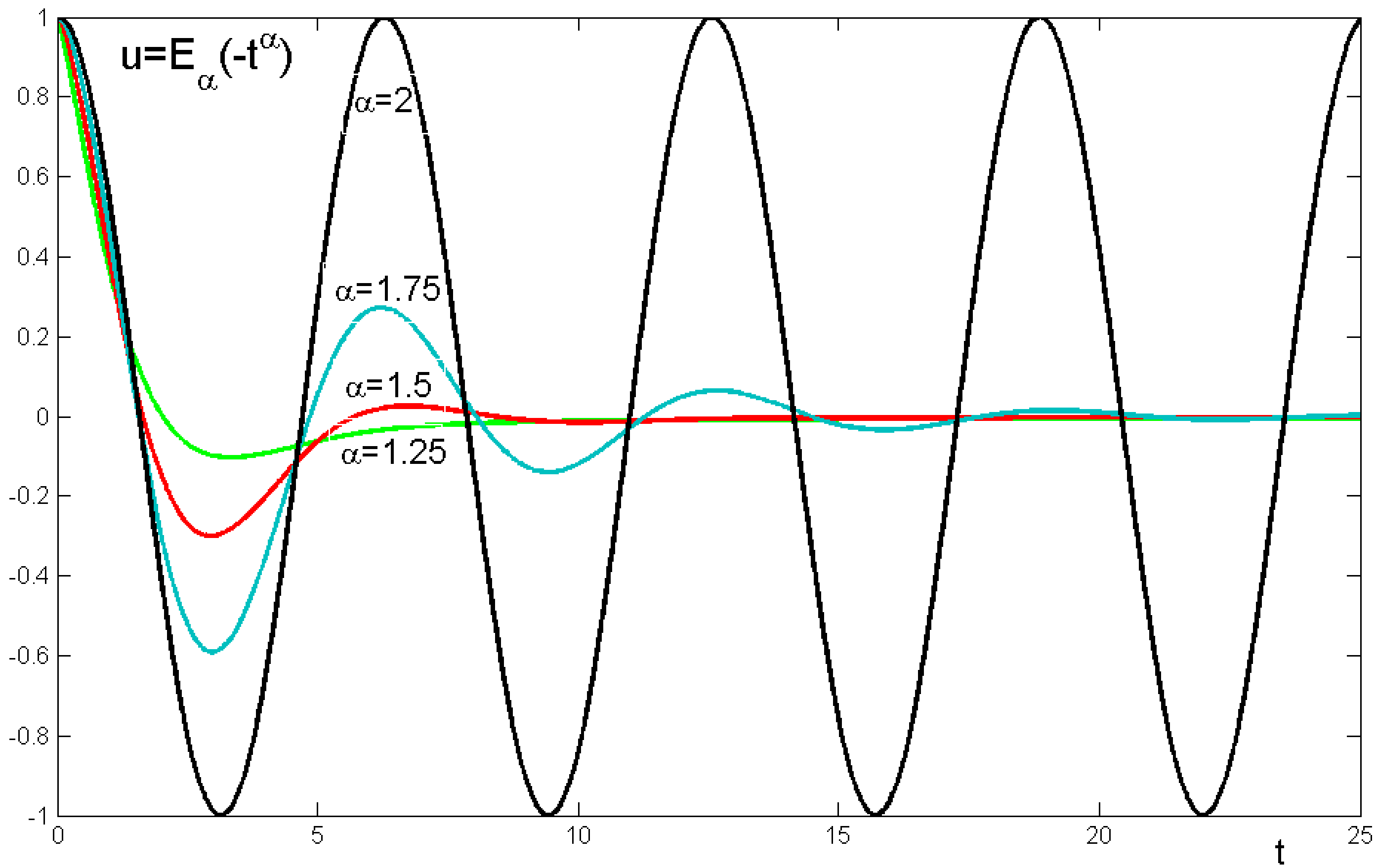
Solution:

$\alpha = 1$: $u(t) = \exp(-\lambda t)$ - ordinary (exponential) relaxation,

$\alpha = 2$: $u(t) = \cos(\sqrt{\lambda} t)$ - oscillations.

$1 < \alpha \leq 2$: $u(t) = E_{\alpha}(-\lambda t^{\alpha})$ - damped oscillations.

$\alpha \in (1,2)$: Fractional (damped) oscillations



Plots of $E_\alpha(-t^\alpha)$ for different values of $\alpha \in (1,2]$.

Mittag-Leffler functions

$E_\alpha(z) = E_{\alpha,1}(z)$, where

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}$$ – two-parameter Mittag-Leffler function

Entire function. Asymptotic expansion:

$$E_{\alpha,\beta}(-t) = \frac{t^{-1}}{\Gamma(\beta - \alpha)} + O(t^{-2}), \quad t \to +\infty, \alpha \in (0,2), \beta \in \mathbb{R}.$$

Laplace transform:

$$\mathcal{L}\left\{t^{\beta-1} E_{\alpha,\beta}(-\lambda t^\alpha)\right\} = \frac{s^{\alpha-\beta}}{s^\alpha + \lambda}$$

Completely monotone functions

A function $f : (0, \infty) \to \mathbb{R}$ is called **completely monotone function** ($\mathcal{CMF}$) if

$$(-1)^n f^{(n)}(t) \geq 0, \text{ for all } t > 0, \ n = 0, 1, ...$$

The simplest example: $f(t) = e^{-t}$

Mittag-Leffler function ($\alpha, \beta \in \mathbb{R}, \ \alpha > 0$):

$$E_{\alpha,\beta}(-t) = \sum_{k=0}^{\infty} \frac{(-t)^k}{(\alpha k + \beta)}, \quad E_\alpha(-t) = E_{\alpha,1}(-t).$$

$E_1(-t) = e^{-t} \in \mathcal{CMF}$

$E_\alpha(-t) \in \mathcal{CMF}$, iff $0 < \alpha < 1$ (Pollard, 1948)

$E_{\alpha,\beta}(-t) \in \mathcal{CMF}$, iff $0 \leq \alpha \leq 1$, $\alpha \leq \beta$ (Schneider, 1996; Miller, 1999)

