On March 11, 2015, **a workshop on fractional calculus** was held, at the Department of Mathematics and Physics, Roma Tre University. The purpose of this one-day event was to present few contributions by several experts to lighten some recent advances on numerical treatment of fractional differential equations, modelling of problems through fractional calculus, and applications involving probabilistic approaches, special functions, and other analytical methods.

Below, we show the Program, and then the slides of all seminars, in the same order they were presented.

Renato Spigler

WORKSHOP ON FRACTIONAL CALCULUS AND ITS APPLICATIONS

Roma Tre, March 11, 2015

PROGRAM

h. 9:00-11:00 am, **Numerical methods**:

• Diethelm, "Numerical methods for terminal value problems of fractional order"

• Yuste: "High order adaptive methods for fractional PDEs"

• Garrappa: "Numerical methods for fractional operators involved in anomalous polarization processes"

h. 11:30-13:00, **Models with memory**:

• Caputo: "Why new fractional derivatives?"

• Fabrizio: "Damage and fatigue by a fractional model"

• Cavallaro: "Approach to equilibrium of a sphere in a Stokes fluid"

14:00-16:00, **Anomalous diffusion and probabilistic applications**:

• Beghin: “From fractional diffusion equations to fractional shift operators”

• Pagnini: “Generalized grey Brownian motion: from classical diffusion to Erdelyi-Kober fractional diffusion”

• Agliari: “Levy flights with power-law absorption”

• Concezzi: “Numerical solution of two-dimensional fractional diffusion equations by a high-order ADI method”

16:30-17:30, **Special Functions and analytical methods**:

• Cesarano: “Special polynomials in the description of fractional calculus”

• Garra:“Fractional diffusions with time-varying coefficients”

• Taverna: “Overview of the Fractional Calculus of Variations and its application to non-standard Lagragians”

Numerical Methods for Terminal Value Problems of Fractional Order

Kai Diethelm

Gesellschaft für numerische Simulation mbH Braunschweig

and

AG Numerik
Institut Computational Mathematics
Technische Universität Braunschweig

Recent Advances and Trends in Fractional Calculus and its Applications
Università Roma 3 — March 11, 2015

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Fundamental Task

Investigation of a real process governed by fractional order differential equation:

$$D_{*a}^{\alpha} y(t) = f(t, y(t)), \qquad t \geq a$$

where

D_{*a}^{α} = Caputo differential operator of order α with starting point a.

Fundamental Task

Investigation of a real process governed by fractional order differential equation:

$$D^{\alpha}_{*a} y(t) = f(t, y(t)), \qquad t \geq a$$

where

D^{α}_{*a} = Caputo differential operator of order α with starting point a.

Frequent obstacle

State of system can only be observed at time $t = b > a$.

Concrete Application Example

Fractional Maxwell model for viscoelastic material:

$$D^{\alpha}_{*0}\sigma(t) = \tau^{-\alpha}\sigma(t) + E \cdot D^{\alpha}_{*0}\epsilon(t) \quad (1)$$

- Task: Find shear stress $\sigma(t)$ for $t \geq 0$.

Concrete Application Example

Fractional Maxwell model for viscoelastic material:

$$D^{\alpha}_{*0}\sigma(t) = \tau^{-\alpha}\sigma(t) + E \cdot D^{\alpha}_{*0}\epsilon(t) \tag{1}$$

- Task: Find shear stress $\sigma(t)$ for $t \geq 0$.
- Measurement:

$$\sigma(b) = \sigma^* \text{ with some } b > 0 \tag{2}$$

Concrete Application Example

Fractional Maxwell model for viscoelastic material:

$$D^{\alpha}_{*0}\sigma(t) = \tau^{-\alpha}\sigma(t) + E \cdot D^{\alpha}_{*0}\epsilon(t) \tag{1}$$

- Task: Find shear stress $\sigma(t)$ for $t \geq 0$.
- Measurement:

$$\sigma(b) = \sigma^* \text{ with some } b > 0 \tag{2}$$

- Known data:
  - shear strain $\epsilon(t)$
  - relaxation time τ
  - order $\alpha \in (0, 1)$
  - shear modulus E

Concrete Application Example

Fractional Maxwell model for viscoelastic material:

$$D^{\alpha}_{*0}\sigma(t) = \tau^{-\alpha}\sigma(t) + E \cdot D^{\alpha}_{*0}\epsilon(t) \tag{1}$$

- Task: Find shear stress $\sigma(t)$ for $t \geq 0$.
- Measurement:

$$\sigma(b) = \sigma^{*} \text{ with some } b > 0 \tag{2}$$

- Approach:
  - solve (1) subject to (2) on $[0, b]$ (terminal value problem)
  - compute initial value $\sigma(0)$ from this solution
  - construct initial value problem from (1) and initial condition
  - if desired, solve initial value problem on $[0, T]$ with $T > b$

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Analytical Fundamentals

Task: Find solution to fractional order terminal value problem

$$\begin{aligned} D_{*a}^{\alpha} y(t) &= f(t, y(t)) \\ y(b) &= y^* \end{aligned}$$

for $t \in [a, b]$.

In this talk: $0 < \alpha \leq 1$
(generalization to $\alpha > 1$ requires additional terminal conditions)

Existence and Uniqueness of Solutions

General assumptions on right-hand side of differential equation:

- continuity
- boundedness
- Lipschitz condition w. r. t. second variable

Existence and Uniqueness of Solutions

General assumptions on right-hand side of differential equation:

- continuity
- boundedness
- Lipschitz condition w. r. t. second variable

Theorems:

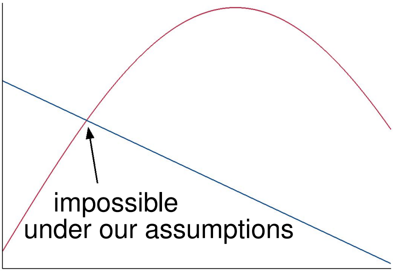
- Uniqueness of continuous solution to terminal value problem.
- Existence of continuous solution if interval $[a, b]$ is sufficiently small.

(Di. 2008, Di. & Ford 2012)

Existence and Uniqueness of Solutions

Corollary:

The graphs of two solutions to *the same differential equation* subject to *different initial or terminal conditions* never meet or cross each other.



(Di. & Ford 2012)

Integral Equation Formulation

Terminal value problem can be rewritten as Fredholm integral equation

$$y(t) = y^* + \frac{1}{\Gamma(\alpha)} \int_a^b G(t,s) f(s, y(s))\, \mathrm{d}s$$

with

$$G(t,s) = \begin{cases} -(b-s)^{\alpha-1} & \text{for } s > t, \\ (t-s)^{\alpha-1} - (b-s)^{\alpha-1} & \text{for } s \le t. \end{cases}$$

(Di. 2010)

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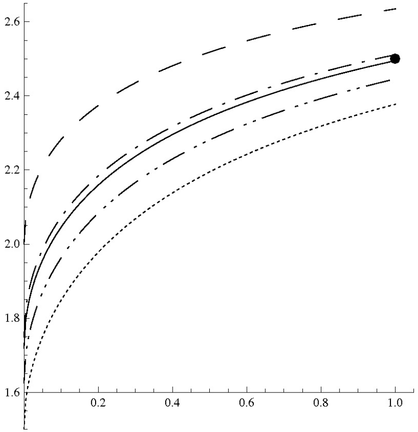
Shooting Methods

Rationale:



Shooting Methods

Fundamental approach:

1. Guess initial value $y(a)$
2. Solve fractional differential equation (numerically) with this initial value
3. Compare solution $y(b)$ with required terminal value y^*:
    - if $|y(b) - y^*| < \epsilon$ then accept y as approximate solution to terminal value problem,
    - if $y(b) \gg y^*$ then replace guess for initial value $y(a)$ by smaller number and go back to step 2,
    - if $y(b) \ll y^*$ then replace guess for initial value $y(a)$ by larger number and go back to step 2.

Shooting Methods

Questions:

1. Good initial guess for $y(a)$?
2. Algorithm for numerical solution of initial value problem?
3. Step size?
4. Strategy for finding improved value for $y(a)$?

Shooting Methods

Questions:

1. Good initial guess for $y(a)$?
   Use terminal value y^* (unless additional information available)
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   Use Adams-Bashforth-Moulton scheme
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   Depends on required accuracy of final result
   and on quality of starting value
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3. Step size?
   Depends on required accuracy of final result
   and on quality of starting value
4. Strategy for finding improved value for $y(a)$?
   Bisection method (Ford, Morgado & Rebelo 2014)
   or Newton iteration

Shooting Methods

Step size selection strategy:

1. Error of fractional initial value problem solver = $\epsilon^{\mathrm{I}} + \epsilon^{\mathrm{N}}$:
    - $\epsilon^{\mathrm{I}} =$ error due to incorrectly chosen initial value
    - $\epsilon^{\mathrm{N}} =$ error introduced by numerical approximation scheme
2. Early iterations:
    - approximation of correct initial value is poor
    - ϵ^{I} is large
    - no need to have very small ϵ^{N}
    - coarse discretization of interval suffices
    - reduction of computation cost

(Di. 2015)

Shooting Methods

Step size selection strategy:

1. Error of fractional initial value problem solver = $\epsilon^{\mathrm{I}} + \epsilon^{\mathrm{N}}$:
   - $\epsilon^{\mathrm{I}} =$ error due to incorrectly chosen initial value
   - $\epsilon^{\mathrm{N}} =$ error introduced by numerical approximation scheme
2. Later iterations:
   - approximation of correct initial value is good
   - ϵ^{I} is small
   - ϵ^{N} should be small as well
   - fine discretization of interval is required
   - accurate solution can be achieved

(Di. 2015)

Shooting Methods

Example problem:

$$D_{*0}^{\alpha} y(t) = \Gamma(2+\alpha)t + \frac{1}{4}\left(y(t) - w - t^{1+\alpha}\right)$$

Exact solution: $y(t) = t^{1+\alpha} + w$

Parameters:

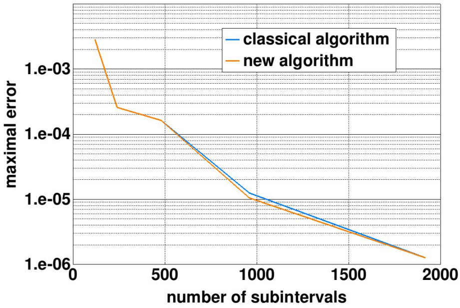
- $\alpha = 7/10$
- $w = -3$
- $b = 12$ (rather long interval)

Shooting Methods

Specific step size selection strategy:

- Define number K of iterations of shooting method
- Define minimal step size h (for last iteration)
- Use step size $h_m = hK/m$ in mth iteration

Computational results:



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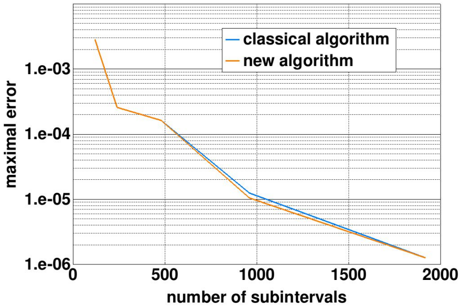

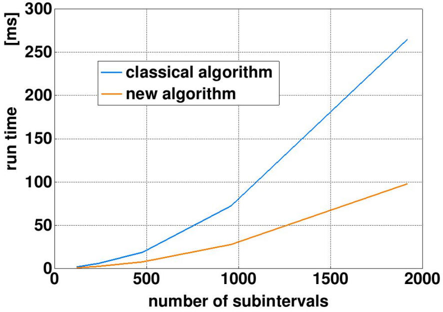

Galerkin Methods

Integral equation form of terminal value problem:

$$y\ \ (t) - y^* - \frac{1}{\Gamma(\alpha)} \int_a^b G(t,s) f(s, y\ \ (s))\, ds \qquad = 0$$

with

$$G(t,s) = \begin{cases} -(b-s)^{\alpha-1} & \text{for } s > t, \\ (t-s)^{\alpha-1} - (b-s)^{\alpha-1} & \text{for } s \le t. \end{cases}$$

Galerkin Methods

Numerical solution y_{G} of integral equation:

$$\int_a^b \left[y_{\mathrm{G}}(t) - y^* - \frac{1}{\Gamma(\alpha)} \int_a^b G(t,s) f(s, y_{\mathrm{G}}(s))\,\mathrm{d}s \right] y_j(t)\,\mathrm{d}t = 0$$

for $j = 1, 2, \dots, n$, where

$$y_{\mathrm{G}}(t) = \sum_{j=1}^{n} a_j y_j(t)$$

Galerkin Methods

- Well established method for boundary value problems ($1 < \alpha < 2$, one condition given at each end of $[a, b]$)
- Can be used for terminal value problems as well
- Especially useful for linear problems, i. e. $f(t, y(t)) = p(t) + r(t)y(t)$
- Classical choice for basis functions y_j: piecewise linear functions on uniform mesh

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Detailed Analysis of Galerkin Scheme

Open questions:

- Optimization of underlying mesh?
- Choice of basis functions:
  - Higher order functions?
  - Combination of integer and non-integer exponents?
  - Globally supported functions?
- “Natural” space of functions for convergence analysis?

Generalized Problem

Terminal Value Problem

$$D_{*a}^{\alpha} y(t) = f(t, y(t)), \qquad y(b) = y^*$$

Generalized Problem

Terminal Value Problem

$$D^{\alpha}_{*a} y(t) = f(t, y(t)), \qquad y(b) = y^*$$

Traditional assumption: Starting time a is known.

Generalized Problem

Terminal Value Problem

$$D^{\alpha}_{*a} y(t) = f(t, y(t)), \qquad y(b) = y^*$$

Traditional assumption: Starting time a is known.

Question: What if a is unknown?

Generalized Problem

Terminal Value Problem

$$D_{*a}^{\alpha} y(t) = f(t, y(t)), \qquad y(b) = y^*$$

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Question: What if a is unknown?

1. Existence of solution?

Generalized Problem

Terminal Value Problem

$$D^{\alpha}_{*a} y(t) = f(t, y(t)), \qquad y(b) = y^*$$

Traditional assumption: Starting time *a* is known.

Question: What if *a* is unknown?

1. Existence of solution?
2. Uniqueness of solution under which additional condition?

Generalized Problem

Terminal Value Problem

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4. Numerical method?

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4. Numerical method?

Partial answers to questions 1, 2, 3 in Di. (2014)

Thank you for your attention!

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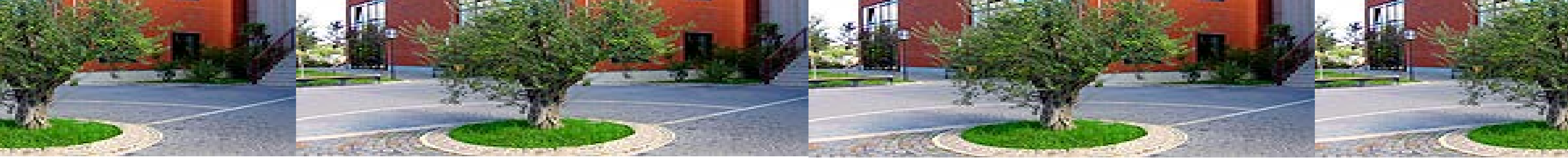


"Workshop on Fractional Calculus and its Applications"
Roma Tre University, March 11, 2015

High order adaptive methods for fractional PDEs

Santos Bravo Yuste and Joaquín Quintana-Murillo

Dpt. Física, Univ. Extremadura, Badajoz, Spain

UNIÓN EUROPEA
Fondo Europeo de Desarrollo Regional
Una manera de hacer Europa

GOBIERNO DE EXTREMADURA

Outline

1. *Very short presentation of the* L1 finite difference scheme with non-uniform timesteps (stability? Be aware!)

2. Why variable timesteps?

3. How to choose the size of the timesteps? → adaptive methods

4. L1 adaptive method in action 

new

5. A naïve way to improve the L1 adaptive method: let's use a X discretization scheme of higher order than L1

   5.1 X=Cao-Xu(2013) [as expected]

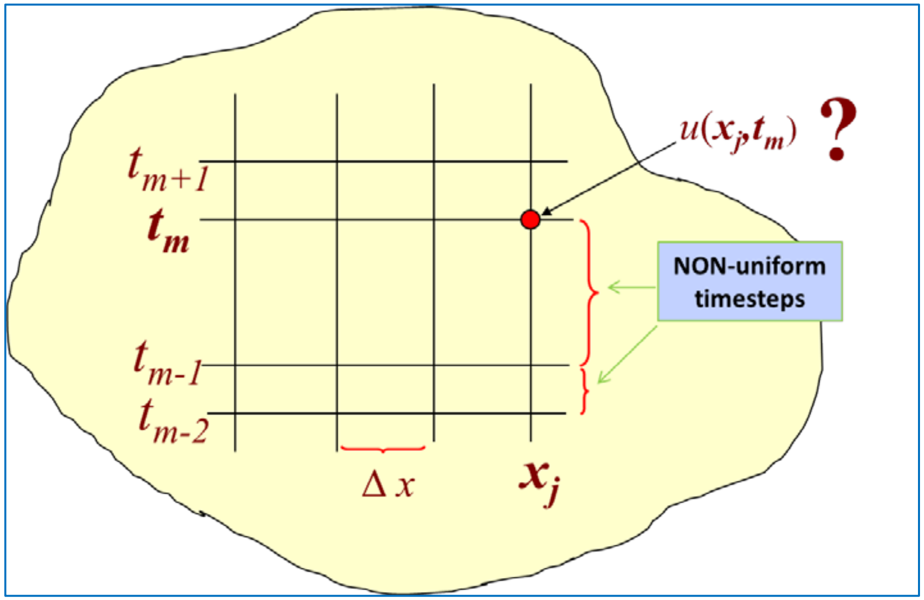
   5.2 X=Gao-Sun-Zhang(2014) [surprise!]

6. Conclusions

L1 finite difference scheme
Discretization of the FPDE

$\partial u = F$

Continuous integro-differential equation → Finite difference equation



exact → approx.

$u(x_j,t_m)$ → U_j^m

$\partial u = F$ → $\delta U = F$

FPDE → finite difference eq.

$$\partial \equiv \frac{\partial^\gamma}{\partial t^\gamma} - K\frac{\partial^2}{\partial x^2} \rightarrow \delta \equiv \delta_t^\gamma - K\delta_x^2$$

L1 finite difference method. Spatial discretization

$$\left[\frac{\partial^\gamma}{\partial t^\gamma} - K\frac{\partial^2}{\partial x^2}\right] u(x,t) = F(x,t) \longrightarrow \left[\delta_t^\gamma - K\delta_x^2\right] U_j^n = F(x_j, t_n)$$

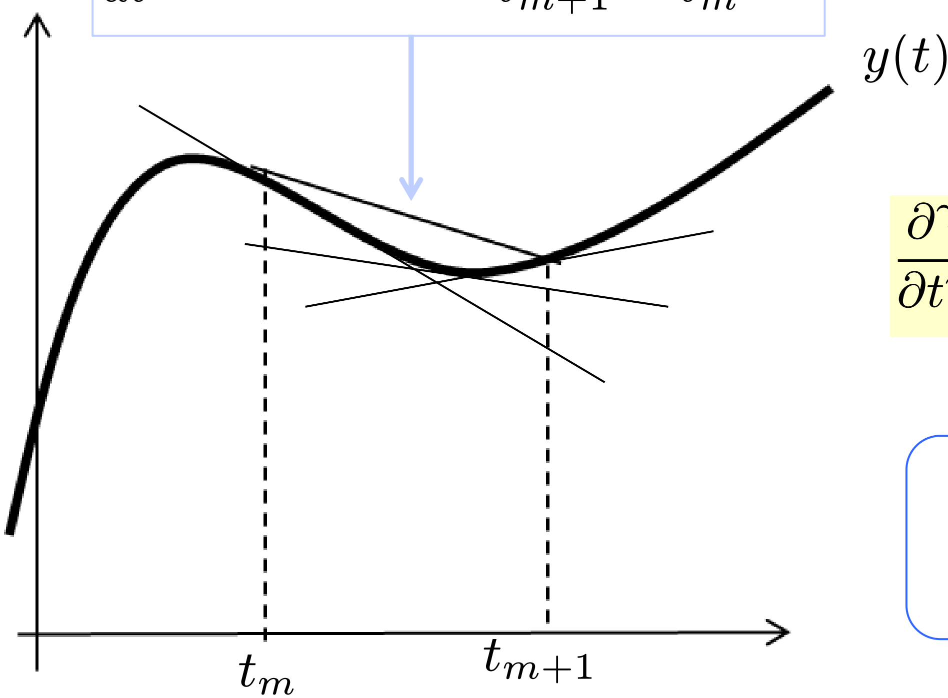
Discretization of the Laplacian: three point centered formula

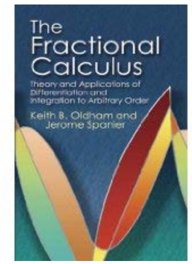
$$\frac{\partial^2 u}{\partial x^2} \Longrightarrow \delta_x^2 u(x_j,t) = \frac{u(x_{j+1},t) - 2u(x_j,t) + u(x_{j-1},t)}{(\Delta x)^2}$$

L1 discretization of the Caputo operator, $0<\gamma<1$, with **not-fixed timesteps**

L1 approx. of the Caputo derivative $\Leftrightarrow$ piecewise constant approximation of $\dfrac{dy}{dt}$

$$\frac{dy}{dt} \approx \text{slope} = \frac{y(t_{m+1}) - y(t_m)}{t_{m+1} - t_m}$$





$$\frac{\partial^\gamma}{\partial t^\gamma} y(t) \equiv \frac{1}{\Gamma(1-\gamma)} \int_0^t d\tau \frac{1}{(t-\tau)^\gamma} \boxed{\frac{dy(\tau)}{d\tau}}$$

$$t_{n+1} - t_n = \Delta_n = \Delta$$

Discretization error: $O\left(\Delta^{2-\gamma}\right)$

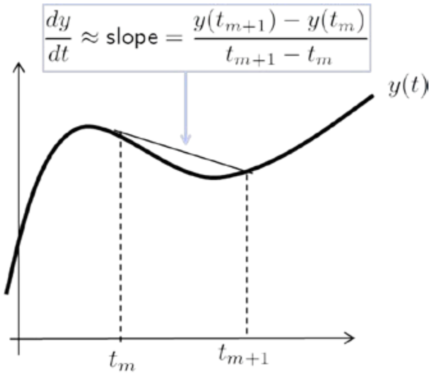
Simple idea: we can increase the size of the steps without losing accuracy if we use discretizations of order higher than 2-γ

L1 finite difference method.
Non-homogeneus discretization of the Caputo derivative

0<γ <1

$$\frac{\partial^\gamma}{\partial t^\gamma} y(t) \equiv \frac{1}{\Gamma(1-\gamma)} \int_0^t d\tau \frac{1}{(t-\tau)^\gamma} \frac{dy(\tau)}{d\tau}$$

straightforward



$$\delta_t^\gamma y(t_n) = \frac{1}{\Gamma(2-\gamma)} \sum_{m=0}^{n-1} T_{m,n}^{(\gamma)} \left[y(t_{m+1}) - y(t_m) \right]$$

L1 approximation with variable timesteps

$$T_{0,1}^{(\gamma)} = (t_1 - t_0)^{-\gamma},$$

$$T_{m,n}^{(\gamma)} = \frac{(t_n - t_m)^{1-\gamma} - (t_n - t_{m+1})^{1-\gamma}}{t_{m+1} - t_m}, \quad m \le n-1,$$

Finite difference method: numerical scheme

$$\left[\delta_t^\gamma - K\delta_x^2\right] U_j^n = F(x_j, t_n)$$

$$\delta_x^2 u(x_j,t) = \frac{u(x_{j+1},t) - 2u(x_j,t) + u(x_{j-1},t)}{(\Delta x)^2}$$

$$\delta_t^\gamma U_j^n = \frac{1}{\Gamma(2-\gamma)} \sum_{m=0}^{n-1} T_{m,n}^{(\gamma)} \left[U_j^{m+1} - U_j^m\right]$$

Substituting and reordering:

$$-S_n U_{j+1}^n + (1+2S_n)U_j^n - S_n U_{j-1}^n = \mathcal{M}U_j^n + \tilde{F}(x_j,t_n)$$

$$S_n = \Gamma(2-\gamma)K\frac{(t_n - t_{n-1})^\gamma}{(\Delta x)^2},$$

$$\mathcal{M}U_j^n \equiv U_j^{n-1} - \sum_{m=0}^{n-2} \tilde{T}_{m,n}^{(\gamma)} \left[U_j^{m+1} - U_j^m\right]$$

Implicit method

$$AU^{(n)} = \mathcal{M}U^{(n)} + \tilde{F}^{(n)}$$

Tridiagonal linear system
(Thomas algorithm)

Does the method always work?
Stability

The L1 method with *variable* timesteps is *unconditionally* stable (stable for any t_m, x_j, γ)
(**Yuste&Quintana-Murillo**, Computer Physics Communications, 2012)

$$\boxed{-S_n\, U_{j+1}^n + (1+2S_n)U_j^n - S_n\, U_{j-1}^n = \mathcal{M}U_j^n + \tilde{F}(x_j, t_n)}$$

$$\widehat{U}_j^{(m)} - U_j^{(m)} = v_j^{(m)}$$

perturbed solution

perturbation

It is proved there that

$$\boxed{\left\| v^{(n)} \right\|_2 \;\square\; \left\| v^{(0)} \right\|_2}$$

always!

Outline

1. *Very short presentation of the* L1 finite difference scheme with non-uniform timesteps (stability? Be aware!)

2. Why variable timesteps?

3. How to choose the size of the timesteps? → adaptive methods

4. L1 adaptive method in action 

new

5. A naïve way to improve the L1 adaptive method: let's use a X discretization scheme of higher order than L1

   5.1 X=Cao-Xu(2013) → unstable→ not surprising

   5.2 X=Gao-Sun-Zhang(2014) → unstable!!→ surprise!!

6. Conclusions

Difficulties

Fractional (***sub***)diffusion equation (FDE)

$$\frac{\partial^\gamma}{\partial t^\gamma} u(\vec{r},t) = \nabla^2 u(\vec{r},t) + F(\vec{r},t) \qquad 0 < \gamma < 1$$

Two main drawbacks of *standard* finite difference methods with fixed timesteps:

1. Slooooooooooowness

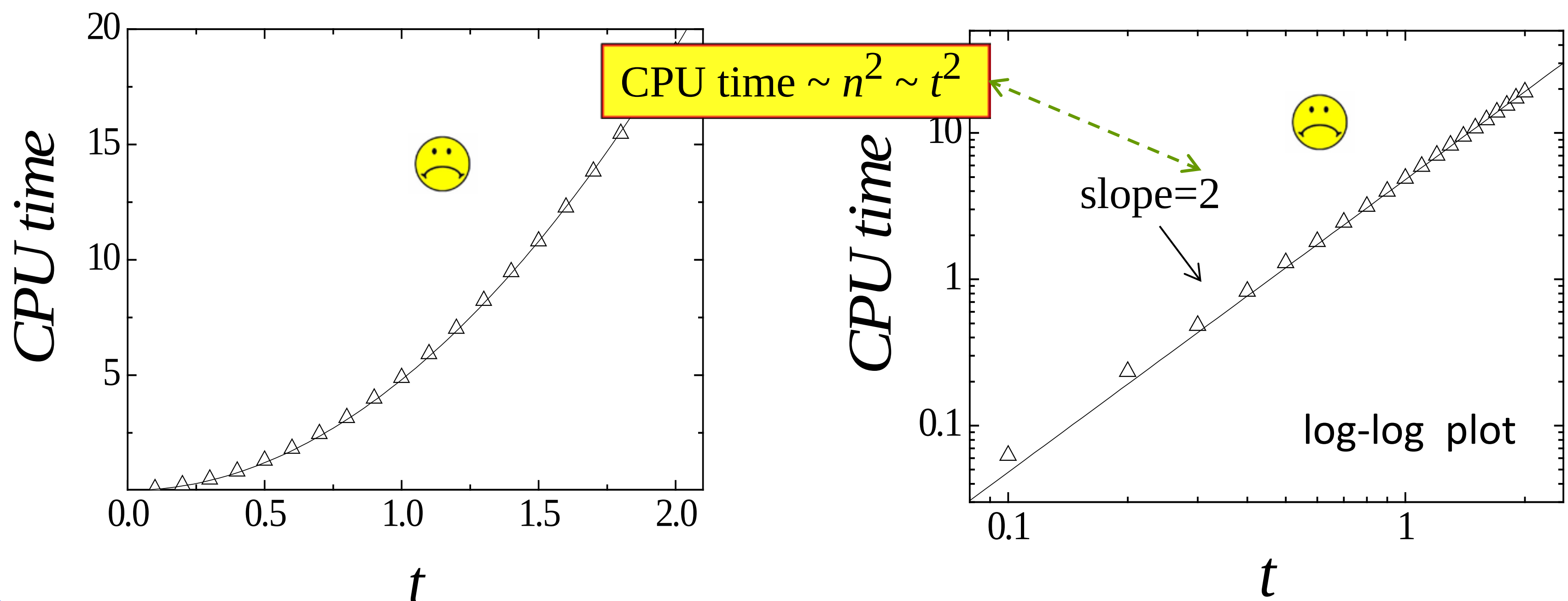
2. Inconsistent accuracy

1. These methods become sloooooooooooower as time increases

Fact: computational cost ~ [number of timesteps]^2

EXAMPLE

Standard finite difference methods, fixed timestesps



Example:

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2}$$

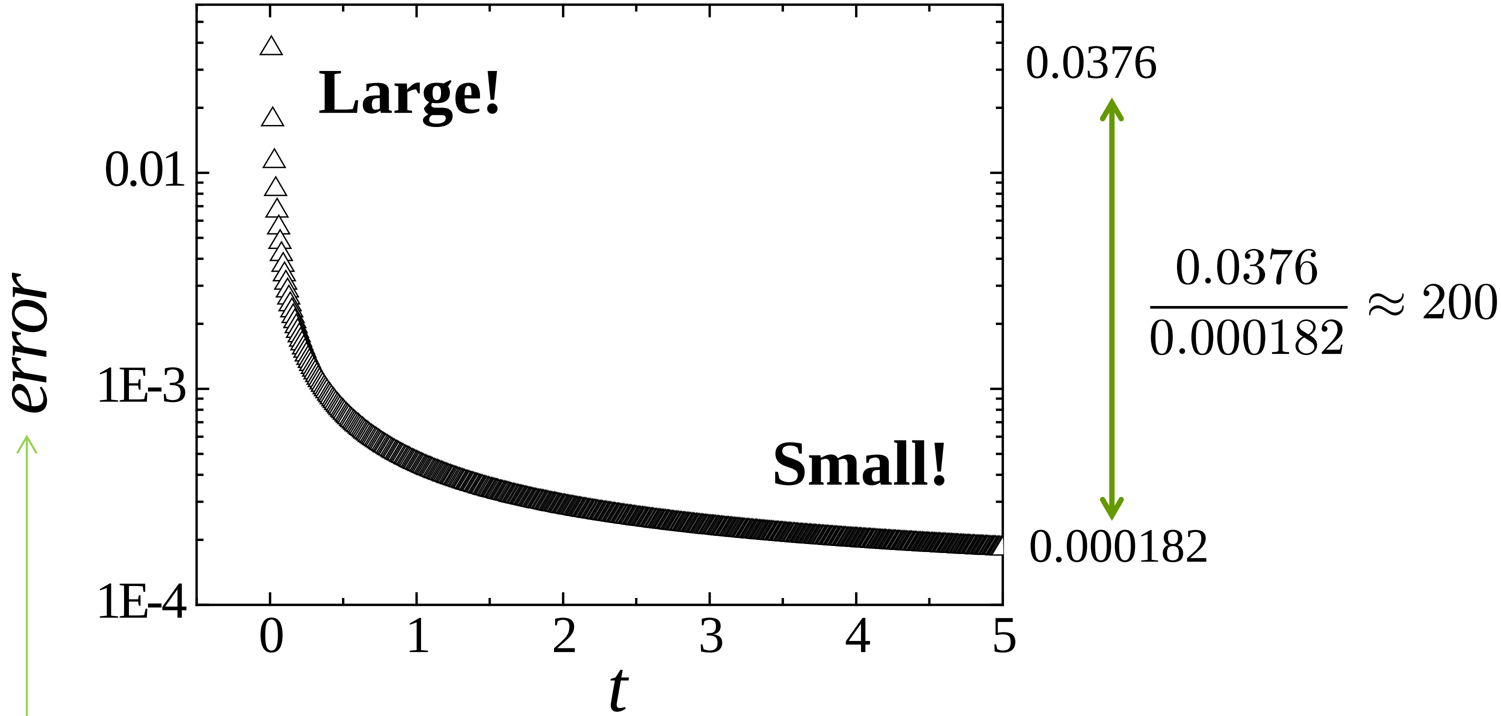
$0 \leq x \leq \pi$

BC: $u(x=0,t) = u(x=\pi,t) = 0$

IC: $u(x,0) = \sin x$

γ=1/4

2. The accuracy of these methods is not consistent



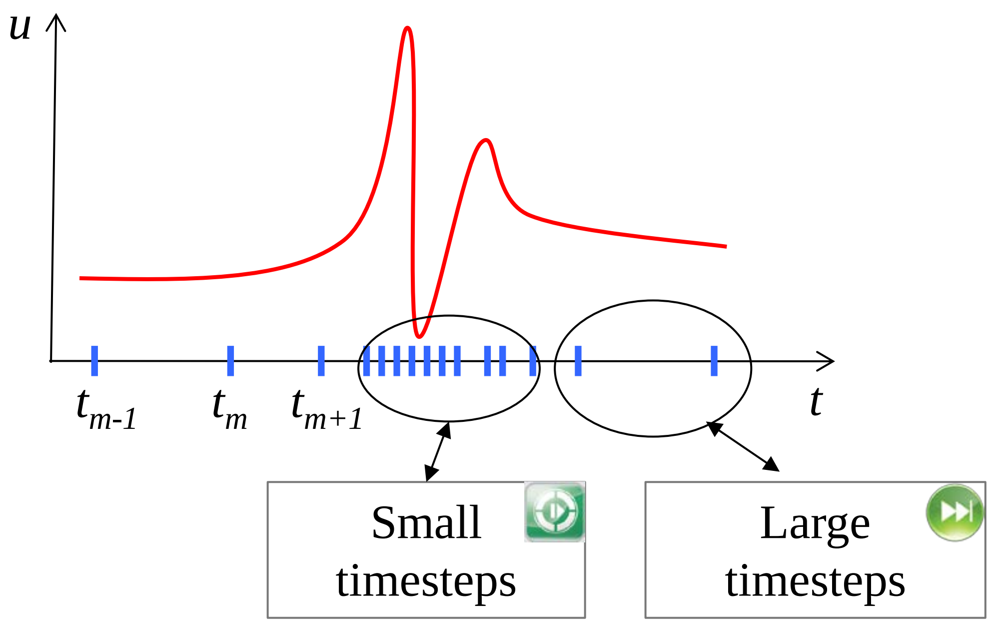
Errors of a *standard* finite difference methods with fixed timestesps for the problem:

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} \qquad \text{BC: } u(x=0,t) = u(x=\pi,t) = 0$$

$$0 \leq x \leq \pi \qquad \text{IC: } u(x,0) = \sin x$$

γ=1/4

What to do?
Variable/**adaptive** timestesps



A good ***ODE*** integrator should exert some adaptive control over its own progress, making frequent changes in its stepsize. […] Many small steps should **tiptoe** through treacherous terrain, while a few **great strides** should speed through smooth uninteresting countryside. The resulting gains in efficiency are not mere tens of percents or factors of two; they can sometimes be factors of ten, a hundred, or more

Press,Teukolsky, Vetterling & Flannery. *Numerical recipes.The Art of Scientific Computing*

Adaptive methods
- ***more reliable***: via thorough sampling of difficult regions
- ***faster*** : via sparse sampling of quiet regions

What do we need?

1. A finite difference method that can work with *variable* timesteps

2. A method for choosing the right size of the timesteps … *according to* the behaviour of the solution

$\Downarrow$

adaptive method

What do we need?

1. **Finite difference method with *variable* timesteps (*an example: the L1 method*).**

Discretization : temporal → L1 (Oldham-Spanier) spatial → three point centred formula	
Fixed timesteps: Liu, Anh & Turner (2006), Murio (2008)	

$$\frac{\partial^\gamma}{\partial t^\gamma} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) + F(x,t)$$

$$u(x_j, t_n) \to U_j^n$$

Generalization for variable timesteps

SBY & Quintana-Murillo, Comput. Phys. Commun. **183** (2012) 2594

$$-S_n U_{j+1}^n + (1+2S_n)U_j^n - S_n U_{j-1}^n = \mathcal{M}U_j^n + \tilde{F}(x_j, t_n)$$

where:

$$\mathcal{M}U_j^n \equiv U_j^{n-1} - \sum_{m=0}^{n-2} \tilde{T}_{m,n}^{(\gamma)} \left[U_j^{m+1} - U_j^m\right]$$

$$S_n = \Gamma(2-\gamma) K \frac{(t_n - t_{n-1})^\gamma}{(\Delta x)^2},$$

$$T_{m,n}^{(\gamma)} = \frac{(t_n - t_m)^{1-\gamma} - (t_n - t_{m+1})^{1-\gamma}}{t_{m+1} - t_m}$$

Implicit method

$$AU^{(n)} = \mathcal{M}U^{(n)} + \tilde{F}^{(n)}$$

Tridiagonal linear system

What do we need?

2. **A method for choosing the right size of the timesteps … *according to* the behaviour of the solution.**

$\Downarrow$

adaptive method

What do we need?

2. **A method for choosing the right size of the timesteps … *according to* the behaviour of the solution**

adaptive method

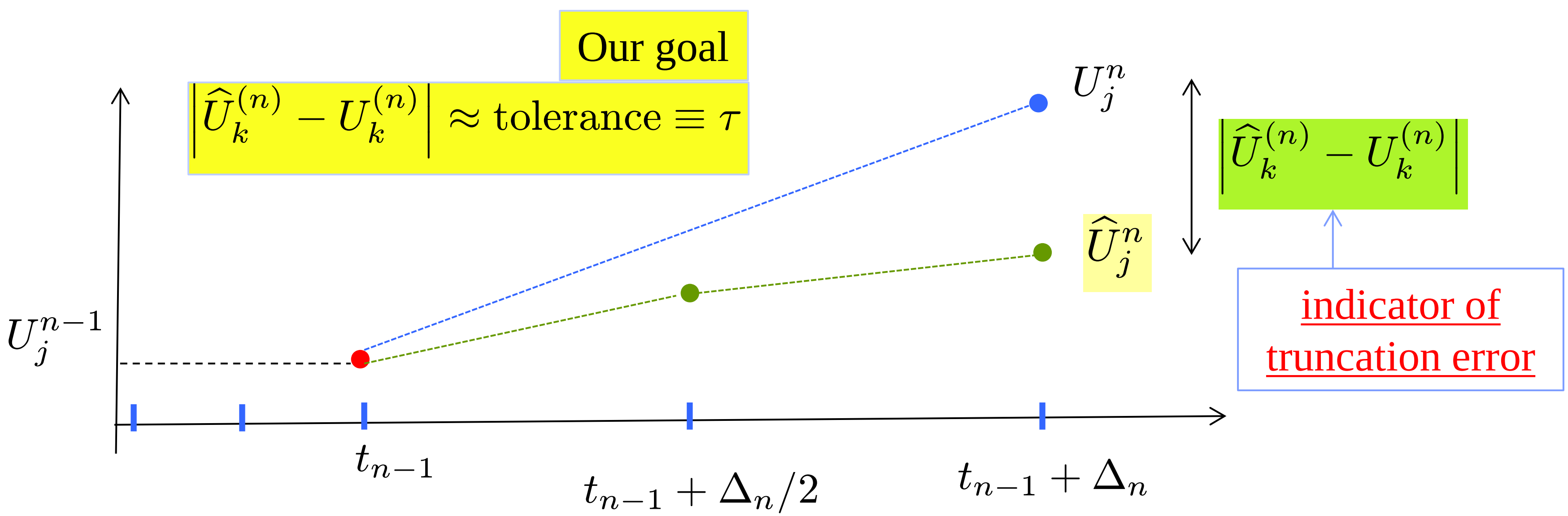
Adaptive procedures:

- **Trial and error** *step-doubling* algorithm ⇨ **This talk**
- **Predictive** *step-doubling* algorithm
- ……………………………………

Step-doubling technique for FDE (notation)

$$\left(t_m, U_j^m\right) \quad m = 0, 1, \cdots, n-1 \quad \Longleftrightarrow \quad \left[t_{\{n-1\}}, U_j^{\{n-1\}}\right] \xrightarrow{?} \left(t_n, U_j^n\right)$$

Some definitions	$\Delta_n \equiv t_n - t_{n-1}$ *n* -th timestep	$U_j^{\{n-1\}} \xrightarrow{\Delta_n} U_j^n$ $U_j^{\{n-1\}} \xrightarrow[\text{2 steps}]{\Delta_n/2} \widehat{U}_j^n$



Trial and error (t&e) step-doubling algorithm for FDE

$$\boxed{(t_m, U_j^m) \quad m = 0, 1, \cdots, n-1} \Longleftrightarrow \left[t_{\{n-1\}}, U_j^{\{n-1\}}\right] \xrightarrow{?} (t_n, U_j^n)$$

Some definitions	$\Delta_m \equiv t_m - t_{m-1}$ *m*-th timestep	$U_j^{\{n-1\}} \xrightarrow{\Delta_n} U_j^n$ $U_j^{\{n-1\}} \xrightarrow[\text{2 steps}]{\Delta_n/2} \widehat{U}_j^n$

t&e step-doubling algorithm

1. Bootstrap of step *n:* $\Delta_n = \Delta_{n-1}$ and $\left|\widehat{U}_k^{(n)} - U_k^{(n)}\right| \overset{?}{>} \boxed{\text{tolerance}} \equiv \tau$

2a. True: then $\Delta_n \to \Delta_n/2$ until $\left|\widehat{U}_k^{(n)} - U_k^{(n)}\right| < \tau$ then $t_n = t_{n-1} + \Delta_n$

2b. False: then $\Delta_n \to 2\Delta_n$ until $\left|\widehat{U}_k^{(n)} - U_k^{(n)}\right| > \tau$ then $t_n = t_{n-1} + \Delta_n/2$

3. Repeat [i.e., $n \to n+1$ and go to 1]

Outline

1. *Very short presentation of the* L1 finite difference scheme with non-uniform timesteps (stability? Be aware!)

2. Why variable timesteps?

3. How to choose the size of the timesteps? → adaptive methods

4. L1 adaptive method in action 

new

5. A naïve way to improve the L1 adaptive method: let's use a X discretization scheme of higher order than L1

   5.1 X=Cao-Xu(2013) [as expected]

   5.2 X=Gao-Sun-Zhang(2014) [surprise!]

6. Conclusions

The method works!

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} + f(x,t)$$

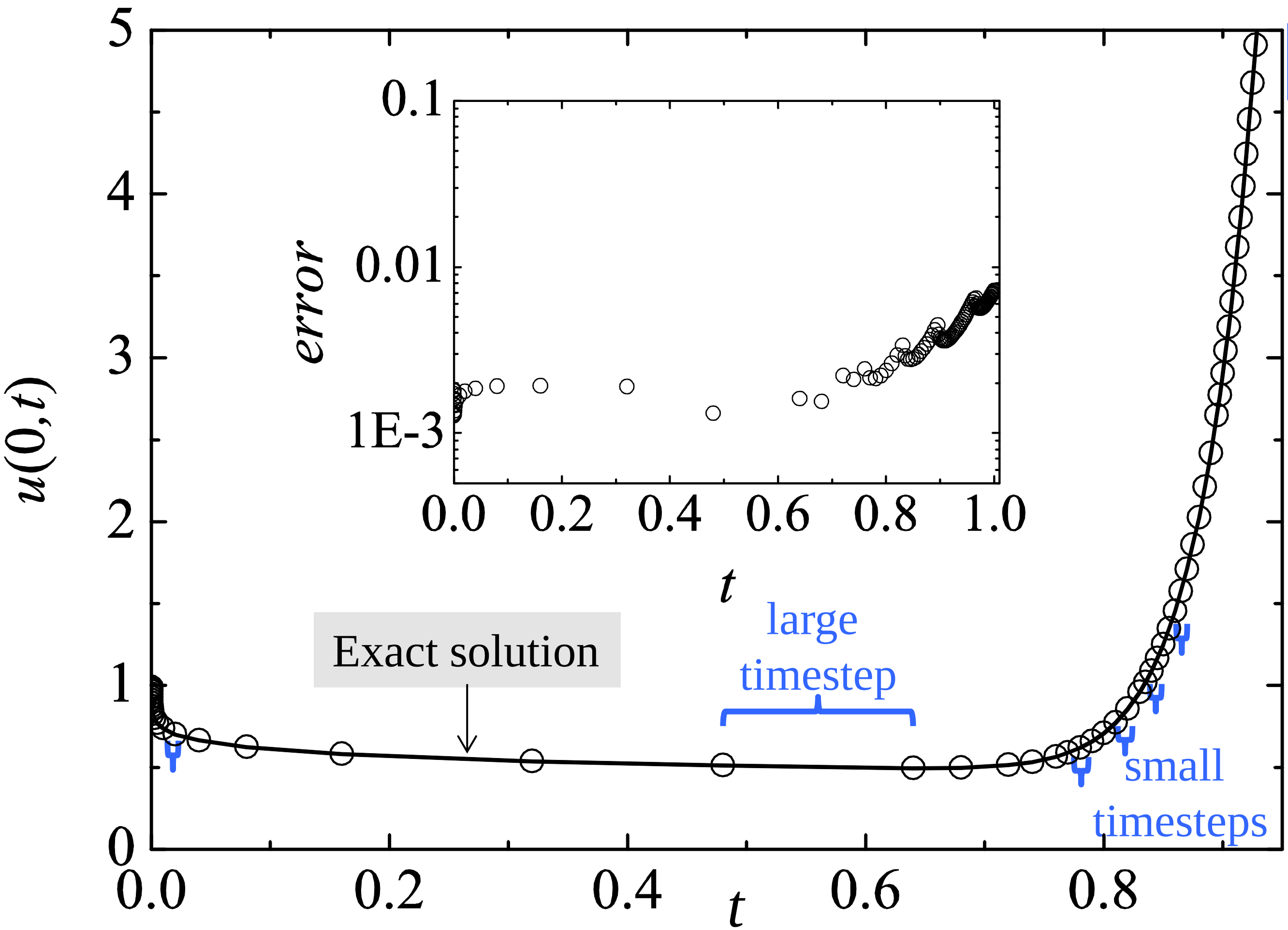
$$u(x=0,t) = u(x=\pi,t) = 0$$

$$u(x,0) = \sin x$$

$$f(x,t) = \left[1 + \frac{\Gamma(1+p)t^\gamma}{\Gamma(1+p-\gamma)}\right] a t^p \sin x$$

$$a = p = 20$$

$$\tau = 10^{-3}$$



How good is the t&e method ?

Is the new t&e method an improvement over standard non-adaptive methods?

1. How fast is the t&e method?

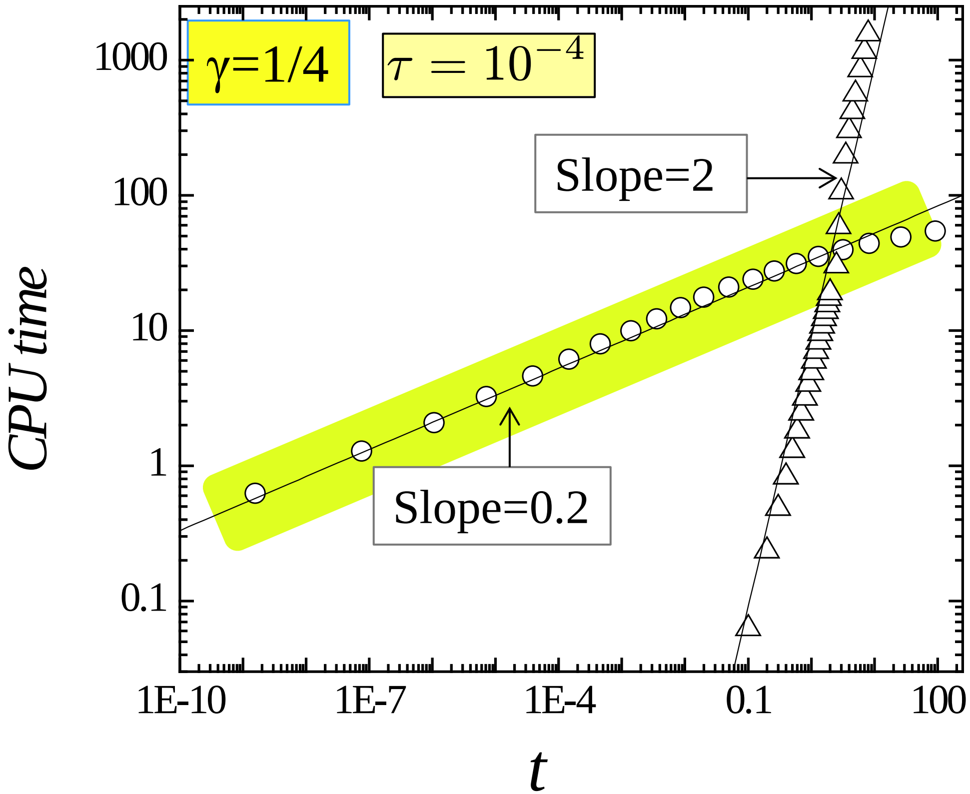
2. How are the numerical errors?

How fast is the t&e method?

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} \qquad \text{BC: } u(x=0,t) = u(x=\pi,t) = 0$$

$$0 \le x \le \pi \qquad \text{IC: } u(x,0) = \sin x$$

Really fast!!

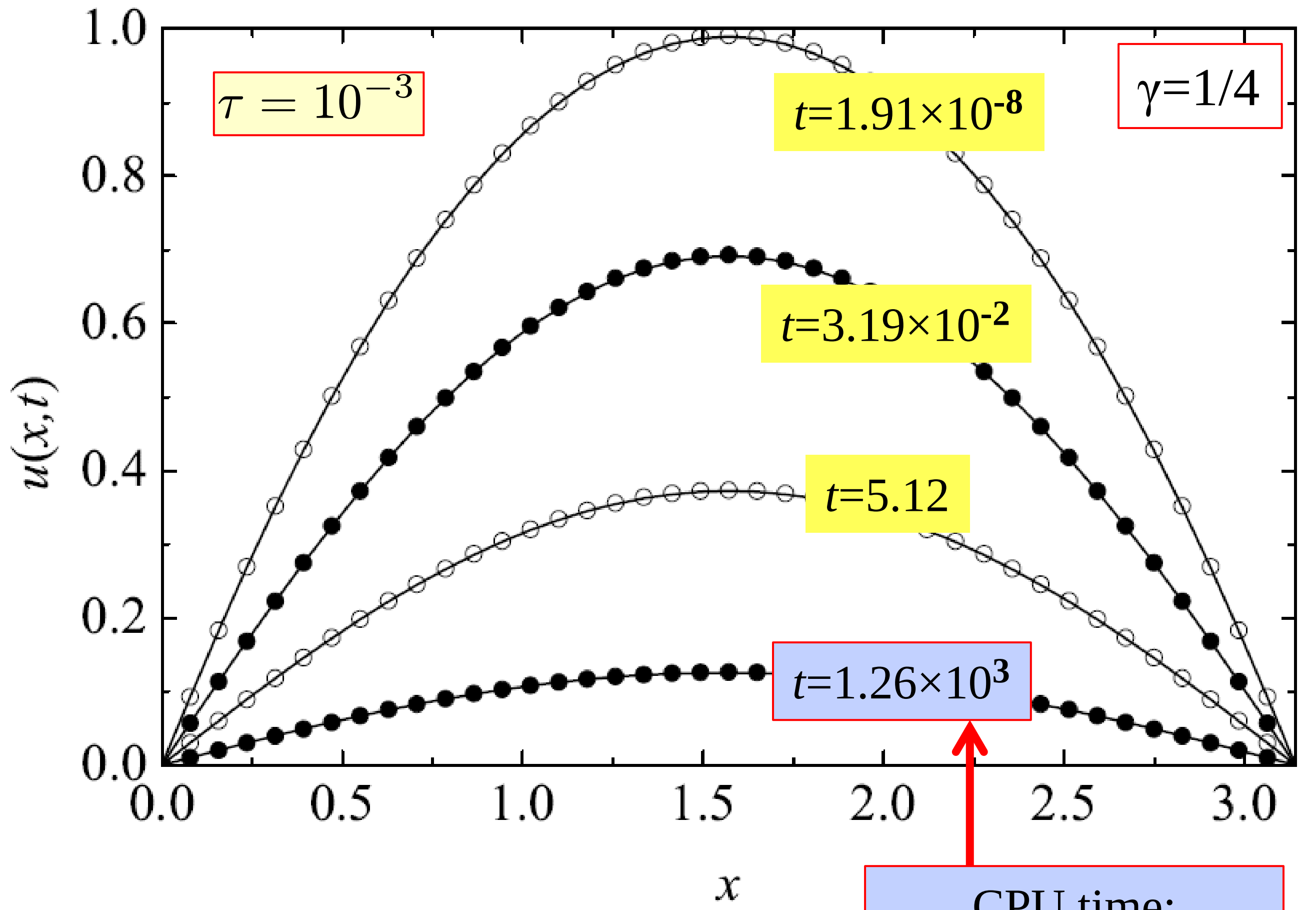


(*) estimation

t	1.30	8.34	92.82
CPU time Δ_n=0.01	8 s	50 minutes	≈ 5 days (*)
CPU time *adaptive*	35 s	44 s	54 s

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} \qquad \text{BC: } u(x=0,t) = u(x=\pi,t) = 0$$

$$0 \le x \le \pi \qquad \text{IC: } u(x,0) = \sin x$$



CPU time:
1 minute (adaptive)
vs
3 years (Δ_n=0.01)

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} \qquad \text{BC: } u(x=0,t) = u(x=\pi,t) = 0$$

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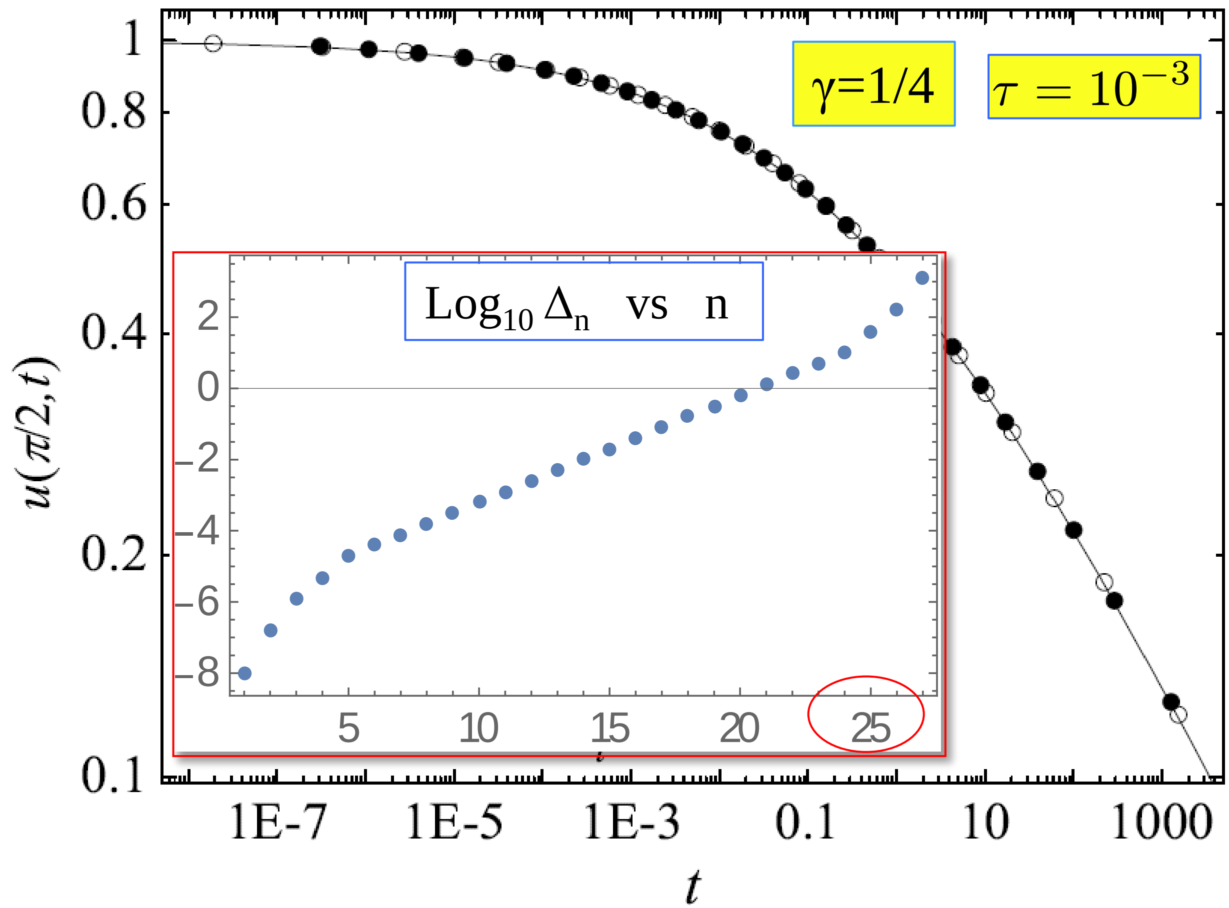


Really fast!!

Solution at the midpoint $u(\pi/2,t)$ vs. t for $\gamma = 1/4$. The symbols are the numerical solution. In all cases $\tau = 0.001$, $\Delta x = \pi/40$, $\Delta_0 = 0.01$. The line is the exact solution .

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} + f(x,t) \qquad 0 \,\square\, x \,\square\, \pi$$

$$f(x,t) = a\left[\sin(\nu t) + \nu^\gamma \sin\left(\nu t + \gamma\pi/2\right)\right]\sin x$$

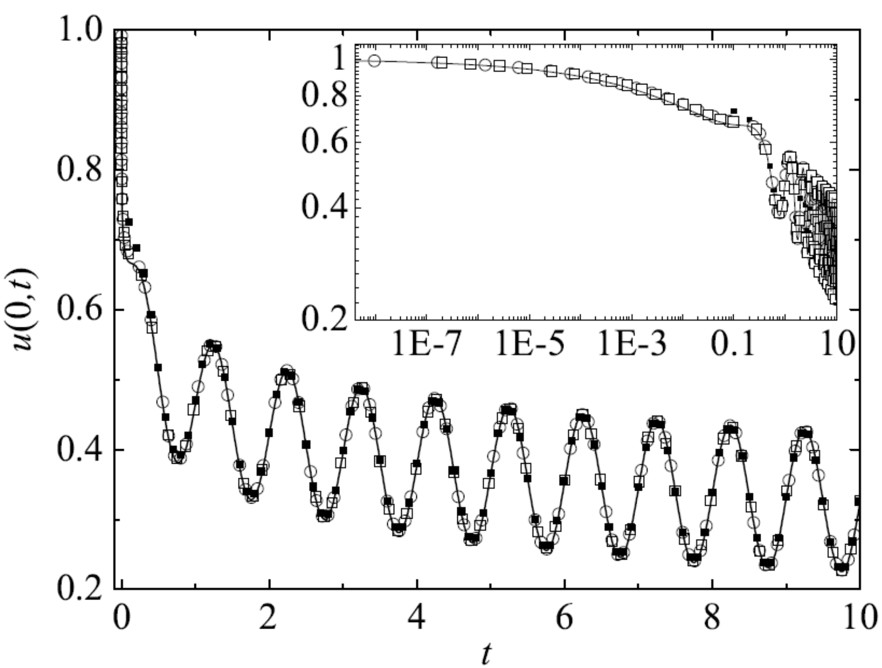
$$u(x=0,t) = u(x=\pi,t) = 0$$

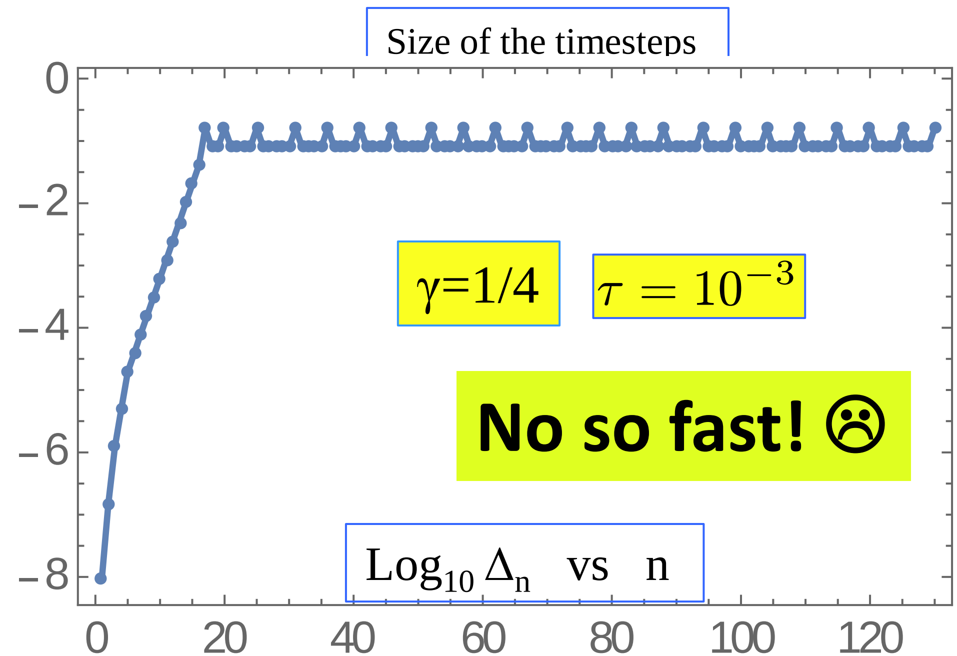
$$u(x,0) = \sin x$$

Exact solution

$$u(x,t) = \left[E_\gamma(-t^\gamma) + a\sin(\nu t)\right]\,\sin x$$

Mittag-Leffler function





Solution at the midpoint $u(\pi/2,t)$ vs. time for $\gamma = 1/4$, $\nu = 2\pi$ and $a = 1/10$. Solid squares: numerical method with $\Delta_n = 0.1$; Open symbols: numerical solution with tolerance $\tau = 10^{-3}$; line: exact solution. In all cases $\Delta x = \pi/40$ and $\Delta_0 = 0.01$. Inset: detail of the solution $u(\pi/2,t)$ for short times.

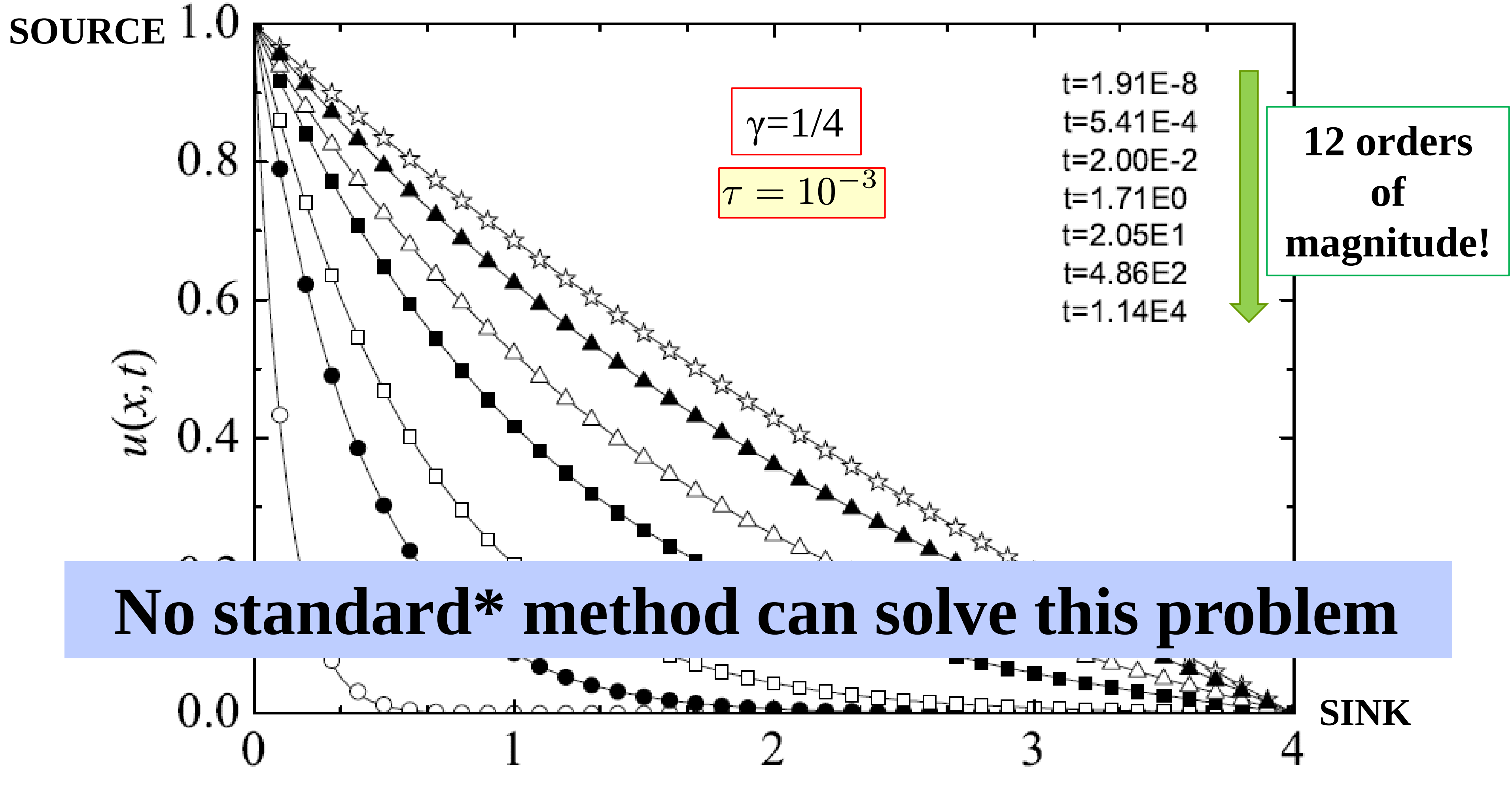
Last example: source and sink of subdiffusive particles

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2}$$

$u(x=0,t)=1$

$u(x=4,t)=0$

$u(x,0)=0$



No standard* method can solve this problem

* Finite difference method with fixed timesteps

Is the new t&e method an improvement over standard non-adaptive methods?

1. How fast is the t&e method?

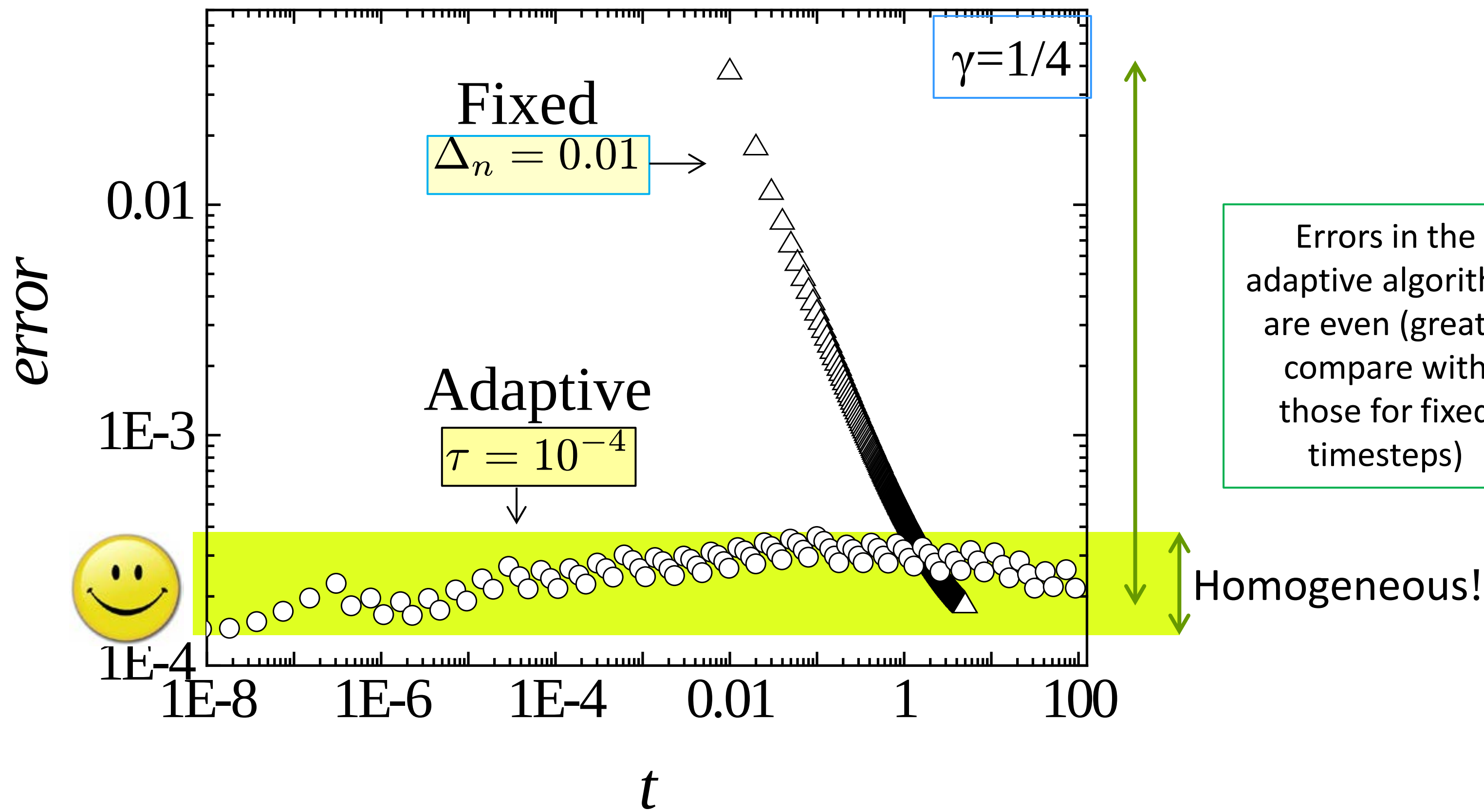
2. How are the numerical errors?

How are the errors?

Homogeneous!

$$\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} \qquad \text{BC: } u(x=0,t) = u(x=\pi,t) = 0$$

$$0 \le x \le \pi \qquad \text{IC: } u(x,0) = \sin x$$



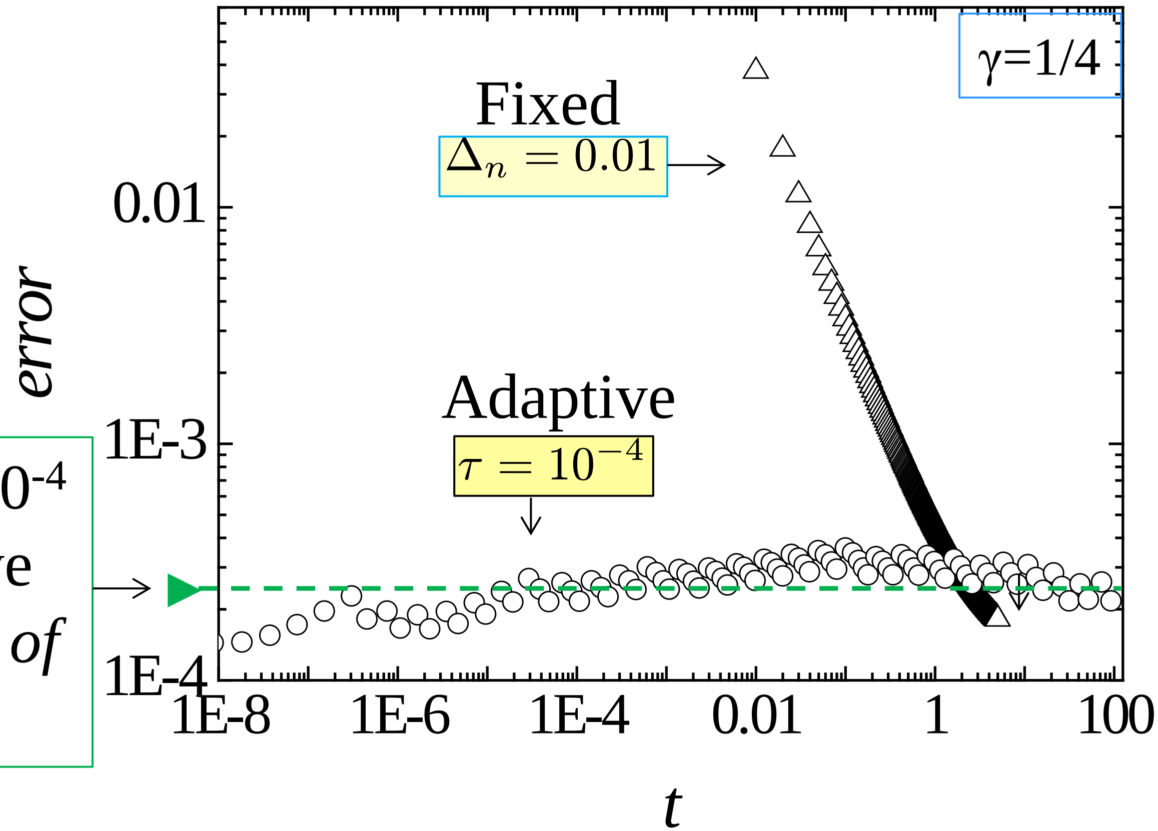
Errors in the adaptive algorithm are even (great!, compare with those for fixed timesteps)

Numerical errors at the mid-point of (i) the adaptive method with $\tau = 10^{-4}$ and $\Delta_0 = 0.01$ (circles), and (ii) the method with constant timesteps of size $\Delta_n = 0.01$ (triangles). In all cases $\gamma = 1/4$ and $\Delta x = \pi/20$.

How are the errors?

The *tolerance* is a convenient indicator of truncation error !

☞ Tolerance=10^{-4} and errors have the *same order of magnitude*



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5. A naïve way to improve the L1 adaptive method: let’s use a X discretization scheme of higher order than L1

   5.1 X=Cao-Xu(2013) [as expected]

   5.2 X=Gao-Sun-Zhang(2014) [surprise!]

6. Conclusions

A naïve way to improve the L1 adaptive method:
let's use a X discretization scheme of higher order than L1

Program of activities:

1) Select a discretization formula of order higher than L1
2) Generalize this formula to variable timesteps
3) Employ this formula to build finite difference schemes for the PDE
4) Is the numerical method stable?
5) Check the numerical method with some standard examples.

Program for the Cao-Xu (*) dicretization scheme of order $3+\gamma$:

1) Select a discretization formula of order higher than L1 ✓

2) Generalize this formula to variable timesteps ✓

3) Employ this formula to build finite difference schemes for the PDE ✓

4) Is the numerical method stable?

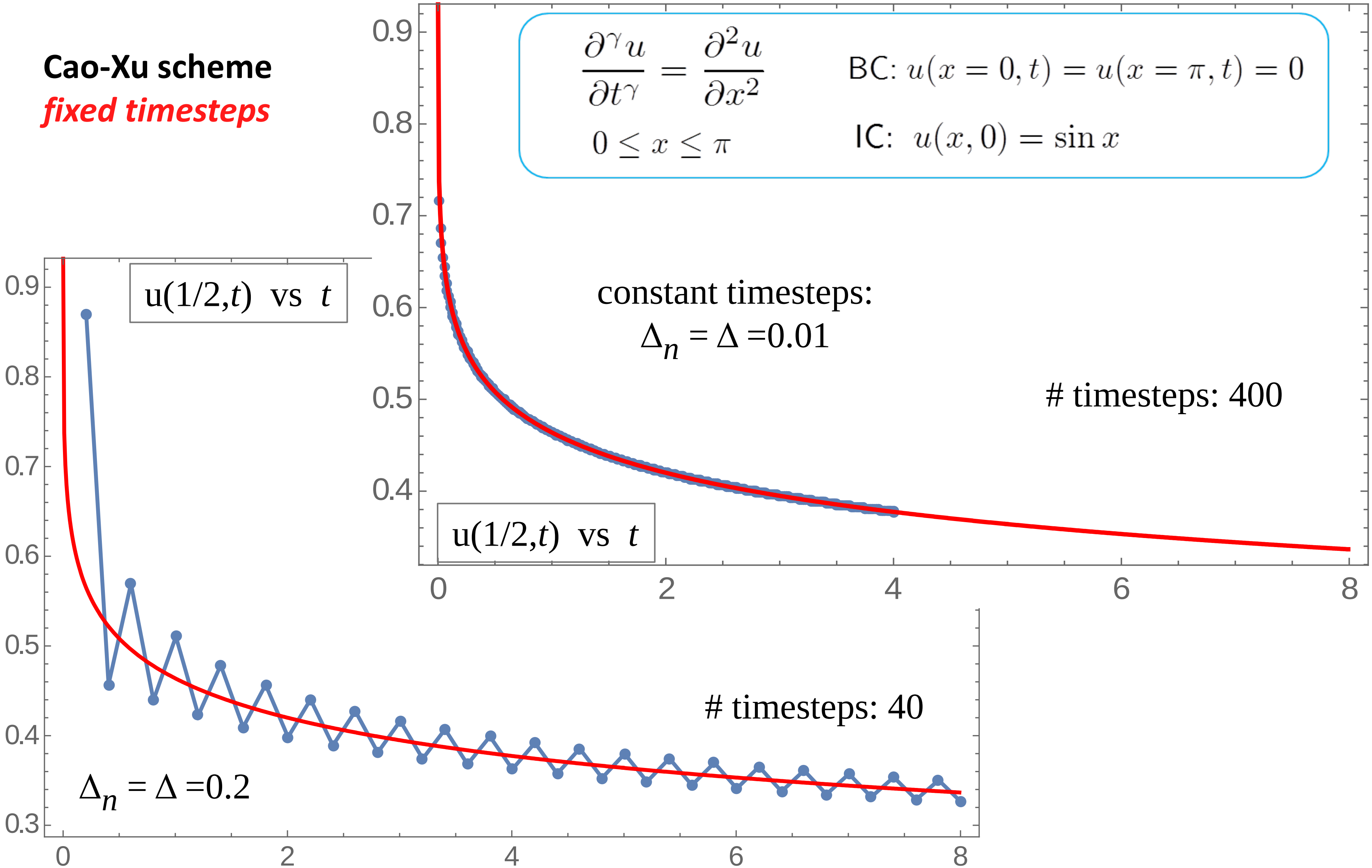
5) Check the numerical method with some standard examples.

4) The method with *fixed* timesteps of size Δ is *not* unconditionally stable (*) ⇔
For a given spatial discretization, the method becomes **unstable** for Δ large enough ⇨
one has to expect **difficulties** for the method with **variable** timesteps if Δ_n is large.

(*) Cao, J. & Xu, C. A high order schema for the numerical solution of the fractional ordinary differential equations. J. Comput. Phys. 238, 154–168 (2013).

Cao-Xu scheme

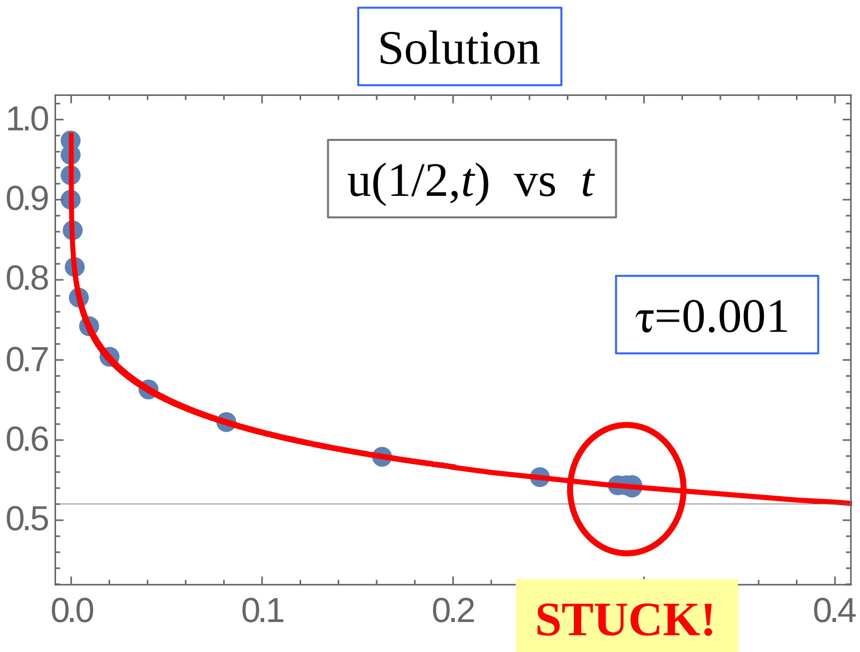
fixed timesteps

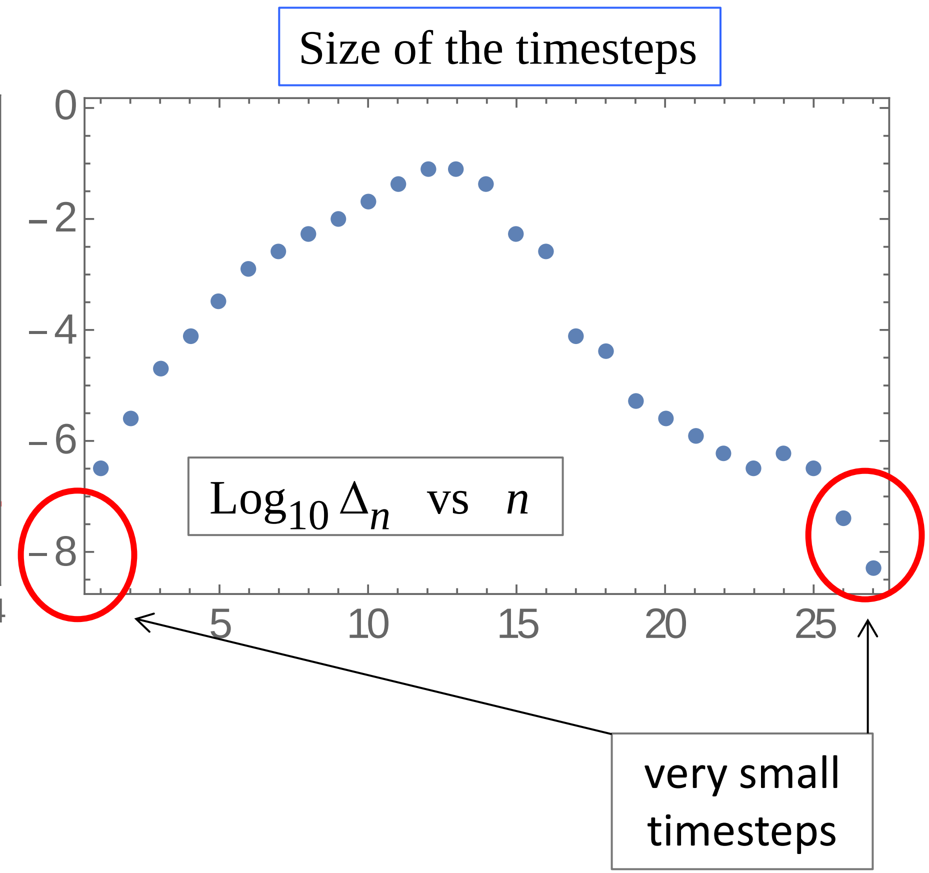


Cao-Xu scheme

Variable adaptative timesteps

How does the T&E algorithm deal with the onset of instability?





Program for the L1-2 dicretization scheme of order 3-γ by Gao-Sun-Zhang (*) :

1) Select a discretization formula of order higher than L1 ✓
2) Generalize this formula to variable timesteps ✓
3) Employ this formula to build finite difference schemes for the PDE ✓
4) Is the numerical method stable?
5) Check the numerical method with some standard examples.

4) The method with *fixed* timesteps of size Δ "is" ***unconditionally*** stable ⇔
For a given spatial discretization, the method "is" ***always stable* for arbitrarily large** Δ ⇨
One **does not expect difficulties** for the method with *variable timesteps* for any $\{\Delta_n\}$.

(*) Gao, G., Sun, Z. & Zhang, H. A new fractional numerical differentiation formula to approximate the Caputo fractional derivative and its applications. J. Comput. Phys. 259, 33–50 (2014).