Inhomogeneous fractional relaxation equation

Let $\lambda > 0,\ 0 < \alpha \leq 1.$

$$\mathbf{D}_t^\alpha u(t) + \lambda u(t) = f(t), \quad t > 0,$$
$$u(0) = 1.$$

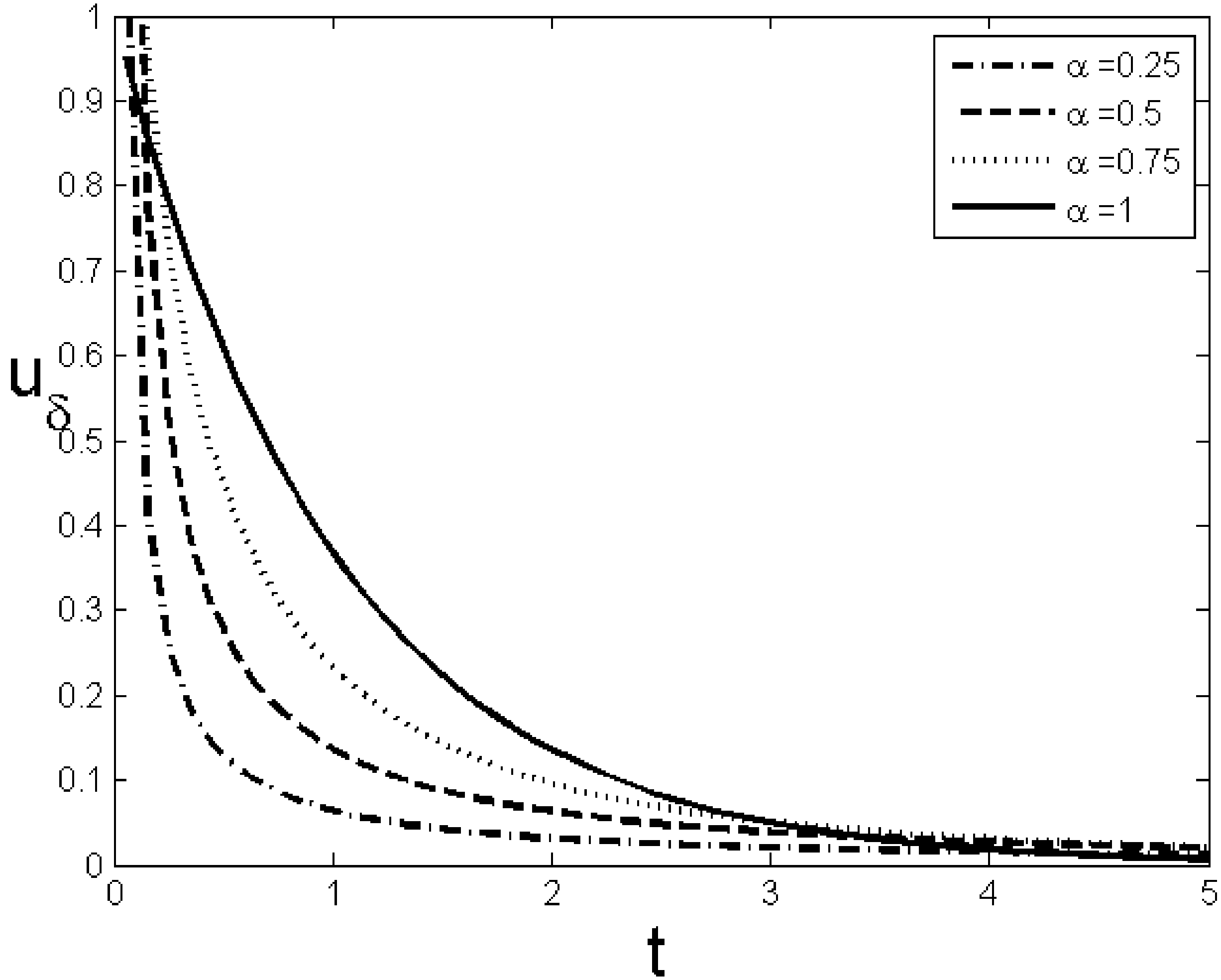
The solution is obtained by applying Laplace transform and is given by:

$$u(t) = E_\alpha(-\lambda t^\alpha) + \int_0^t \tau^{\alpha-1} E_{\alpha,\alpha}(-\lambda \tau^\alpha) f(t-\tau)\, d\tau.$$

$E_\alpha(-\lambda t^\alpha)$ and $t^{\alpha-1}E_{\alpha,\alpha}(-t^\alpha)$ are completely monotone functions.

$E_\alpha(-\lambda t^\alpha) = O(1/t^\alpha)$ as $t \to \infty$

$t^{\alpha-1}E_{\alpha,\alpha}(-t^\alpha) = O(1/t^{\alpha+1})$ as $t \to \infty$



Plots of $t^{\alpha-1}E_{\alpha,\alpha}(-t^{\alpha})$ for different values of $\alpha \in (0,1]$.
Completely monotone functions. Algebraic decay $\sim 1/t^{\alpha+1}$ as $t \to \infty$.

Multi-term fractional relaxation equation

$$\mathbf{D}_t^{\alpha} u(t) + \sum_{j=1}^{m} \lambda_j \mathbf{D}_t^{\alpha_j} u(t) + \lambda u(t) = f(t), \quad t > 0,$$

$$u(0) = 1,$$

where $0 < \alpha_m < ... < \alpha_1 < \alpha \leq 1, \quad \lambda, \lambda_j > 0, \ j = 1, ..., m, \ m \in \mathbb{N}.$

By applying Laplace transform we can find the solution:

$$u(t) = u_0(t) + \int_0^t u_\delta(t-\tau) f(\tau)\, d\tau,$$

where

$$\mathcal{L}\{u_0\}(s) = \frac{s^{\alpha-1} + \sum_{j=1}^m \lambda_j s^{\alpha_j - 1}}{s^\alpha + \sum_{j=1}^m \lambda_j s^{\alpha_j} + \lambda}, \quad \mathcal{L}\{u_\delta\}(s) = \frac{1}{s^\alpha + \sum_{j=1}^m \lambda_j s^{\alpha_j} + \lambda}.$$

Note that

$$\mathcal{L}\{E_\alpha(-\lambda t^\alpha)\}(s) = \frac{s^{\alpha-1}}{s^\alpha + \lambda}, \quad \mathcal{L}\{t^{\alpha-1} E_{\alpha,\alpha}(-\lambda t^\alpha)\}(s) = \frac{1}{s^\alpha + \lambda}.$$

$u_0(t)$ and $u_\delta(t)$ - **generalizations of the Mittag-Leffler type functions**

$$E_\alpha(-\lambda t^\alpha) \text{ and } t^{\alpha-1} E_{\alpha,\alpha}(-\lambda t^\alpha)$$

Aim: Study the properties of $u_0(t)$ and $u_\delta(t)$

Theorem.

$$u_0(t) = \int_0^\infty e^{-rt} K_0(r)\, dr \quad \text{and} \quad u_\delta(t) = \int_0^\infty e^{-rt} K_\delta(r)\, dr, \quad \text{where}$$

$$K_0(r) = \frac{\lambda}{\pi r} \cdot \frac{B(r)}{(A(r)+\lambda)^2 + (B(r))^2} \quad \text{and} \quad K_\delta(r) = \frac{1}{\pi} \cdot \frac{B(r)}{(A(r)+\lambda)^2 + (B(r))^2}$$

$$A(r) = r^\alpha \cos\alpha\pi + \sum_{j=1}^m \lambda_j r^{\alpha_j} \cos\alpha_j\pi, \;\; B(r) = r^\alpha \sin\alpha\pi + \sum_{j=1}^m \lambda_j r^{\alpha_j} \sin\alpha_j\pi.$$

Proof: Take the inverse Laplace integral of $\widehat{u}_0(s)$ and $\widehat{u}_\delta(s)$, i.e.

$$u_0(t) = \frac{1}{2\pi i} \int_{Br} e^{st} \frac{s^{\alpha-1} + \sum_{j=1}^m \lambda_j s^{\alpha_j - 1}}{s^\alpha + \sum_{j=1}^m \lambda_j s^{\alpha_j} + \lambda}\, ds,$$

(and similarly for $u_\delta(t)$), where $Br = \{s;\ \mathrm{Re}\, s = \sigma,\ \sigma > 0\}$ is the Bromwich path.

Remark: The obtained representations of $u_0(t)$ and $u_\delta(t)$ are appropriate for numerical computation.

Other properties

Theorem. The functions $u_0(t)$ and $u_\delta(t)$ have the following properties

$$0 < u_0(t) < 1,\ u_\delta(t) > 0,\ \text{strictly decreasing for } t > 0, \tag{1}$$

$$u_0(0) = 1,\ u_\delta(0) = +\infty, \tag{2}$$

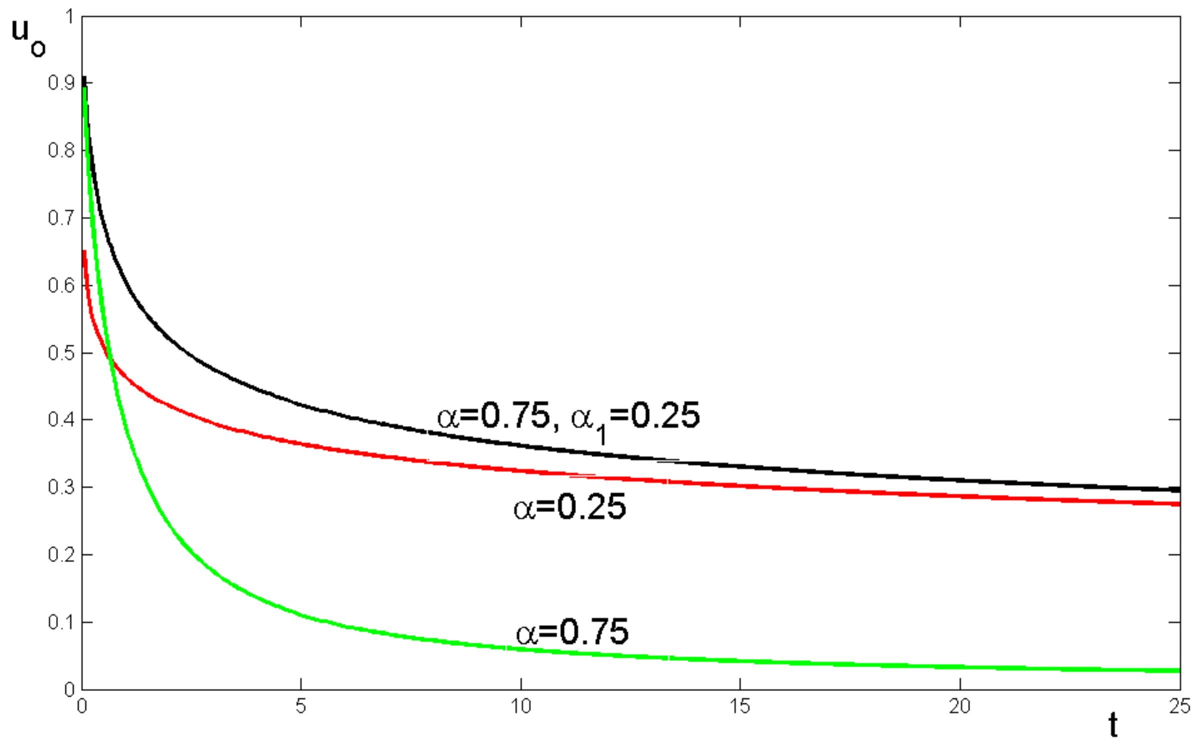
$$u_0(t) \text{ and } u_\delta(t) \text{ are completely monotone functions for } t > 0, \tag{3}$$

$$u_0'(t) = -\lambda u_\delta(t), \quad t > 0, \tag{4}$$

$$\int_0^T u_\delta(t)\, dt < \frac{1}{\lambda}, \quad T > 0, \tag{5}$$

$$u_0(t) \sim 1 - \lambda \frac{t^\alpha}{\Gamma(\alpha+1)}, \quad u_\delta(t) \sim \frac{t^{\alpha-1}}{\Gamma(\alpha)}, \quad t \to 0, \tag{6}$$

$$u_0(t) \sim \frac{\lambda_m t^{-\alpha_m}}{\lambda \Gamma(1-\alpha_m)}, \quad u_\delta(t) \sim -\frac{\lambda_m t^{-\alpha_m-1}}{\lambda^2 \Gamma(-\alpha_m)}, \quad t \to +\infty. \tag{7}$$



Solution $u_0(t)$ (black) of the two-term equation with $\alpha = 0.75$, $\alpha_1 = 0.25$

$$\mathbf{D}_t^{\alpha} u_0(t) + \mathbf{D}_t^{\alpha_1} u_0(t) + u_0(t) = 0, \quad t > 0, \; u_0(0) = 1,$$

compared to the functions $E_\alpha(-t^\alpha)$ for $\alpha = 0.75$ (green) and $\alpha = 0.25$ (red).
For $t \to 0$ the asymptotic behavior of u_0 is determined by the largest order (0.75), and for $t \to \infty$ by the smallest order (0.25).

Fractional relaxation of distributed order

$$\int_0^1 \mu(\beta)\mathbf{D}_t^{\beta} u(t)\, d\beta = -\lambda u(t), \quad t > 0, \lambda > 0, \quad u(0) = 1.$$

$\mu \in C[0,1],\ \mu(\beta) \geq 0,\ \beta \in [0,1]$, and $\mu(\beta) \neq 0$ on a set of a positive measure.

Applying Laplace transform:

$$\widehat{u}(s) = \frac{h(s)}{s(h(s)+\lambda)}, \text{ where } \quad h(s) = \int_0^1 \mu(\beta) s^{\beta}\, d\beta.$$

$u(t)$ is again completely monotone function; the main difference: in the asymptotic behaviour at $t \to \infty$

Example: uniform distribution $\mu(\beta) = 1$. Then

$$h(s) = \frac{s-1}{\log s} \quad \Rightarrow \quad u(t) \sim \frac{1}{\lambda \log t}, \ t \to \infty$$

Ultraslow relaxation: **logarithmic decay**.

Two-term fractional relaxation-oscillation equation

Let $1 < \alpha \leq 2$, $0 < \beta < \alpha$, $c \geq 0$.

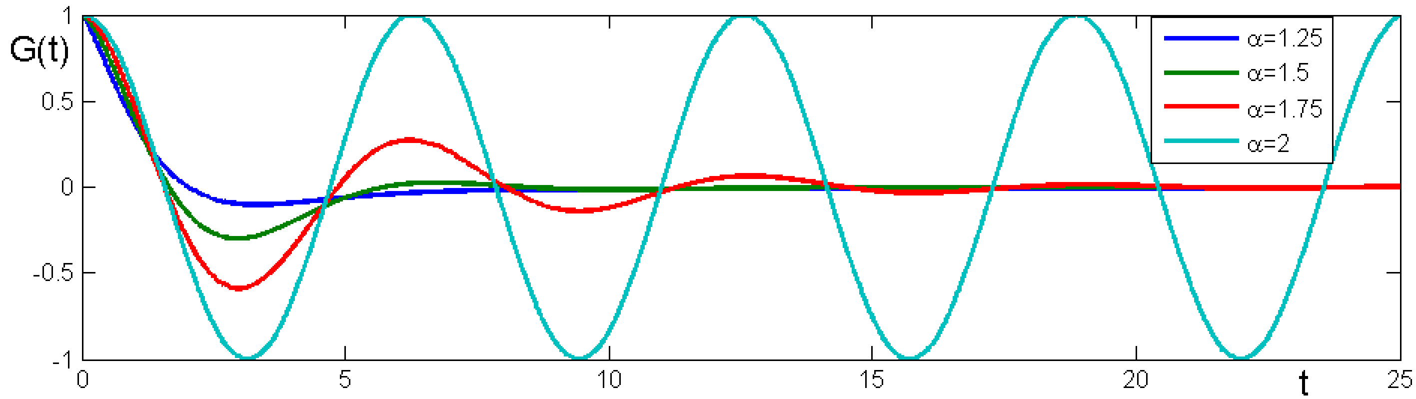
$$\mathbf{D}_t^{\alpha} G(t) + c\mathbf{D}_t^{\beta} G(t) = -\omega G(t),$$
$$G(0) = 1, \quad G'(0) = 0.$$