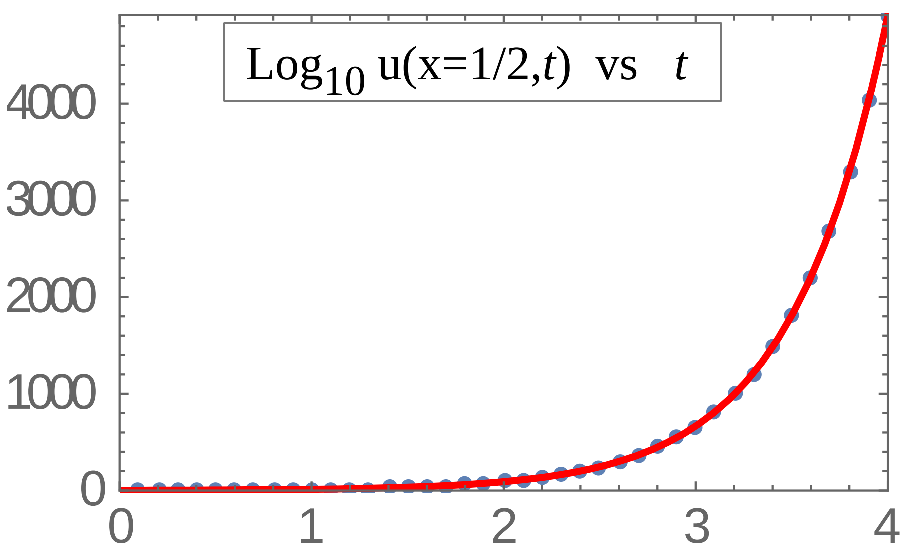
Check of

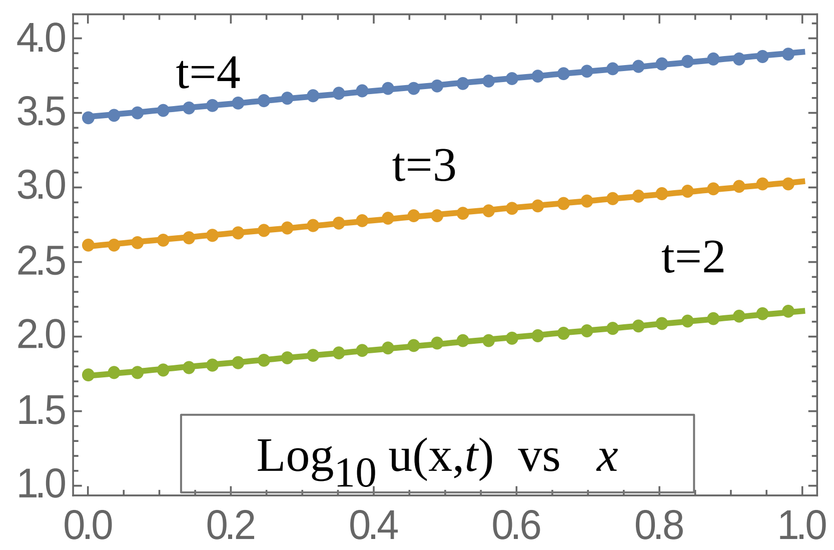
"The L1-2 method with *fixed* timesteps *is* *unconditionally* stable"

$$
\begin{aligned}
&{}_0^C\mathcal{D}_t^\alpha u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \quad x \in (0,1),\ t \in (0,T],\\
&u(0,t) = \phi(t), \qquad u(1,t) = \varphi(t), \quad t \in (0,T],\\
&u(x,0) = u^0(x), \quad x \in [0,1],
\end{aligned}
$$

$$
f(x,t) = \mathrm{e}^x[2t^{1-\alpha}E_{1,2-\alpha}(2t) - \mathrm{e}^{2t}],\ \phi(t) = \mathrm{e}^{2t},\ \varphi(t) = \mathrm{e}^{1+2t},\ u^0(x) = \mathrm{e}^x
$$

Case: $\gamma=\alpha=1/2$, $\mathbf{\Delta_n = 0.1}$, $\Delta x=1/200$





Check of

“The L1-2 method with *fixed* timesteps is *unconditionally* stable”

$$
{}_0^C\mathcal{D}_t^{\alpha} u(x,t) = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \quad x \in (0,1),\ t \in (0,T],
$$
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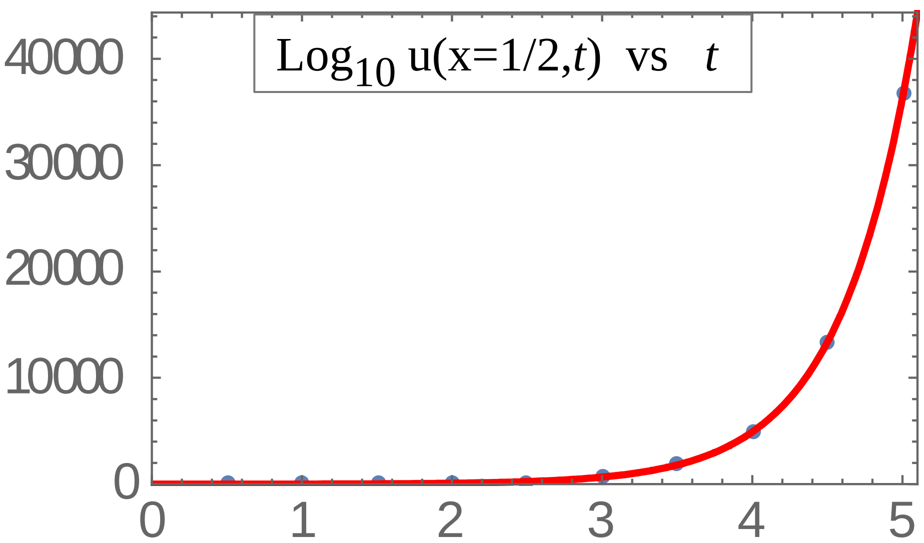
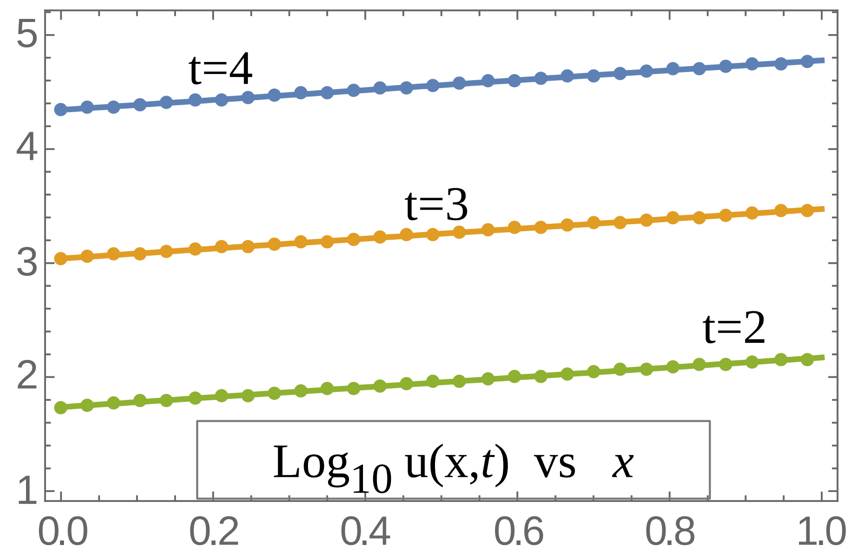
u(0,t) = \phi(t), \qquad u(1,t) = \varphi(t), \quad t \in (0,T],
$$
$$
u(x,0) = u^0(x), \quad x \in [0,1],
$$
$$
f(x,t) = e^x[2t^{1-\alpha} E_{1,2-\alpha}(2t) - e^{2t}],\ \phi(t) = e^{2t},\ \varphi(t) = e^{1+2t},\ u^0(x) = e^x
$$

Case: $\gamma=\alpha=1/2$, $\mathbf{\Delta_n = 0.5}$, $\Delta x=1/200$





L1-2
fixed timesteps

$$\boxed{\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} + f(x,t)} \qquad 0 \,\square\, x \,\square\, \pi$$

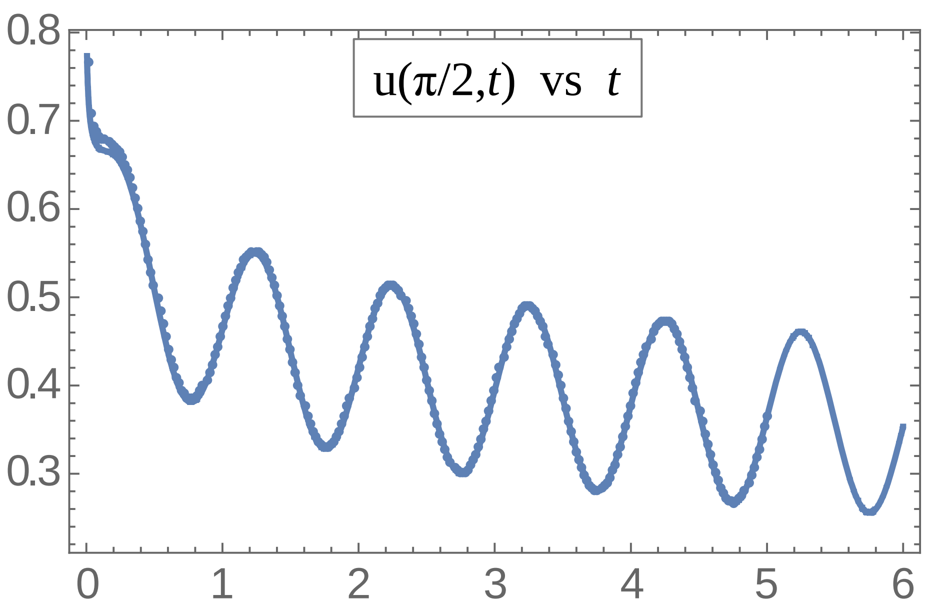
$$f(x,t) = a\left[\sin(\nu t) + \nu^\gamma \sin\left(\nu t + \gamma\pi/2\right)\right]\sin x$$

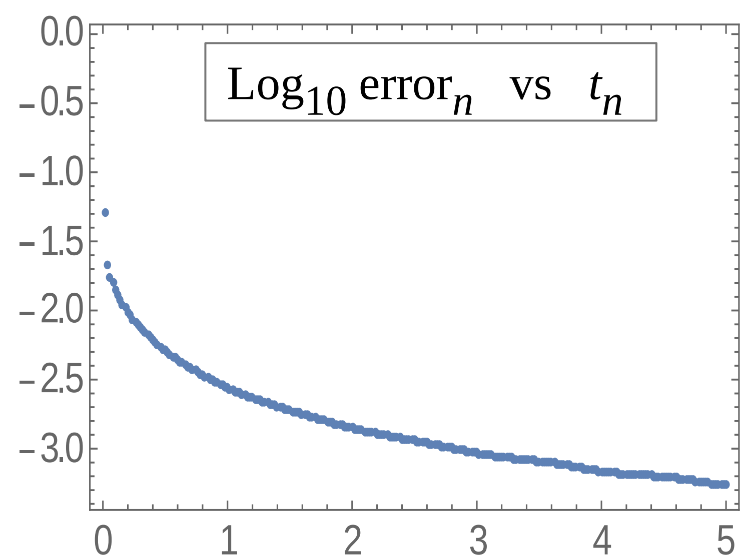
$$u(x=0,t) = u(x=\pi,t) = 0$$

$$u(x,0) = \sin x$$

Stable

Case: $\gamma=1/4$, $\boldsymbol{\Delta_n = 0.02}$, $\Delta x=1/200$, $a=1/10$, $\omega=2\pi$





L1-2
fixed timesteps

$$\boxed{\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} + f(x,t)} \qquad 0 \le x \le \pi$$

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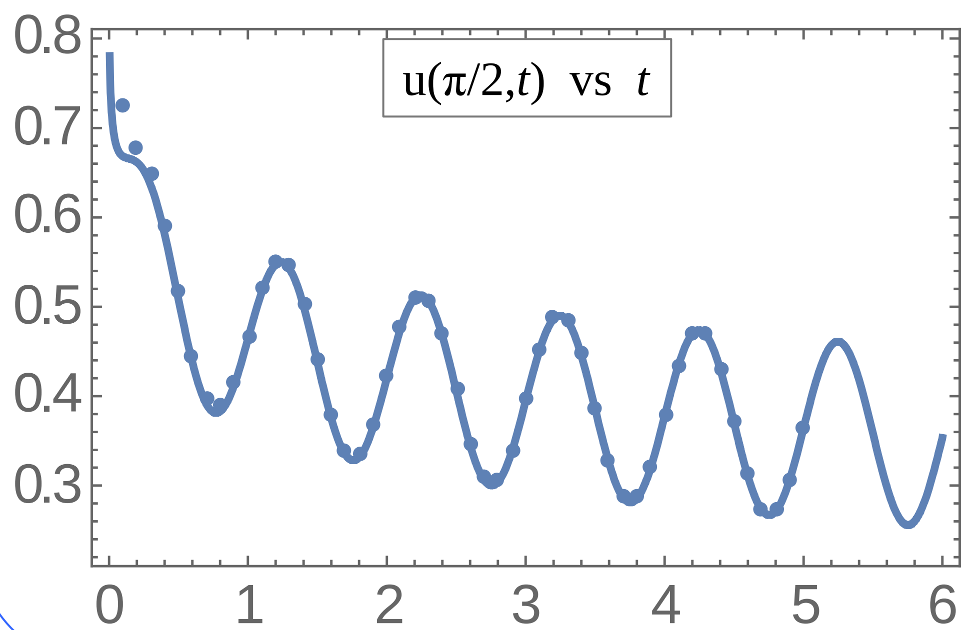
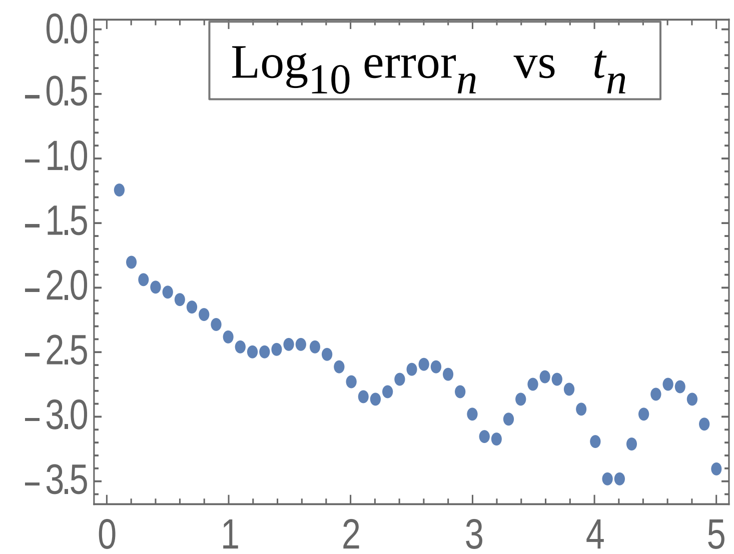
Stable

Case: γ=1/4, $\mathbf{\Delta_n = 0.1}$, Δx=1/200, a=1/10, ω=2π





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fixed timesteps

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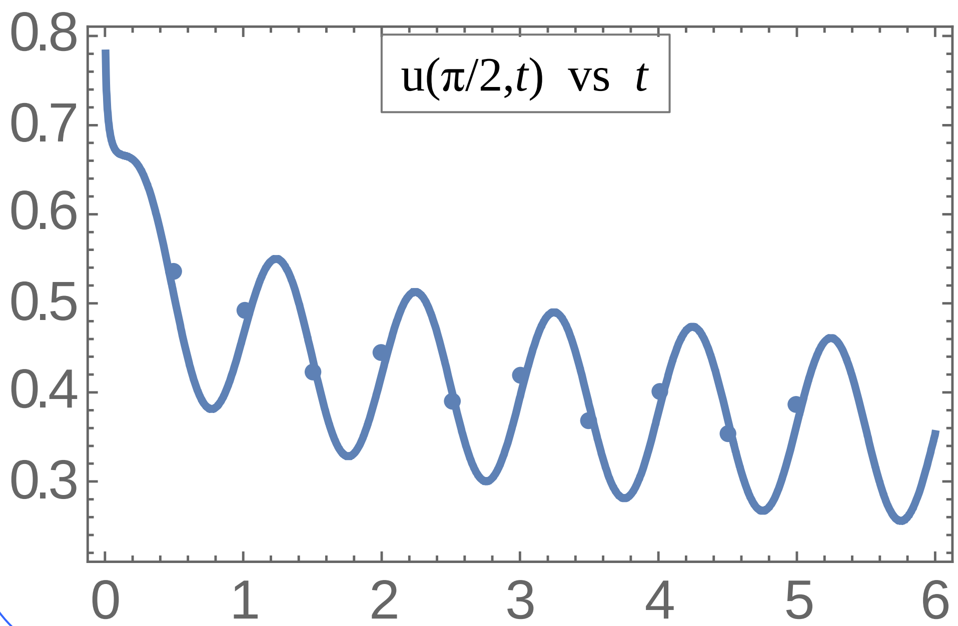
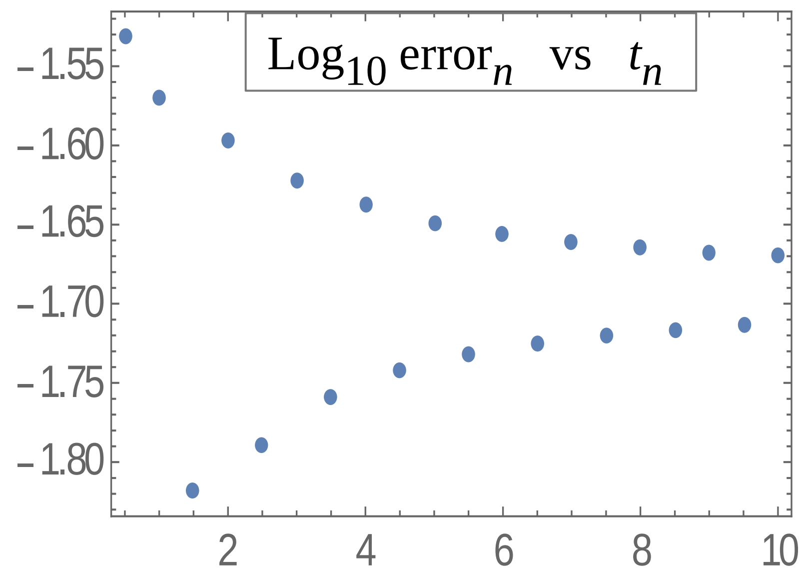
Stable

Case: $\gamma=1/4$, $\boldsymbol{\Delta_n = 0.5}$, $\Delta x=1/200$, $a=1/10$, $\omega=2\pi$





L1-2
variable timesteps

$$\boxed{\frac{\partial^\gamma u}{\partial t^\gamma} = \frac{\partial^2 u}{\partial x^2} + f(x,t)} \qquad 0 \le x \le \pi$$

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$$u(x=0,t) = u(x=\pi,t) = 0$$

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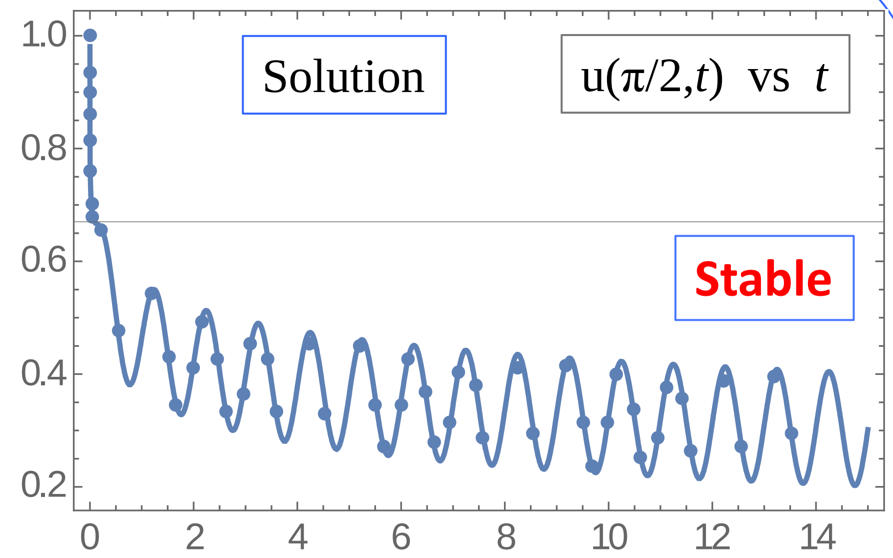
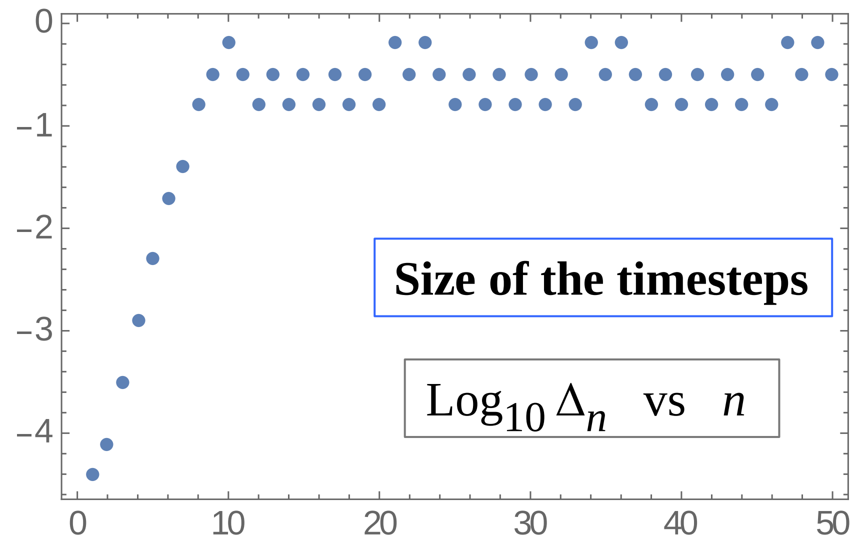
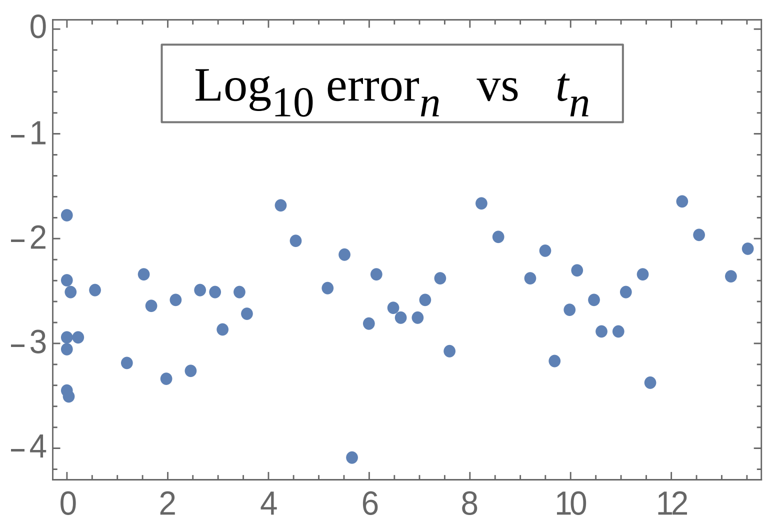
Case: $\gamma=1/4$, **τ= 0.01,**
$\Delta x=1/200$, $a=1/10$, $\omega=2\pi$







L1-2
variable timesteps

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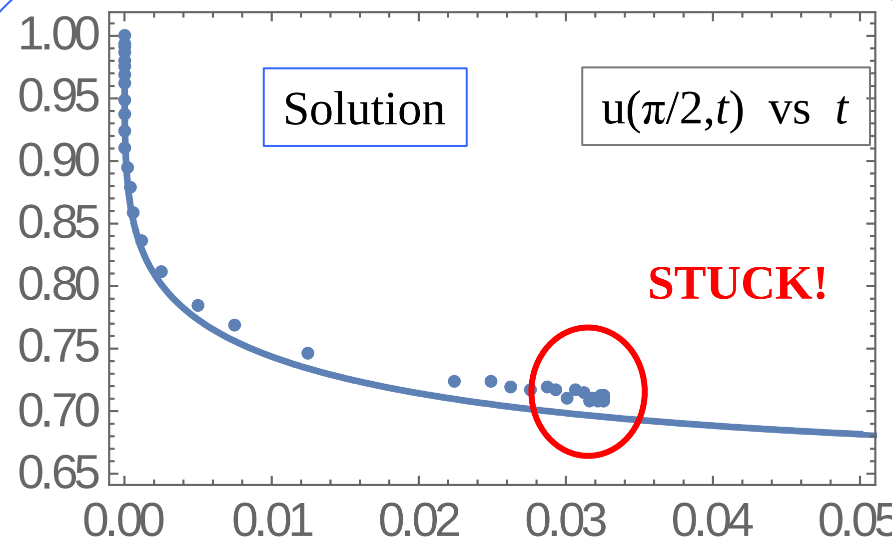
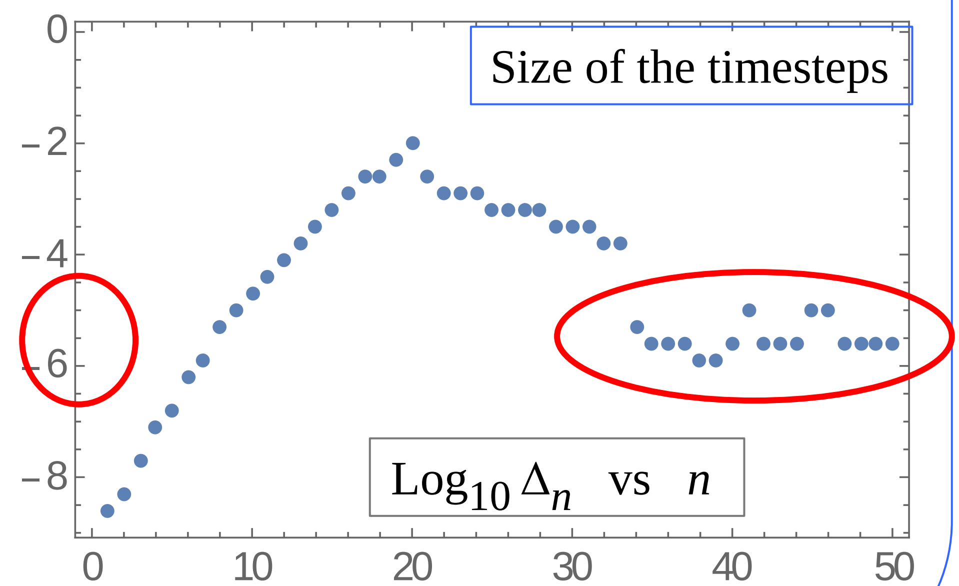
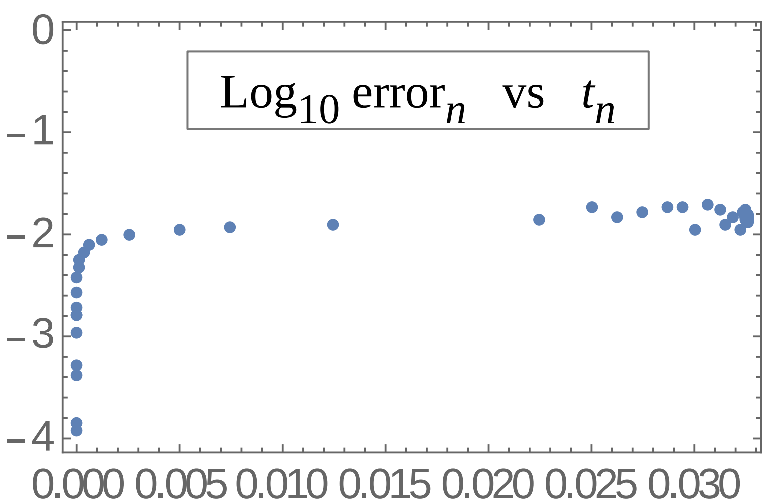
Case: $\gamma=1/4$, **τ= 0.001**, $\Delta x=1/200$, $a=1/10$, $\omega=2\pi$

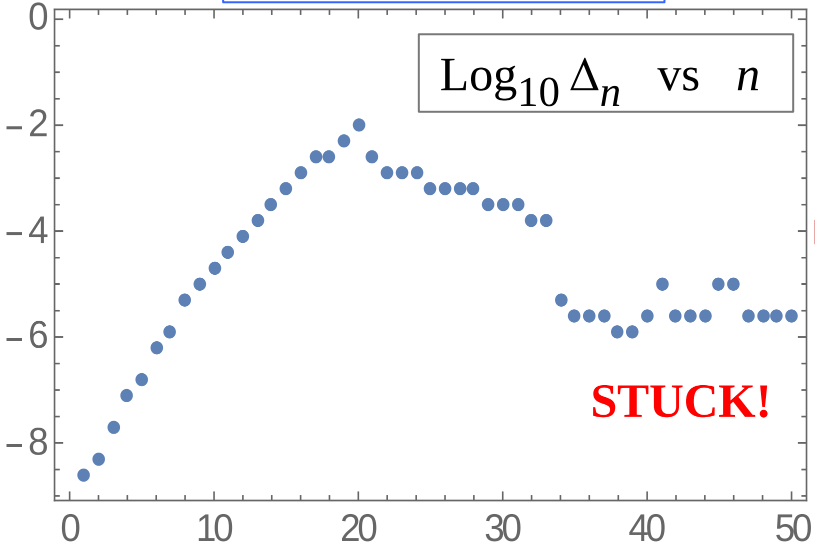




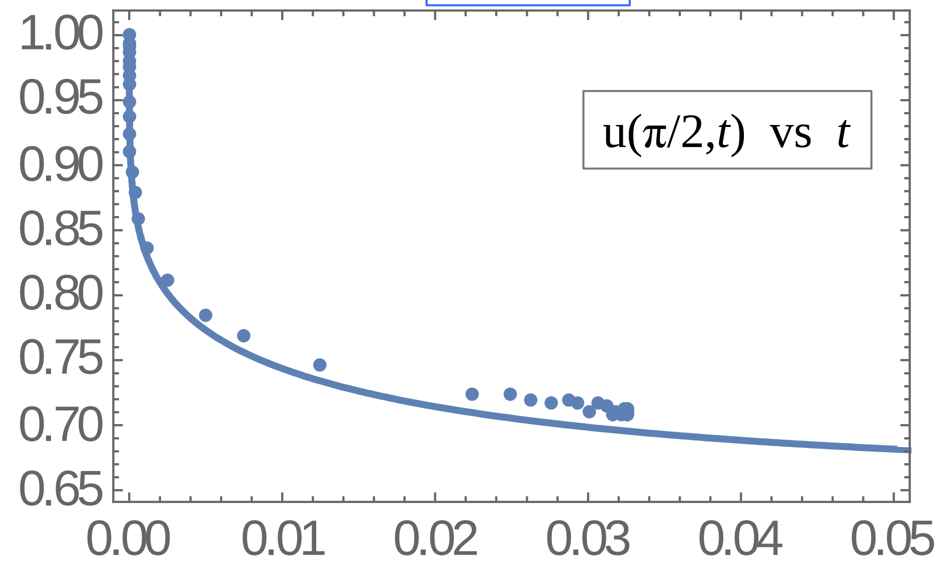


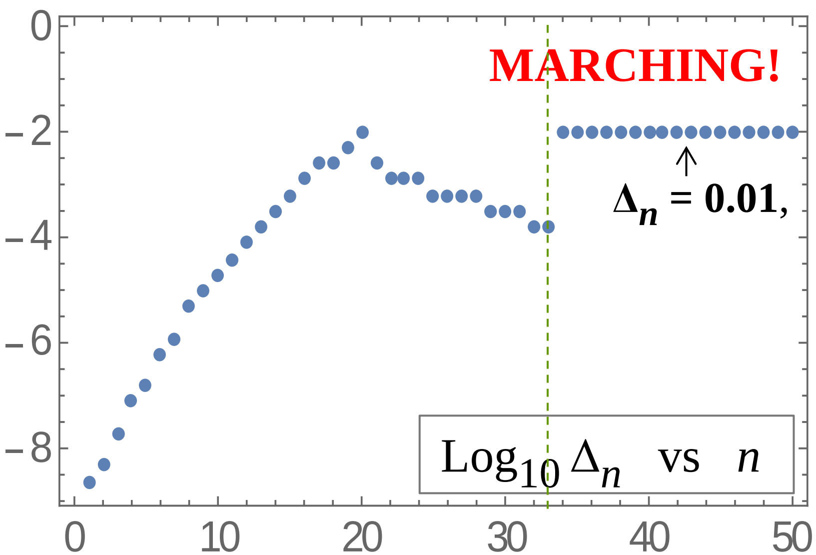
L1-2

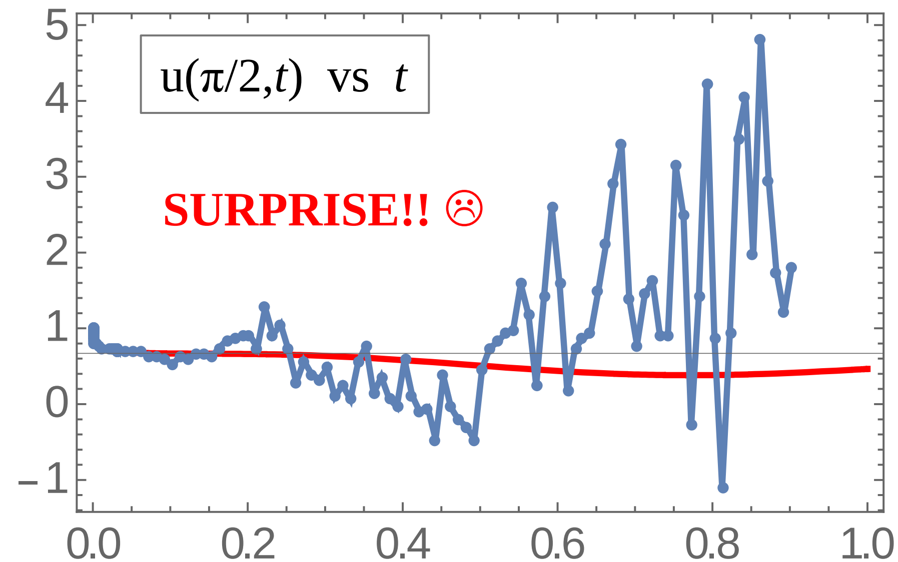
Size of the timesteps



Solution



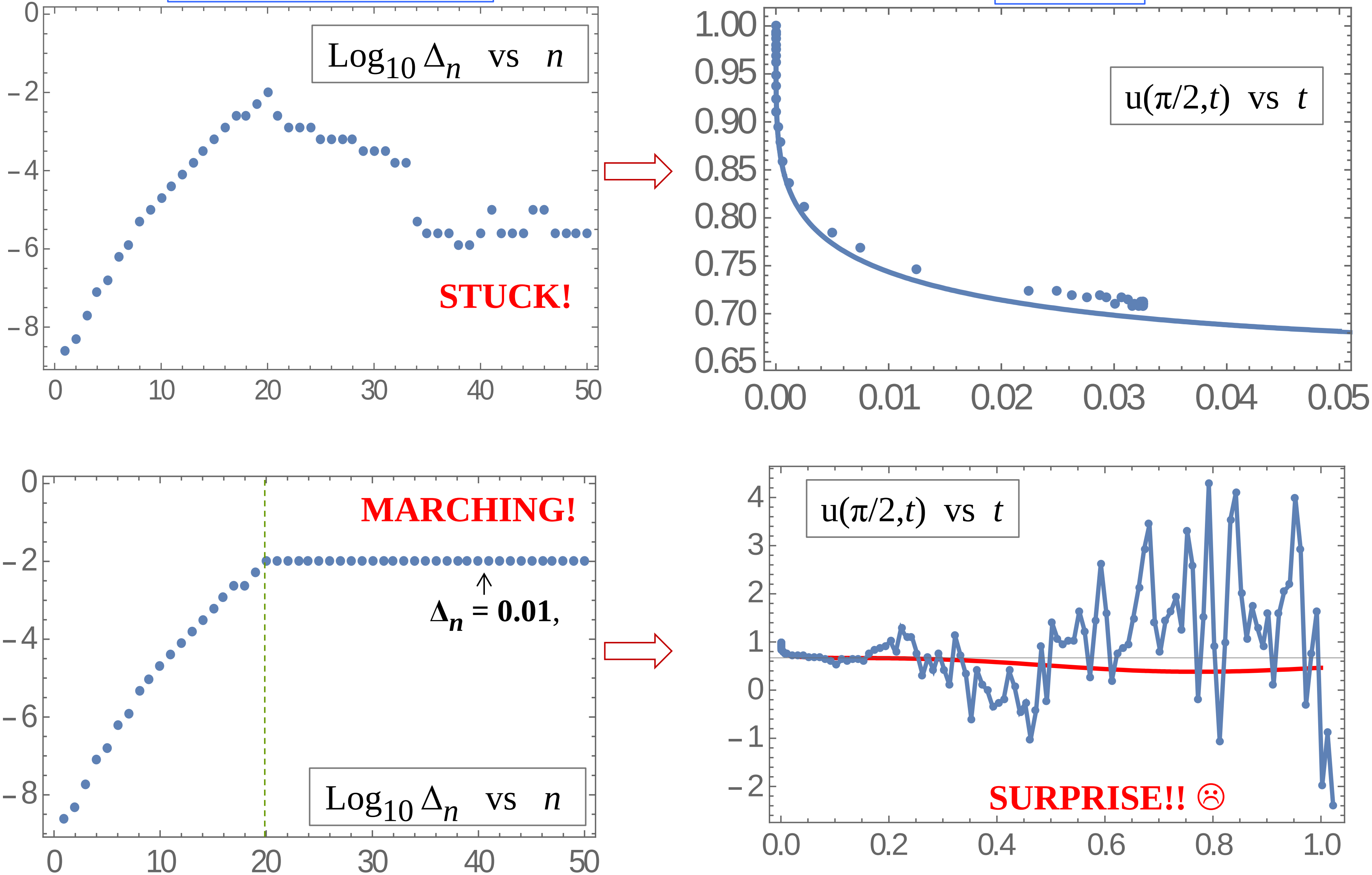




L1-2

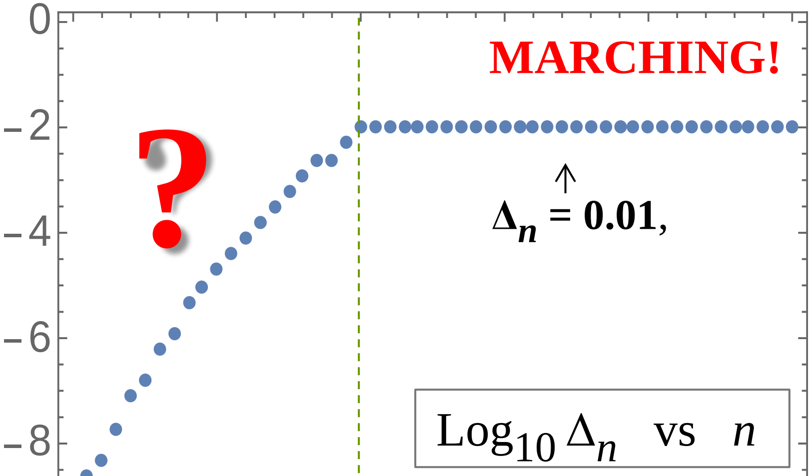
Size of the timesteps

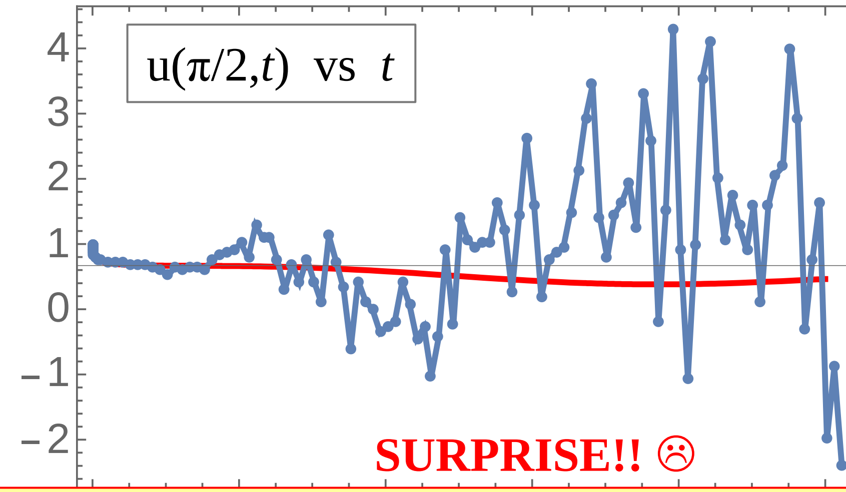
Solution



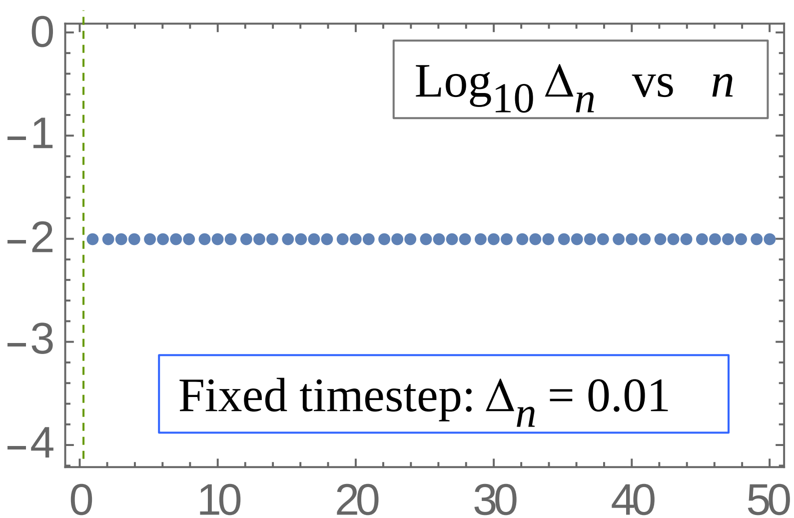
Size of the timesteps

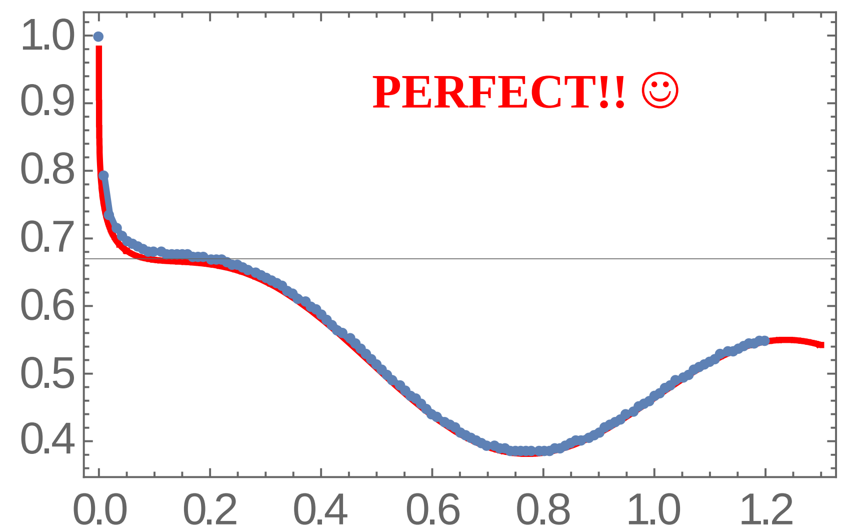
Solution





Large fixed timesteps can lead to better solutions than smaller variable timesteps!





Conclusions

- L1 adaptive method : excellent in many cases → fast and accurate ☺

- L1 method with variable timesteps is unconditionally stable ☺

- *Large fixed timesteps can lead to better solutions than* smaller *variable timesteps!* ☹

- *High-order methods developed for fixed timesteps should be use with care when variable timesteps are employed* ☹

Take away idea

To build higher order* adaptive *methods is harder than one may think

Numerical methods for fractional operators involved in anomalous polarization processes

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INdAM GNCS Project 2015

Workshop on Fractional Calculus and its Applications
Roma Tre, March 11, 2015

Outline

1. Introduction and motivations
2. Havriliak–Negami: a general overview
3. New formalization (of GL type) for Havriliak–Negami operators
   - Continuous operators
   - Discretized operators
4. Numerical experiments and Matlab codes

Havriliak-Negami models

Maxwell's equations:

$$\begin{cases} \nabla \times \mathbf{H} = \epsilon_0 \dfrac{\partial}{\partial t}\mathbf{E} + \dfrac{\partial}{\partial t}\mathbf{P} & \text{Ampere's law} \\ \nabla \times \mathbf{E} = -\mu_0 \dfrac{\partial \mathbf{H}}{\partial t} & \text{Faraday's law} \end{cases}$$

E: electric field **H**: magnetic field

Real-world applications: antenna design, nano–optical storage devices, medical diagnosis (MRI), cancer therapy, ...

Description of polarization (in the frequency domain)

$$\hat{\mathbf{P}} = \hat{\mathcal{X}}(\omega)\hat{\mathbf{E}}$$

$\hat{\mathcal{X}}(\omega)$: dielectric response

Determined from experimental data on the basis of some suitable model !

What model for the dielectric response ?

Relaxation properties: return to equilibrium after an external force

In the frequeny domain (Fourier or Laplace transform):

$$Y(s) = G(s)F(s)$$

$F(s)$: external stimulation $\qquad$ $Y(s)$: output of the system
$G(s)$: Susceptibility ($s = i\omega$) or Transfer function ($s \in \mathbb{C}$)

In the time domain (integral or differential operators)

$$y(t) = \int_0^t g(t-u)f(u)\,du$$

Relaxation function $g(t)$ is the (Fourier or Laplace) inverse of $G(s)$

$g(t)$ difficult or no differential operators: problem for numerical simulation !