By applying Laplace transform it follows

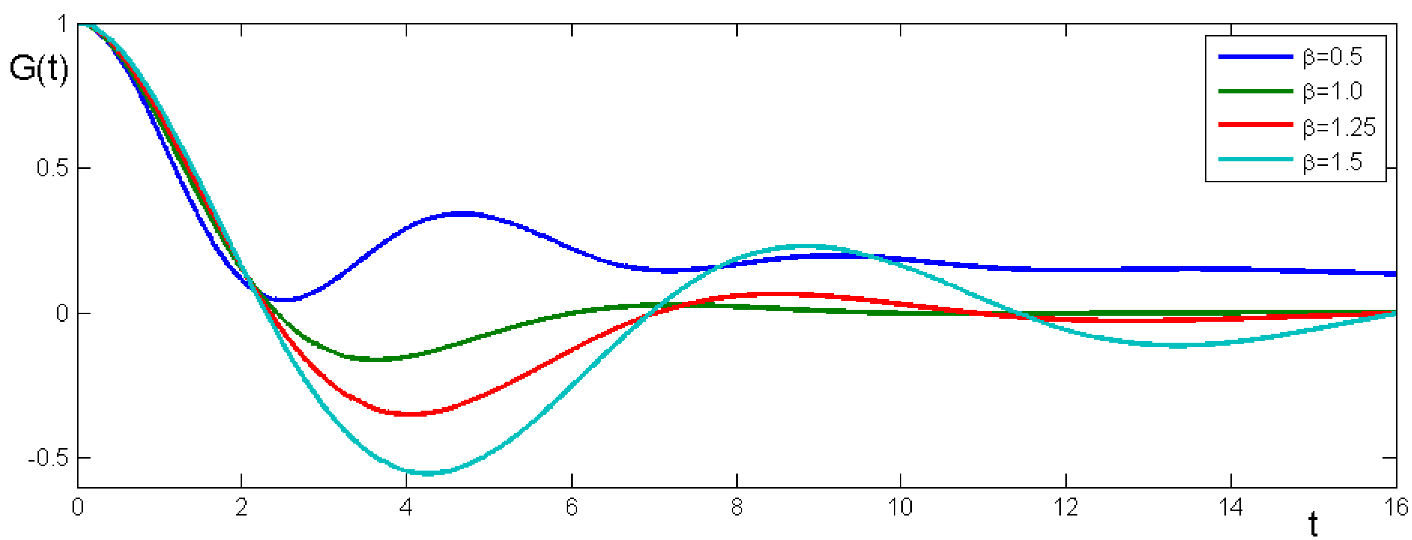
$$\widehat{G}(s) = \frac{s^{\alpha-1} + cs^{\beta-1}}{s^{\alpha} + cs^{\beta} + \omega}$$

$$G(t) = 1 - \sum_{n=0}^{\infty} \sum_{p=0}^{n} (-1)^n \binom{n}{p} c^p \omega^{n-p+1} \frac{t^{\alpha n - \beta p + \alpha}}{\Gamma(\alpha n - \beta p + \alpha + 1)}$$

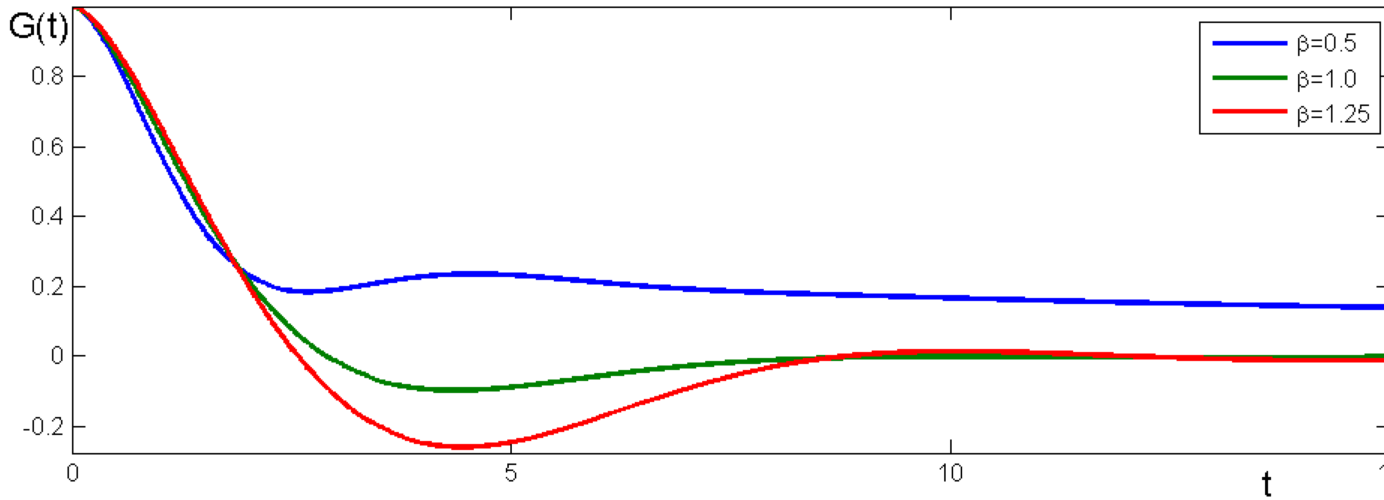
$$G(t) \sim \frac{t^{-\alpha}}{\omega \Gamma(1-\alpha)} + \frac{ct^{-\beta}}{\omega \Gamma(1-\beta)}, \quad t \to \infty.$$



Plots of $G(t)$ for $\omega = 1$, $c = 0$ and different values of α.



Plots of $G(t)$ for $\omega = c = 1$, $\alpha = 2$ and different values of β.



Plots of $G(t)$ for $\omega = c = 1$, $\alpha = 1.75$ and different values of β.

Transition from ODE to PDE

An example: a time-fractional diffusion-wave equation

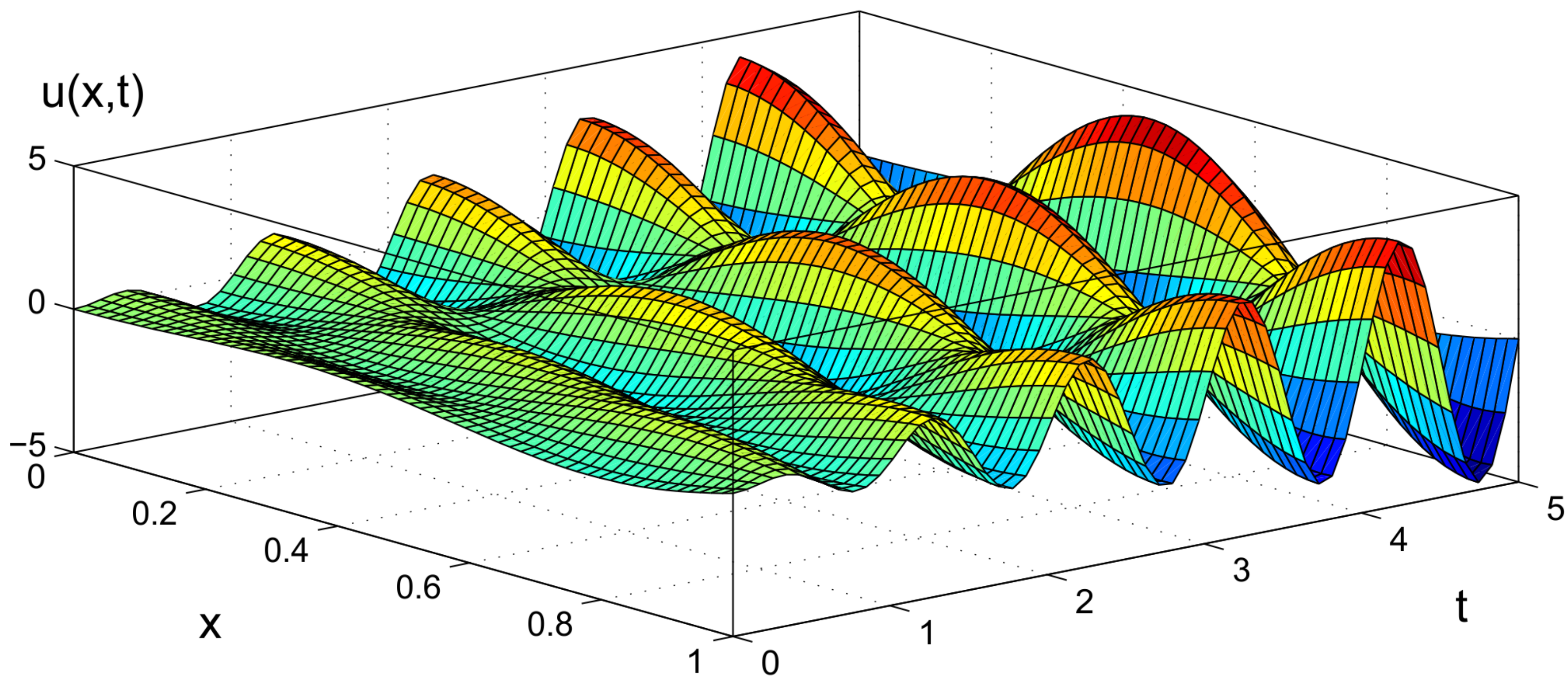
Let $1 < \alpha \leq 2$. Consider the IBVP on $(0,1) \times (0,\infty)$:

$$\begin{aligned}
&\mathbf{D}_t^{\alpha} u(x,t) = u_{xx}(x,t),\\
&u_x(0,t) = 0, \qquad u(0,t) = u(1,t),\\
&u(x,0) = f(x), \quad u_t(x,0) = 0.
\end{aligned}$$