A simple model: the Debye relaxation

$$G(s) = \frac{1}{s+\lambda} \qquad \frac{1}{\lambda} > 0 \quad \text{relaxation time}$$

From frequency–domain to time–domain

	Frequency	Time
Relaxation func.	$G(s) = \dfrac{1}{s+\lambda}$	$g(t) = e^{-\lambda t}$
Integral eq.	$Y(s) = G(s)F(s)$	$y(t) = \int_0^t e^{-\lambda(t-u)} f(u)\, du$
ODE	$\left[G(s)\right]^{-1} Y(s) = F(s)$	$y'(t) + \lambda y(t) = f(t)$

No memory in Debye relaxation: uncommon in practice!

Introducing memory preservation

$$\text{Debye}: \quad \frac{1}{s+\lambda} \qquad e^{-\lambda t}$$

$$\text{Cole-Cole}: \quad \frac{1}{s^{\alpha}+\lambda} \qquad t^{\alpha-1}E_{\alpha,\alpha}(-t^{\alpha}\lambda)$$

$$\text{Havriliak–Negami}: \quad \frac{1}{(s^{\alpha}+\lambda)^{\gamma}} \qquad t^{\alpha\gamma-1}E^{\gamma}_{\alpha,\alpha\gamma}(-t^{\alpha}\lambda)$$

Other models: Cole–Davidson, Excess wing (Hilfer and Nigmatullin et al.), ecc.

$$E_{\alpha\,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k+\beta)} \qquad E^{\gamma}_{\alpha,\beta}(z) = \frac{1}{\Gamma(\gamma)} \sum_{k=0}^{\infty} \frac{\Gamma(\gamma+k)z^k}{k!\Gamma(\alpha k+\beta)}$$

$$0 < \alpha < 1, \quad 0 < \gamma < \frac{1}{\alpha}$$

E.Capelas, F.Mainardi and J.Vaz "Models based on ML functions for anomalous relaxation in dielectrics". In: *Eur. Phys. J. ST* 193 (2013)

F.Mainardi and R.Garrappa "On complete monotonicity of the Prabhakar function and non–Deby relaxation in dielectrics". In: *J. Comput. Phys.* (2014)

Differential operators in the time domain

$$\text{Debye}: \quad \frac{1}{s+\lambda} \qquad \big(D_t + \lambda\big) y(t) = f(t)$$

$$\text{Cole-Cole}: \quad \frac{1}{s^{\alpha}+\lambda} \qquad \big({}_0D_t^{\alpha} + \lambda\big) y(t) = f(t)$$

$$\text{Havriliak–Negami}: \quad \frac{1}{(s^{\alpha}+\lambda)^{\gamma}} \qquad \big({}_0D_t^{\alpha} + \lambda\big)^{\gamma} y(t) = f(t) \quad ???$$

A Pseudo Fractional Differential operator

Differential operators in the time domain

$$\text{Debye}: \quad \frac{1}{s+\lambda} \qquad \big(D_t + \lambda\big) y(t) = f(t)$$

$$\text{Cole-Cole}: \quad \frac{1}{s^{\alpha}+\lambda} \qquad \big({}_0D_t^{\alpha} + \lambda\big) y(t) = f(t)$$

$$\text{Havriliak–Negami}: \quad \frac{1}{(s^{\alpha}+\lambda)^{\gamma}} \qquad \big({}_0D_t^{\alpha} + \lambda\big)^{\gamma} y(t) = f(t) \quad ???$$

$$\big({}_0D_t^{\alpha} + \lambda\big)^{\gamma} = \exp\left(-\frac{\lambda t}{\alpha}\, {}_0D_t^{1-\alpha}\right) \cdot {}_0D_t^{\alpha\gamma} \cdot \exp\left(\frac{\lambda t}{\alpha}\, {}_0D_t^{1-\alpha}\right) \qquad ^{a}$$

Useful for theoretical investigations

[a] R.R.Nigmatullin and Y.E.Ryabov "Cole–Davidson dielectric relaxation as a self–similar relaxation process". In: *Physics of the Solid State* 39.1 (1997)

Differential operators in the time domain

$$\text{Debye}: \quad \frac{1}{s+\lambda} \qquad \big(D_t + \lambda\big) y(t) = f(t)$$

$$\text{Cole-Cole}: \quad \frac{1}{s^{\alpha}+\lambda} \qquad \big({}_0D_t^{\alpha} + \lambda\big) y(t) = f(t)$$

$$\text{Havriliak–Negami}: \quad \frac{1}{(s^{\alpha}+\lambda)^{\gamma}} \qquad \big({}_0D_t^{\alpha} + \lambda\big)^{\gamma} y(t) = f(t) \quad ???$$

$$\big({}_0D_t^{\alpha} + \lambda\big)^{\gamma} = \sum_{k=0}^{\infty} \binom{\gamma}{k} \lambda^k {}_0D_t^{\alpha(\gamma-k)}$$ [a] [b]

No satisfactory for error control

[a] V.Novikov et al. "Anomalous relaxation in dielectrics. Equations with fractional derivatives". In: *Mater. Sci. Poland* 23.4 (2005)

[b] P.Bia et al. "A novel FDTD formulation based on fractional derivatives for dispersive Havriliak–Negami media". In: *Signal Processing*, 107 (2015) 312–318

An operator for Havriliak–Negami models

$$Y(s) = \frac{1}{\big(s^\alpha + \lambda\big)^\gamma} F(s) \qquad \Longleftrightarrow \qquad y(t) = \int_0^t e^{\gamma}_{\alpha,\alpha\gamma}(\tau; -\lambda) f(t-\tau)\, d\tau$$

In terms of a suitable operator:

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} f(t)$$

$$\mathbf{E}^{\gamma}_{\alpha,\beta,\omega,a+} f(t) = \int_a^t e^{\gamma}_{\alpha,\beta}(\tau;\omega) f(t-\tau)\, d\tau \qquad e^{\gamma}_{\alpha,\beta}(t;\omega) = t^{\beta-1} E^{\gamma}_{\alpha,\beta}(t^\alpha \omega)$$

Studied in :

1. Prabhakar [Yokohama Math. J., 1971]
2. Kilbas, Saigo & Saxena [Integr. Transf. Spec. Funct., 2004]
3. Garra, Gorenflo, Polito & Tomovski [Appl. Math. Comput., 2014]

An operator for Havriliak–Negami models

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} f(t)$$

Some properties:

- Bounded operator
- Composition with functions and operators of fractional calculus
- Left-inversion (derivative)

$$f(t) = \mathbf{D}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} y(t) = \frac{d^m}{dt^m} \mathbf{E}^{-\gamma}_{\alpha,m-\alpha\gamma,-\lambda,0+} y(t), \quad m = \lceil \alpha\gamma \rceil$$

- Caputo-type derivative for Havriliak–Negami models

$$\begin{aligned} {}^{C}\mathbf{D}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} y(t) &= \mathbf{E}^{-\gamma}_{\alpha,m-\alpha\gamma,-\lambda,0+} \frac{d^m}{dt^m} y(t) \\ &= \mathbf{D}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} \left(y(t) - \sum_{k=0}^{m-1} \frac{t^k}{k!}\, y^{(k)}(0^+) \right) \end{aligned}$$

R.Garra, R.Gorenflo, F.Polito and Z.Tomovski "Hilfer-Prabhakar derivatives and some applications". In: *Appl. Math. Comput.* 242 (2014)

Havriliak–Negami operator of Grünwald–Letnikov type

$$\mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} f(t) = \lim_{h\to 0} \sum_{k=0}^{\infty} W_k^{(\gamma)} f(t-kh)$$

$$W_k^{(\gamma)} \equiv W_k^{(\gamma)}(\alpha,\lambda,h)$$

Riemann–Liouville operators

$$\begin{array}{llll} \gamma=1 \quad \lambda=0 & \mathbf{E}^{1}_{\alpha,\alpha,0,0+} = \frac{t^{\alpha-1}}{\Gamma(\alpha)} * = J_0^{\alpha} & \text{(RL integral)} \\ \gamma=-1 \quad \lambda=0 & \mathbf{E}^{-1}_{\alpha,-\alpha,0,0+} = \frac{t^{-\alpha-1}}{\Gamma(-\alpha)} * = D_0^{\alpha} & \text{(RL derivative)} \end{array}$$

Consistence with traditional Grünwald–Letnikov operators ($\gamma = \pm 1$ and $\lambda = 0$)

$$\begin{array}{ll} \text{GL integral :} & W_k^{(1)} = h^{\alpha} \omega_k^{(-\alpha)} \\ \text{GL derivative :} & W_k^{(-1)} = \dfrac{1}{h^{\alpha}} \omega_k^{(\alpha)} \end{array} \qquad \omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k}$$

Havriliak–Negami operator of Grünwald–Letnikov type

$$\mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} f(t) = \lim_{h\to 0} \sum_{k=0}^{\infty} W_k^{(\gamma)} f(t-kh)$$

$$\begin{cases} W_k^{(\gamma)} = \dfrac{h^{\alpha\gamma}}{(1+h^{\alpha}\lambda)^{\gamma}} w_k^{(\gamma)} \\ w_0^{(\gamma)} = 1, \quad w_k^{(\gamma)} = \displaystyle\sum_{j=1}^{k} \left(\frac{(1-\gamma)j}{k} - 1 \right) \frac{\omega_j^{(\alpha)}}{1+h^{\alpha}\lambda} w_{k-j}^{(\gamma)} \end{cases}$$

$\omega_j^{(\alpha)}$: coefficients of standard Grünwald–Letnikov operators

Consistence with standard GL operators

$\gamma = +1$	$\lambda = 0$	$W_k^{(1)} = h^{\alpha}\omega_k^{(-\alpha)}$	GL integral
$\gamma = -1$	$\lambda = 0$	$W_k^{(-1)} = \dfrac{1}{h^{\alpha}}\omega_k^{(\alpha)}$	GL derivative

Why these coefficients $W_k^{(\gamma)}$?

Discretization of convolution integrals

$$y(t_n) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} f(t) = \int_0^{t_n} e^{\gamma}_{\alpha,\alpha\gamma}(\tau;-\lambda) f(t_n-\tau)\,d\tau \qquad \text{Convol. integral}$$

$$y_n = \sum_{k=0}^{n} W_k^{(\gamma)} f(t_n - kh) \qquad \text{Convol. quadrature}$$

$$\text{Convergence : } \lim_{h\to 0} \sum_{k=0}^{\infty} W_k^{(\gamma)} f(t_n-kh) = \int_0^{t_n} e^{\gamma}_{\alpha,\alpha\gamma}(\tau;-\lambda) f(t_n-\tau)\,d\tau$$

How to compute weights $W_k^{(\gamma)}$ (kernel $e^{\gamma}_{\alpha,\alpha\gamma}(t;-\lambda)$ difficult) ?

Convolution quadratures by Lubich [Lubich, 1988]

- Use only the LT $\dfrac{1}{\left(s^\alpha+\lambda\right)^\gamma}$ and not $e^{\gamma}_{\alpha,\alpha\gamma}(t;-\lambda)$
- Based on classical linear multistep methods for ODEs

Lubich's convolution quadratures

Consider a k-step linear multistep method for ODEs

$$\alpha_0 y_n + \alpha_1 y_{n-1} + \cdots + \alpha_k y_{n-k} = h\left(\beta_0 f_n + \beta_1 f_{n-1} + \cdots + \beta_k f_{n-k}\right)$$

Characteristic polynomials:

- $\rho(\xi) = \alpha_0 + \alpha_1 \xi + \cdots + \alpha_k \xi^k$
- $\sigma(\xi) = \beta_0 + \beta_1 \xi + \cdots + \beta_k \xi^k$

Generating function: $\Delta(\xi) = \dfrac{\rho(1/\xi)}{\sigma(1/\xi)}$

$$\sum_{n=0}^{\infty} W_n^{(\gamma)} \xi^n = G\left(\frac{\Delta(\xi)}{h}\right) = \frac{1}{\left(\left(\frac{\Delta(\xi)}{h}\right)^{\alpha} + \lambda\right)^{\gamma}}$$

Theorem ([Lubich, 1988])

Let $\Delta(\xi)$ be the generating function of a linear multistep method of order p. Then

$$\left|y(t_n) - y_n\right| \leq C t_n^{\alpha\gamma - 1} h^p$$

Grünwald–Letnikov scheme

Implicit Euler method: $$y_n = y_{n-1} + hf(t_n, y_n)$$

Generating function: $$\Delta(\xi) = \frac{\rho(1/\xi)}{\sigma(1/\xi)} = 1 - \xi$$

Application to RL fractional integrals $G(s) = 1/s^{\alpha}$

$$G\left(\frac{\Delta(\xi)}{h}\right) = \frac{h^{\alpha}}{\left(1-\xi\right)^{\alpha}} = h^{\alpha}\sum_{n=0}^{\infty} \omega_n^{(-\alpha)} \xi^n$$

Grünwald–Letnikov integral: $${}_0J_t^{\alpha} y(t_n) \approx h^{\alpha} \sum_{k=0}^{n} \omega_k^{(-\alpha)} y(t_n - kh)$$

Grünwald–Letnikov derivative: $${}_0D_t^{\alpha} y(t_n) \approx \frac{1}{h^{\alpha}} \sum_{k=0}^{n} \omega_k^{(\alpha)} y(t_n - kh)$$

Grünwald–Letnikov scheme for Havriliak–Negami

Generating function: $$\Delta(\xi) = \frac{\rho(1/\xi)}{\sigma(1/\xi)} = 1 - \xi$$

$$G(s) = \frac{1}{s^\alpha} \quad \longleftrightarrow \quad G(s) = \frac{1}{\big(s^\alpha + \lambda\big)^\gamma}$$

Grünwald–Letnikov scheme for the Havriliak-Negami operator

$$G\left(\frac{\Delta(\xi)}{h}\right) = \frac{h^{\alpha\gamma}}{\big((1-\xi)^\alpha + h^\alpha\lambda\big)^\gamma} = \sum_{n=0}^{\infty} W_n^{(\gamma)} \xi^n$$

How to compute W_n ?

Evaluation of convolution weights

Miller's Formula: power $\beta \in \mathbb{C}$ of a Formal Power Series

$$\left(1 + a_1\xi + a_2\xi^2 + a_3\xi^3 + \dots\right)^\beta = v_0^{(\beta)} + v_1^{(\beta)}\xi + v_2^{(\beta)}\xi^2 + v_3^{(\beta)}\xi^3 + \dots$$

where coefficients $v_n^{(\beta)}$ are recursively evaluated as

$$v_0^{(\beta)} = 1, \quad v_n^{(\beta)} = \sum_{j=1}^{n} \left(\frac{(\beta+1)j}{n} - 1 \right) a_j v_{n-j}^{(\beta)}.$$

Application to $\dfrac{h^{\alpha\gamma}}{\left((1-\xi)^\alpha + h^\alpha\lambda\right)^\gamma}$

1. Miller's formula for $(1-\xi)^\alpha$
2. Add $h^\alpha\lambda$ to the first weight
3. Miller's formula for power $-\gamma$ of the resulting series

Computational cost: $N^2 + 3N$
Explicit recursive relationship

Grünwald–Letnikov operators for Havrialiak–Negami

Integral operator

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} f(t) = \lim_{h\to 0} \sum_{k=0}^{\infty} W_k^{(\gamma)} f(t-kh)$$

First order approx. $$y(t_n) = \sum_{k=0}^{n} W_k^{(\gamma)} f(t_n - kh)$$

Differential operator

$$\mathbf{D}^{-\gamma}_{\alpha,m-\alpha\gamma,-\lambda,0+} y(t) = \lim_{h\to 0} \sum_{k=0}^{\infty} W_k^{(-\gamma)} y(t-kh) = f(t)$$

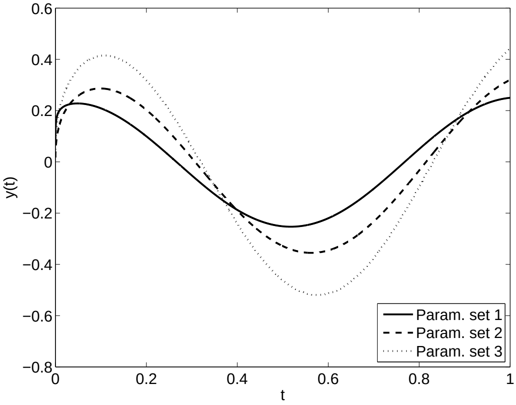
First order approx. $$\sum_{k=0}^{n} W_k^{(-\gamma)} y(t_n - kh) = f(t_n)$$

$\gamma \to 1$, $\lambda \to 0$: classic Grünwald–Letnikov operators and schemes

Numerical experiments

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} \cos(2\pi t), \quad t \in [0,1]$$

	α	γ	λ
Set 1	0.3	0.8	4.0
Set 2	0.6	0.7	4.0
Set 3	0.9	0.4	4.0



Numerical experiments

Errors and EOC for the test problem

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+} \cos(2\pi t), \quad t \in [0,1]$$

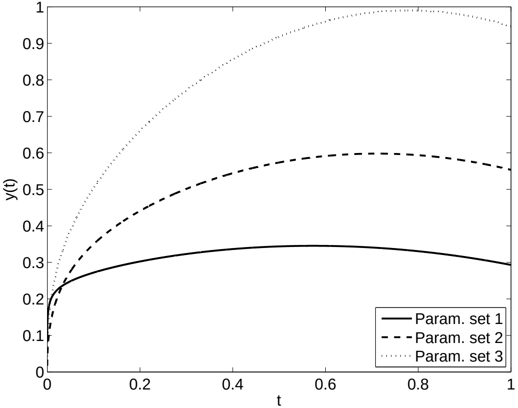
h	Param. set 1 Error	Param. set 1 EOC	Param. set 2 Error	Param. set 2 EOC	Param. set 3 Error	Param. set 3 EOC
2^{-4}	2.63(−4)		2.94(−3)		1.49(−2)	
2^{-5}	1.73(−4)	0.601	1.34(−3)	1.133	7.45(−3)	0.998
2^{-6}	9.70(−5)	0.837	6.37(−4)	1.075	3.72(−3)	1.001
2^{-7}	5.09(−5)	0.929	3.09(−4)	1.044	1.86(−3)	1.004
2^{-8}	2.59(−5)	0.975	1.51(−4)	1.031	9.21(−4)	1.011
2^{-9}	1.29(−5)	1.005	7.38(−5)	1.033	4.53(−4)	1.023

$$\mathrm{EOC} = \log_2\big(E(h)/E(\tfrac{h}{2})\big)$$

Numerical experiments

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+}\Big(1 + t(1-t)\Big), \quad t \in [0,1]$$

	α	γ	λ
Set 1	0.3	0.8	4.0
Set 2	0.6	0.7	4.0
Set 3	0.9	0.4	4.0



Numerical experiments

Errors and EOC for the test problem

$$y(t) = \mathbf{E}^{\gamma}_{\alpha,\alpha\gamma,-\lambda,0+}\Big(1 + t(1-t)\Big), \quad t \in [0,1]$$

	Param. set 1		Param. set 2		Param. set 3	
h	Error	EOC	Error	EOC	Error	EOC
2^{-4}	2.46(−4)		1.82(−3)		3.62(−3)	
2^{-5}	1.23(−4)	1.000	9.15(−4)	0.990	1.82(−3)	0.990
2^{-6}	6.13(−5)	1.002	4.58(−4)	0.997	9.14(−4)	0.997
2^{-7}	3.05(−5)	1.005	2.29(−4)	1.003	4.56(−4)	1.003
2^{-8}	1.52(−5)	1.011	1.14(−4)	1.010	2.26(−4)	1.010
2^{-9}	7.46(−6)	1.023	5.59(−5)	1.022	1.12(−4)	1.022

$$\mathrm{EOC} = \log_2\big(E(h)/E(\frac{h}{2})\big)$$

Mittag–Leffler and Prabhakar functions

$$\mathbf{E}^{\gamma}_{\alpha,\beta,\omega,a+} f(t) = \int_a^t e^{\gamma}_{\alpha,\beta}(\tau;\omega) f(t-\tau)\, d\tau$$

$e^{\gamma}_{\alpha,\beta}(t;\omega)$ Laplace transform inverse of $\dfrac{s^{\alpha\gamma-\beta}}{\left(s^{\alpha}-\omega\right)^{\gamma}}$

The Prabhakar function

$$e^{\gamma}_{\alpha,\beta}(t;\omega) = t^{\beta-1} E^{\gamma}_{\alpha,\beta}(t^{\alpha}\omega) \qquad E^{\gamma}_{\alpha,\beta}(z) = \frac{1}{\Gamma(\gamma)} \sum_{k=0}^{\infty} \frac{\Gamma(\gamma+k) z^k}{k! \Gamma(\alpha k + \beta)}$$

When $\gamma = 1$, $E^{\gamma}_{\alpha,\beta}(z)$ is the Mittag–Leffler function

How to compute this functions ?

Mittag–Leffler and Prabhakar functions

$$E_{\alpha,\beta}^{\gamma}(z) = \frac{1}{\Gamma(\gamma)} \sum_{k=0}^{\infty} \frac{\Gamma(\gamma + k) z^k}{k! \Gamma(\alpha k + \beta)}$$

Use of the series expansion only for very small $|z|$:

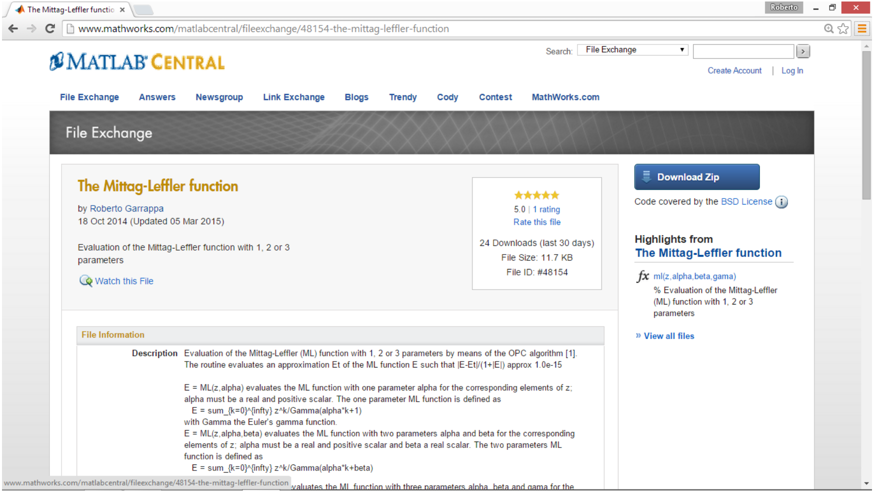
- Convergence is very slow
- Round-off and overflow errors

Numerical inversion of the Laplace transform $\dfrac{s^{\alpha\gamma-\beta}}{\left(s^{\alpha}-\omega\right)^{\gamma}}$:

- Deformation of the Bromwich line in a suitable contour
- Application of a quadrature rule
- Error analysis to choose parameters

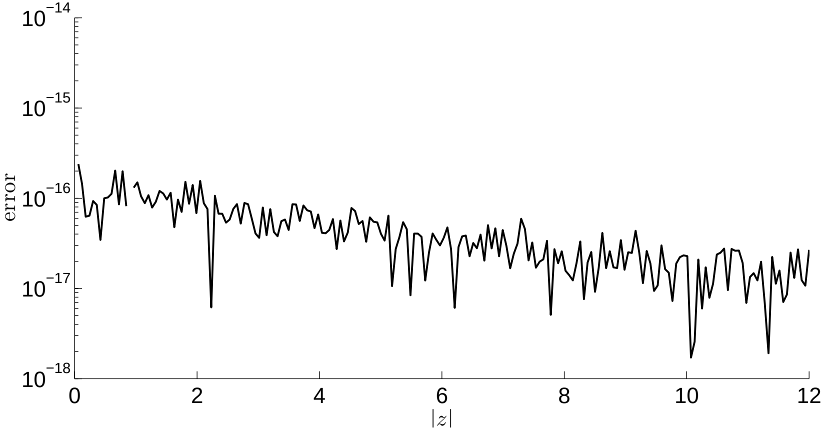
OPC: Optimal parabolic contour

Mittag–Leffler and Prabhakar functions



The Prabhakar function: accuracy

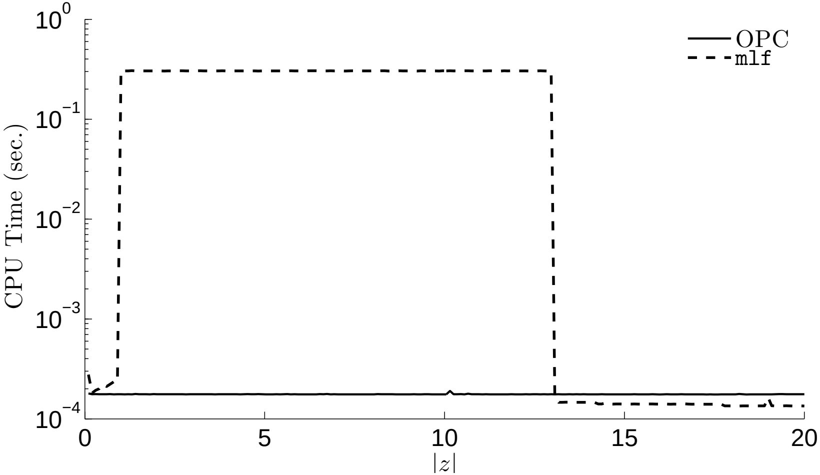
$$E^{\gamma}_{\alpha,\beta}(z) \quad : \quad \alpha = 0.6 \qquad \beta = 0.9 \qquad \gamma = 1.2 \qquad \arg(z) = \frac{3}{4}\pi$$



Reference values: Maple with variable precision arithmetic (100 digits)

The Mittag–Leffler function: fast algorithm

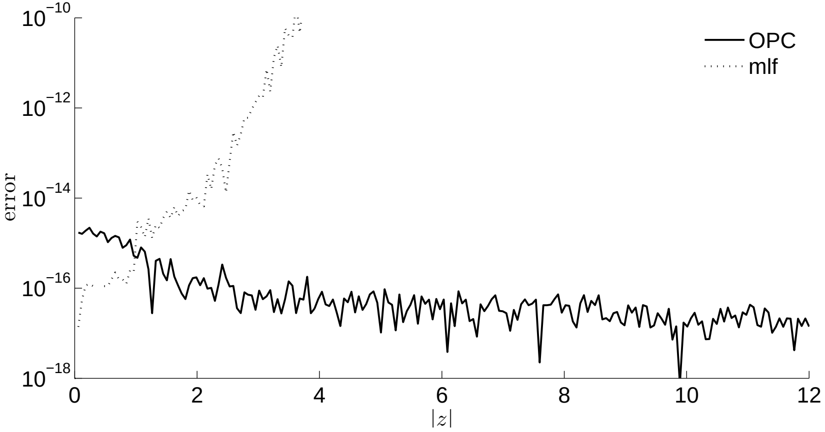
$$E_{\alpha,\beta}(z) \quad : \quad \alpha = 0.7 \qquad \beta = 1.0 \qquad \arg(z) = \pi$$



mlf : Matlab code by Podlubny and Kacenak

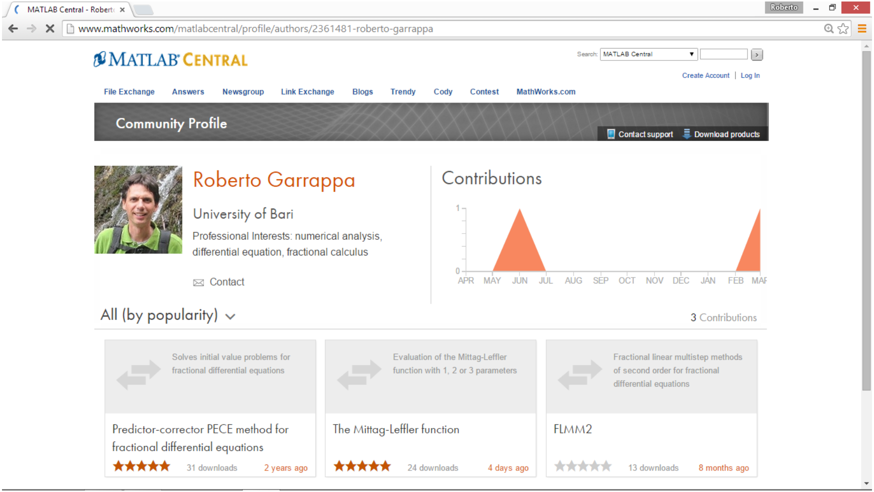
The Mittag–Leffler function: fast algorithm

$$E_{\alpha,\beta}(z) \quad : \quad \alpha = 0.5 \qquad \beta = 1.0 \qquad \arg(z) = \frac{\pi}{2}$$



Reference values: Maple with variable precision arithmetic (100 digits)

Other codes for FDEs



Concluding remarks

The Havriliak–Negami model:

- Applications in describing polarization processes
- Pseudo fractional differential operator (not well known)

The Grünwald–Letnikov scheme:

- Convolution quadrature rule
- Weights evaluable in an explicit way

Further developments:

- Higher order methods
- Different methods for computing the weights
- Maxwell's equations (FDTD, Yee algorithm)

Some references

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- Lubich C. "Convolution quadrature and discretized operational calculus I and II", In: *Numer. Math.* 52, 129–145 and 413–425 (1998).
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Workshop on Fractional Calculus and its Applications

Rome - 11 March 2015

Why new fractional derivatives?

Michele Caputo (Accademia dei Lincei)

The title of my presentation may sound ambiguous because is transparent to the idea that there be a need of new fractional derivatives or may sound an instigation to produce new derivatives or that there are already new fractional derivatives.

As a matter of fact there are already new fractional derivative, what I will say of the new derivatives concerns a note in collaboration with M. Fabrizio in the journal: *Progress in fractional calculus and applications.*

I will later briefly sketch the new derivatives with some of their properties and differences relative to that commonly used. I will say almost no math, which is available in the note in the web, but some discussion on fractional derivatives.

Let me say that I was not completely satisfied with my derivative from the very beginning and always hoped to take care of it, but never did because of that monster called priority and I was attracted by more urgent matters or applications and postponed it at retirement time.

But I had also the fear that as we say "better" is an enemy of "good" and new fractional derivatives could cause confusion.

What cause my embarrassment and needed help is that the derivative of elementary transcend functions turning into a series and not into a somewhat elegant closed form formula, the singularity it has in the time domain and the consequent singularity in the frequency domain the sometime exaggerate use in some problems and fields of science without a sufficient justification some colleagues complaining that it is too complicate handle its use in some 3D problems.

After the use of fractional derivative in problems of physics, economy and finance, in rheology and biology. I did all this also myself but the force for what I will say comes from the results of the others with the deep detailed research appeared in many excellent books, I was surprised by how it would help in so many different fields.

Only time will say if it is an appropriate approach

It would be possible that model of the various phenomena need a different derivative,

I am for this conclusion, it will not generate confusion, probably a progress as when it was found that diffusion in 1D some phenomena requires models with 2 parameters and not only one and we are lazy to adjust to this new reality .

We are not yet used to this. The same would be in radioactive decay since impurities are always present and memory represents them. Just as the decrease of diffusivity in sand is a measure of the assessment of the grains of sand and of the quantity of fluid went through it

Is clear what I mean, in spite of what I said. But I have more about it concerning the fractional derivative

We have a concept and translate it into a model or a formula.

But we do not know which part of the concept is left out of the formula nor what is in the formula which was not in the concept.

Both are important, also for the fractional derivative, which most of us are using in applications.

I must also say that perhaps Mauro and myself do not want to have the remorse of not having reacted after our feelings. So it is already known that the new derivatives exist and let me sketch them to you.

Classical Fractional Derivative

$$D^{(\alpha)}f(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{f'(\tau)}{(t-\tau)^\alpha}d\tau \ , \ \alpha \in (0,1)$$

New Fractional Derivative with a exponential kernel

$$\mathcal{D}^{(\alpha)}f(t) = \frac{M(\alpha)}{(1-\alpha)}\int_0^t f'(\tau)\,\mathrm{exp}(-\frac{\alpha}{1-\alpha}(t-\tau))d\tau \ , \ \alpha \in (0,1)$$

with $M(\alpha)$ a normalization factor, such that $M(0) = M(1) = 1$.

Fractional derivative of $\sin \omega t$

$$\mathcal{D}^{(\alpha)}\sin \omega t = \frac{\cos c}{1-\alpha}\left[\sin(\omega t + c) - \mathrm{exp}(-\frac{\alpha}{1-\alpha}t)\sin c\right]$$

where

$$\cos c = \frac{\omega}{\left(\frac{\alpha}{(1-\alpha)^2} + \omega^2\right)^{0.5}} \quad , \quad \sin c = \frac{\frac{\alpha}{(1-\alpha)}}{\left(\frac{\alpha}{(1-\alpha)^2} + \omega^2\right)^{0.5}}$$

By a change of variable

$$\sigma = \frac{1-\alpha}{\alpha} \in [0, \infty]$$

as a function of σ, the new fractional derivative assume the form

$$\mathcal{R}^{(\sigma)} f(t) = \frac{N(\sigma)}{\sigma} \int_0^t f'(\tau) \exp(-\frac{(t-\tau)}{\sigma}) d\tau$$

with $N(0) = N(\infty) = 1$. For $\sigma = 0$ we have

$$\mathcal{R}^{(0)} f(t) = f'(t)$$

for $\sigma = \infty$

$$\mathcal{R}^{(\infty)} f(t) = f(t)$$

Related with new definition of fractional derivative, we can introduce the distributed-order fractional derivative

$$ {}_aP_b^{(\alpha)} f(t) = \int_a^b g(z)dz \left[P^{(\alpha)} f(t) \right] $$

$$ LT_a P_b f(t) = F(p) \int_a^b \frac{pg(z)}{\log(p+z)} dz $$

$$ g(z) = 1 $$

$$ LT_a P_b f(t) = \left[p \log \frac{p+b}{p+a} \right] F(p) $$

Fractional Gradient of $\alpha-$order with a Gaussian kernel

$$\nabla^{(\alpha)}u(x) = \frac{\alpha}{(1-\alpha)\pi^{\frac{\alpha}{2}}}\int_{\Omega}\nabla u(y)\,\mathrm{exp}\left(-\frac{\alpha^2(x-y)^2}{(1-\alpha)^2}\right)dy$$

Fractional Divergence of $\alpha-$order with a Gaussian kernel

$$\nabla^{(\alpha)}u(x) = \frac{\alpha}{(1-\alpha)\pi^{\frac{\alpha}{2}}}\int_{\Omega}\nabla\cdot\mathbf{u}(y)\,\mathrm{exp}\left(-\frac{\alpha^2(x-y)^2}{(1-\alpha)^2}\right)dy$$

Fractional Laplacian of $\alpha-$order with a Gaussian kernel

$$(\nabla^2)^{(\alpha)}u(x) = \frac{\alpha}{(1-\alpha)\pi^{\frac{\alpha}{2}}}\int_{\Omega}\nabla\cdot\nabla u(y)\,\mathrm{exp}\left(-\frac{\alpha^2(x-y)^2}{(1-\alpha)^2}\right)dy$$

$Fourier\ Trasnform$ of gradient and divergence

$$FT(\nabla^{(\alpha)}u)(\xi) = \pi^{\frac{1-\alpha}{2}} FT(\nabla u)(\xi) \exp\left[-\frac{\pi^2(1-\alpha)^2\xi^2}{\alpha^2}\right]$$

$$FT(\nabla^{(\alpha)} \cdot \mathbf{u})(\xi) = \pi^{\frac{1-\alpha}{2}} FT(\nabla \cdot \mathbf{u})(\xi) \exp\left[-\frac{\pi^2(1-\alpha)^2\xi^2}{\alpha^2}\right]$$

Response of kernel $exp(-at)$

$$a = \frac{\alpha}{1-\alpha}$$

$$m(\omega) = \frac{M}{(1-\alpha)} \frac{\omega}{(\omega^2 + a^2)^{0,5}}$$

which is monotonic increasing with $m(0) = 0$, $m(\infty) = \frac{N}{1-\alpha}$.
In the Laplace domain, if $u(0) = 0$, we have

$$TL\mathcal{D}^{(\alpha)}u(t) = \frac{p}{p+a}U = (1 - \frac{a}{p+a})U$$

then, by the Laplace inversion

$$\mathcal{D}^{(\alpha)}u(t) = u(t) - au(t) * exp(-\alpha t)$$

In the case of old fractional derivative with module

$$m(\omega) = \frac{\omega^{\alpha}}{\Gamma(1-\alpha)}$$

which is monotonic increasing with $m(\infty) = 0, \; m'(0) = \infty.$

FT with Gaussian kernel.

$$U = \omega \left[\pi^{\frac{1-\alpha}{\alpha}} \right] \exp(-\frac{\pi^2 \omega^2 (1-\alpha)^2}{\alpha^2})$$

$$\omega_m = \frac{\alpha}{2\pi(1-\alpha)}\ , \quad \omega_f = \frac{3\alpha}{2\pi(1-\alpha)}$$

where ω_m is frequency of maximum and ω_f is frequency of inflection. Which is bed shape $m(0) = 0$, $m(\infty) = 0$, $m'(0) = \pi^a$.

$$\omega_f = 3\omega_m$$

$$\frac{U(\omega_f)}{U(\omega_m)} = 3\exp(-2)$$

It could include rheology with the work of Kornig and Muller for the postglacial rebound and underground nuclear explosions.

It could be used as Bagley and Torvik who at the Wright Patterson Air Force Institute of Technology successfully tested 143 materials for the blades of the rotors of the jets and for the vibration abatement

Wenn $v = z$ wir haben classic Cole and Cole often used for Maxwell equations.

Deeper studies and experimental data may say which is best to use in the single cases.

But most important the second principle of thermodynamics is always included, which is a matter of substance.

It could be used for the evolution of he planetary systems as for the evolution of our planet with Moon

The fractional derivative is now spreading also in economy which in quiet period could evolve following the entropy rule of physical systems.

Workshop on Fractional Calculus and its Applications

Rome - 11 March 2015

A fractional model for damage and fatigue phenomena

Mauro Fabrizio (University of Bologna)

Fatigue and damage in the material science are consequence to loading and unloading processes, which produces a gradual and progressive damage effects, involving crack nucleation, creep rupture and then rapid fracture . Since during damage processes, we observe a change of the internal structure. So we describe such structural variation by an order parameter denoted by $\alpha \in [0,1]$.

It is well known that inside the fractional models, a linear viscoelastic body $\mathcal{B}$, can be defined by

$$\tilde{\sigma}(x,t) = \mathbf{A}(x)\,{}_{t_0}^{C}D_t^{\alpha}\ \varepsilon(x,t)\ , \quad \alpha \in [0,1] \tag{1}$$

where $\sigma(x,t)$ and $\varepsilon(x,t)$ are the stress and strain tensors respectively. The operator ${}_{t_0}^{C}D_t^{\alpha}$ denotes the Caputo derivative of $\alpha-$order)

Fatigue and damage can be described by a variation of the coefficient $\alpha(x,t)$ of the fractional derivative. In this framework, the virgin material, supposed as an elastic body, is described by the coefficient $\alpha = 0$. Then, fatigue consequence of loading and unloading processes, produces an increase of damage and of coefficient $\alpha(x,t)$ accordingly.

Therefore, the material show viscous effects, which will increase with the increments of α, until reaching a limit value $\alpha_{\mathsf{C}}(x) < 1$, wherein the stress goes to zero, with the subsequent fracture. Then in this pattern, the fraction α is a function of (x,t) able to represent the evolution of the material system. For this reason, in addition to the equation of motion, we have to consider a new equation for the $\alpha(x,t)$ variable.

Here, the stress is given by

$$\sigma(t) = (\alpha_{\mathsf{C}} - \alpha(t))^2 \mathbf{A}(x) {}_{t_0}^{C}D_t^{\alpha} \varepsilon(x,t). \tag{2}$$

The coefficient $\alpha_{\mathsf{C}} < 1$ is such that $0 \leq \alpha(t) \leq \alpha_{\mathsf{C}}$, when $\alpha(t) = \alpha_{\mathsf{C}}$ we have fracture. Moreover, the function $\mathcal{F}(t)$ that describes fatigue, is defined by

$$\mathcal{F}(\varepsilon(t_0), P_{[0,t)})) = \int_{t_0}^{t} (\alpha_{\mathsf{C}} - \alpha(\tau)) \mathbf{A}(x) {}_{t_0}^{C}D_t^{\alpha} \varepsilon(x,\tau) \cdot \dot{\varepsilon}(x,\tau) d\tau \tag{3}$$

here $\varepsilon(t_0)$ denotes the initial virgin state and $P_{[0,t)}$ the process restricted to the interval $[0,t)$.

The differential system describing fatigue phenomenon is given by the motion equation

$$\rho_0(x)\dot{\mathbf{v}}(x,t) = \nabla \cdot \sigma(x,t) + \rho_0(x)\mathbf{b}(x,t) \tag{4}$$

where $\mathbf{v}$ is the velocity, ρ_0 the density and $\mathbf{b}$ the external source.

Now we introduce the Ginzburg-Landau (G-L) equation, which is able to describe the material structural variations by a phase field or order parameter, given by the field $\alpha(x,t)$.

Then, we consider the functions

$$F(\alpha) = \alpha_c - \bar{\alpha} \quad , \qquad G(\alpha) = 8\alpha_c(\bar{\alpha}^2 - \frac{3}{4}\bar{\alpha}^4) \tag{5}$$

where the variable $\bar{\alpha}$ is given by

$$\bar{\alpha} = \begin{cases} 0 & if \quad \alpha < 0 \\ \alpha & if \quad 0 \leq \alpha \leq \alpha_c \\ \alpha_c & if \quad \alpha > \alpha_c \end{cases}$$

For this purpose, we use a modified representation of the Ginzburg-Landau equation,

$$
\begin{aligned}
\rho_0(x)\dot{\alpha}(x,t) \;&=\; \gamma(x)\nabla^2\alpha(x,t) + \mathcal{F}_0(x)G'(\alpha(x,t)) \\
&\quad -\mathcal{F}(s(x,t_0), P_{[0,t)}(x))F'(\alpha(x,t))
\end{aligned} \tag{6}
$$

where γ is a positive coefficient.

For the study of damage and fatigue is crucial that the system satisfies the dissipation restrictions and admits the existence of a free energy with features and properties in agreement with the laws of thermodynamics. Because, we are working with isothermal processes, the thermodynamic restrictions are given by the Dissipation Principle, which is obtained from the Second Law of the Thermodynamics with constant temperature.

Dissipation Principle

On any pair (σ, P), there exists a state function $\psi(\cdot)$, called free energy, such that

$$
\rho_0(x)\dot{\psi}(x,t) \le \mathcal{P}^i_m(x,t) + \mathcal{P}^i_s(x,t) \tag{7}
$$

where $\mathcal{P}_m^i(x,t)$ denotes the internal mechanical power and $\mathcal{P}_s^i(x,t)$ the internal structural power.

By the use of the equations (4) and (6) we have

$$\begin{aligned} \mathcal{P}_m^i(x,t) &= \sigma(x,t) \cdot \dot{\varepsilon}(x,t) = \\ &\qquad (\alpha_{\mathsf{C}} - \alpha(x,t))^2 \mathbf{A}(x) {}^C D_{t_0}^\alpha \ \varepsilon(x,t) \cdot \dot{\varepsilon}(x,t) \end{aligned} \tag{8}$$

$$\begin{aligned} \mathcal{P}_s^i(x,t) &= \rho_0(x)\dot{\alpha}^2(x,t) + \gamma(x)\nabla\alpha(x,t) \cdot \nabla\dot{\alpha}(x,t) - \\ &\quad \mathcal{F}(s(x,t_0), P_{[0,t)}(x))\alpha(x,t) + \mathcal{F}_0(x)\dot{G}(\alpha(x,t)) \end{aligned} \tag{9}$$

From (7), (8) and (9) we obtain

$$\rho_0\dot{\psi}(t) \leq (\alpha_{\mathsf{C}} - \alpha(t))^2 \mathbf{A} {}^C D_{t_0}^\alpha \varepsilon(t) \cdot \dot{\varepsilon}(t) + \rho_0\dot{\alpha}^2(t) +$$

$$\gamma\nabla\alpha(t) \cdot \nabla\dot{\alpha}(t) - \mathcal{F}(s(t_0), P_{[0,t)}))\dot{F}(\alpha(t)) + \mathcal{F}_0\dot{G}(\alpha(t))$$

So, if we suppose that $\tilde{\sigma}(t)$ is the stress defined in (1), we have

$$\rho_0\dot{\psi}(t) \leq (\alpha_{\mathsf{C}} - \alpha(t))\frac{\partial}{\partial t}\int_{t_0}^t (\alpha_{\mathsf{C}} - \alpha(\tau))\tilde{\sigma}(\tau) \cdot \dot{\varepsilon}(\tau)d\tau +$$

$$+\mathcal{F}_0\dot{G}(\alpha(t) + \frac{\gamma}{2}\frac{\partial}{\partial t}(\nabla\alpha(t))^2 + \dot{F}(\alpha(t))\mathcal{F}(s(t_0), P_{[0,t)})) \quad (10)$$

$$= \frac{\partial}{\partial t}(F(\alpha(t))\mathcal{F}(s(t_0), P_{[0,t)}) + \frac{\gamma}{2}(\nabla\alpha(t))^2 + \mathcal{F}_0 G(\alpha(t)))$$

The two terms $\frac{\gamma}{2}(\nabla\alpha(t))^2$ and $\mathcal{F}_0 G(\alpha(t))$ of the inequality (10) are conservative quantities and belong to the free energy ψ.

For the study of simulation processes, fixed a time $t^* > 0$, we introduce the potential

$$V_{t^*}(\alpha(t)) = F(\alpha(t))\mathcal{F}(t^*) + \mathcal{F}_0 G(\alpha(t))$$

for an assigned fatigue value $\mathcal{F}(t^*) = \mathcal{F}(s(t_0), P_{[0,t^*)})$ for all $t \geq t^*$. It is evident, that the behavior of the phase field $\alpha(t)$ depends on the function $V'_{t^*}(\alpha(t))$, because

$$\rho_0(x)\dot{\alpha}(x,t) = \gamma\,(x))\,\nabla^2\alpha(x,t) - V'_{t^*}(\alpha(t)) \qquad (11)$$

So that, for understand the evolution of $\alpha(t)$ is crucial to study the behavior of the function $V'_{t^*}(\alpha(t))$ for different values of t^*. Therefore, in the Fig.1 and 2, we have represented the behavior of $V_{t^*}(\alpha(t)$ at different values of fatigue.

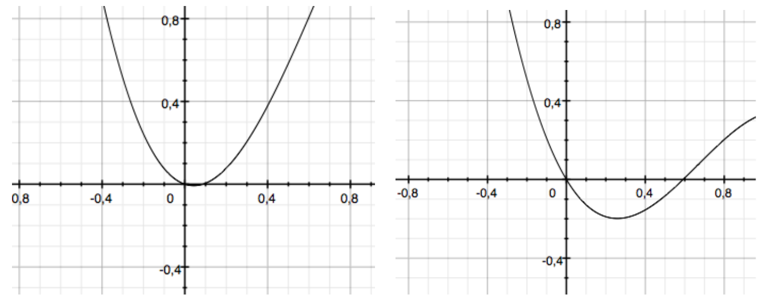


Fig.1. The first graphic, in the space (α, V), describes the behavior of the function $V_{t^*}(\alpha(0))$ at the initial time $t = 0$, corresponding to virgin state, so fatigue $\mathcal{F}(t = 0)$ is zero. In the second graphic, fatigue occurs at the time t_1, for which $\mathcal{F}(t_1) > 0$.

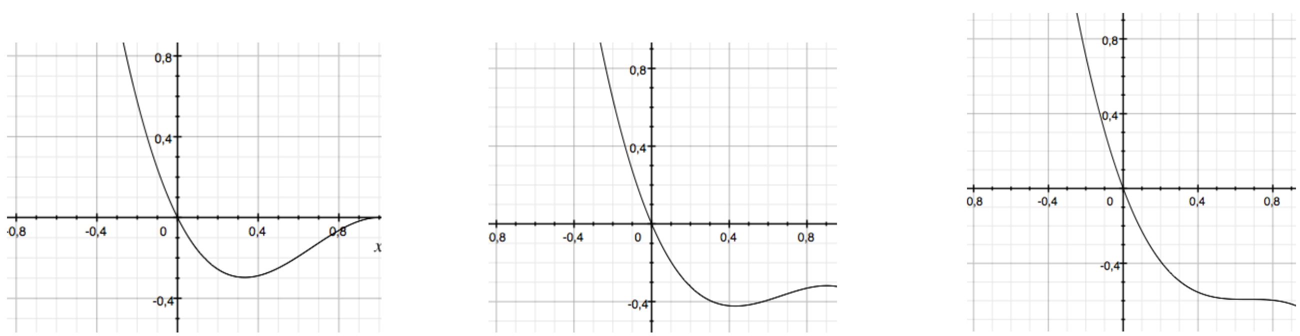


Fig. 2. These graphics (V_{t^*}, α) describe the behavior of $V_{t^*}(\alpha(t))$ corresponding at the time $t_2 < t_3 < t_4$, for which $\mathcal{F}(t_2) < \mathcal{F}(t_3) < \mathcal{F}(t_4)$ and such that $t_2 > t_1$ and $\mathcal{F}(t_2) > \mathcal{F}(t_1)$.

Now, we study the behavior with the potential $V_{t^*}(\alpha(t))$ related to the functions F and G defined with different coefficients. By the simulations represented in the Fig. 3, we confirm a more rapid damage process as a function of fatigue behavior. While for small fatigue values we observe a greater material tenacity.

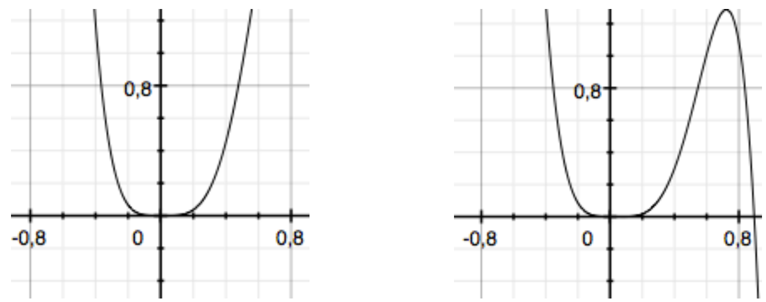


Fig. 3. The graphics of $V_{t^*}(\alpha)$ show material tenacity in the first part of the fatigue process.

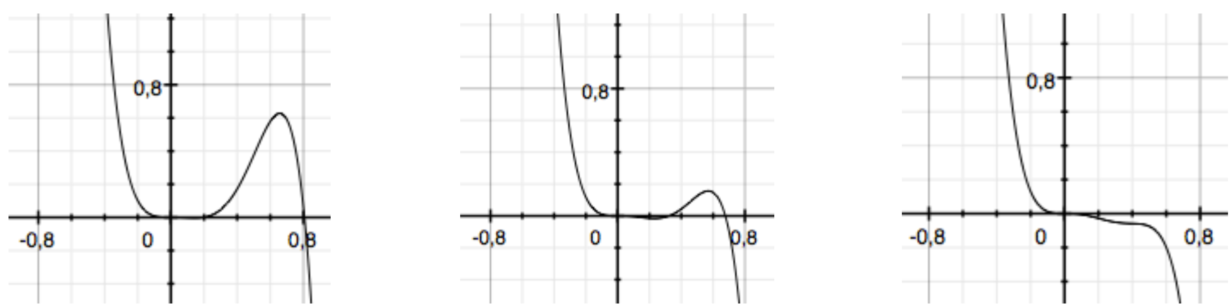


Fig. 4. The graphics of $V_{t^*}(\alpha)$ show the rapid damage process in the final part of the fatigue process.

Maximum theorem

The maximum theorem for the damage variable α is crucial in order to describe a natural fatigue problem. For the proof, we start from a differential system defined by the equations (4), (6), and (5) in a smooth domain $\Omega \subset \mathbb{R}^3$ and time interval $I = [0, T] \subset \mathbb{R}$, with the initial and boundary conditions

$$\mathbf{u}(x,0) = \mathbf{u}_0(x)\ ,\ \mathbf{v}(x,0) = \mathbf{v}_0(x)\ ,\ \alpha(x,0) = \alpha_0(x) \qquad (12)$$

$$\mathbf{u}(x,t)|_{\partial\Omega} = \mathbf{0} \quad , \quad \nabla\alpha(x,t)|_{\partial\Omega} = 0 \qquad (13)$$

where $\mathbf{u}(x,t)$ is the displacement, so that $\dot{\mathbf{u}}(x,t) = \mathbf{v}(x,t)$.

Theorem. Any solution of the equation (6), with initial conditions (12) such that $0 \leq \alpha_0(x) \leq \alpha_c$, with boundary conditions (13), satisfies the restriction

$$0 \leq \alpha(x,t) \leq \alpha_c\ ,\ for\ all\ \ t > 0\ and\ a.e.\ \ x \in \Omega \qquad (14)$$

then using $\alpha\_\alpha_t = -\alpha\_\alpha\_{t}$ and $\nabla\alpha\_ \cdot \nabla\alpha = -\nabla\alpha\_ \cdot \nabla\alpha\_$ we have

$$\int_0^T \int_\Omega \rho\alpha\_(t)\alpha\_{t}(t) + \gamma(\nabla\alpha\_(t))^2 +$$

$$+\alpha\_(t)\mathcal{F}_0\left\langle 2\alpha(t)-\frac{\alpha^2}{2}(t)\right\rangle dxdt \geq 0$$

so by the initial conditions we obtain

$$\int_\Omega \frac{1}{2}\rho\left(\alpha\_(T)\right)^2 + \tag{15}$$

$$+\int_0^T\left[\gamma\left(\nabla\alpha\_(t)\right)^2-\alpha\_(t)\mathcal{F}_0\left\langle 2\alpha(t)-\frac{\alpha^2}{2}(t)\right\rangle\right]dtdx \leq 0$$

because

$$\int_0^T\int_\Omega \alpha\_(t)\mathcal{F}_0\left\langle 2\alpha(t)-\frac{\alpha^2}{2}(t)\right\rangle dxdt = 0$$

then from (15), $\alpha\_(x,T)=0$ for any $T\in[0,\infty]$ and a.e. $x\in\Omega$. Hence, it is satisfied the restriction that $\alpha(x,t)\geq 0$..

To show that $\alpha(x,t)\leq\alpha_{\text{c}}$, let us to consider the function

$$(\alpha-\alpha_{\text{c}})_+ = \begin{cases} \alpha-\alpha_{\text{c}} & \forall\alpha>\alpha_{\text{c}} \\ 0 & \forall\alpha\leq\alpha_{\text{c}} \end{cases}$$

and suppose that $\alpha(x,t)>1$.

Thus, multiplying (6) by $(\alpha-\alpha_{\text{c}})_+$, after an integration on

Ω, we have

$$\int_\Omega \Big[\rho(\alpha-\alpha_\mathsf{c})_+\,\alpha_t+\gamma\nabla(\alpha-\alpha_\mathsf{c})_+\cdot\nabla\alpha$$
$$+(\alpha-\alpha_\mathsf{c})_+\mathcal{F}_0\left\langle 2\alpha-\frac{\alpha^2}{2}\right\rangle\Big]\,dx$$
$$=-\int_\Omega\langle -1\rangle\,(\alpha-\alpha_\mathsf{c})_+\int_0^t[1-\alpha(\tau)]\,\mathbf{A}\nabla\mathbf{u}(\tau)\cdot\nabla\dot{\mathbf{u}}(\tau)d\tau dx$$

then because

$$\int_\Omega\langle -1\rangle\,(\alpha-\alpha_\mathsf{c})_+\int_0^t[1-\alpha(\tau)]\,\mathbf{A}\nabla\mathbf{u}(\tau)\cdot\nabla\dot{\mathbf{u}}(\tau)d\tau dx=0$$

after a time integration on $[0,T]$, we obtain

$$\int_0^T\int_\Omega\Big[\rho(\alpha-\alpha_\mathsf{c})_+(\alpha-\alpha_\mathsf{c})_t+\gamma\nabla(\alpha-\alpha_\mathsf{c})_+\cdot\nabla(\alpha-1)$$
$$+(\alpha-1)\mathcal{F}_0\left\langle 2\alpha-\frac{\alpha^2}{2}\right\rangle\Big]\,dxdt=0$$

So,

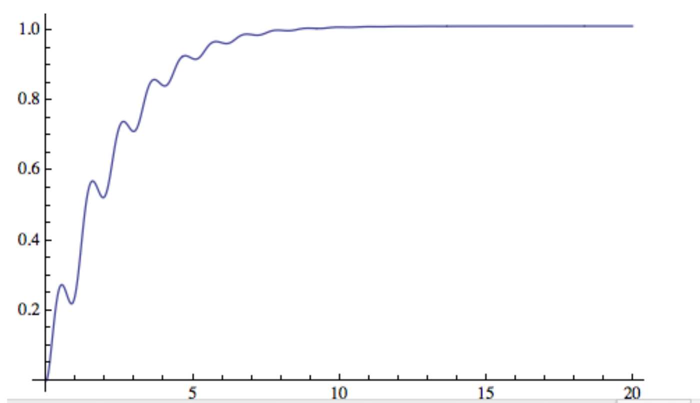
$$\int_\Omega\left\{\frac{1}{2}\rho\left[(\alpha-\alpha_\mathsf{c})_+(T)\right]^2+\gamma\int_0^T\left[\nabla(\alpha-\alpha_\mathsf{c})_+(t)\right]^2dt+\right.$$
$$\left.(\alpha-\alpha_\mathsf{c})_+\mathcal{F}_0\left\langle 2\alpha-\frac{\alpha^2}{2}\right\rangle dt\right\}dx=0, \tag{16}$$

because we have the sum of three positive quantities, it follows that $(\alpha-\alpha_{\text{C}})_{+}(x,T)=0$, $\nabla(\alpha-\alpha_{\text{C}})_{+}(t)=\mathbf{0}$ and $(\alpha-\alpha_{\text{C}})_{+}(x,t)=0$ for any $T\in[0,\infty]$. Therefore, the hypothesis $\alpha(x,t)>\alpha_{\text{C}}$ is inconsistent, from which the restriction (14) is proved.

Some simulations of fatigue and stress

Finally, we study the behavior of fatigue and stress submit to processes of loading and unloading on the strain, which confirm the results of the paper.

So that, the simulations represented in Fig 5, 6, 7 and 8 correspond to several selections of the critical threshold α_{C} of order parameter, frequency ω and process time T, which plot fatigue and stress of the equations (2) and (3), corresponding to periodic processes with the same amplitude.



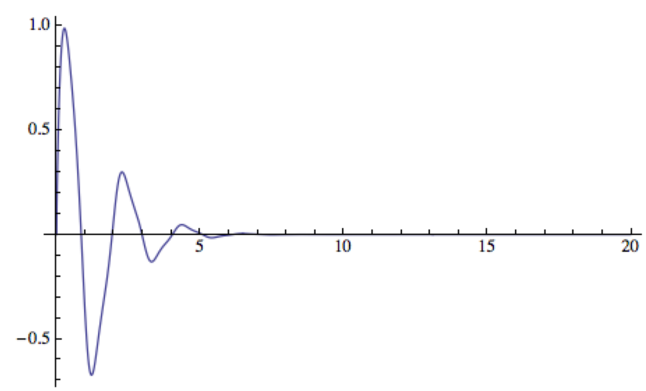


Fig.5. In the pictures $(\mathcal{F}, t)$ and (σ, t), the behavior of fatigue $\mathcal{F}(t)$ and stress $\sigma(t)$ as a funtion of t are respectively plotted corresponding to the following values of order parameter $\alpha_{\rm C} = \frac{\pi}{6}$, frequency $\omega = 3$, and process time $T = 20\frac{\pi}{\omega}$,

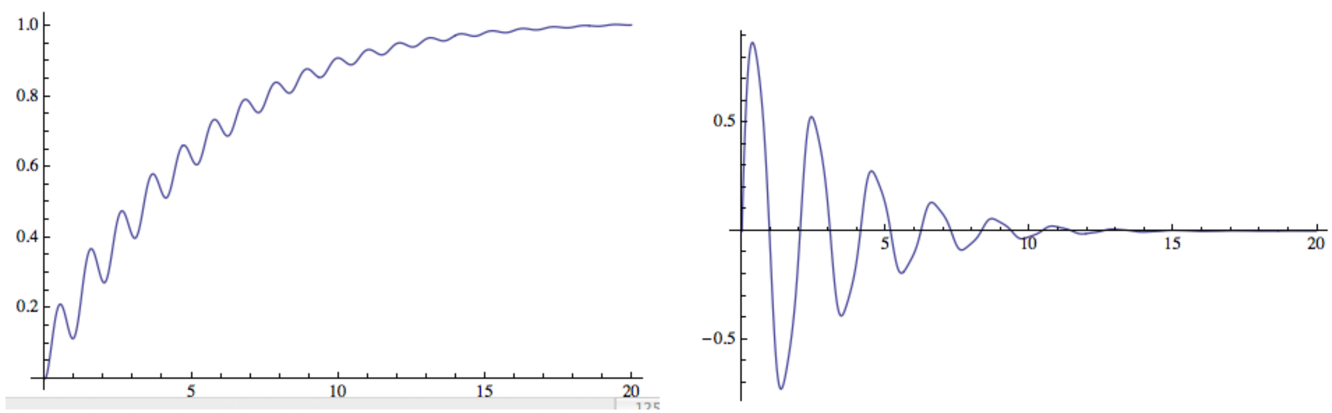


Fig.6. The behavior of fatigue $\mathcal{F}(t)$ and stress $\sigma(t)$ are respectively plotted corresponding to the following values of order parameter $\alpha_{\rm C} = \frac{\pi}{12}$.

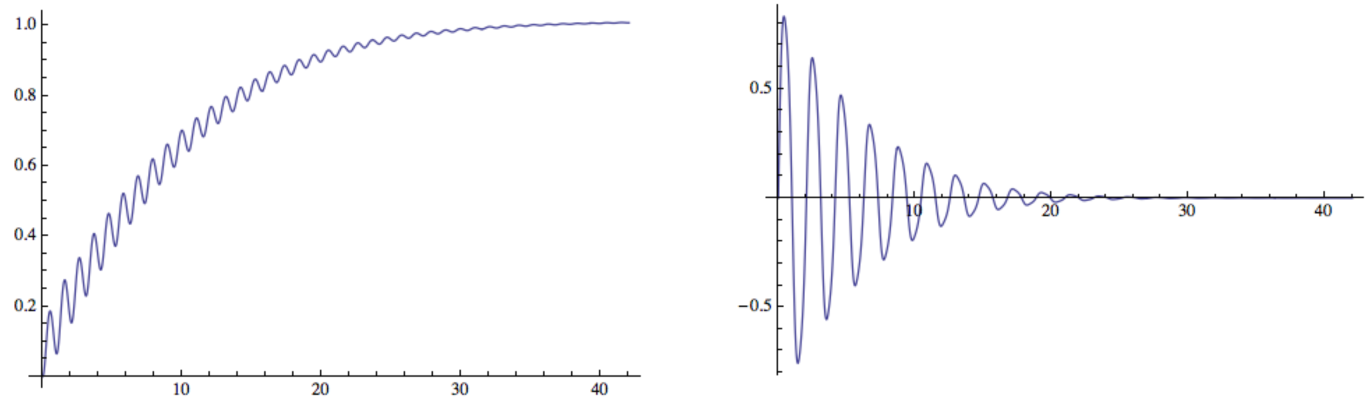


Fig.7. The behavior of fatigue $\mathcal{F}(t)$ and stress $\sigma(t)$ are respectively plotted corresponding to the following values of order parameter $\alpha_{\mathrm{C}} = \frac{\pi}{22}$.

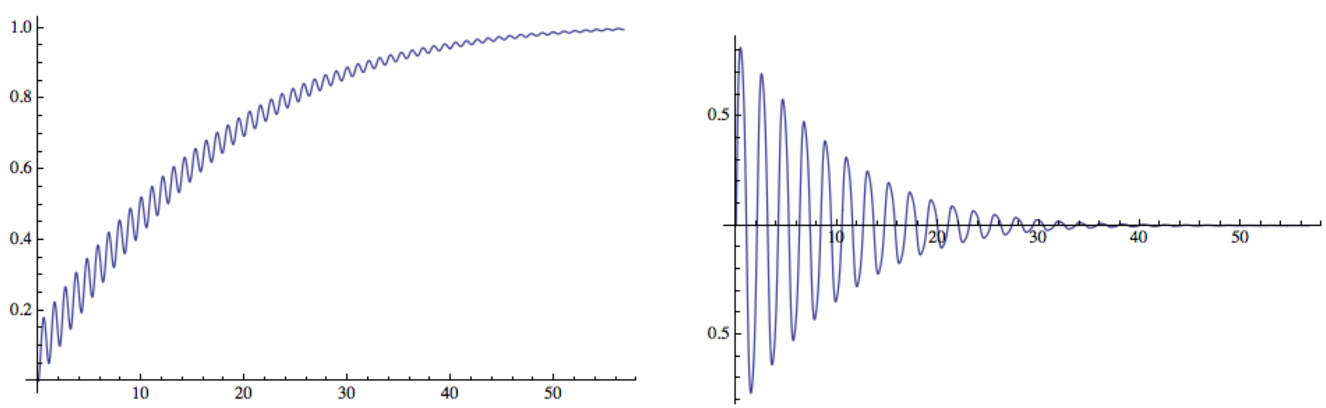


Fig. 8. The behavior of fatigue $\mathcal{F}(t)$ and stress $\sigma(t)$ are respectively plotted corresponding to the following values of order parameter $\alpha_{\mathrm{C}} = \frac{\pi}{36}$.

Thank you for your attention

Approach to equilibrium of a sphere in a Stokes fluid

Guido Cavallaro

Sapienza Università di Roma

March 11, 2015

Workshop on Fractional Calculus and its Applications
Roma Tre University

We consider a fluid governed by the Navier-Stokes equation, which in dimensionless form is

$$\begin{cases} \frac{\partial \vec{u}}{\partial t} + Re(\vec{u} \cdot \nabla)\vec{u} = -\nabla p + \Delta \vec{u} \\ \operatorname{div} \vec{u} = 0 \end{cases}$$

where $\vec{u}(\vec{x}, t)$ is the velocity field of the fluid, $p(\vec{x}, t)$ is the pressure,

$$Re = \frac{\rho L V}{\mu} \qquad \text{Reynolds number.}$$

The approximation $Re = 0$ is the so called Stokes approximation, which gives origin to the Stokes equation.

The first solution to the Stokes equation in case of a sphere moving at constant velocity V was obtained by Stokes (1851), and it gives a drag force of the medium expressed by the well known formula

$$F = 6\pi\mu RV$$

with R radius of the sphere.

It can be obtained by the following steps:

• we put in the reference frame in which the sphere is at rest, hence the stationary equation to be solved is

$$-\nabla p + \mu \Delta \vec{u} = 0, \quad \mathrm{div}\, \vec{u} = 0, \quad \vec{u} = -V\hat{x} \quad \text{at infinity}$$

• we impose on the surface of the sphere: $\vec{u} = 0$

• we then obtain the velocity field $\vec{u}$ and the pressure field p.

• we compute the force per unit area on the sphere, to be integrated over the whole surface of the sphere:

$$P_i = -\sigma_{ik} n_k = p\, n_i - \sigma'_{ik} n_k$$

with σ_{ik} *stress tensor*. In the first term it appears the ordinary pressure, the second term (σ'_{ik}) includes the friction effects due to viscosity.

For a sphere forced to oscillate at given frequency ω, the Stokes equation can be solved exactly, giving a hydrodynamical drag force

$$F = 6\pi\mu R \left(1 + \frac{R}{\delta}\right) V(t) + 3\pi R^2 \rho\delta \left(1 + \frac{2R}{9\delta}\right) \frac{dV}{dt} \tag{1}$$

where $\delta = \sqrt{\frac{2\mu}{\omega\rho}}$

Let us obtain by the last formula the force acting on a sphere with arbitrary velocity $V(t)$. We represent $V(t)$ as a Fourier integral

$$V(t) = \int_{-\infty}^{\infty} V_\omega e^{-i\omega t} d\omega, \quad V_\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} V(\tau) e^{i\omega\tau} d\tau.$$

Since the equations are linear, the total force can be written as the integral over the forces which are the Fourier components $V_\omega e^{-i\omega t}$ (putting $\nu = \frac{\mu}{\rho}$):

$$\pi\rho R^3 V_\omega e^{-i\omega t} \left\{ \frac{6\nu}{R^2} - \frac{2i\omega}{3} + \frac{3\sqrt{2\nu}}{R}(1-i)\sqrt{\omega} \right\}.$$

Noting that $\left(\frac{dV}{dt}\right)_\omega = -i\omega V_\omega$, we can rewrite it as

$$\pi\rho R^3 e^{-i\omega t} \left\{ \frac{6\nu}{R^2} V_\omega + \frac{2}{3}\left(\dot{V}\right)_\omega + \frac{3\sqrt{2\nu}}{R}\left(\dot{V}\right)_\omega \frac{1+i}{\sqrt{\omega}} \right\}.$$

Integrating over all the frequences ω, the first and second term give respectively $V(t)$ and $\dot{V}(t)$. To integrate the third term, we note that for $\omega < 0$ this term must be substituted by the complex conjugate, putting $\frac{(1-i)}{\sqrt{|\omega|}}$ in place of $\frac{(1+i)}{\sqrt{\omega}}$; this because the equation (1) has been obtained for a velocity $A\, e^{-i\omega t}$ with $\omega > 0$, and for a velocity $A\, e^{i\omega t}$ we have to obtain the complex conjugate. Instead of an integral from $\omega = -\infty$ to $+\infty$, we can take twice the real part of the integral from $\omega = 0$ to $+\infty$.

We have then

$$2\Re\left\{(1+i)\int_0^\infty \frac{\left(\dot V\right)_\omega e^{-i\omega t}}{\sqrt{\omega}}d\omega\right\}$$

$$=\frac{1}{\pi}\Re\left\{(1+i)\int_{-\infty}^\infty\int_0^\infty \frac{\dot V(\tau)e^{i\omega(\tau-t)}}{\sqrt{\omega}}d\omega d\tau\right\}$$

$$=\frac{1}{\pi}\Re\left\{(1+i)\int_{-\infty}^t\int_0^\infty \frac{\dot V(\tau)e^{-i\omega(t-\tau)}}{\sqrt{\omega}}d\omega d\tau\right.$$

$$\left.+(1+i)\int_t^\infty\int_0^\infty \frac{\dot V(\tau)e^{i\omega(\tau-t)}}{\sqrt{\omega}}d\omega d\tau\right\}$$

$$=\sqrt{\frac{2}{\pi}}\Re\left\{\int_{-\infty}^t \frac{\dot V(\tau)}{\sqrt{(t-\tau)}}d\tau+i\int_t^\infty \frac{\dot V(\tau)}{\sqrt{(\tau-t)}}d\tau\right\}$$

$$=\sqrt{\frac{2}{\pi}}\int_{-\infty}^t \frac{\dot V(\tau)}{\sqrt{(t-\tau)}}d\tau.$$

Hence we get for the force on a sphere moving with arbitrary velocity

$$
\begin{aligned}
F_{drag} &= 6\pi\mu R\, V(t) + \frac{1}{2} M_f \frac{dV}{dt} \\
&+ 6\pi R^2 \sqrt{\frac{\mu}{\pi\rho}} \int_{-\infty}^{t} \frac{\dot{V}(s)}{\sqrt{t-s}}\, ds
\end{aligned}
$$

1° term: stationary force term

2° term: added mass term (force due to accelerate the surrounding fluid)

3° term: *Basset memory term*.

The solution for a sphere immersed in a Stokes fluid and also subjected to its own weight is well known

$$
M_s \dot{V}(t) = M_s g - F_{drag}(t)
$$

the solution can be explicitly computed via Laplace transform. The equation of motion is

$$\dot{V}(t) + V(t) + \alpha \int_0^t \frac{\dot{V}(s)}{\sqrt{t-s}}\, ds = 1$$
$$V(0) = 0$$

$$\mathcal{L}\{V\}(s) = \frac{1}{s(s + \alpha\sqrt{s} + 1)}$$

$$V(t) = 1 + \frac{\alpha}{\lambda_1 - \lambda_2} \left\{ \frac{e^{\lambda_1 t}\mathrm{Erfc}\sqrt{\lambda_1 t}}{\sqrt{\lambda_1}} - \frac{e^{\lambda_2 t}\mathrm{Erfc}\sqrt{\lambda_2 t}}{\sqrt{\lambda_2}} \right\}$$

$$|V(t) - V_\infty| \approx \frac{C}{\sqrt{t}} \qquad \text{for } \ t \to \infty$$

moreover $V(t)$ turns out to be monotone.

In this setting we have analyzed the approach to equilibrium of an harmonic oscillator immersed in a Stokes fluid:

$$M_s \ddot{X}(t) = -K\, X(t) - F_{drag}(t)$$

which in dimensionless form looks like

$$\ddot{X}(t) + \dot{X}(t) + K\, X(t) + \alpha \int_0^t \frac{\ddot{X}(s)}{\sqrt{t-s}}\, ds = 0$$

$$X(0) = X_0, \quad \dot{X}(0) = V_0, \quad \alpha = \sqrt{\frac{9\rho}{2\rho_s + \rho}}$$

assuming the following integral equal zero

$$\int_{-\infty}^0 \frac{\ddot{X}(s)}{\sqrt{t-s}}\, ds = 0 \qquad (2)$$

(if the system has been prepared in a stationary state)

G. C. and C. Marchioro, *On the approach to equilibrium for a pendulum immersed in a Stokes fluid*, Math. Models Methods Appl. Sci. **20**, 1999–2019 (2010).

By applying the Laplace transform we get

$$\mathcal{L}\{\dot{X}\}(s) = \frac{V_0 s + \alpha V_0 \sqrt{s} - K X_0}{s(s + \alpha\sqrt{s} + 1) + K}$$

which cannot be (easily) anti-transformed. We have to perform an asymptotic study to established the law with which $X(t) \to 0$ for $t \to \infty$. The result is

$$X(t) \sim \frac{C}{t^\gamma} \qquad \text{for } \ t \to \infty$$

with $\gamma = 3/2$ if $V_0 = 0$ and $X_0 \neq 0$, $\gamma = 1/2$ if $V_0 \neq 0$ for any X_0.

We give a sketch of the proof.
The main difficulty is to exclude that $X(t)$ performs infinitely many oscillations, situation in which we can say nothing about the rate of decay. It turns out that this is not the case, $X(t)$ turns out to be monotone for large times.
We transform the IDE into an ODE (thanks to "Abel Theorem"):

$$\begin{aligned} & X'''' + (2 - \pi\alpha^2) X''' + (2K+1) X'' + 2KX' + K^2 X \\ = & \quad -\frac{\alpha}{2t^{3/2}} (KX_0 + V_0) + K\alpha \frac{V_0}{t^{1/2}} \\ \stackrel{def}{=} & \quad f(t) \end{aligned}$$

whose solution is

$$X(t) = \sum_{i=1}^{4} C_i \, e^{\lambda_i t} + \int_{t_0}^{t} K(t-s) \, f(s) \, ds$$

$$\text{where} \qquad K(t-s) = \sum_{j=1}^{4} F_j(\{\lambda_i\}) \, e^{\lambda_j (t-s)}$$

A priori the characteristic polynomial could have roots λ_i with $\Re(\lambda_i) > 0$, anyway $X(t)$ behaves, for $t \to \infty$, as $f(t)$.
This can be seen by plugging $X(t)$, obtained as a solution of the ODE, into the original IDE, and deducing some conditions on the coefficients C_i, which assure that $X(t)$ is also a solution of the IDE. Such conditions assure that the behavior of $X(t)$, for $t \to \infty$, is the same as $f(t)$.

In case that the system is prepared, for $t < 0$, in such a way that

$$\int_{-\infty}^{0} \frac{\ddot{X}(s)}{\sqrt{t-s}}\, ds \neq 0 \tag{3}$$

the asymptotic behavior of the solution is affected.
If the system (fluid + sphere) is prepared for $t < 0$ in such a way that the sphere is brought from rest up to the velocity $\dot{X}(0)$ in a finite time interval, then

$$X(t) \sim \frac{C}{t^{3/2}} \qquad \text{per} \;\; t \to \infty \tag{4}$$

if this happens in the interval $(-\infty, 0]$ then

$$\frac{C_1}{t^{3/2}} \leq X(t) \leq \frac{C_2}{\sqrt{t}} \qquad \text{per} \;\; t \to \infty \tag{5}$$

with any possible behavior between $t^{-3/2}$ and $t^{-1/2}$.

Let us consider now a rotating sphere in a Stokes fluid. If the sphere rotates with angular velocity of the form

$$\Omega_0 e^{-i\omega t} \tag{6}$$

then the fluid exerts on the sphere a torque of the form

$$M = -\frac{8\pi}{3}\mu R^3 \Omega_0 e^{-i\omega t} A(\omega), \tag{7}$$

with

$$A(\omega) = 3 + \frac{2\omega\left[\sqrt{\omega} - i(\sqrt{\omega}+1)\right]}{1 + 2\sqrt{\omega} + 2\omega}. \tag{8}$$

For a sphere rotating with arbitrary angular velocity $\Omega(t)$, we obtain via Fourier transform the resulting torque

$$M = -8\pi\mu R^3 \left(\Omega(t) + \frac{2}{3\pi} \int_{-\infty}^{\infty} \dot{\Omega}(\tau) F(t-\tau)\, d\tau \right),$$

with

$$F(t-\tau) = \int_0^\infty \cos(\omega(t-\tau)) \frac{\sqrt{\omega}+1}{1+2\sqrt{\omega}+2\omega}\, d\omega + \int_0^\infty \sin(\omega(t-\tau)) \frac{\sqrt{\omega}}{1+2\sqrt{\omega}+2\omega}\, d\omega.$$

It's not trivial to notice that the two integrals, for $(t-\tau) > 0$, are equal and their value is

$$\frac{\sqrt{2\pi}}{4\sqrt{t}} - \frac{\pi}{4} e^{t/2} \mathrm{Erfc}\sqrt{t/2}$$

on the contrary for $(t-\tau) < 0$ they are opposite in sign, whence $F(t-\tau) = 0$ and the torque M takes the form

$$M = -8\pi\mu R^3 \left(\Omega(t) + \frac{2}{3\pi} \int_{-\infty}^{t} \dot{\Omega}(\tau) F(t-\tau)\, d\tau \right)$$

The equation of motion

$$I\,\dot{\Omega}(t) = M$$

in dimensionless form is

$$\dot{\Omega}(t) + \Omega(t) + \int_0^t \dot{\Omega}(s)\,F(t-s)\,ds = 0, \tag{9}$$

with $\Omega(s) = \Omega_0$ for $s \leq 0$. Equation (9) has the same structure of the equation for the rectilinear case, with a more complicated convolution kernel, which prevent to transform the IDE into an ODE.

The asymptotic behavior of the solution to (9) is

$$\Omega_0 \frac{\sqrt{\pi}}{\sqrt{2}\,t^{3/2}}$$

We proceed by applying the Laplace transform to the IDE (9)

$$\mathcal{L}\left\{\Omega\right\}(s) = \frac{\Omega_0 + \Omega_0 \mathcal{L}\{F\}(s)}{s + s\mathcal{L}\{F\}(s) + 1} \tag{10}$$

which explicitly reads

$$\mathcal{L}\left\{\Omega\right\}(s) = \Omega_0 \frac{\sqrt{2}\sqrt{s} + 1 + \pi}{\sqrt{2}s\sqrt{s} + (1+\pi)s + \sqrt{2}\sqrt{s} + 1}$$

and it can be decomposed by simple fractions

$$\Omega_0 \left(\frac{A_1}{\sqrt{s} + B_1} + \frac{A_2}{\sqrt{s} + B_2} + \frac{A_3}{\sqrt{s} + B_3} \right)$$

with

$$\begin{cases} B_1 + B_2 + B_3 = \frac{1+\pi}{\sqrt{2}} \\ B_1 B_2 + B_1 B_3 + B_2 B_3 = 1 \\ B_1 B_2 B_3 = \frac{1}{\sqrt{2}}, \end{cases}$$

$$\begin{cases} A_1 + A_2 + A_3 = 0 \\ A_1(B_2 + B_3) + A_2(B_1 + B_3) + A_3(B_1 + B_2) = 1 \\ A_1(B_2 B_3) + A_2(B_1 B_3) + A_3(B_1 B_2) = \frac{1+\pi}{\sqrt{2}}. \end{cases}$$

In order to determine the asymptotic behavior of the solution $\Omega(t) = \mathcal{L}^{-1}\left\{\Omega\right\}(t)$ we use the result

$$\begin{aligned} \mathcal{L}^{-1}\left\{\frac{1}{\sqrt{s}+a}\right\}(t) &= \frac{1}{\sqrt{\pi t}} - a\, e^{a^2 t}\,\mathrm{Erfc}(a\sqrt{t}) \\ &\overset{t\to\infty}{\sim} \frac{1}{2a^2\sqrt{\pi}\, t^{3/2}}, \end{aligned}$$

keeping into account the asymptotic expansion of Erfc

$$e^{z^2}\,\mathrm{Erfc}\, z \overset{z\to\infty}{\sim} \frac{1}{\sqrt{\pi}\, z}\left[1 + \sum_{m=1}^{\infty}(-1)^m \frac{1\cdot 3\cdots(2m-1)}{(2z^2)^m}\right].$$

Hence, for $t \to \infty$, $\Omega(t)$ results equal to

$$
\begin{aligned}
& \Omega_0 \left(\frac{A_1}{2B_1^2 \sqrt{\pi}\, t^{3/2}} + \frac{A_2}{2B_2^2 \sqrt{\pi}\, t^{3/2}} + \frac{A_3}{2B_3^2 \sqrt{\pi}\, t^{3/2}} \right) \\
= \quad & \Omega_0 \frac{A_1 B_2^2 B_3^2 + A_2 B_1^2 B_3^2 + A_3 B_1^2 B_2^2}{2B_1^2 B_2^2 B_3^2 \sqrt{\pi}\, t^{3/2}} \\
= \quad & \Omega_0 \frac{\sqrt{\pi}}{\sqrt{2}\, t^{3/2}}
\end{aligned}
$$

In case that the rotating sphere is also subjected to an external torque of the form $-K\,\theta$ (*torsion pendulum*) the equation of motion takes the form

$$\ddot{\theta}(t) + \dot{\theta}(t) + K\theta(t) + \int_0^t \ddot{\theta}(s)\, F(t-s)\, ds = 0,$$

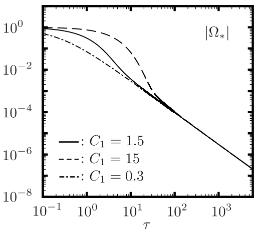
with $\theta(0) = \theta_0$, $\dot{\theta}(0) = \Omega_0$.
The solution $\theta(t)$ has the asymptotic behavior

$$\frac{\bar{C}}{t^{3/2}}, \tag{11}$$

(with a constant $\bar{C} \neq 0$), if $\Omega_0 \neq 0$, otherwise the asymptotic behavior turns out to be

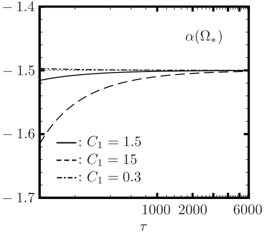
$$\frac{\widetilde{C}}{t^{5/2}}, \tag{12}$$

(with a constant $\widetilde{C} \neq 0$), if $\Omega_0 = 0$ and $\theta_0 \neq 0$.



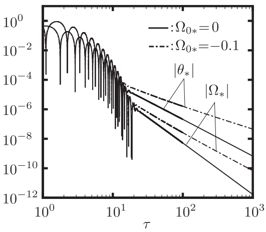
$|\Omega_*|$
: $C_1 = 1.5$
: $C_1 = 15$
: $C_1 = 0.3$
τ

(a)



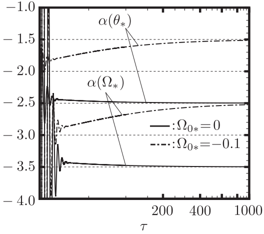
$\alpha(\Omega_*)$
: $C_1 = 1.5$
: $C_1 = 15$
: $C_1 = 0.3$
τ

(b)



:$\Omega_{0*} = 0$
:$\Omega_{0*} = -0.1$
$|\theta_*|$
$|\Omega_*|$
τ

(a)



$\alpha(\theta_*)$
$\alpha(\Omega_*)$
:$\Omega_{0*} = 0$
:$\Omega_{0*} = -0.1$
τ

(b)

From fractional diffusion equations to fractional shift operators

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Some notation

- **Shift (or translation) operator**

$$e^{cD_x}f(x) := \sum_{n=0}^{\infty} \frac{c^n D_x^n}{n!} f(x) = f(x+c),$$

for any analytic function $f : \mathbb{R} \to \mathbb{R}$ and $c \in \mathbb{R}$, where $D_x^n := d^n/dx^n$, for any $n \in \mathbb{N}$.

- **Symbol of pseudo-differential operator**
A pseudo-differential operator $\mathcal{A}$, w.r.t. $x \in \mathbb{R}$, is defined through its Fourier representation, i.e.

$$\mathcal{F}\{\mathcal{A}f(x);\xi\} = \int_{-\infty}^{+\infty} e^{ix\xi}\mathcal{A}f(x)dx = \widetilde{\mathcal{A}}(\xi)\widetilde{f}(\xi), \qquad \xi \in \mathbb{R},$$

where $\widetilde{\mathcal{A}}(\xi)$ is the symbol of $\mathcal{A}$.

- **Right-sided R.L. fractional derivative**

  $D^{\alpha}_{+,x}u(x) := \frac{1}{\Gamma(1-\alpha)}\frac{d}{dx}\int_{-\infty}^{x}\frac{u(s)}{(x-s)^{\alpha}}ds$, for $0 < \alpha < 1$, with symbol

  $$\widetilde{D}^{\alpha}_{+,x}(\xi) = (-i\xi)^{\alpha} = |\xi|^{\alpha} e^{-i\pi\alpha\, sign\xi/2}$$

- **Left-sided R.L. fractional derivative**

  $D^{\alpha}_{-,x}u(x) := \frac{1}{\Gamma(m-\alpha)}\left(-\frac{d}{dx}\right)^{m}\int_{x}^{+\infty}\frac{u(s)}{(s-x)^{1+\alpha-m}}ds$, for $x > 0$ and $\lfloor\alpha\rfloor = m$, with symbol

  $$\widetilde{D}^{\alpha}_{-,x}(\xi) = (i\xi)^{\alpha} = |\xi|^{\alpha} e^{i\pi\alpha\, sign\xi/2}$$

- **Riesz-Feller fractional derivative**

$\mathcal{D}^{\alpha}_{x,\theta}$ defined by

$$\mathcal{F}\left\{\mathcal{D}^{\alpha}_{x,\theta}u(x);\xi\right\} = \psi^{\alpha}_{\theta}(\xi)\mathcal{F}\left\{u(x);\xi\right\}, \quad \alpha \in (0,2],$$

with symbol

$$\psi^{\alpha}_{\theta}(\xi) := -|\xi|^{\alpha} e^{i\, sign\xi\, \theta\pi\alpha/2}, \qquad \theta = \arctan\left[-\beta \tan \pi\alpha/2\right]$$

which coincides with the Lévy exponent of an α-stable r.v. $\mathcal{S}^{\beta}_{\alpha}$ with asymmetry parameter β.