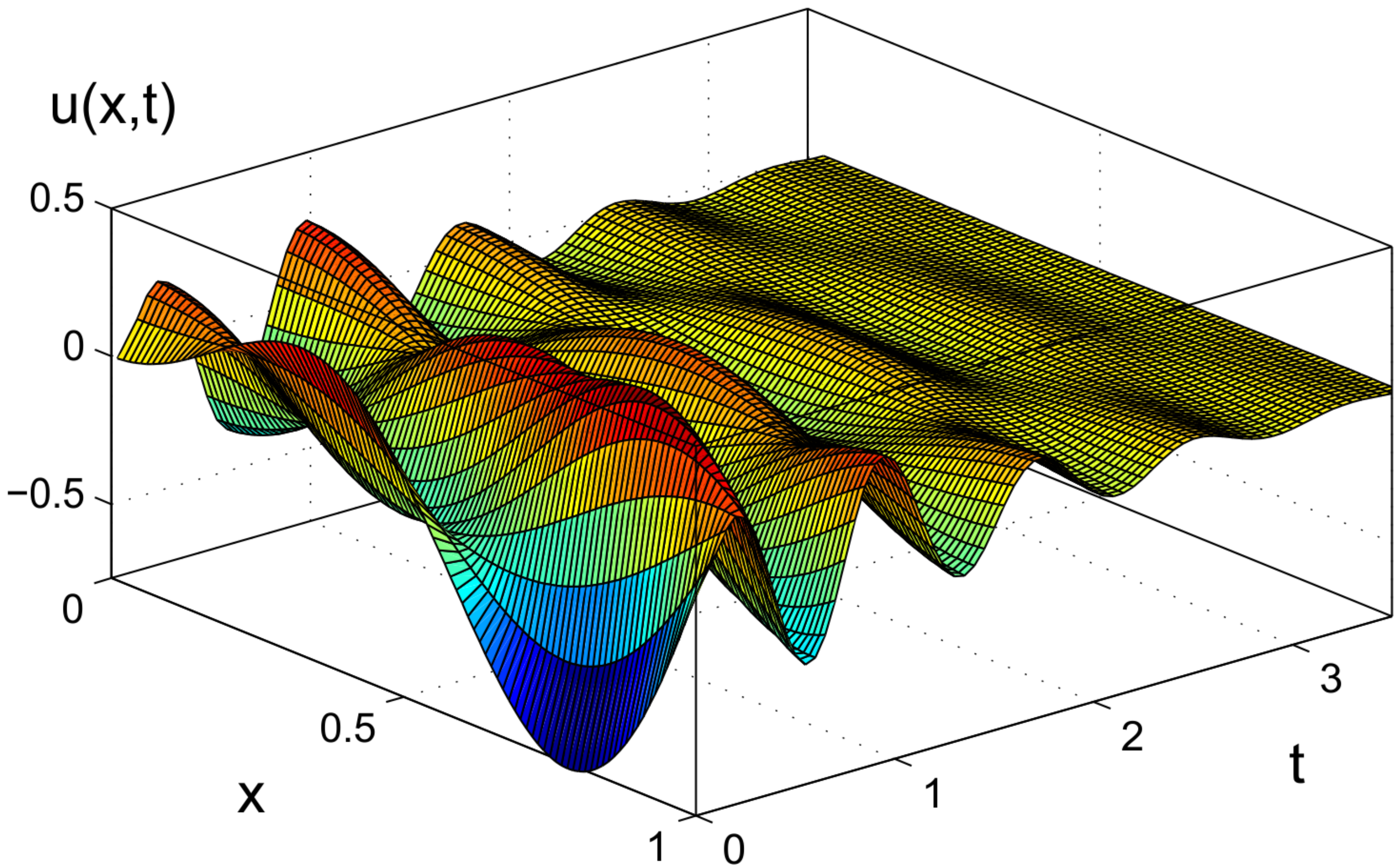
$f(x)$ is a given sufficiently smooth function, satisfying the compatibility conditions

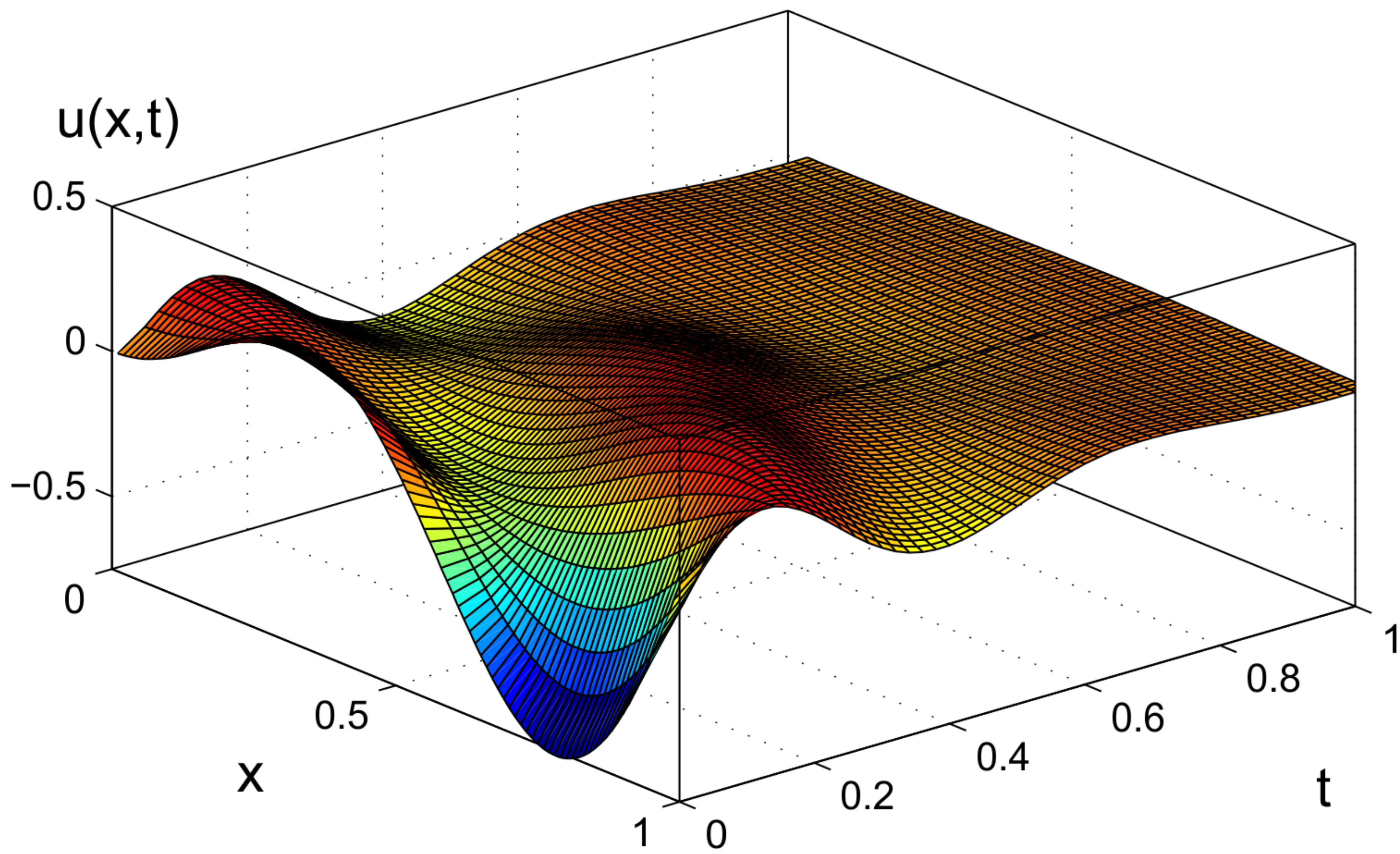
$$f(0) = f(1), \;\; f'(0) = 0.$$

Solution for $\alpha = 2,\ f(x) = x\sin(2\pi x)$



Solutions for $\alpha = 1.75$ and $\alpha = 1.5,\ f(x) = x\sin(2\pi x)$





Observation: the time evolution of solution of a PDE is determined by the behaviour of solution of corresponding ODE, obtained by replacing of the operator acting in space by a constant (eigenvalue)

Time-fractional diffusion equation (TFDE)

Describes **diffusion in complex media**: porous, highly heterogeneous (e.g. underground diffusion of contaminants), amorphous; in colloids, dielectrics, biological systems, polymers, etc.

Diffusion of contaminants under the ground $\to$ impact for the environment: better simulations and predictions of the density of the contaminant over time is needed (the real size is in kilometers; laboratory experiments with meter sizes)

Classical diffusion-convection equation:

$$\rho(x)\frac{\partial u}{\partial t}(x,t) = \mathrm{div}(p(x)\nabla u(x,t)) + b(x).\nabla u(x,t),$$

where $u(x,t)$ denotes the density at time t and the location x.

Field data show anomalous diffusion in heterogeneous aquifer which **can not be interpreted by the classical convection-diffusion equation**:

E.E. Adams and L.W. Gelhar, Field study of dispersion in a heterogeneous aquifer 2. spatial moments analysis, Water Resources Research 28 (1992) 3293 3307.

Pollutants take longer times to travel than expected from classical diffusion, due to trapping caused by stagnant regions of zero velocity of the mean flow of the groundwater.

The diffusion is observed to be slower than the prediction on the basis of the classical convection-diffusion equation, and such anomalous diffusion is called **slow diffusion**.

The continuous-time random walk is a microscopic model for the anomalous diffusion, and by an argument similar to the derivation of the classical diffusion equation from the random walk, one can derive **fractional diffusion models**.

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Y. Hatano, N. Hatano, Dispersive transport of ions in column experiments: an explanation of long-tailed profiles, Water Resources Research 34 (1998) 1027 1033.

R. Metzler, J. Klafter, The random walks guide to anomalous diffusion:a fractional dynamics approach, Phyics Reports 339 (2000) 177.

Time-fractional diffusion equation on a bounded domain

$$\mathbf{D}_t^\alpha u(x,t) = L_x u(x,t) + F(x,t),\ (x,t) \in G \times (0,T),$$
$$u(x,t) = 0, \quad x \in \partial G, t \in (0,T),$$
$$u(x,0) = a(x), \quad x \in G.$$

$0 < \alpha \leq 1$;

$G \subset \mathbb{R}^d$ - bounded domain with sufficiently smooth boundary ∂G;

L_x - symmetric uniformly elliptic operator;

$$L_x(u) = \mathrm{div}(p(x)\nabla u) - q(x)u,$$

where $p \in C^1(\overline{G}), q \in C(\overline{G}), p(x) > 0, q(x) \geq 0, x \in \overline{G}$,

$F(x,t), a(x)$ - given functions.

Eigenfunction expansion of the solution

$\{\mu_n(x)\}_{n\in\mathbb{N}}$ - eigenvalues of $-L_x$, $0 < \mu_1 \le \mu_2 \le \ldots$,
$\{\varphi_n(x)\}_{n\in\mathbb{N}}$ - eigenfunctions form orthonormal basis in $L^2(G)$.
Eigenfunction decomposition implies:

$$u(x,t) = \sum_{n=1}^{\infty} \left(a_n E_\alpha(-\mu_n t^\alpha) + \int_0^t F_n(t-\tau)\tau^{\alpha-1} E_{\alpha,\alpha}(-\mu_n \tau^\alpha)\, d\tau \right) \varphi_n(x),$$

$a_n = (a, \varphi_n),\ F_n(t) = (F(.,t), \varphi_n),\quad (.,.)$ - inner product in $L^2(G)$.
(Prove convergence of the series!)

Eigenfunction expansion is useful for:
- study of the qualitative properties of the solution (e.g **asymptotic behavior**) related to different parameters,
- obtaining **regularity estimates** for the solution, necessary for error estimates in numerical methods (e.g. FEM),
- study of **inverse problems**: identification of source term $F(x)$ from given initial and final data, parameter identification (e.g. $\alpha \sim$ anomaly of diffusion, $p(x)\sim$heterogeneity of the medium), or **problems backward in time**.

Main characteristics of TFDE:

Although the time-fractional diffusion equation inherits certain properties from the classical diffusion equation, it differs considerably from it, especially in the sense of

- slow decay in time,
- limited smoothing effect in space.

Regularity in space is determined by estimates of the form

$$\|\Delta u\|_{L^2(G)} + \|\mathbf{D}_t^\alpha u\|_{L^2(G)} \leq C t^{-\alpha} \|a\|_{L^2(G)}$$

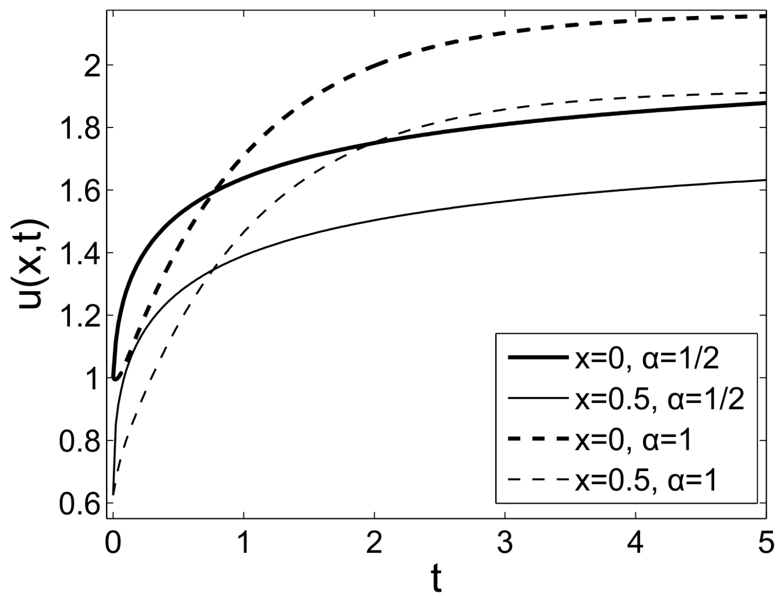
Fractional Thornley's problem

Model of **spiral phyllotaxis in botany**: $u(x,t)$ - morphogen concentration

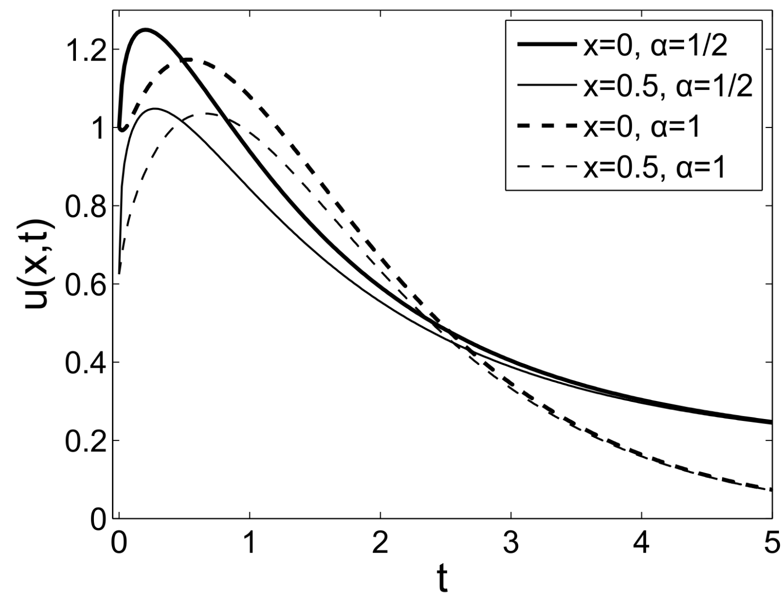
$$\mathbf{D}_t^\alpha u(x,t) = u_{xx}(x,t) - \gamma^2 u(x,t), \quad 0 < \alpha \le 1, \; x \in (0,1), t > 0,$$