Gorenflo R., Kilbas A.A., Mainardi F., Rogosin S.V. (2014), *Mittag-Leffler Functions, Related Topics and Applications*, Springer.

Well-known result (Mainardi et al. (2001)): for $\alpha \in (0,2]$, $\nu \in (0,1]$,

$$\begin{cases} D^{\nu}_{+,t} u(x,t) = c\mathcal{D}^{\alpha}_{x,\theta} u(x,t) \\ u(x,0) = \delta(x) \\ \lim_{|x|\to\infty} u(x,t) = 0 \\ \frac{\partial}{\partial t} u(x,t)\Big|_{t=0} = 0, if \alpha > 1 \end{cases} \tag{1}$$

with $x \in \mathbb{R}$, $t \geq 0$.

- $\alpha = 2$, $\nu = 1$: (*standard diffusion eq.*) $\Rightarrow W(t)$ Brownian motion
- $\alpha \in (0,2)$, $\nu = 1$: (*space-fractional diffusion eq.*) $\Rightarrow \mathcal{S}^{\theta}_{\alpha}(t)$ α-stable process
- $\alpha = 2$, $\nu \in (0,1)$: (*time-fractional diffusion eq.*) $\Rightarrow W(\mathcal{L}_{\nu}(t))$ Brownian motion time-changed by the inverse of the ν-stable subordinator $\mathcal{L}_{\nu}$.

Mainardi F., Luchko Y., Pagnini G. (2001), The fundamental solution of the space-time fractional diffusion equation, *Fract. Calc. Appl. Analysis*, 4 (2),

First extension

Eq. (1) for $\nu > 1$: "*Higher-order fractional diffusion*" with $\alpha \in (0, 2]$:

$$\begin{cases} D^{\nu}_{-,t} u(x,t) = c\mathcal{D}^{\alpha}_{x,\theta} u(x,t) \\ u(x,0) = \delta(x) \\ \lim_{|x|\to\infty} u(x,t) = 0 \\ \frac{\partial}{\partial t} u(x,t)\big|_{t=0} = 0, if\, \alpha > 1 \end{cases}$$

with $x \in \mathbb{R}$, $t \geq 0$.

We obtain the subordinated stable process $\mathcal{S}^{\theta}_{\alpha}(\mathcal{A}_{1/\nu}(t))$.

- Lévy process (infinitely divisible for any t, stochastically continuous, stationary and independent increments) with symbol $[\psi^{\alpha}_{\theta}(\xi)]^{1/\nu}$
- Infinite variance, even for $\alpha = 2$
- For $\alpha = 2 \Rightarrow W(\mathcal{A}_{1/\nu}(t))$ subordinated Brownian motion

The proof is based on the following result (B.- D'Ovidio (2014)): the transition density of the stable process, i.e. $h_{1/\nu}$, is solution to the equation

$$\begin{cases} D^{\nu}_{-,\,t} h_{1/\nu}(x,t) = \frac{\partial}{\partial x} h_{1/\nu}(x,t) \\ h_{1/\nu}(x,0) = \delta(x) \end{cases},$$

for $x, \; t \geq 0$, $\nu \geq 1$.

B.-D'Ovidio (2014), Poisson processes with random drift, *Electr. J. Probab.*, 19 (122), 1-26.

Further extensions

What happens if we consider eq. (1)

- adding the pseudo-differential operator $e^{\mathcal{D}^{\alpha}_{x,\theta}}$?

  or

- replacing the time-fractional derivatives $D^{\nu}_{+,t}$ or $D^{\nu}_{-,t}$ with the fractional shift operator $e^{D^{\nu}_{+,t}}$ (for $\nu \in (0,1)$) or $e^{D^{\nu}_{-,t}}$ (for $\nu \geq 1$) respectively?

Definition

Fractional shift operators (FCO's)

Let $f : \mathbb{R}^+ \to \mathbb{R}$ be a continuous function, $c \in \mathbb{R}$, then

$$e^{cD^\nu_{+,x}} f(x) := \sum_{n=0}^{\infty} \frac{c^n}{n!} \underbrace{D^\nu_{+,x} \dots D^\nu_{+,x}}_{n-times} f(x),$$

for $\nu \in (0,1]$, while

$$e^{-cD^\nu_{-,x}} f(x) := \sum_{n=0}^{\infty} \frac{(-c)^n}{n!} \underbrace{D^\nu_{-,x} \dots D^\nu_{-,x}}_{n-times} f(x),$$

for $\nu \geq 1$, provided that the series converge.

For $\nu = 1 \Rightarrow$ standard shift operator.

B.- Fractional Gamma and Gamma-subordinated processes, arXiv (2014).

Properties of the FCO's

- The operators $e^{cD_x^\nu}$ and $e^{-cD_{-,x}^\nu}$ are well-defined in the *class of ν-analytic functions*, for which the fractional Taylor's expansion holds:

$$g(x) = \sum_{j=0}^{\infty} \frac{c_j x^{(j+1)\nu-1}}{\Gamma(\nu(j+1))},$$

where $\nu \in (0,1]$, $c_j = \Gamma(\nu)[x^{1-\nu} D_x^{j\nu} g(x)]$ and $D_x^{j\nu}$ is the sequential fractional derivative defined as $D_x^{j\nu} := \underbrace{D_x^\nu \ldots D_x^\nu}_{j-times}$.

Trujillo J. J., Rivero M., Bonilla, B. (1999), On a Riemann–Liouville generalized Taylor's formula, *J. Math. Anal. Appl.*, 231, 255–265.

- **Symbols of FSO's**

  Since

$$\mathcal{F}\{e^{cD_x^\nu} g(x);\theta\} = e^{c(-i\theta)^\nu}\widetilde{g}(\theta),$$

  and

$$\mathcal{F}\{e^{-cD_{-,x}^\nu} g(x);\theta\} = e^{-c(i\theta)^\nu}\widetilde{g}(\theta),$$

  for a "sufficiently good function" g. Thus the symbols are

$$\widetilde{e^{D_{\pm,x}^\nu}}(\xi) = e^{(\mp i\xi)^\nu}$$

- **Comparison with "generalized shift operators"**

  The fractional generalization of the shift operator is defined as follows: for an analytic function g,

$$e^{c(\partial/\partial x)^{\nu}} g(x) = \sum_{n=0}^{\infty} a_n H_n^{(\nu)}(x,c), \quad \nu > 0 \qquad (2)$$

where a_n are the coefficients of the usual series expansion $g(x) = \sum_{n=0}^{\infty} a_n x^n$ and $H_n^{(\nu)}$ are the Hermite-Kampé de Fériet polynomial of fractional order ν defined as

$$H_n^{(\nu)}(x,c) = n! \sum_{r=0}^{\infty} \frac{c^r x^{n-\nu r}}{\Gamma(n-\nu r+1) r!}.$$

In the special case of an integer order ν the operator in (2) coincides with the fractional shift operators defined here.

Dattoli G, Ricci P.E., Sacchetti D. (2003), Generalized shift operators and pseudo-polynomials of fractional order, *Appl. Math. Comput.*, 141, 215-224.

- **Eigenfunctions of $e^{cD^{\nu}_{+,x}}$ and $e^{-cD^{\nu}_{-,x}}$**

  Let $E_{\nu}(-\lambda x) = \sum_{j=0}^{\infty} \frac{x^j}{\Gamma(\nu j+1)}$ be the Mittag-Leffler function. For $\nu \in (0,1]$, $E_{\nu}(-\lambda x^{\nu})$ is the eigenfunction of $e^{cD^{\nu}_{+,x}}$ with scaling factor $e^{-c\lambda}$, i.e.

  $$e^{cD^{\nu}_{+,x}} E_{\nu}(-\lambda x^{\nu}) = e^{-c\lambda} E_{\nu}(-\lambda x^{\nu}).$$

  On the other hand, for $\nu > 1$, the eigenfunction of $e^{-cD^{\nu}_{-,x}}$ (with scaling factor $e^{-c\lambda}$) is represented by $e^{-x\lambda^{1/\nu}}$, i.e.

  $$e^{-cD^{\nu}_{-,x}} e^{-x\lambda^{1/\nu}} = e^{-c\lambda} e^{-x\lambda^{1/\nu}}.$$

- For $\alpha \in (0, 1]$, an alternative definition of FSO is given in D'Ovidio-Garra (2014), as follows:

$$e^{-cD_x^\alpha} f(x) = \int_0^{+\infty} f(x-s) h_\alpha(s,c) ds, \qquad t, c, x > 0,$$

where D_x^α is the Caputo fractional derivative and h_α is the transition density of an α-stable subordinator.

D'Ovidio M., Garra R. (2014), Multidimensional fractional advection-dispersion equations and related stochastic processes, *Electr. J. Probab.*, 19, n.61, 1-31.

In the Riesz-Feller case

Definition

Fractional R.-F. shift operator

Let $f : \mathbb{R}^+ \to \mathbb{R}$ be a continuous function, then

$$e^{c\mathcal{D}^{\alpha}_{x,\theta}} f(x) := \sum_{n=0}^{\infty} \frac{c^n}{n!} \underbrace{\mathcal{D}^{\alpha}_{x,\theta} \dots \mathcal{D}^{\alpha}_{x,\theta}}_{n-times} f(x),$$

for $\alpha \in (0,2]$, provided that the series converges.

The symbol of $e^{\mathcal{D}^{\alpha}_{x,\theta}}$ is $e^{\psi^{\alpha}_{\theta}(\xi)}$ and thus coincides with the Fourier transform of the α-stable r.v.

Second extension of eq. (1)

$$\begin{cases} D^{\nu}_{+,t} u(x,t) = [\mathcal{D}^{\alpha}_{x,\theta} - \lambda(I - e^{\mathcal{D}^{\alpha}_{x,\theta}})] u(x,t) \\ u(x,0) = \delta(x) \\ \lim_{|x|\to\infty} u(x,t) = 0 \\ \frac{\partial}{\partial t} u(x,t)\Big|_{t=0} = 0, \, if \, \alpha > 1 \end{cases}$$

with $x \in \mathbb{R}$, $t \geq 0$.

- $\alpha \in (0,2]$, $\nu = 1$: (*space-fractional*) $\Rightarrow \mathcal{S}^{\theta}_{\alpha}(t + N(t))$ α-stable process with drifted Poisson time
- $\alpha = 2$, $\nu \in (0,1]$: (*time-fractional*) $\Rightarrow W(\mathcal{L}_{\nu}(t) + N(\mathcal{L}_{\nu}(t)))$ Brownian motion with randomly-drifted Poisson time.

For $\lambda = 0$ we obtain eq. (1): $\Rightarrow \mathcal{S}^{\theta}_{\alpha}(\mathcal{L}_{\nu}(t))$.

Definition

Poisson process with drift

Let, for any $a > 0$ and $t \geq 0$,

$$N(t) + at$$

be the process with the following transition semigroup, for $\lambda > 0$ and $x \geq at$,

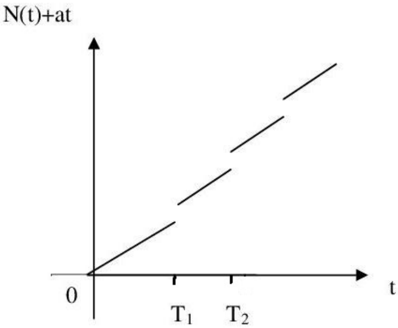
$$P_t f(x) = \mathbb{E} f(x - N(t) - at) = e^{-\lambda t} \sum_{k=0}^{\infty} \frac{(\lambda t)^k}{k!} f(x - k - at),$$

with initial datum $f \in L^1(\mathbb{R}_+)$.

- for $a = 0 \Rightarrow$ standard homogeneous Poisson process
- non-decreasing (a.s.) Lévy process $\Rightarrow$ subordinator.

B.-D'Ovidio (2014), Poisson processes with random drift, *Electr.J.Prob.*, 19 (122), 1-26.

Figure: Poisson process with drift



- For $\alpha \in (0,2]$, $\nu = 1$: $\mathcal{S}_\alpha^\theta(t + N(t))$ is a Lévy process with symbol

$$\psi_\theta^\alpha(\xi) - \lambda(1 - e^{\psi_\theta^\alpha(\xi)})$$

while the Lévy measure is given by

$$M(dx) = \lambda p_\alpha^\theta(x,1)dx + \frac{P}{x^{1+\alpha}} 1_{(0,+\infty)}(dx) + \frac{Q}{|x|^{1+\alpha}} 1_{(-\infty,0)}(dx),$$

where $p_\alpha^\theta(x,t)$ is the transition density of the stable process $\mathcal{S}_\alpha^\theta$.

Third extension of eq. (1)

$$\begin{cases} [I - e^{c_1 D^{\nu}_{\pm,t}}] u(x,t) = c_2 \mathcal{D}^{\alpha}_{x,\theta} u(x,t) \\ u(x,0) = \delta(x) \\ \lim_{|x|\to\infty} u(x,t) = 0 \\ \frac{\partial}{\partial t} u(x,t)\Big|_{t=0} = 0, if\, \alpha > 1 \end{cases} \qquad (3)$$

with $x \in \mathbb{R}$, $t \geq 0$, $c_i \in \mathbb{R}$, for $i = 1, 2$, $\alpha \in (0, 2]$ and $e^{c_1 D^{\nu}_{+,t}}$ when $\nu \in (0, 1)$, while $e^{c_1 D^{\nu}_{-,t}}$, when $\nu \geq 1$.

- $\alpha \in (0, 2]$, $\nu = 1$: (*space-fractional*) $\Rightarrow \mathcal{GS}^{\theta}_{\alpha}(t)$ Geometric stable process
- $\alpha \in (0, 2]$, $\nu \in (0, 1)$: (*time and space-fractional*) $\Rightarrow \mathcal{GS}^{\nu,\theta}_{\alpha}(t)$ fractional Geometric stable process
- $\alpha = 2$, $\nu \in (0, 1)$: (*time-fractional*) $\Rightarrow VG^{\nu}(t)$ fractional Variance Gamma process.

For $\alpha \in (0,2]$, $\nu = 1$: (*space-fractional*) $\Rightarrow \mathcal{GS}_\alpha^\theta(t)$:

Geometric stable process

- large class including Linnik, Laplace, Mittag-Leffler distributions
- weak limit of geometric compound sums of i.i.d. r.v.'s
- one-to-one correspondence with stable law: $\mathbb{E}e^{i\xi\mathcal{GS}_\alpha^\theta} = \frac{1}{1 - log \mathbb{E}e^{i\xi\mathcal{S}_\alpha^\theta}}$
- Lévy process
- heavy tails, unboundedness at zero: useful in modelling financial data (especially in cases of extreme changes of the fundamentals of a financial asset and market crashes).

For $\alpha \in (0,2]$, $\nu \in (0,1)$: (*time and space-fractional*) $\Rightarrow \mathcal{GS}_{\alpha}^{\nu,\theta}(t)$

Definition

Fractional Geometric Stable process

Let $\Gamma(t)$, $t > 0$ be the Gamma subordinator, then we define $\mathcal{S}_{\alpha}^{\theta}(\Gamma_{\nu}(t))$, $t \geq 0$, for $\alpha \in (0,2]$ and $\theta \leq min[\alpha, 2-\alpha]$, where

$$\begin{cases} \Gamma_{\nu}(t) := \Gamma(\mathcal{L}_{\nu}(t)), 0 < \nu < 1, \\ \Gamma_{\nu}(t) := \Gamma(\mathcal{A}_{1/\nu}(t)), \nu > 1, \end{cases}$$

for $\mathcal{L}_{\nu}$ and $\mathcal{A}_{1/\nu}$ independent of Γ.

Its transition density is solution to eq. (3).

B.(2014), Geometric stable processes and related fractional differential equations, *Electron. Commun. Probab.* 19, no. 13, 114.

For $\alpha = 2$, $\nu \in (0,1)$: (*time-fractional*) $\Rightarrow$ $VG^{\nu}(t)$

Definition

Fractional Variance Gamma process

Let $\Gamma(t)$, $t > 0$ be the Gamma subordinator, then we define $VG^{\nu}(t) := W(\Gamma_{\nu}(t))$, $t \geq 0$, $\theta \leq min[\alpha, 2-\alpha]$ where

$$\begin{cases} \Gamma_{\nu}(t) := \Gamma(\mathcal{L}_{\nu}(t)), 0 < \nu < 1, \\ \Gamma_{\nu}(t) := \Gamma(\mathcal{A}_{1/\nu}(t)), \nu > 1, \end{cases}$$

for $\mathcal{L}_{\nu}$ and $\mathcal{A}_{1/\nu}$ independent of Γ.

Its transition density is solution to

$$\begin{cases} [I - e^{c_1 D^{\nu}_{\pm,t}}]u(x,t) = c_2 \frac{\partial^2}{\partial x^2} u(x,t) \\ u(x,0) = \delta(x) \\ \lim_{|x| \to \infty} u(x,t) = 0 \\ \frac{\partial}{\partial t} u(x,t)\Big|_{t=0} = 0, \end{cases}$$

Important feature for applications (to model the logarithm of stock prices):

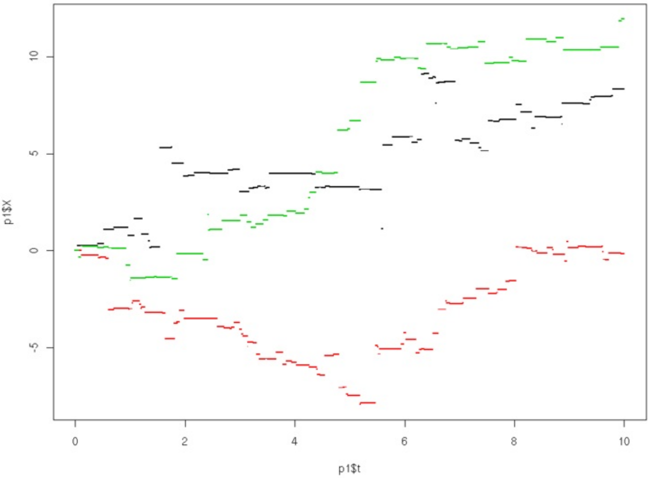
$$VG^{\nu}(t) \stackrel{d}{=} \Gamma_{\nu}(t)Z, \text{ for } \nu < 1 \text{ and } VG^{\nu}(t) \stackrel{d}{=} \overline{\Gamma}_{\nu}(t)Z, \text{ for } \nu > 1,$$

where Z is a standard normal r.v. independent of Γ_ν and $\stackrel{d}{=}$ denotes equality of f.d.d.'s. Thus $VG^{\nu}(t)$ is suitable to represent the stochastic variance or volatility, in financial models.

Alternative definition of fractional VG process (Kozubowski et al. (2006)): as $B_H(\Gamma(t))$ (where B_H is the fractional Brownian motion), for $H = 1/2$.

Kozubowski T.J., Meerschaert M.M., Podgorski K. (2006), Fractional Laplace motion, *Adv. Appl. Probab.*, 38, 451-464.

Figure: Variance Gamma process



Last extension:

Definition

Let $f : \mathbb{R}^+ \to \mathbb{R}$ be a continuous function, then

$$\mathcal{P}_x^{\alpha,\theta} f(x) := \sum_{n=1}^{\infty} \frac{1}{n} \underbrace{\mathcal{D}_{x,\theta}^{\alpha}, \ldots, \mathcal{D}_{x,\theta}^{\alpha}}_{n-times} f(x),$$

for $\alpha \in (0,2]$, $\theta \leq min[\alpha, 2-\alpha]$, provided that the series converges.

For $\alpha = 1$ and $\theta = 0 \Rightarrow \mathcal{P}_x^{1,0} f(x) = -log(1 - f(x))$.

The symbol of $\mathcal{P}_x^{\alpha,\theta}$ is given by $\widetilde{\mathcal{P}_x^{\alpha,\theta}}(\xi) = -log(1 - \psi_\theta^\alpha(\xi))$, for $|\xi| \leq 1$.

Then we consider the equation:

$$\begin{cases} \frac{\partial}{\partial t}u(x,t) = \mathcal{D}^{\alpha}_{x,\theta}u(x,t) + \mathcal{P}^{\alpha,\theta}_{x}u(x,t) \\ u(x,0) = \delta(x) \\ \lim_{|x|\to\infty} u(x,t) = 0 \\ \frac{\partial}{\partial t}u(x,t)\Big|_{t=0} = 0. \end{cases}$$

The solution is the transition density of the process

$$\mathcal{S}^{\theta}_{\alpha}(t+\Gamma(t)), t \geq 0,$$

where Γ is independent from $\mathcal{S}^{\theta}_{\alpha}$.

Lévy flights with absorption and collisions in combs

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Università Campus Bio-Medico, Rome, Italy

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In collaboration with

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Alexander Blumen, Freiburg Universität, Germany

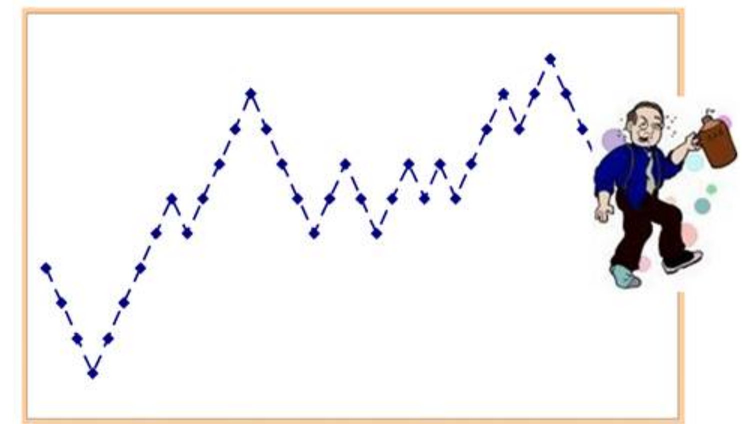
Luca Cattivelli, Scuola Normale, Pisa, Italy

Fabio Sartori, Università di Parma, Italia

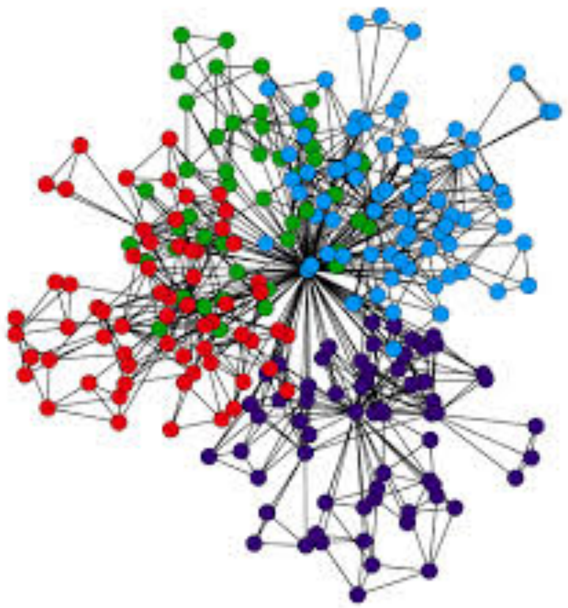
Workshop on Fractional Calculus and its Applications

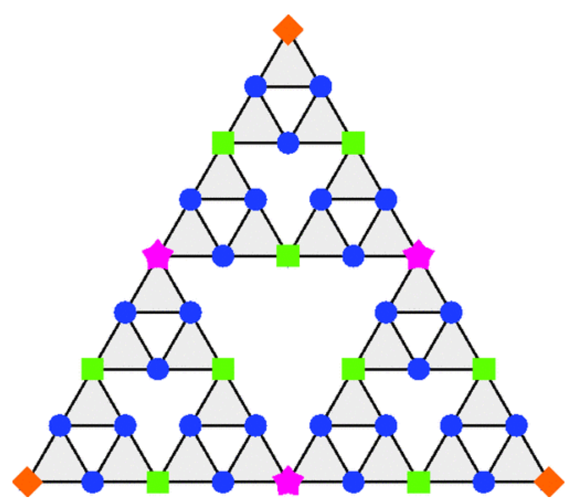
Roma3, March 11, 2015

An introductory statement



Simple random walks
Interacting random walks





in “complex graphs"

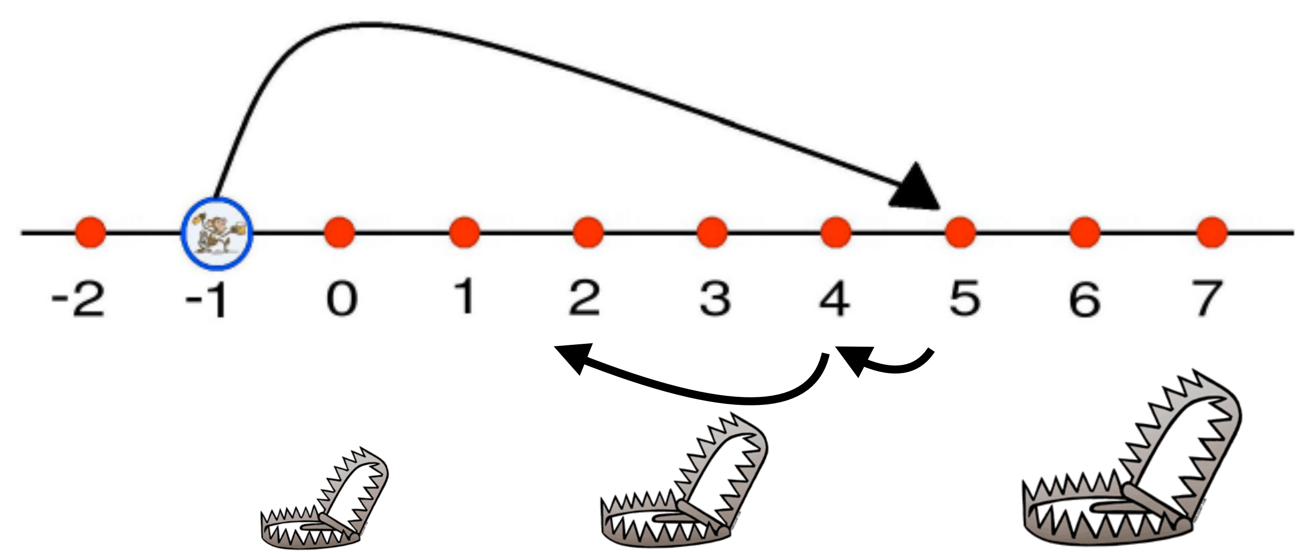
$$A_{ij} = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are adjacent;} \\ 0 & \text{otherwise.} \end{cases}$$

$$p_{ij} = \frac{A_{ij}}{z_i} = (\mathbf{Z}^{-1}\mathbf{A})_{ij}, \quad Z_{ii} = \sum_{j=1}^{V} A_{ij}$$

$$P_{ij}(t) = (\mathbf{p}^t)_{ij};$$

fractional calculus...

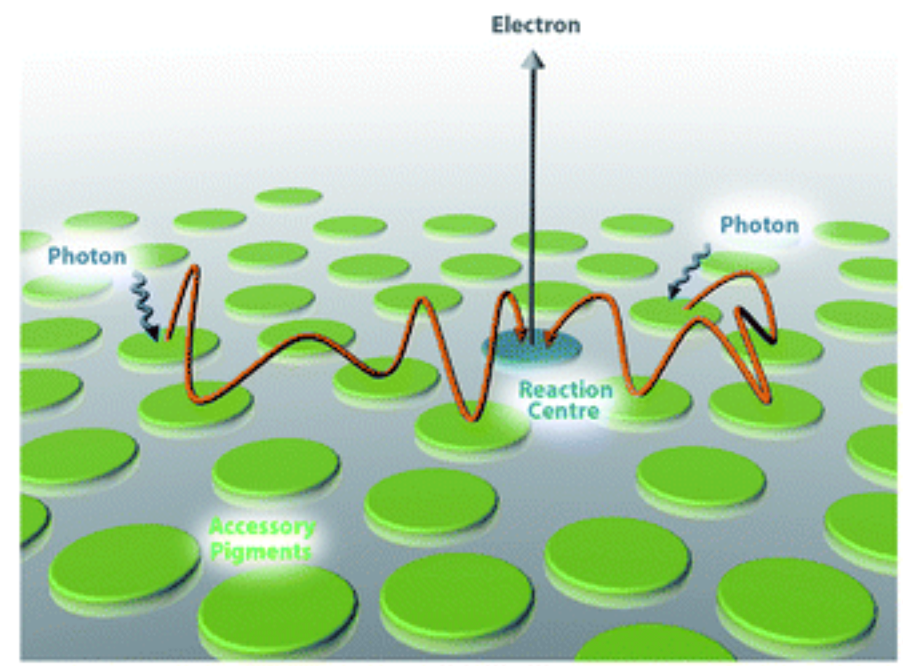
$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial^\mu \rho(x,t)}{\partial x^\mu} - a(x)\rho(x,t)$$



The type problem and its extension

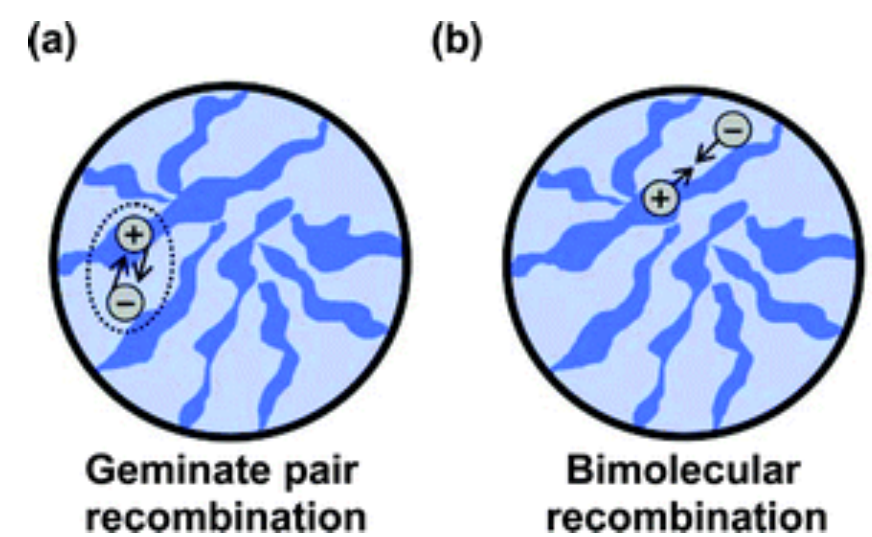
Type problem: determining whether a RW, embedded in a given structure, is certain to eventually visit a given site

Number of phenomena triggered by a diffusive particle reaching a reaction center, or a random observable reaching a threshold



Two particle Type problem: determining whether two RWs, embedded in a given structure, are certain to eventually meet

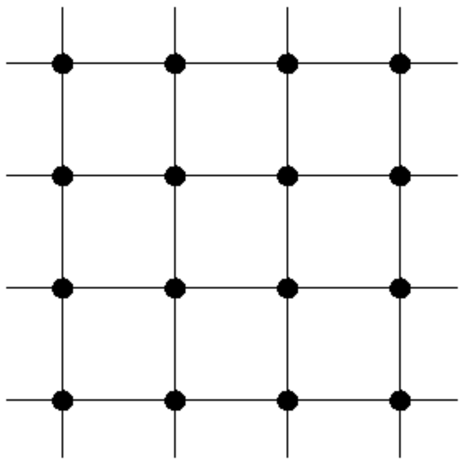
Number of phenomena described as encounters between entities performing random motion on an appropriate structure (e.g., prey-predator, chemical reaction kinetics, foraging)



Homogeneous structures

one-particle problem ↔ two-particle problem

→ the likelihood of a reaction is independent of whether both reactants are moving or only one



d ≤2 → certain return to origin

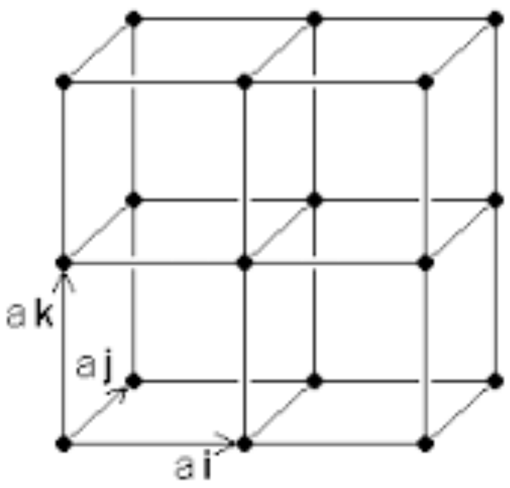
→ certain meeting

→ recurrent

d≥3 → finite probability to never return to origin

→ finite probability never meet

→ transient



There exist a wide class of structures (ubiquitous in nature) where different strategies bear qualitatively different results

There exist a wide class of structures (ubiquitous in nature) where different strategies bear qualitatively different results

One-particle recurrent & Two-particle transient

Chemical reaction kinetics → Reactions favored when either of the reagents is immobilized

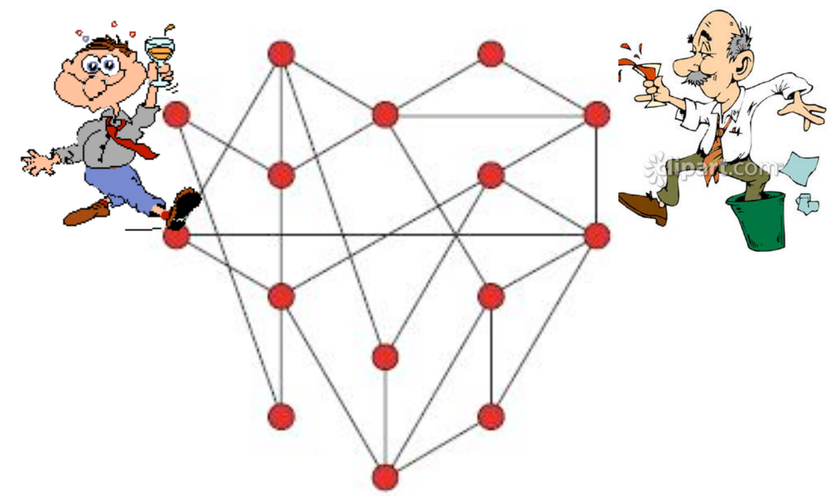
Pharmacokinetics → Drugs affect mobile and static traps differently

Foraging → Possible dynamic of food resource affects animal's fitness

Prey-predator interaction → Prey more likely to survive if keep moving

General results on multiple random walks

Very few rigorous results available



Graph: $\mathcal{G} = (\mathcal{V}, \mathcal{L})$

$\mathcal{V}$ **Collection of vertices**

$\mathcal{L} \in \mathcal{V} \times \mathcal{V}$ **Set of unoriented links between the vertices**

Simple Random Walk (RW) on $\mathcal{G}$ **:** **Markov chain that jumps from one vertex to a neighbor isotropically**

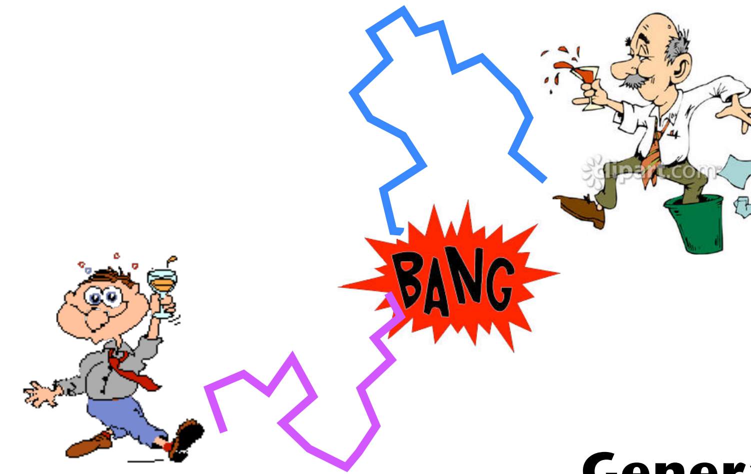
$$P_{vv'}(t) = (p^t)_{vv'}$$

Probability to move from v to v' in t steps
p: one step transition probability matrix

$$\mathcal{P}_{(vw)\to(v'w')}(t) = P_{vv'}(t) P_{ww'}(t)$$

Two RWs starting in v e w
Joint probability in t steps
If v'=w' →probability that the two walkers meet at time t

First-encounter Probability



Recall one-particle problem

$$\tilde{P}_{v\to v'}(\lambda) = \tilde{F}_{v\to v'}(\lambda)\tilde{P}_{v'\to v'}(\lambda) + \delta_{vv'}$$

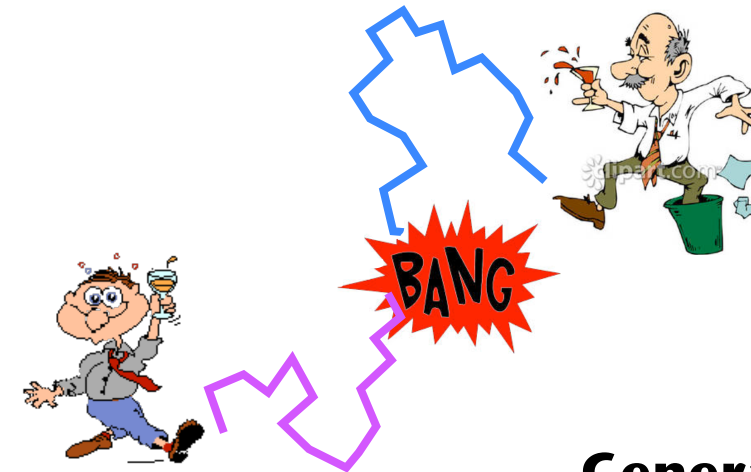
$$\tilde{F}_{vv'}(1) = 1 \Leftrightarrow \tilde{P}_{vv'}(1) = \infty$$

Generating function

$$\tilde{f}(\lambda) = \sum_{t=0}^{\infty} f(t)\lambda^t$$

A walk is recurrent (transient) iff
(any) site is visited an infinite (finite) number of times

First-encounter Probability



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A walk is recurrent (transient) iff (any) site is visited an infinite (finite) number of times

Two-particle problem... $\mathcal{F}_{(vw)\to(v')}(t)$

$$\tilde{\mathcal{P}}_{(vw)\to(v')}(\lambda) = \sum_{l\in\mathcal{V}} \tilde{\mathcal{F}}_{(vw)\to(l)}(\lambda)\tilde{\mathcal{P}}_{(ll)\to(v')}(\lambda) + \delta_{vv'}\delta_{wv'}$$

→ **Matricial relation between** $\tilde{\mathcal{P}}$ **and** $\tilde{\mathcal{F}}$

$\mathcal{F}_{(vw)\to(v')}(t)$ **First-encounter Probability**

Generating function

$$\tilde{f}(\lambda) = \sum_{t=0}^{\infty} f(t)\lambda^t$$

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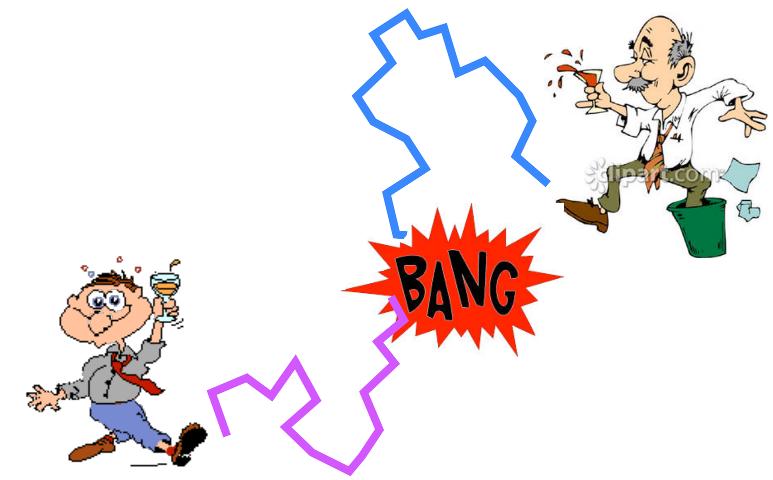
→ **Matricial relation between** $\tilde{\mathcal{P}}$ **and** $\tilde{\mathcal{F}}$



Two-particle type problem

Definition. A graph is two-particle recurrent if the probability that two particles will ever meet is 1, i.e.

$$\sum_{t=0}^{\infty}\sum_{v'\in\mathcal{V}} \mathcal{F}_{(vw)\to v'}(t) = \sum_{v'\in\mathcal{V}} \tilde{\mathcal{F}}_{(vw)\to v'} = 1 \qquad \forall(v,w)\in\mathcal{V}$$

Should the graph not satisfy this condition → two-particle transient

Special case: homogeneous infinite graphs

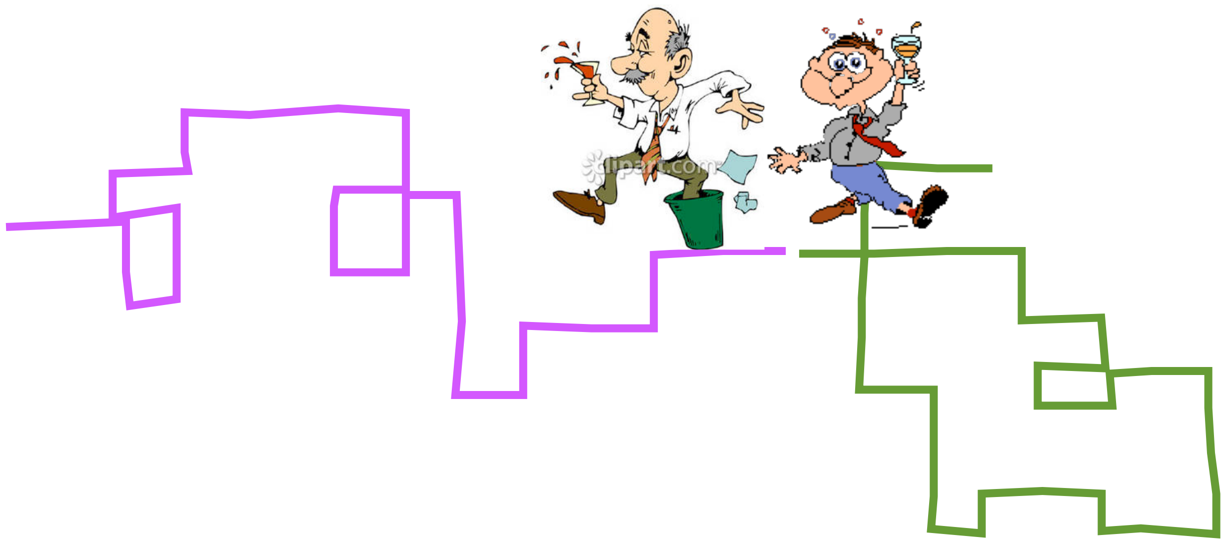
$$\mathcal{P}_{(vw)}(t) = \sum_{v' \in \mathcal{V}} P_{vv'}(t) P_{wv'}(t) = P_{vw}(2t)$$

Recurrent graph is two-particle recurrent
Transient graph is two-particle transient

General case

Transient graph with bounded degree ⇒ Finite probability that two independent walkers never meet

There exist graphs
one-particle recurrent
but two-particle transient



Finite Collision property

Definition. A graph has the finite collision property if the probability that two random walkers will meet only a finite number of times is 1.

$$\mathcal{P}_{(vw)}(N < \infty) = 1,\ \forall v, w \in \mathcal{V} \quad \Rightarrow \quad \mathcal{G} \qquad \textbf{finite collision property}$$

$$\mathcal{P}_{(vw)}(N = \infty) = 1,\ \forall v, w \in \mathcal{V} \quad \Rightarrow \quad \mathcal{G} \qquad \textbf{infinite collision property}$$

[0-1 Law: $\mathcal{P}_{(vw)}(N = \infty) \in \{0, 1\}$ **]**

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[0-1 Law: $\mathcal{P}_{(vw)}(N = \infty) \in \{0, 1\}$ **]**

$$\forall (v, w) \in \mathcal{V}$$

$$\mathcal{P}_{(vw)}(N = \infty) = 1 \quad \Longleftrightarrow \quad \sum_{v' \in \mathcal{V}} \tilde{\mathcal{F}}_{(vw) \to v'} = 1$$

$\mathcal{G}$ **infinite collision property** — $\mathcal{G}$ **two-particle recurrent**

$$\not\Uparrow$$

$\mathcal{G}$ **one-particle recurrent**

Th. A graph has the infinite collision property iff it is two-particle recurrent.