$$u_x(0,t) = g(t), \quad u(0,t) = u(1,t), \quad u(x,0) = f(x),$$

$(g(t) = -\frac{1}{2}S_0(t)$, S_0 - strength of morphogen source at $x = 0)$



$g(t) = -1$



$g(t) = -\exp(-t)$

$\alpha = 1/2$ (solid line) compared to $\alpha = 1$ (dashed line).

Other fractional differential equations

-**Fractional diffusion equation of distributed order**:

$$\text{in TFDE replace } \mathbf{D}_t^{\alpha},\ \alpha \in (0,1),\ \text{with } \int_0^1 \mu(\beta)\mathbf{D}_t^{\beta}\, d\beta.$$

-**Multi-term fractional diffusion equation**:

take $\mu(\beta) = \delta(\beta - \alpha) + \sum_{j=1}^{m} \lambda_j \delta(\beta - \alpha_j), \quad 0 < \alpha_j < \alpha \le 1, \lambda_j > 0:$

$$\mathbf{D}_t^{\alpha} u(x,t) + \sum_{j=1}^{m} \lambda_j \mathbf{D}_t^{\alpha_j} u(x,t) = L_x u(x,t) + F(x,t).$$

-**Fractional telegraph equation (diffusion-wave equation with damping)**:

$$\mathbf{D}_t^{\alpha} u(x,t) + c\mathbf{D}_t^{\beta} u(x,t) = a u_{xx}, \quad 1 < \alpha \le 2, \quad 0 < \beta < \alpha, \quad a, c > 0.$$

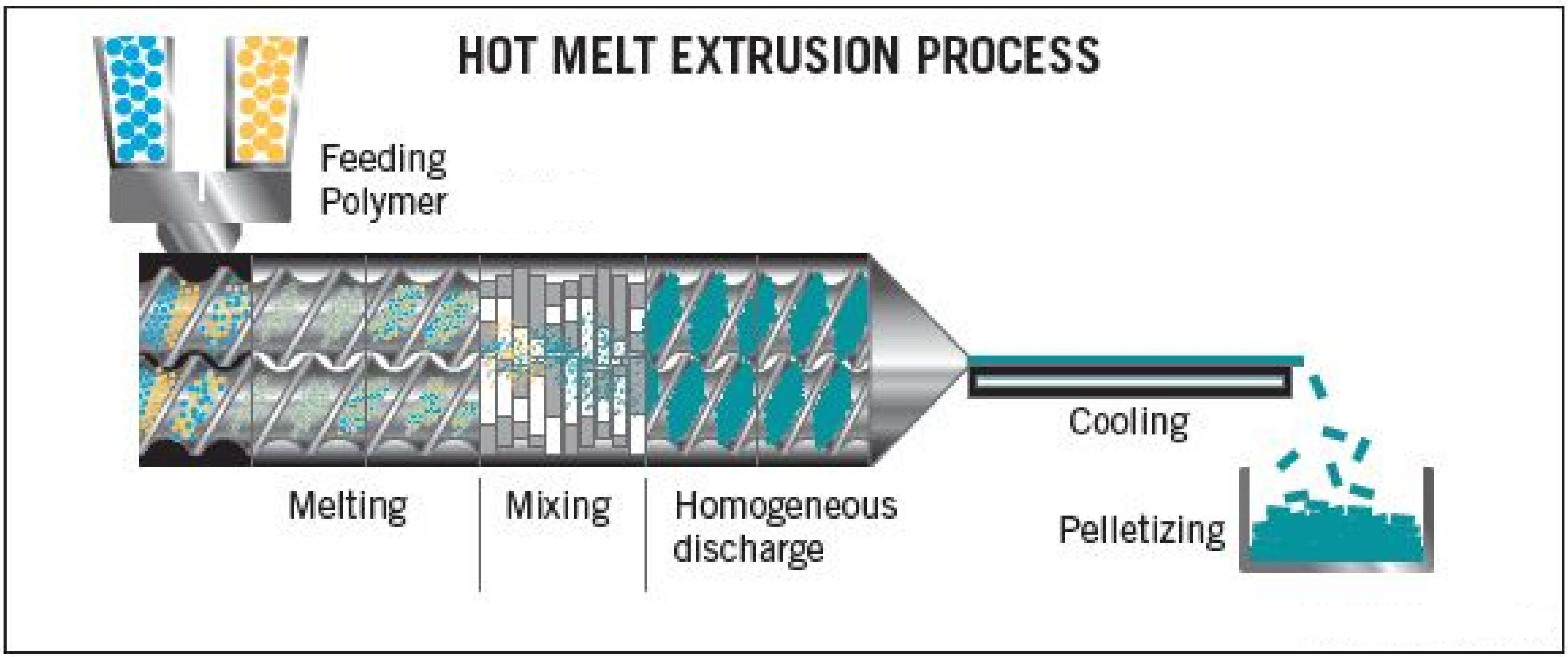
-**Fractional cable equation** (describes electrodiffusion in nerve cells):

$$u_t = D_t^{\alpha}(u_{xx}) - \gamma D_t^{\beta} u,\ 0 < \alpha, \beta < 1, \gamma > 0.$$

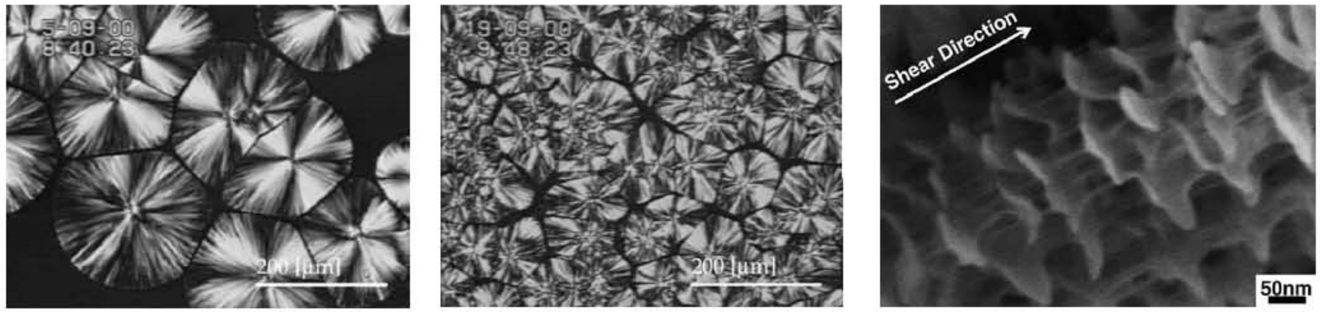
Modelling of flows of viscoelastic fluids

Many industrial and natural processes can be modelled as viscoelastic flows: from polymer extrusion to processes in geophysics.

The main reason for the theoretical development is the wide use of **polymers** in various fields of engineering.



Polymer crystallization



depending on the molecular mobility → flow strength

	quiescent	mild	strong
formed structure:	*point-like nuclei, f(T)*	*more point-like nuclei*	*oriented nuclei*

Crystallization of polymers is a process associated with partial alignment of their molecular chains.
Crystallization structure depends on flow strength and affects **optical, mechanical, thermal and chemical properties of the polymer**.