Finite Collision property

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$\mathcal{G}$ **infinite collision property** $\qquad$ $\mathcal{G}$ **two-particle recurrent**

$$\not\Uparrow$$

$\mathcal{G}$ **one-particle recurrent**

one-particle recurrence $\not\Rightarrow$ **two-particle recurrence**

Th. A graph has the infinite collision property iff it is two-particle recurrent.

Comb lattices

Definition. Given a graph G, let the Comb(G) be the graph with vertex set V(G)xZ and edge set

$$\{[(x,n),(x,m)] : |m-n| = 1\} \cup \{[(x,0),(y,0)] : [x,y] \text{ is an edge in } \mathbf{G}\}$$

➝ we attach a copy of Z at each vertex of the graph G.

Let G be any recurrent infinite graph with constant vertex degree. Then Comb(G) has the finite collision property

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2012, Vol. 48, No. 4, 922–946
DOI: 10.1214/12-AIHP481

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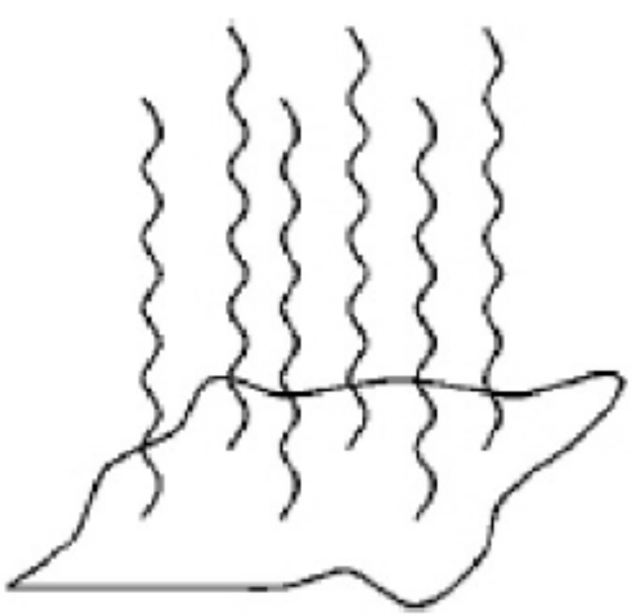
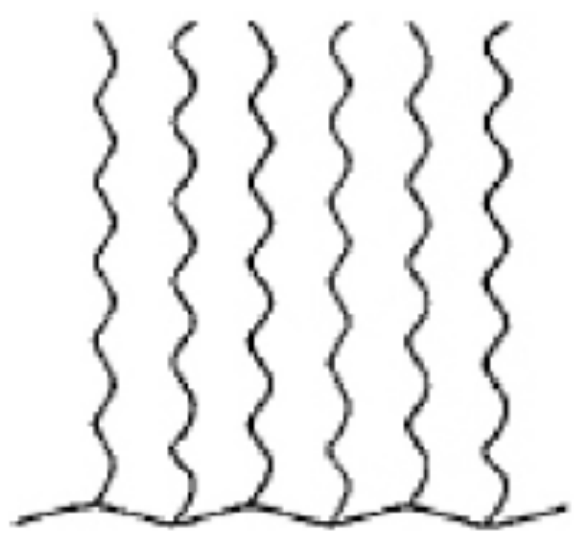
Collisions of random walks

Martin T. Barlow[a,1], Yuval Peres[b] and Perla Sousi[c]



Brush



Comb

Elect. Comm. in Probab. **9** (2004), 72–81
ELECTRONIC COMMUNICATIONS in PROBABILITY

RECURRENT GRAPHS WHERE TWO INDEPENDENT RANDOM WALKS COLLIDE FINITELY OFTEN

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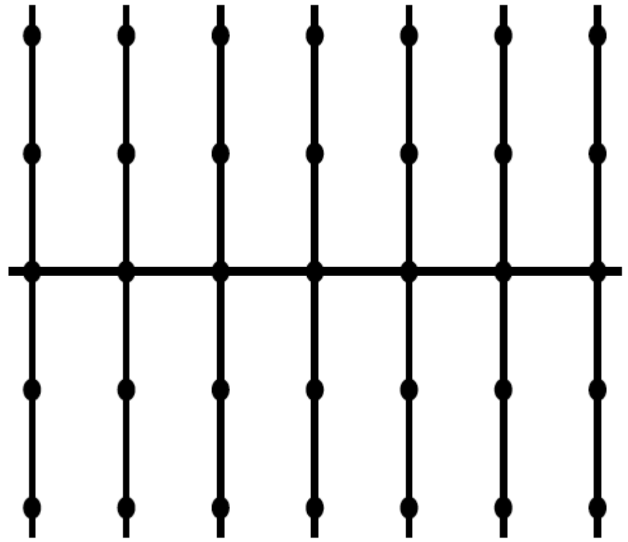
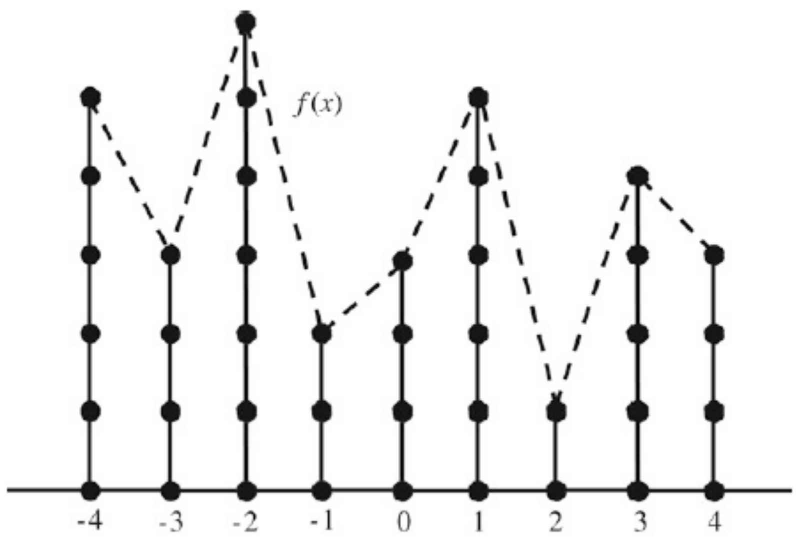
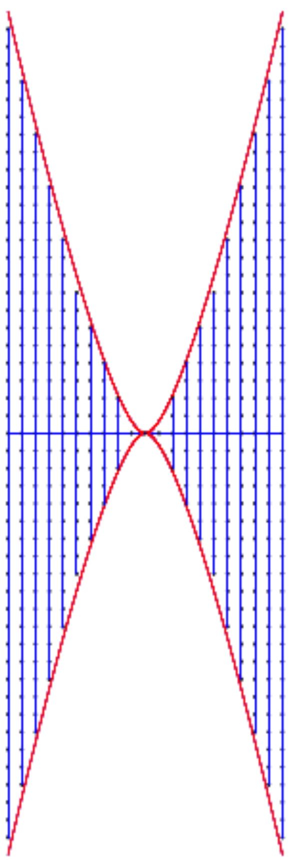
Comb(Z) has the finite collision property



$Z \subset$ Comb(Z) $\subset Z^2$
both Z and Z^2 have infinite collision property
$\Rightarrow$ infinite collision property not simply monotone

→ Probing
subgraphs of Comb(Z)...





2. Let f: Z → R^+. It induces a wedge comb Comb(Z, f), with

$V = \{(x, y) : x, y \in Z, -f(x) \leq y \leq f(x)\}$ vertex set

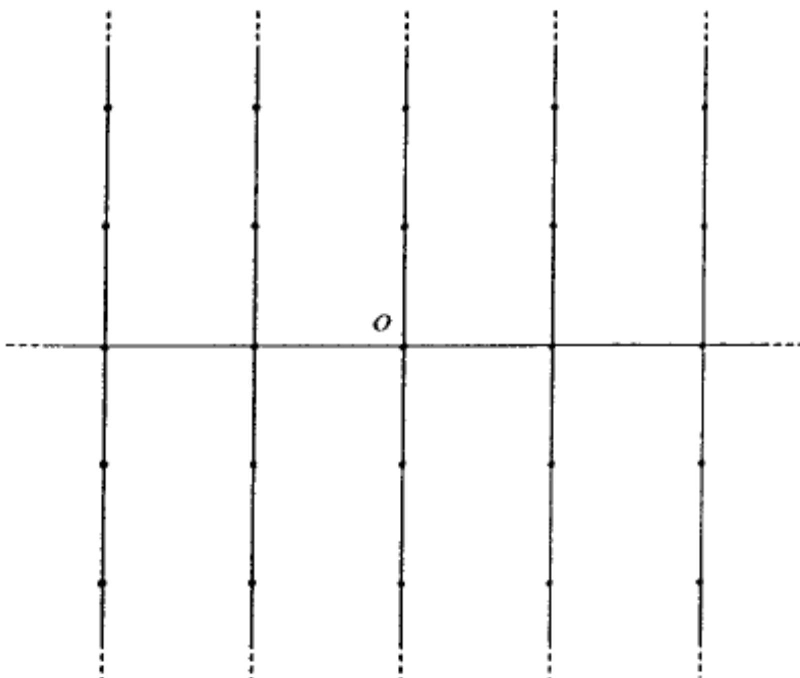
$\{[(x, n), (x,m)] : |m - n| = 1\} \cup \{[(x, 0), (y, 0)] : |x - y| = 1\}$ edge set

Let $\alpha > 0$ and $f(n) = |n|^\alpha$, for each n

Comb(Z, f) infinite collision property $\Leftrightarrow \alpha \leq 1$

Comb lattices

2d-comb



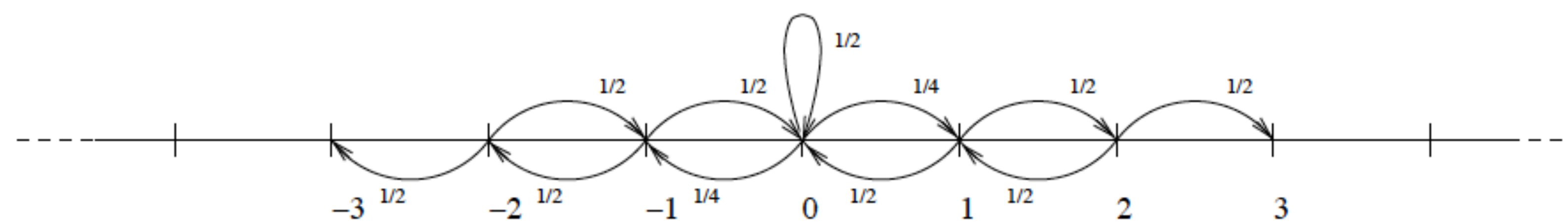
Inhomogeneity → qualitative different behaviors along different dimensions

Eg: 2d, asymptotics of the vertical component coincide (to leading order) with the corresponding estimates for the simple random walk on Z

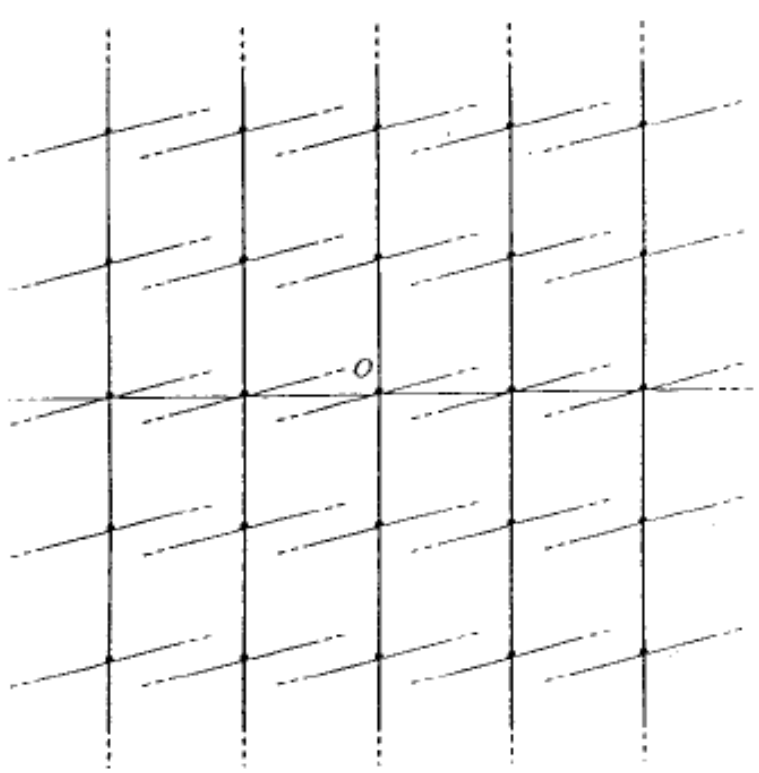
Vol. 11 (2006), Paper no. 45, pages 1184–1203.

Asymptotic behaviour of the simple random walk on the 2-dimensional comb *

Daniela Bertacchi



3d-comb



Eg: Splitting of local spectral dimension (3/2) and average spectral dimension (1)

D. CASSI and S. REGINA, *Mod. Phys. Lett. B* **06**, 1397 (1992). DOI: 10.1142/S0217984992001101

RANDOM WALKS ON d-DIMENSIONAL COMB LATTICES

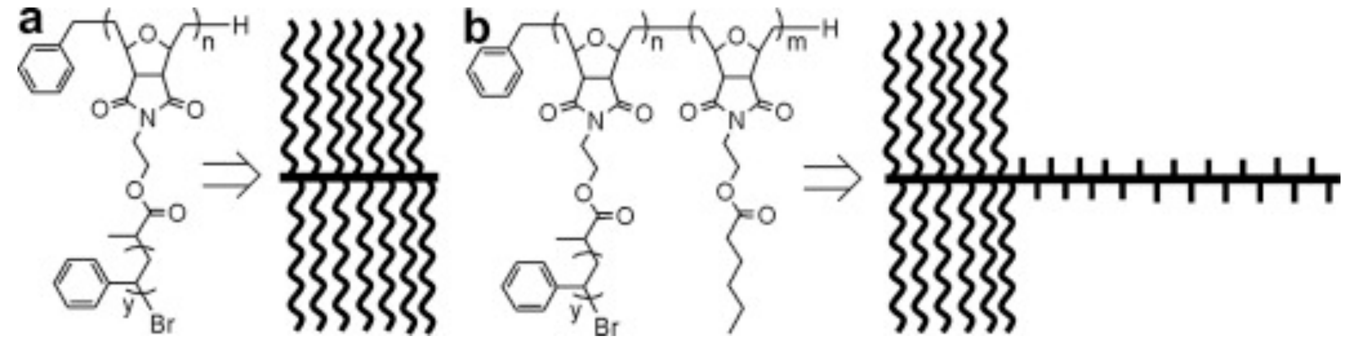
$$\tilde{d} = -2 \lim_{t\to\infty} \frac{\log(^2P_0(t))}{\log t} .$$

$$\tilde{d}_d = 2\left(1 - \frac{1}{2^d}\right) .$$

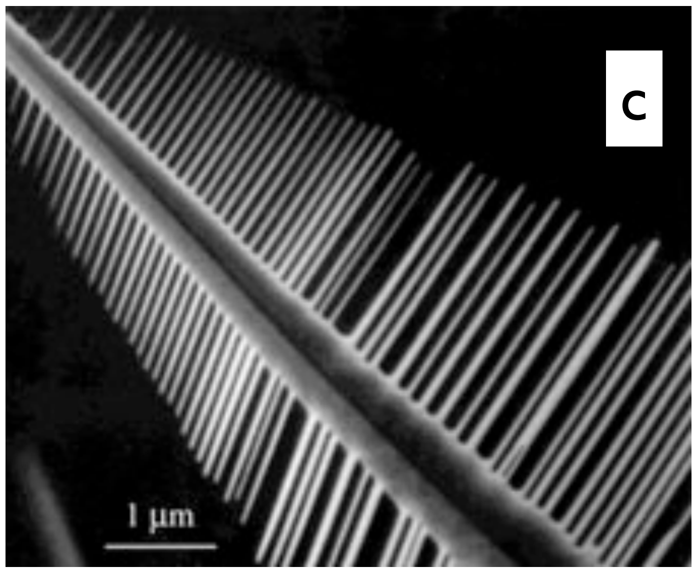
Spectral dimension for the d-dimensional comb

Realizations

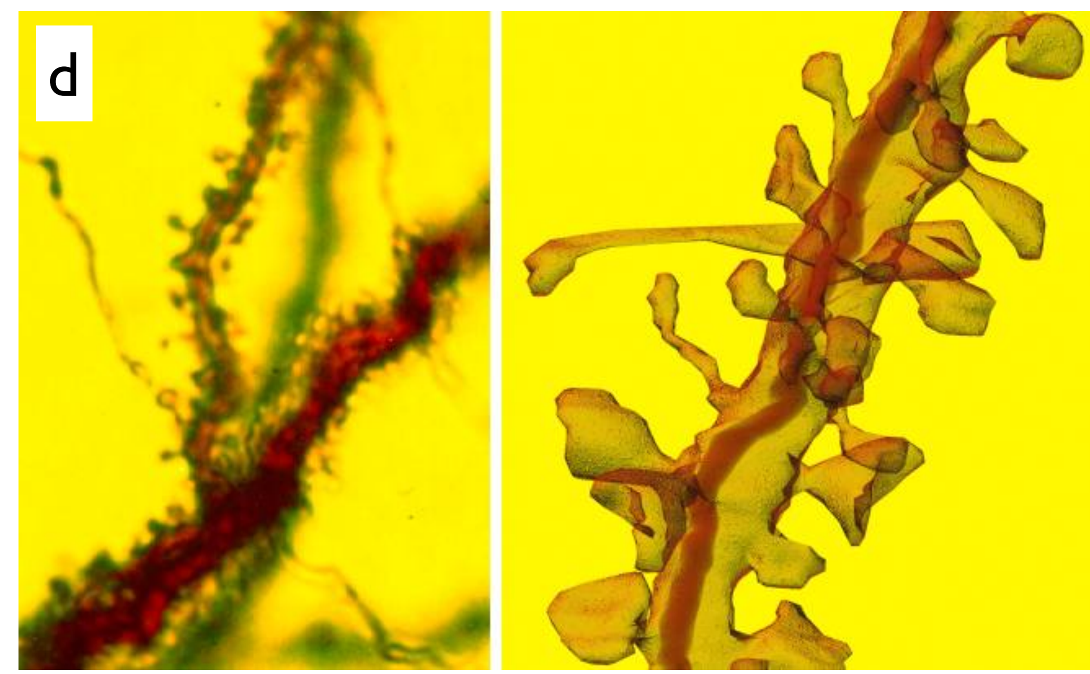
Comb polymers: Molecules consisting of a main chain with branch points and linear side chains. If arms are identical → regular



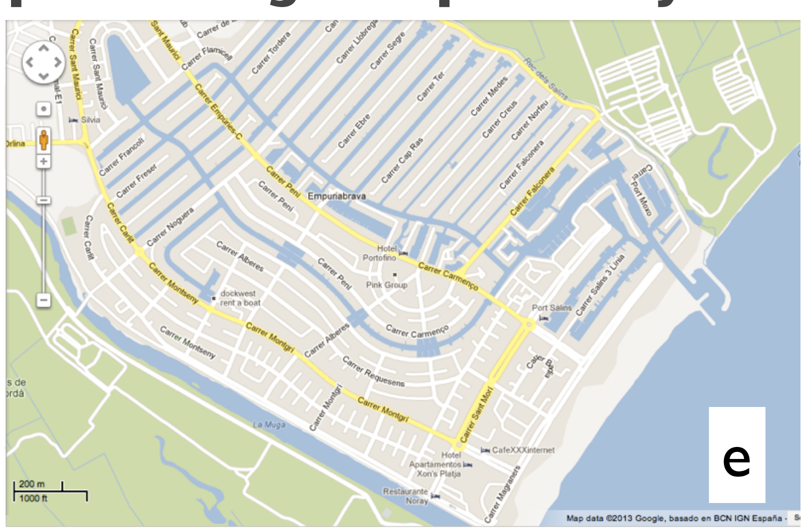
(a) A chemical structure and schematic of a comb polymer with poly(styrene) arms. (b) A comb block copolymer with a schematic of its structure.



(c) Nanowire combs are the products of spontaneous self-organization. One grows needles of zinc oxide, which are decorated with dendritic side-branches regularly spaced



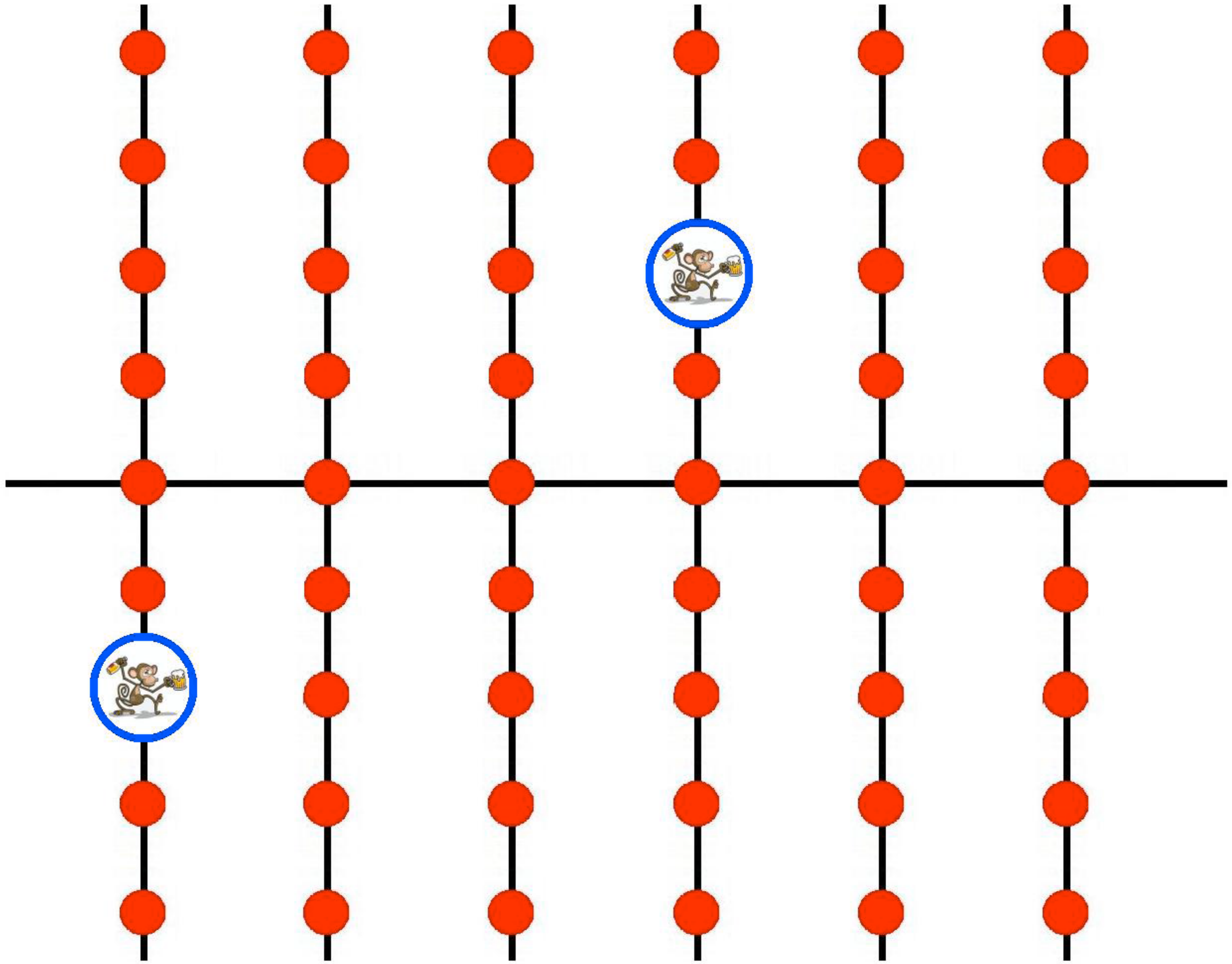
(d) Spiny dendrites are dendrites with lateral small protrusions (dendritic spines) located on the surface. They can be found on the dendrites of most principal neurons in the brain and their physiological role is still unclear although key elements in neuronal information processing and plasticity



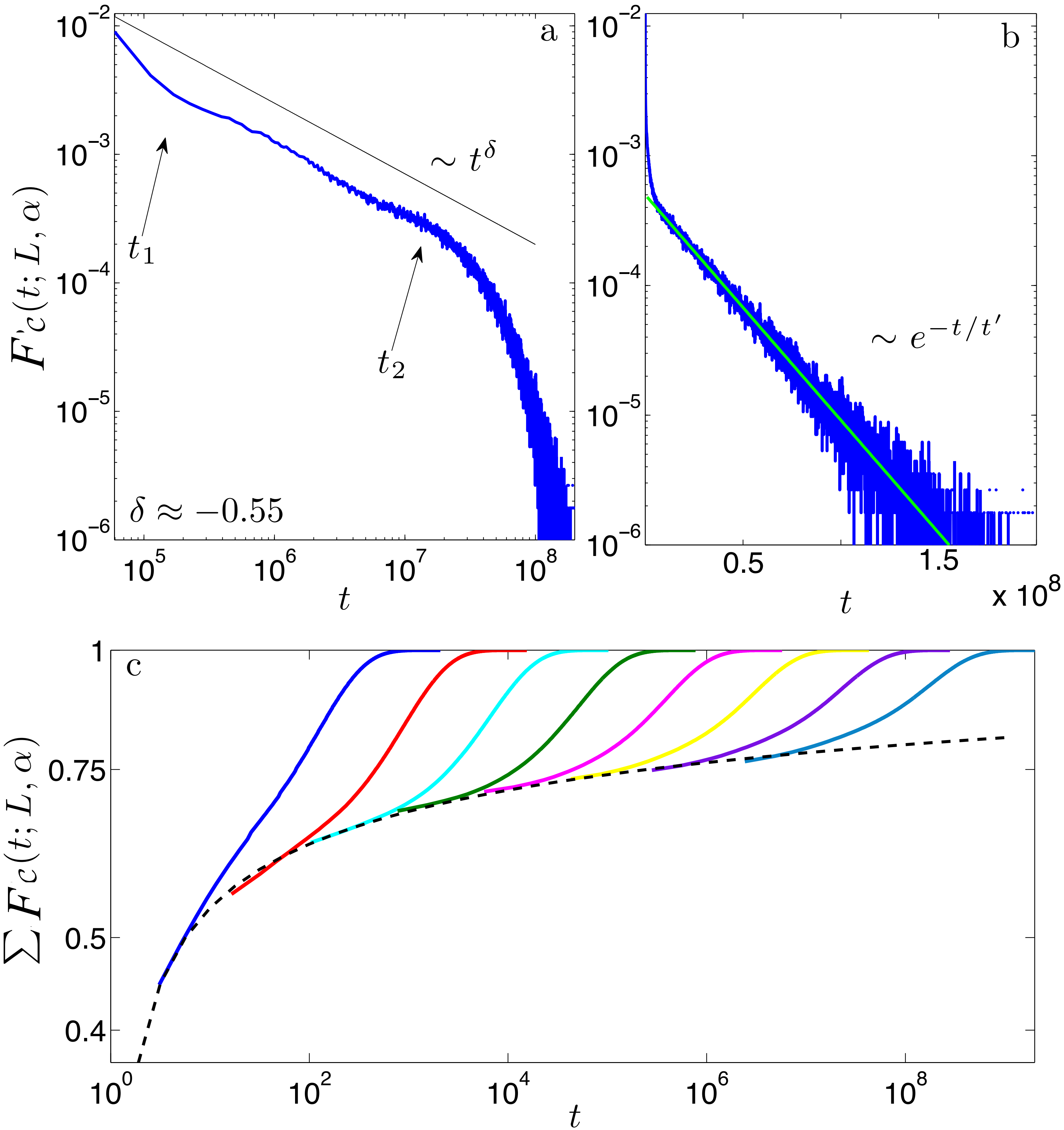
(e) Empuriabrava (Spain)

… Possibility of producing quantum devices, e.g. arrays of Josephson junctions, etc.

First-encounter probability in finite-size systems



First-encounter probability in finite-size systems



t_1<t
Still memory of initial positions

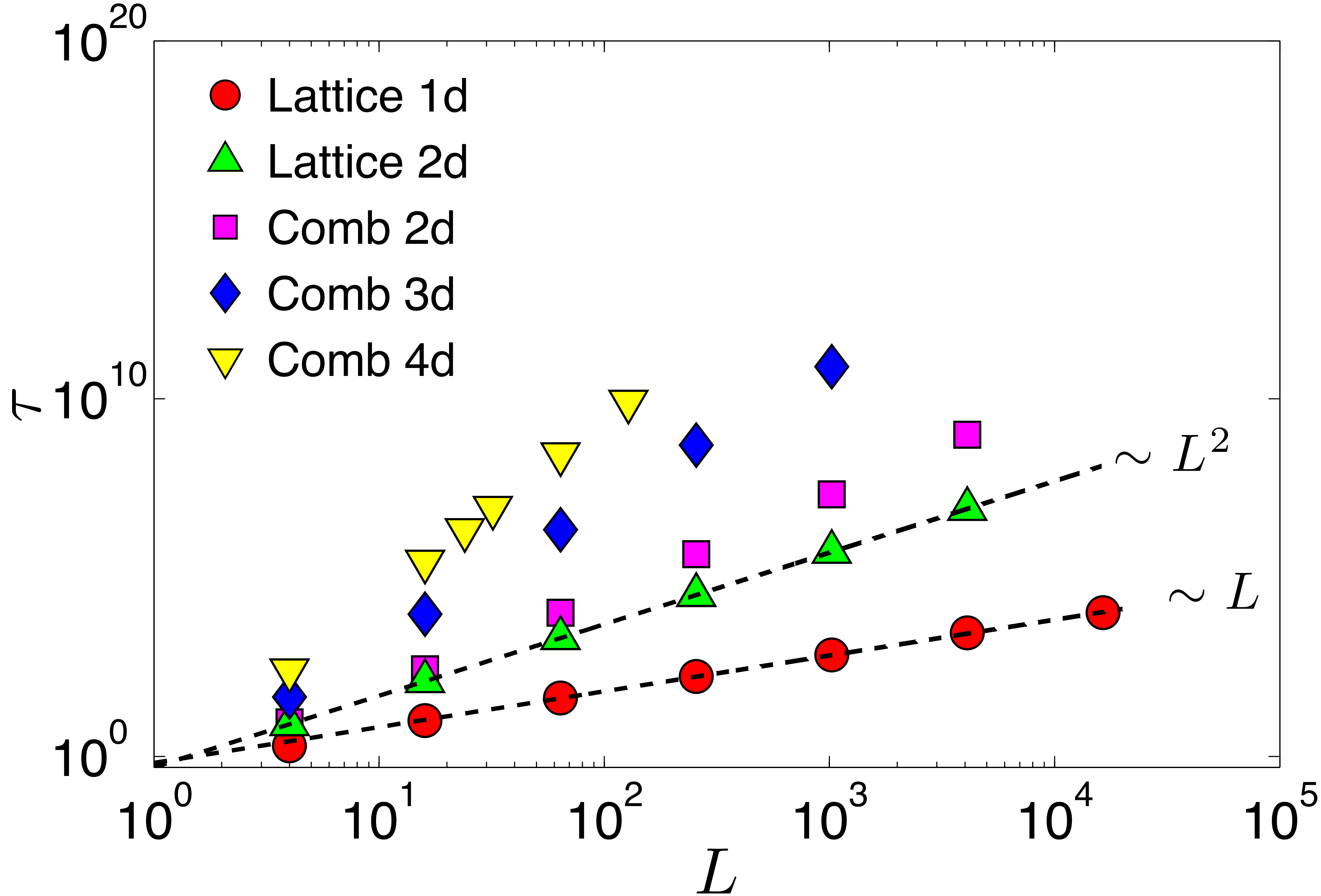
t_1<t<t_2
Probability distribution decays as a power laws, as expected for an infinite structure

t>t_2
Exponential decay, finite size effects emerge

Envelope
Estimate for $F_c(t)$: grows with rate scaling as 1/√logt and saturation value <1

Mean first-encounter time

$$\tau_{\mathcal{C}}(L,\alpha) \equiv \sum_{t=0}^{\infty} t\, F_{\mathcal{C}}(t;L,\alpha)$$



L is linear size
Square lattice/comb
PBC or OBC

Sketch for C_2

#steps for the two CTRWs to first share the same tooth → L

Time taken for each step → L

Probability for the two RWs to first meet before one escapes on the backbone → $P \sim \int_{-L}^{L} \frac{1}{L} \arctan\left(\frac{1}{y}\right) dy \sim \int_0^L \frac{1}{L}\frac{1}{y+1} dy \sim \frac{\log(L)}{L}$

⇒ #trials for the event to occur → L/log(L)

$$\tau \sim L^3 / \log L$$

$\tau \sim L^{d+1} / \log L$ **Mean first-encounter time on C_d**

$\zeta \sim L^d$ **Mean first-passage time on C_d**

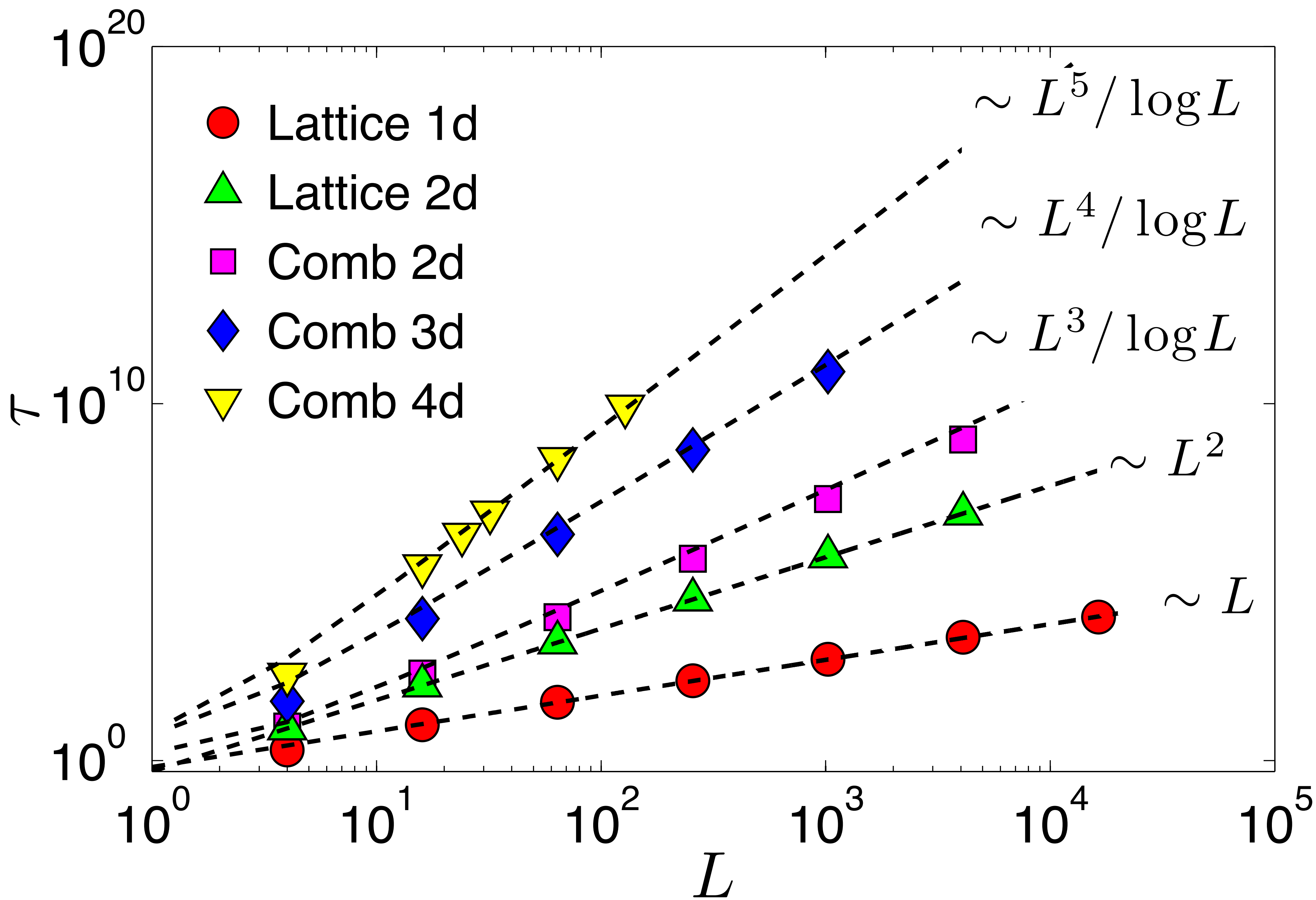
Slow encounters of particle pairs

Mean first-encounter time

$$\tau_{\mathcal{C}}(L,\alpha) \equiv \sum_{t=0}^{\infty} t\, F_{\mathcal{C}}(t; L, \alpha)$$

$\tau \sim L^d$ **d-dimensional lattices**

$\tau \sim L^{d+1}/\log L$ **d-dimensional combs**

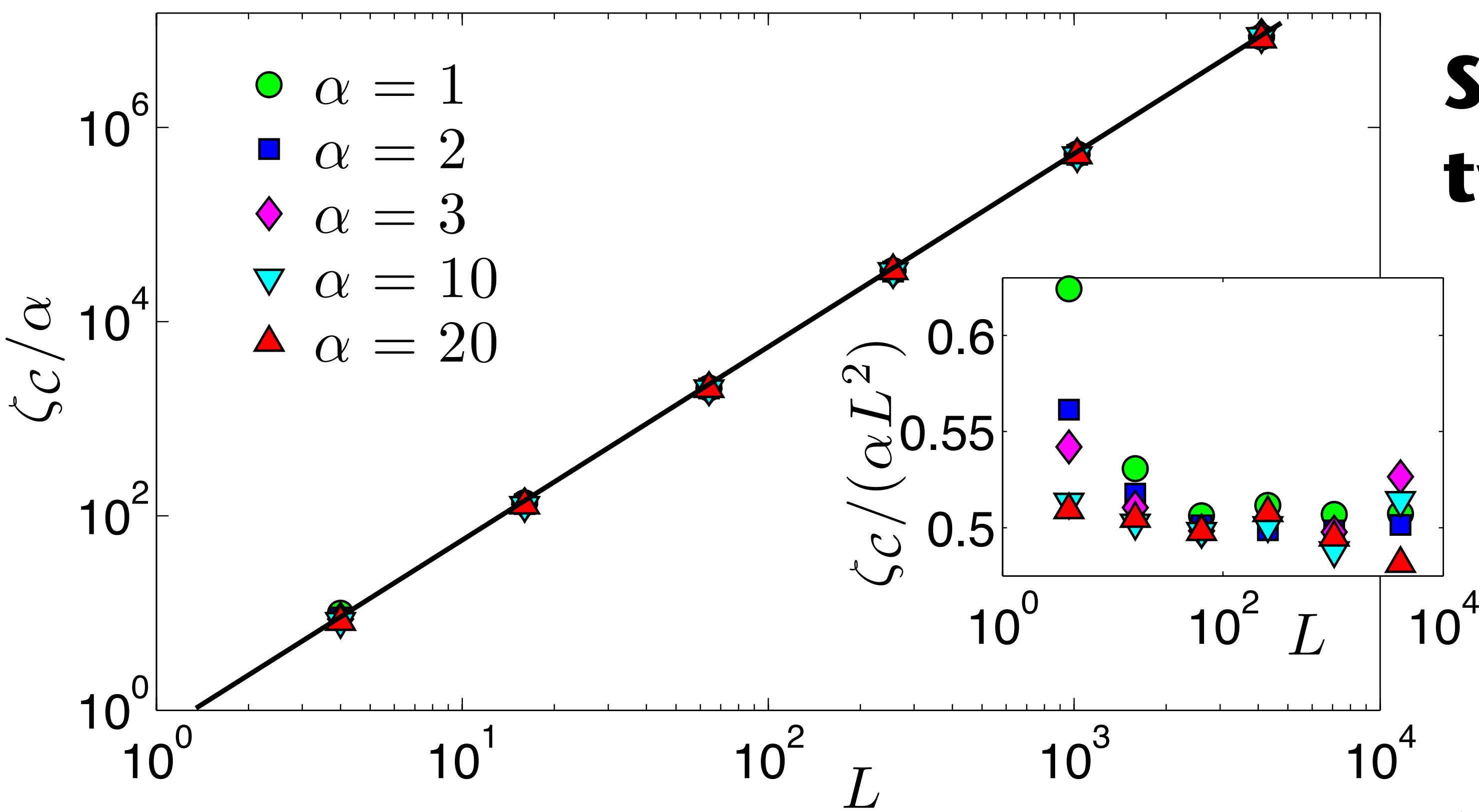


L is linear size
Square lattice/comb
PBC or OBC

$$\tau \sim V$$

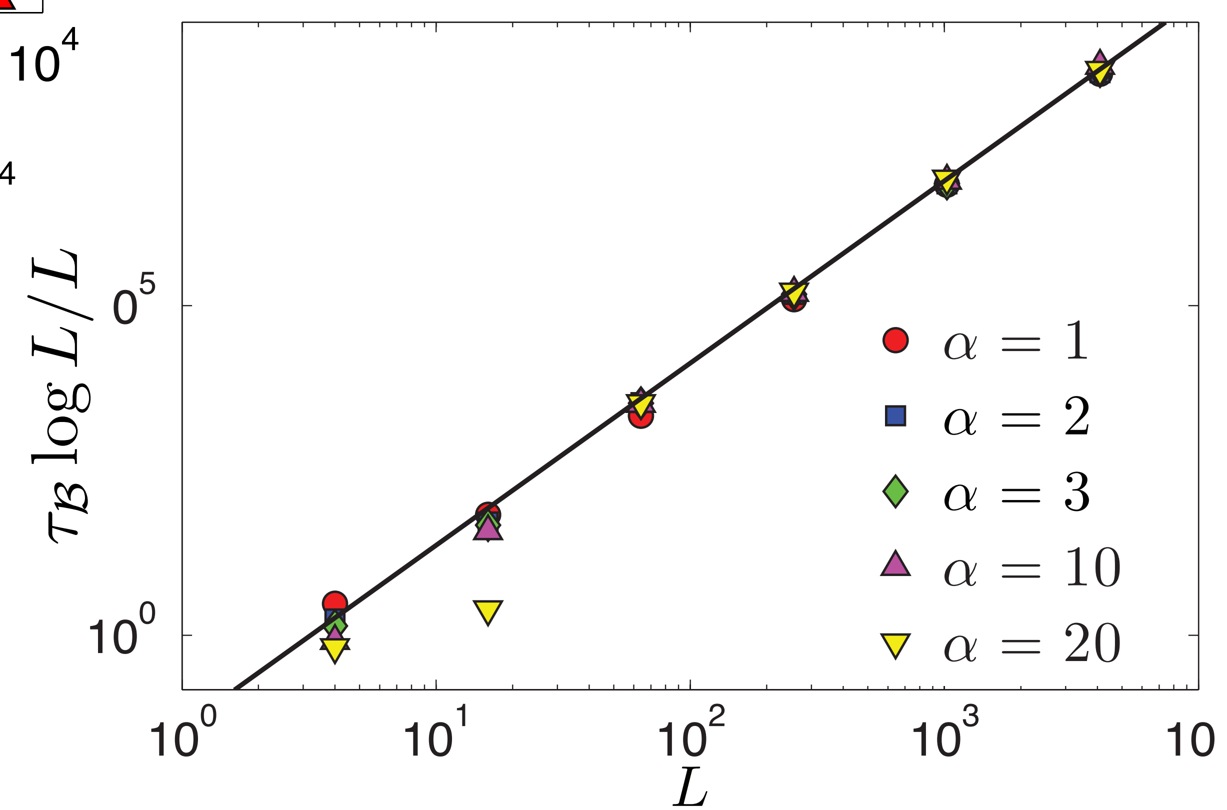
$$\tau \sim V \frac{L}{\log L}$$

On comb there is a correction due to inhomogeneous distribution of encounter sites
→ tau diverges superlinearly with volume