The application of fractional calculus in linear viscoelasticity leads to generalizations of the classical mechanical models: the basic Newton element ($\sigma = \eta\dot{\varepsilon}$) is substituted by the more general Scott-Blair element ($\sigma = aD_t^{\alpha}\varepsilon$).

The **fractional Burgers model** is a linear fractional model of viscoelastic fluids, which can be represented as the combination in series of a fractional KelvinVoigt element and a fractional Maxwell element. The constitutive equation for generalized Burgers fluid is given by:

$$\left(1 + \lambda_1^{\alpha} D_t^{\alpha} + \lambda_2^{\alpha} D_t^{2\alpha}\right) \sigma(t) = \mu \left(1 + \lambda_3^{\beta} D_t^{\beta} + \lambda_4^{\beta} D_t^{2\beta}\right) \dot{\varepsilon}(t),$$

where σ, $\dot{\varepsilon}$ are shear stress, rate of shear strain, $\mu > 0, \lambda_i \geq 0$, $i = 1, 2, 3, 4$, are material constants, the fractional parameters α and β satisfy $0 < \alpha \leq \beta \leq 1$.

Substituting this constitutive equation in the momentum equation leads in the case of **unidirectional flow** to the following equation for the velocity field $u(x, t)$:

$$\left(1 + \lambda_1^{\alpha} D_t^{\alpha} + \lambda_2^{\alpha} D_t^{2\alpha}\right) u_t = \mu \left(1 + \lambda_3^{\beta} D_t^{\beta} + \lambda_4^{\beta} D_t^{2\beta}\right) \Delta u,$$

Fractional Burgers' fluid:

$$\left(1 + \lambda_1^\alpha D_t^\alpha + \lambda_2^\alpha D_t^{2\alpha}\right) u_t = \mu \left(1 + \lambda_3^\beta D_t^\beta + \lambda_4^\beta D_t^{2\beta}\right) \Delta u,$$

where $u(x,t)$ - velocity distribution; μ, λ_i - material parameters;
Δ - Laplace operator acting on space variables.

Particular cases:
- Newtonian fluid: all $\lambda_i = 0$.
- **Generalized second grade fluid**: $\lambda_1, \lambda_2, \lambda_4 = 0$, $\lambda_3 \neq 0$;
- **Fractional Maxwell model**: $\lambda_2, \lambda_3, \lambda_4 = 0$, $\lambda_1 \neq 0$;
- **Fractional Oldroyd-B model**: $\lambda_2, \lambda_4 = 0$, $\lambda_1, \lambda_3 \neq 0$.

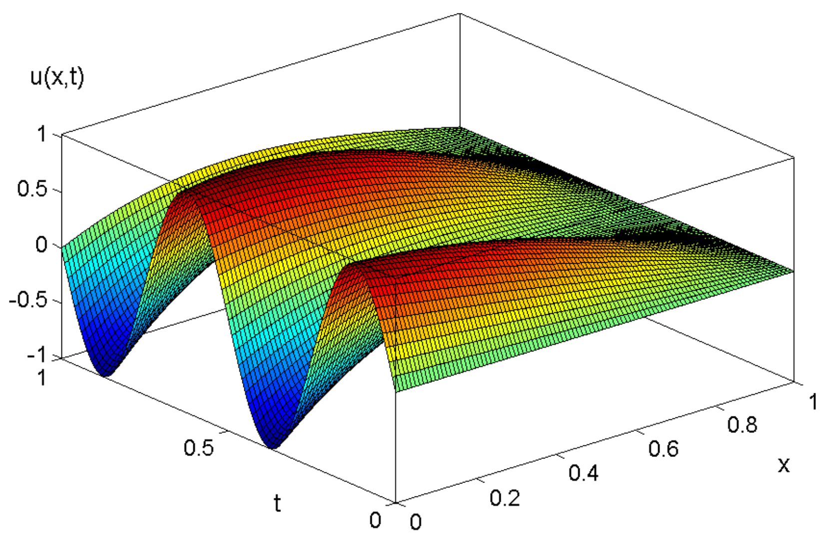
Introducing fractional derivatives in the constitutive equation $\rightarrow$ better description of viscoelastic and memory effects in some materials (e.g polymers and biological liquids). For example: fractional Oldroyd-B model: at least appropriate to describe the behaviour of Xantan gum and Sesbonia gel.
Reference:
Song DY, Jiang TQ, Study on the constitutive equation with fractional derivative for the viscoelastic fluid-modified Jeffreys model and its applications, Rheol. Acta 37 (1998) 512-517.

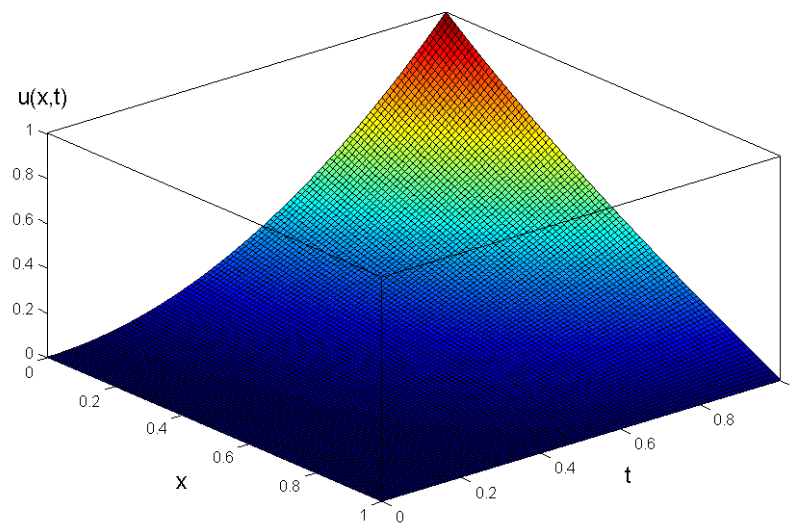
Example: Consider the following Rayleigh-Stokes problem for the fractional second grade fluid

$$u_t = (1 + D_t^{\beta}) u_{xx},$$
$$u(0,t) = \phi(t),\ u(1,t) = 0,\ u(x,0) = 0.$$

It models velocity distribution of a flow between two parallel plates, one of which is moving. The flow is initially at rest.

Two cases: the flow is induced by oscillations ($\phi(t) = \sin(4\pi t)$, left) or by a linear acceleration ($\phi(t) = t^2$, right) of the moving plate, together with a no-slip condition; $\beta = 0.5$.





Numerical methods

Nonlocal character of fractional derivatives $\rightarrow$ ability to model more adequately phenomena with memory. On the other hand, the same nonlocality property makes it difficult to design fast and accurate numerical techniques for fractional order differential equations.

$x \in [0,1], t \in [0,T]$; M, N - number of time and space nodes, $\tau = T/M$ - time step, $h = 1/N$ space step; $x_j = jh, \quad j = 0,1,...,N, \; t_k = k\tau, \quad k = 0,1,...,M$.

One possibility for numerical approximation of the Riemann-Liouville fractional derivative is the Grünwald-Letnikov approximation:

$$(D_t^\alpha u)_j^k = \tau^{-\alpha} \sum_{m=0}^{k} (-1)^m \binom{\alpha}{m} u_j^{k-m} + O(\tau).$$

There is already a vast amount of studies (including numerical studies) of the single-term time-fractional diffusion equation and some recent works on its multi-term and distributed-order generalizations.

Concerning the problems related to viscoelastic models, only the Rayleigh-Stokes problem for the generalized second grade fluid

$$u_t = \mu(1 + D_t^\beta)\Delta u + f(x,t)$$

is well studied numerically as well as theoretically.

The more general problems (for the generalized fractional Oldroyd-B and Burgers' fluids) remain open for future research.

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Thank you for your attention!

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