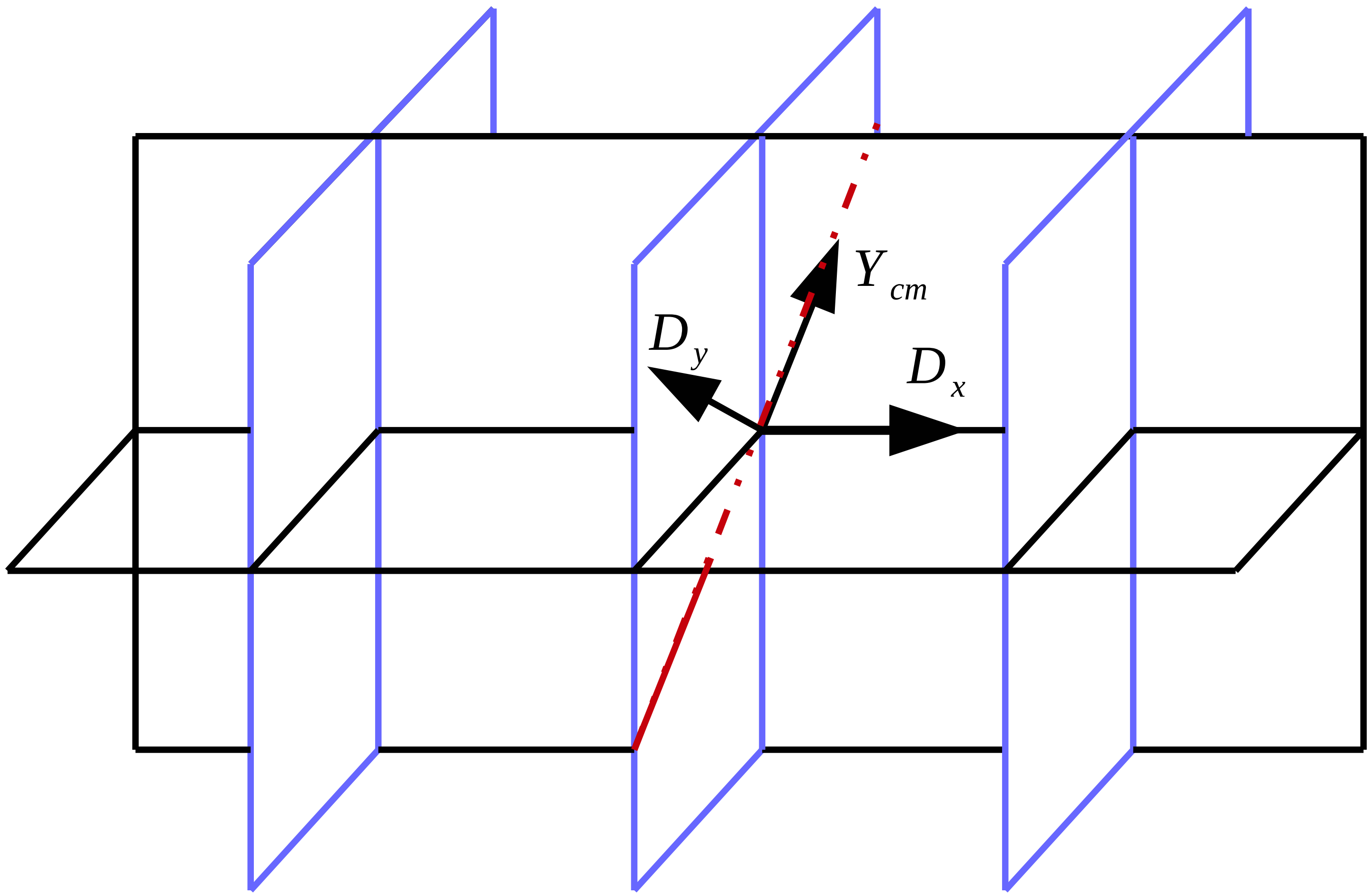


Slowing down genuinely two-particle effect

Robust w.r.t. elements of
- randomness
- disorder
- loops

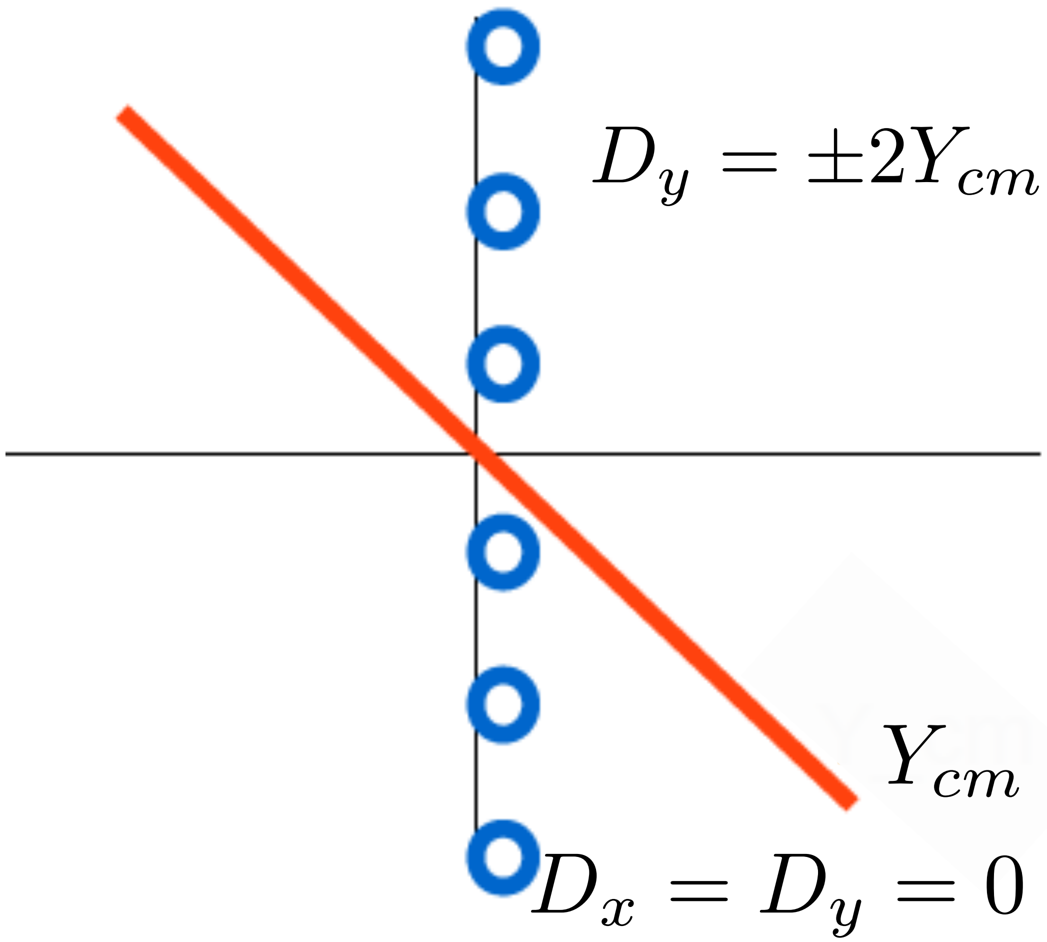


Mapping: two RWs in $\mathcal{C}$ → one RW in $\mathcal{M}$



- D_x and D_y relative distance between the RWs along x e y direction
- X_{cm} and Y_{cm} coordinate for the center of mass
- Exploit translation symmetry along x direction → 3 variables
- Encounter corresponds to red line
- $D_x=0$ → RW on the same tooth → $h(|D_y|) \sim |D_y|^{-3/2}$
- Probability to visit the red line before leaving the plane $D_x=0$
  → $a(|D_y|) \sim 1/|D_y|$

Finite Probability of never crossing the red line
→ Finite collision property



Effective description in terms of 1d Levy flight with power-law absorption

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\partial^\mu \rho(x,t)}{\partial x^\mu} - a(x)\rho(x,t),$$

$$a(x) = \frac{K}{|x|^\alpha + 1} \qquad p(x) \sim \frac{1}{|x|^{1+\mu}}$$

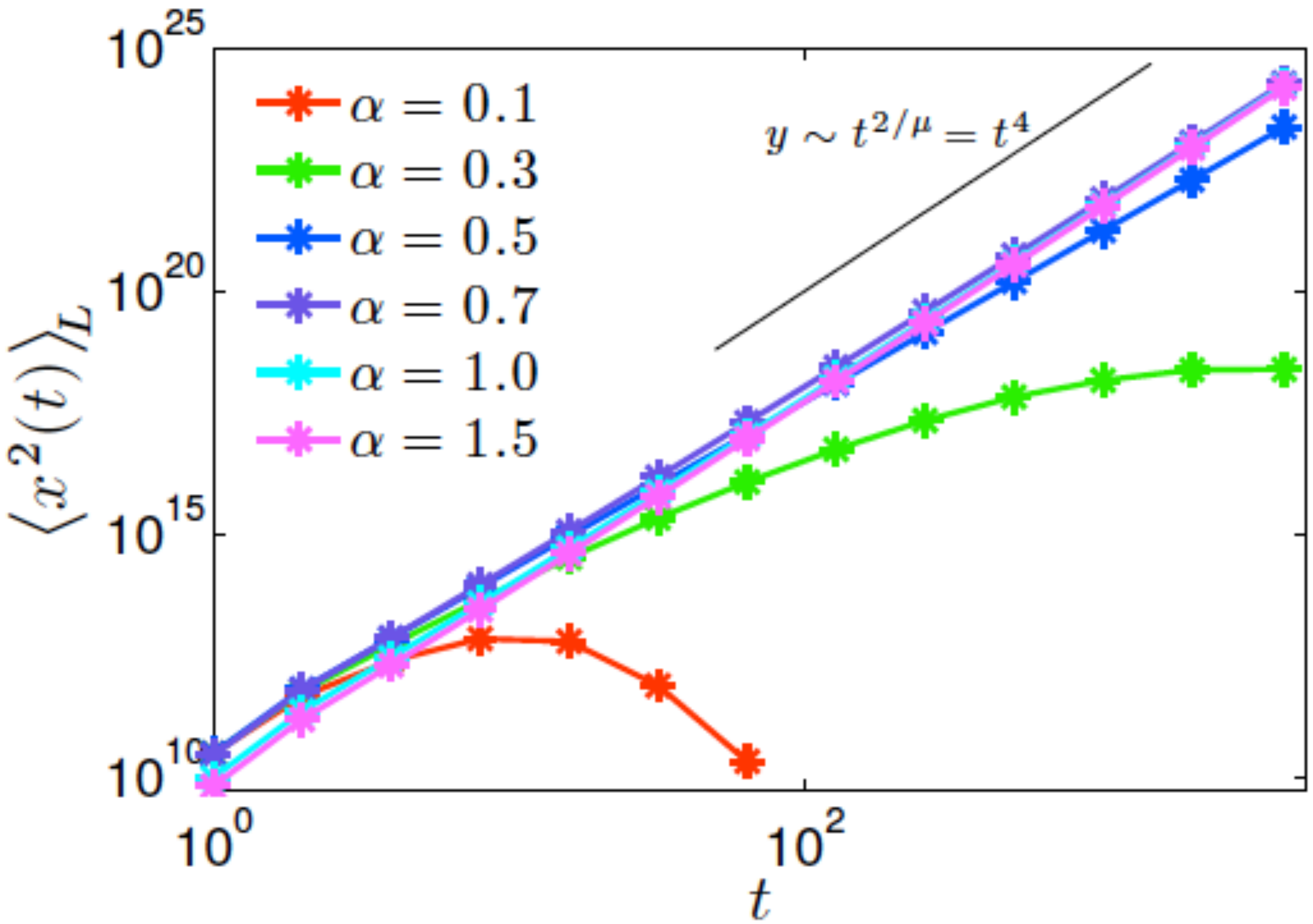
Finite Survival probability
→ Finite collision property

$$h(|D_y|) \sim |D_y|^{-3/2} \;\Rightarrow \mu = 1/2$$

$$a(|D_y|) \sim 1/|D_y| \quad \Rightarrow \alpha = 1$$

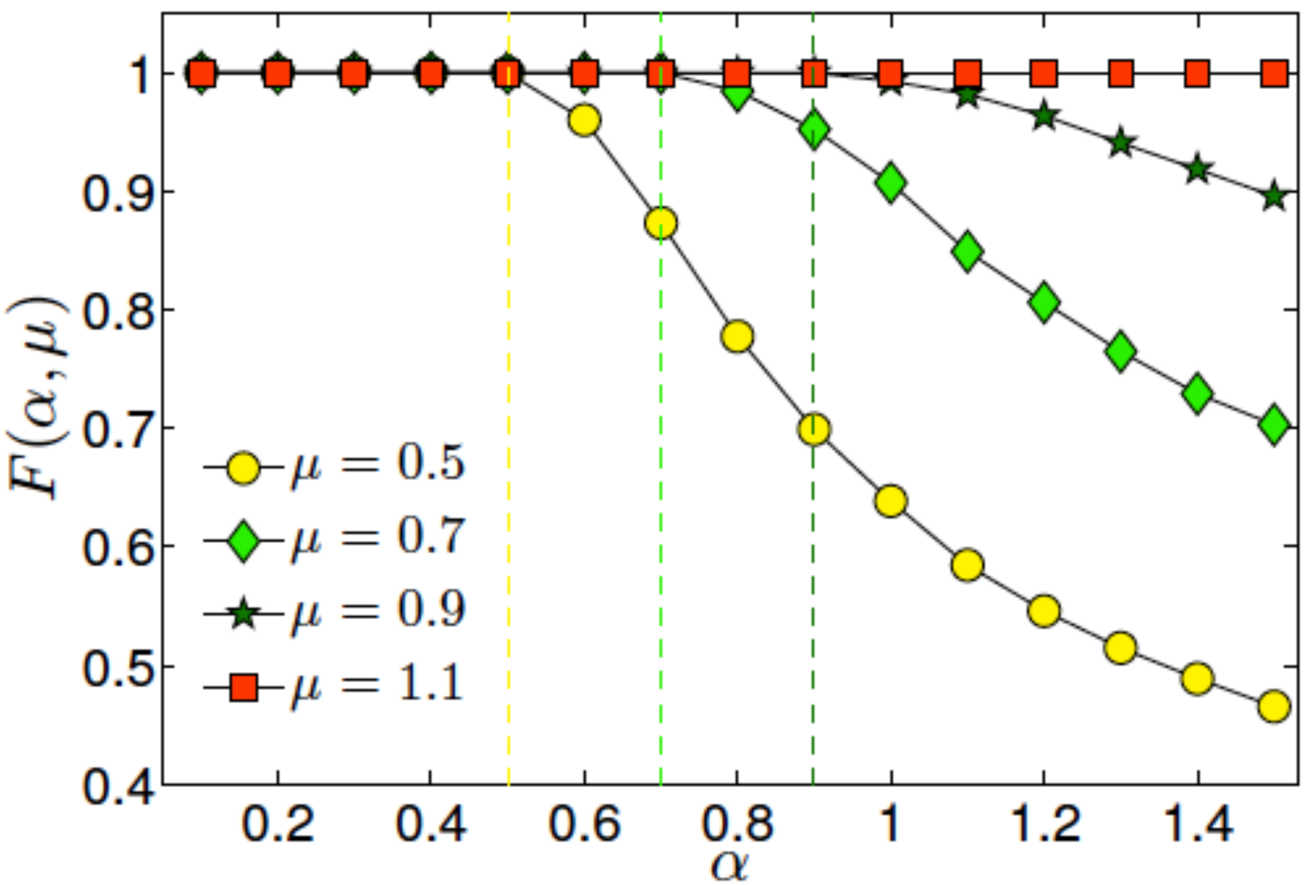
From scaling/intuitive arguments we expect $\mu < 1 \;\&\; \alpha > \mu$ **to avoid certainty of absorption**

Numerical evidence



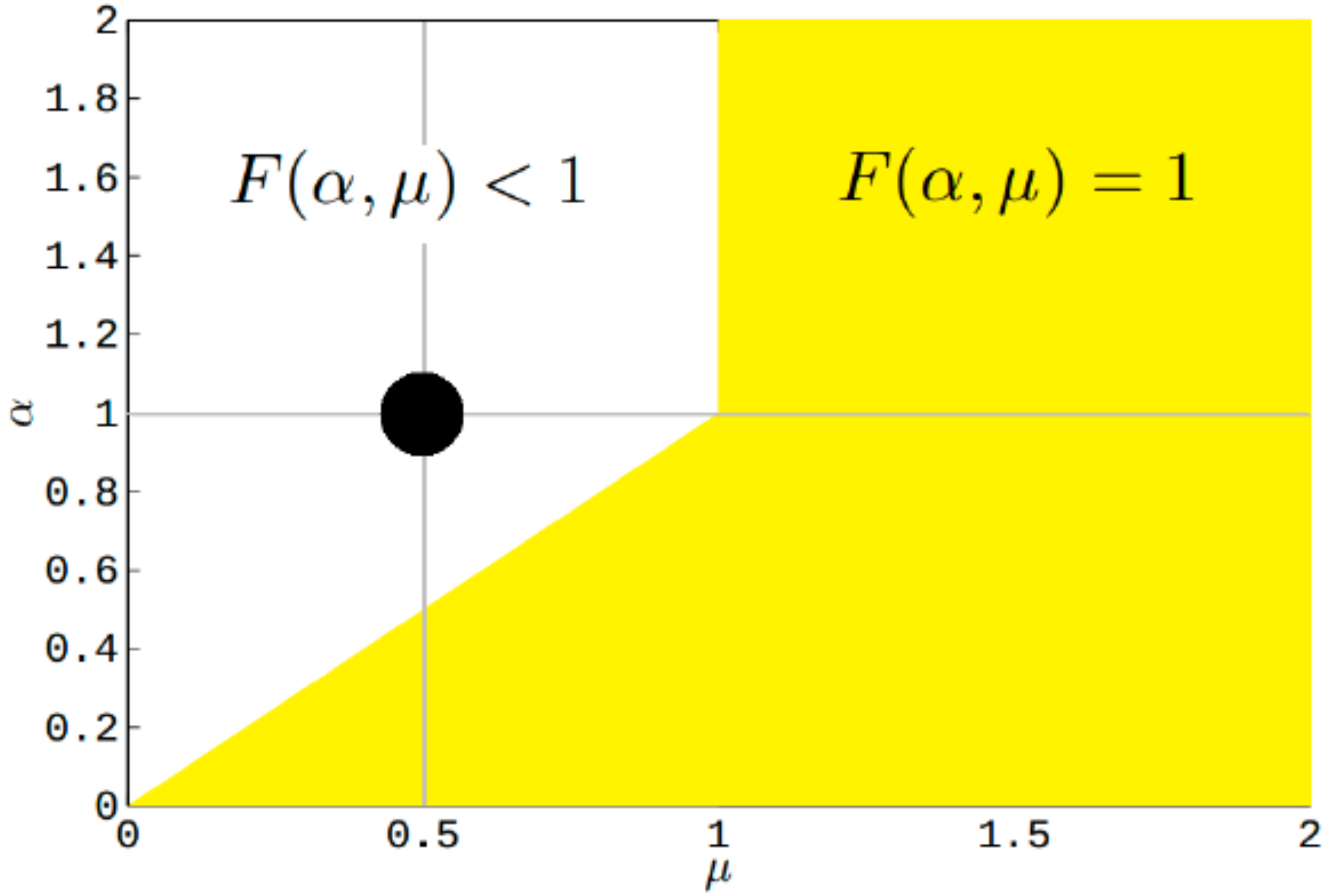
$$\langle x^2(t) \rangle_L \sim \int_{L_1 t^{1/\mu}}^{L_2 t^{1/\mu}} x^2 \rho(x,t)\,\mathrm{d}x \sim t^{2/\mu},$$

Figure 1: Mean-square displacement $\langle x^2(t) \rangle_L$ obtained from Monte Carlo simulations performed on one-dimensional structures for fixed $\mu = 0.5$ and different values of α (as explained by the legend). The parameters of the simulations are $L_1 = 40$ and $L_2 = 100$ and the number of replicas is 10^7.



$$F(\alpha,\mu) = 1 - \lim_{t \to +\infty} \left(\sum_{x=-\infty}^{\infty} \rho_{\alpha,\mu}(x,t) \right)$$

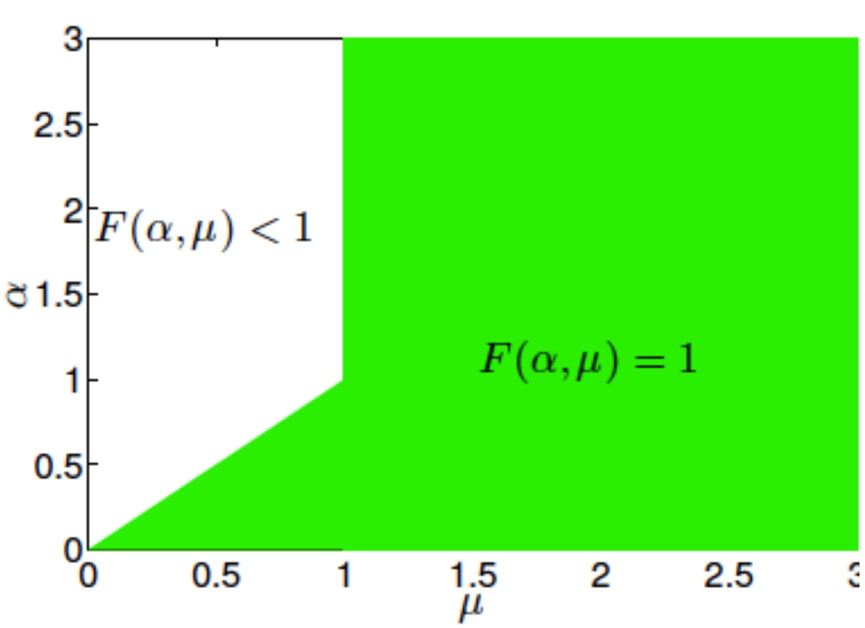
Figure 2: The asymptotic absorption probability found from Monte Carlo simulations. In the figure we notice that the absorption is total with $\alpha \leq \mu$ whit $\mu = 0.5$, $\mu = 0.7$, $\mu = 0.9$ and $\mu = 1.1$. The solid line are guides for the eye. The dotted vertical lines correspond to $\alpha = 0.5$, $\alpha = 0.7$, and $\alpha = 0.9$. The number of replicas is 10^7 and the asymptotic regime is reached tipically around $t_f = 10^6$. The errors on $F(\alpha,\mu)$ are of order 10^{-4}.

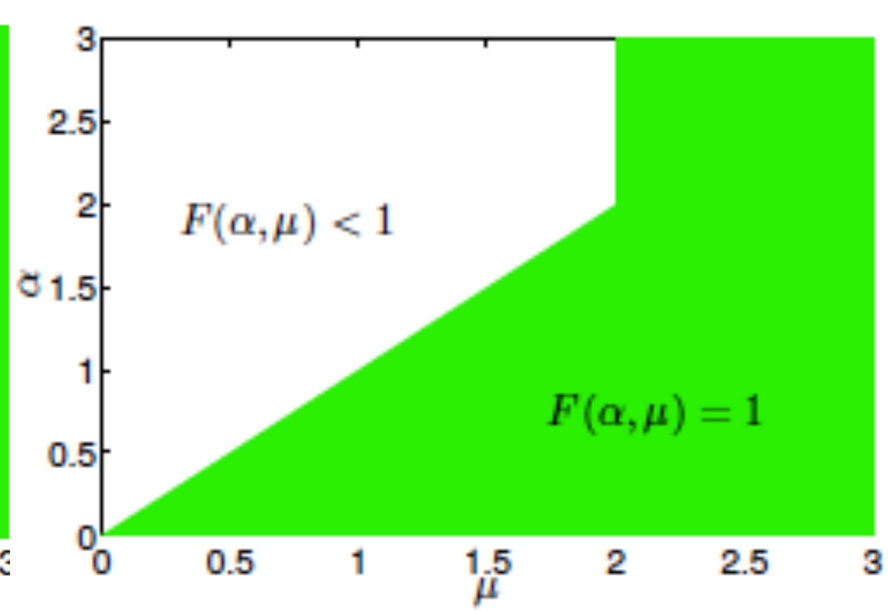


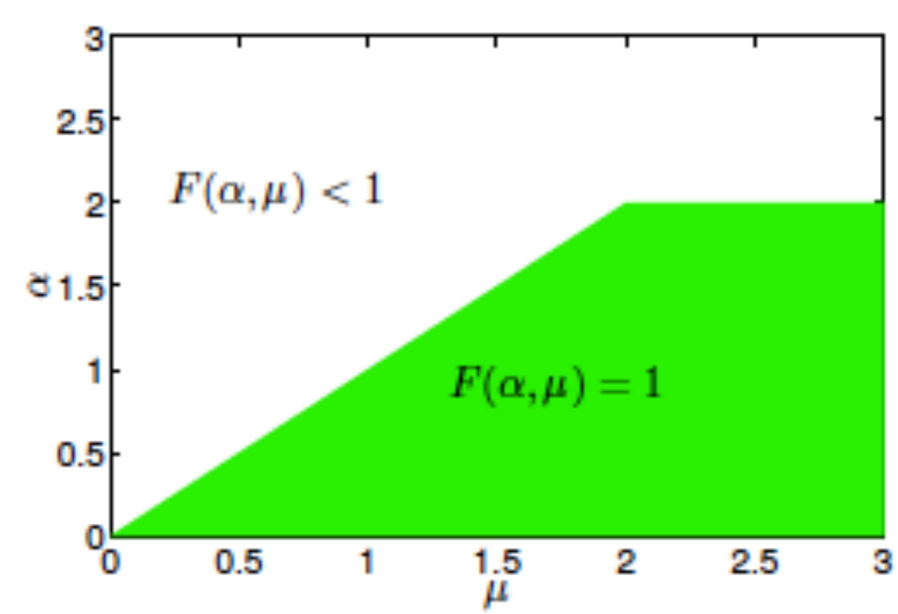
The RW in $\mathcal{M}$ has a finite probability of never crossing the red line → finite encounter probability

Extension to
- **Random combs**
- **Particles with different velocities → (different slope for red line)**
- **"Inverse problem"**

Lévy flight problem possibly extended to higher dimension lattices







Conclusions and Perspectives

There exist signatures of the finite collision property also on finite-size structures → slowing down of reaction

→ New strategy to control reaction kinetics

While in order to increase the survival probability of a species one usually increases the spatial dimension, by adding sites, links or volume to a given structure, in many cases it is possible to obtain a similar or stronger effect by judiciously deleting elements, i.e. by sparing material instead of wasting it.

Extend to other structures (e.g., percolation clusters, hierarchical combs)

How far is two-particle transience independent of local details and disorder?

Extend to the case of more than 2 RWs

Generalized grey Brownian motion: from classical diffusion to Erdélyi–Kober fractional diffusion

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WORKSHOP ON FRACTIONAL CALCULUS AND ITS APPLICATIONS. Roma Tre University, March 11, 2015

Main Goal of the Research

Normal diffusion $\leftrightarrow$ Gaussian process, stationary increments

- Brownian motion or Wiener process
- Standard Random Walk, CTRW with exponential WTs

fractional (anomalous) diffusion $\leftrightarrow$ stochastic process based on a Gaussian process with stationary increments ?

- Time-fractional diffusion $\leftrightarrow$ grey Brownian motion (Schneider 1990, 1992)
- Erdélyi–Kober fractional diffusion $\leftrightarrow$ generalized grey Brownian motion (Mura 2008, Pagnini 2012)
- **Space-time fractional diffusion** $\leftrightarrow$ **???**

The Space-Time Fractional Diffusion Equation

$$ {}_t\mathcal{D}_*^{\beta}\, K_{\alpha,\beta}^{\theta}(x;t) = \,{}_x\mathcal{D}_{\theta}^{\alpha}\, K_{\alpha,\beta}^{\theta}(x;t)\,, \quad K_{\alpha,\beta}^{\theta}(x;0) = \delta(x)\,, \qquad (1)$$

$$0 < \alpha \leq 2\,, \quad |\theta| \leq \min\{\alpha, 2-\alpha\}\,, \qquad (2a)$$

$$0 < \beta \leq 1 \quad \text{or} \quad 1 < \beta \leq \alpha \leq 2\,. \qquad (2b)$$

${}_x\mathcal{D}_{\theta}^{\alpha}$: Riesz–Feller space-fractional derivative

$$\widehat{{}_x\mathcal{D}_{\theta}^{\alpha}}(\kappa)\widehat{f}(\kappa) = \mathcal{F}\left\{{}_x\mathcal{D}_{\theta}^{\alpha}\, f(x);\kappa\right\} = -|\kappa|^{\alpha}\, \mathrm{e}^{i(\mathrm{sign}\,\kappa)\theta\pi/2}\,\widehat{f}(\kappa)\,. \qquad (3)$$

${}_t\mathcal{D}_*^{\beta}$: Caputo time-fractional derivative

$$\mathcal{L}\left\{{}_t\mathcal{D}_*^{\beta}\, f(t);s\right\} = s^{\beta}\,\widetilde{f}(s) - \sum_{j=0}^{m-1} s^{\beta-1-j}\, f^{(j)}(0^+)\,, \qquad (4)$$

with $m-1 < \beta \leq m$ and $m \in N$.

The Green Function $K^{\theta}_{\alpha,\beta}(x;t)$

Self-similarity

$$K^{\theta}_{\alpha,\beta}(x;t) = t^{-\beta/\alpha}\, K^{\theta}_{\alpha,\beta}\left(\frac{x}{t^{\beta/\alpha}}\right) . \tag{5}$$

Symmetry relation

$$K^{\theta}_{\alpha,\beta}(-x;t) = K^{-\theta}_{\alpha,\beta}(x;t)\,, \tag{6}$$

which allows the restriction to $x \geq 0$.

Mellin–Barnes integral representation

$$K^{\theta}_{\alpha,\beta}(x;t) = \frac{1}{\alpha x}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{\Gamma(\frac{q}{\alpha})\Gamma(1-\frac{q}{\alpha})\Gamma(1-q)}{\Gamma(1-\frac{\beta}{\alpha}q)\Gamma(\rho\, q)\Gamma(1-\rho\, q)} \left(\frac{x}{t^{\beta/\alpha}}\right)^{q} dq\,, \tag{7}$$

where $\rho = (\alpha-\theta)/(2\,\alpha)$ and c is a suitable real constant.

Mainardi, Luchko, Pagnini Fract. Calc. Appl. Anal. 2001

Special Cases: $x > 0$

$$K_{2,1}^{0}(x;t) = \frac{1}{\sqrt{4\pi t}}\,\mathrm{e}^{-x^2/(4t)} = G(x;t) = t^{-1/2} G\left(\frac{x}{t^{1/2}}\right) , \qquad (8)$$

$$K_{\alpha,1}^{\theta}(x;t) = L_{\alpha}^{\theta}(x;t) = t^{-1/\alpha} L_{\alpha}^{\theta}\left(\frac{x}{t^{1/\alpha}}\right) , \qquad (9)$$

$$K_{2,\beta}^{0}(x;t) = \frac{1}{2} M_{\beta/2}(x;t) = \frac{1}{2} t^{-\beta/2} M_{\beta/2}\left(\frac{x}{t^{\beta/2}}\right) , \qquad (10)$$

$$K_{\alpha,\alpha}^{\theta}(x;t) = \frac{t^{-1}}{\pi}\, \frac{(x/t)^{\alpha-1} \sin[\frac{\pi}{2}(\alpha-\theta)]}{1 + 2(x/t)^{\alpha} \cos[\frac{\pi}{2}(\alpha-\theta)] + (x/t)^{2\alpha}} , \qquad (11)$$

$$K_{2,2}^{0}(x;t) = \frac{1}{2}\delta(x-t) . \qquad (12)$$

Integral Representation Formulae for $K^{\theta}_{\alpha,\beta}(x;t)$

If $x > 0$ then

$$K^{\theta}_{\alpha,\beta}(x;t) = \int_0^{\infty} L^{\theta}_{\alpha}(x;\tau) L^{-\beta}_{\beta}(t;\tau) \frac{t}{\tau\beta}\, d\tau\,, \quad 0 < \beta \leq 1\,, \qquad (13)$$

$$K^{\theta}_{\alpha,\beta}(x;t) = \int_0^{\infty} L^{\theta}_{\alpha}(x;\tau)\, M_{\beta}(\tau;t)\, d\tau\,, \quad 0 < \beta \leq 1\,, \qquad (14)$$

$$K^{\theta}_{\alpha,\beta}(x;t) = \int_0^{\infty} K^{\theta}_{\alpha,\alpha}(x;\tau)\, M_{\beta/\alpha}(\tau;t)\, d\tau\,, \quad 0 < \beta/\alpha \leq 1\,. \qquad (15)$$

Mainardi, Luchko, Pagnini Fract. Calc. Appl. Anal. 2001

Supplementary Results

From formulae (13) and (14) it follows that

$$\frac{t}{\beta\tau} L_\beta^{-\beta}(t,\tau) = \frac{t}{\beta\tau^{1/\beta+1}} L_\beta^{-\beta}\left(\frac{t}{\tau^{1/\beta}}\right) = \frac{1}{t^\beta} M_\beta\left(\frac{\tau}{t^\beta}\right) \tag{16}$$

$$0 < \beta \leq 1\,, \quad \tau, t > 0\,.$$

From formulae (8) and (9)

$$K_{2,1}^0(x;t) = G(x;t) = L_2^0(x;t)\,. \tag{17}$$

From formulae (8) and (10)

$$K_{2,1}^0(x;t) = G(x;t) = \frac{1}{2} M_{1/2}(x;t)\,. \tag{18}$$

Supplementary Results

$$L_\alpha^\theta(x;t) = \int_0^\infty L_\eta^\omega(x;\xi) L_\nu^{-\nu}(\xi;t)\, d\xi\,, \quad \alpha = \eta\nu\,, \quad \theta = \omega\nu\,, \tag{19}$$

$$0 < \alpha \leq 2\,, \quad |\theta| \leq \min\{\alpha, 2-\alpha\}\,,$$

$$0 < \eta \leq 2\,, \quad |\omega| \leq \min\{\eta, 2-\eta\}\,, \quad 0 < \nu \leq 1\,.$$

In particular it holds

$$\begin{aligned} L_\alpha^0(x;t) &= \int_0^\infty L_2^0(x;\xi) L_{\alpha/2}^{-\alpha/2}(\xi;t)\, d\xi && (20) \\ &= \int_0^\infty G(x;\xi) L_{\alpha/2}^{-\alpha/2}(\xi;t)\, d\xi\,. && (21) \end{aligned}$$

Mainardi, Pagnini, Gorenflo Fract. Calc. Appl. Anal. 2003

Supplementary Results

$$M_\nu(x;t) = \int_0^\infty M_\eta(x;\xi) M_\beta(\xi;t)\, d\xi\,, \quad \nu = \eta\beta\,, \qquad (22)$$

$$0 < \nu, \eta, \beta \leq 1\,.$$

In particular it holds

$$\begin{aligned} M_{\beta/2}(x;t) &= 2\int_0^\infty M_{1/2}(x;\xi) M_\beta(\xi;t)\, d\xi & (23) \\ &= 2\int_0^\infty G(x;\xi) M_\beta(\xi;t)\, d\xi\,. & (24) \end{aligned}$$

Mainardi, Pagnini, Gorenflo Fract. Calc. Appl. Anal. 2003

New Integral Representation Formula for $K_{\alpha,\beta}^{\theta}(x;t)$

Consider formula (14), i.e. $K_{\alpha,\beta}^{\theta}(x;t) = \int_0^\infty L_\alpha^\theta(x;\tau) M_\beta(\tau;t)\, d\tau$, then and by using (19) it follows

$$\begin{aligned}
K_{\alpha,\beta}^{\theta}(x;t) &= \int_0^\infty \left\{ \int_0^\infty L_\eta^\omega(x;\xi) L_\nu^{-\nu}(\xi;t)\, d\xi \right\} M_\beta(\tau,t)\, d\tau \\
&= \int_0^\infty L_\eta^\omega(x;\xi) \left\{ \int_0^\infty L_\nu^{-\nu}(\xi;t) M_\beta(\tau;t)\, d\tau \right\} d\xi \\
&= \int_0^\infty L_\eta^\omega(x;\xi)\, K_{\nu,\beta}^{-\nu}(\xi;t)\, d\xi\,, \quad \alpha = \eta\nu\,, \quad \theta = \omega\nu\,,
\end{aligned}$$

$$0 < \alpha \le 2\,, \quad |\theta| \le \min\{\alpha, 2-\alpha\}\,, \quad 0 < \beta \le 1\,,$$
$$0 < \eta \le 2\,, \quad |\omega| \le \min\{\eta, 2-\eta\}\,, \quad 0 < \nu \le 1\,.$$

New Integral Representation Formula for $K_{\alpha,\beta}^{\theta}(x;t)$

$$K_{\alpha,\beta}^{\theta}(x;t) = \int_0^{\infty} L_{\eta}^{\omega}(x;\xi)\, K_{\nu,\beta}^{-\nu}(\xi;t)\, d\xi\,, \qquad (25)$$

$$0 < x < +\infty\,, \quad \alpha = \eta\nu\,, \quad \theta = \omega\nu\,,$$

$$0 < \alpha \le 2\,, \quad |\theta| \le \min\{\alpha, 2-\alpha\}\,, \quad 0 < \beta \le 1\,,$$

$$0 < \eta \le 2\,, \quad |\omega| \le \min\{\eta, 2-\eta\}\,, \quad 0 < \nu \le 1\,.$$

Spatial symmetric case: $\eta = 2$ and $\omega = 0 \Rightarrow L_2^0 \equiv G$

Hence $\nu = \alpha/2$ and $\theta = 0$ and formula (25) gives

$$K_{\alpha,\beta}^{0}(x;t) = \int_0^{\infty} G(x;\xi)\, K_{\alpha/2,\beta}^{-\alpha/2}(\xi;t)\, d\xi\,. \qquad (26)$$

$$-\infty < x < +\infty\,, \quad 0 < \alpha \le 2\,, \quad 0 < \beta \le 1\,.$$

Special Cases: Time Fractional $\alpha = 2$ and $0 < \beta \leq 1$

From (14) it results that

$$\begin{aligned} K_{1,\beta}^{-1}(\xi;t) &= \int_0^\infty L_1^{-1}(\xi;\tau)\, M_\beta(\tau;t)\, d\tau \\ &= \int_0^\infty \delta(\xi-\tau)\, M_\beta(\tau;t)\, d\tau = M_\beta(\xi;t)\,, \qquad (27) \end{aligned}$$

finally by using (24)

$$K_{2,\beta}^{0}(x;t) = \int_0^\infty G(x;\xi)\, K_{1,\beta}^{-1}(\xi;t)\, d\xi \qquad (28)$$

$$= \int_0^\infty G(x;\xi)\, M_\beta\, d\xi = \frac{1}{2} M_{\beta/2}(x;t)\,. \qquad (29)$$

Special Cases: Space Fractional $0 < \alpha \leq 2$ and $\beta = 1$

From (14) it results that

$$\begin{aligned} K_{\alpha/2,1}^{-\alpha/2}(\xi;t) &= \int_0^\infty L_{\alpha/2}^{-\alpha/2}(\xi;\tau)\, M_1(\tau;t)\, d\tau \\ &= \int_0^\infty L_{\alpha/2}^{-\alpha/2}(\xi;\tau)\, \delta(\tau - t)\, d\tau = L_{\alpha/2}^{-\alpha/2}(\xi;t)\,, \end{aligned} \tag{30}$$

finally by using (21)

$$K_{\alpha,1}^{0}(x;t) = \int_0^\infty G(x;\xi)\, K_{\alpha/2,1}^{-\alpha/2}(\xi;t)\, d\xi \tag{31}$$

$$= \int_0^\infty G(x;\xi)\, L_{\alpha/2}^{-\alpha/2}(\xi;t)\, d\xi = L_{\alpha}^{0}(x;t)\,. \tag{32}$$

Product of Random Variables

- Z_1 and Z_2 are two real independent random variables
- PDFs $p_1(z_1)$ and $p_2(z_2)$, $z_1 \in R$, $z_2 \in R^+$.
- Joint PDF is $p(z_1, z_2) = p_1(z_1)p_2(z_2)$.

Let $Z = Z_1\, Z_2^\gamma$ so that $z = z_1 z_2^\gamma$

Carrying out the variable transformations $z_1 = z/\lambda^\gamma$ and $z_2 = \lambda$,

$$p(z_1, z_2)\, dz_1\, dz_2 = p_1(z/\lambda^\gamma)p_2(\lambda)\, J\, dz\, d\lambda,$$

where $J = 1/\lambda^\gamma$ is the Jacobian of the transformation.

Integration in $d\lambda$ gives

$$p(z) = \int_0^\infty p_1\left(\frac{z}{\lambda^\gamma}\right) p_2(\lambda)\, \frac{d\lambda}{\lambda^\gamma}\,. \tag{33}$$

Product of Random Variables

Hence by applying the changes of variable $z = xt^{-\gamma\Omega}$ and $\lambda = \tau t^{-\Omega}$, integral formula (33) becomes

$$t^{-\gamma\Omega} p\left(\frac{x}{t^{\gamma\Omega}}\right) = \int_0^\infty \tau^{-\gamma} p_1\left(\frac{x}{\tau^\gamma}\right) t^{-\Omega} p_2\left(\frac{\tau}{t^\Omega}\right) d\tau \,. \tag{34}$$

By setting

$$p_1 \equiv G\,, \quad p_2 \equiv K_{\alpha/2,\beta}^{-\alpha/2}\,, \tag{35}$$

$$\gamma = 1/2\,, \quad \Omega = 2\beta/\alpha\,, \tag{36}$$

formula (34) turns out to be identical to (26), i.e.

$$p(x;t) = \int_0^\infty G(x;\tau)\, K_{\alpha/2,\beta}^{-\alpha/2}(\tau;t)\, d\tau\,,$$

hence

$$p(x;t) \equiv K_{\alpha,\beta}^{0}(x;t)\,. \tag{37}$$

Stochastic Solution of Space-Time Fractional Diffusion

$$\int_0^\infty \frac{1}{\tau^{1/2}} G\left(\frac{x}{\tau^{1/2}}\right) \, \frac{1}{t^{2\beta/\alpha}} K_{\alpha/2,\beta}^{-\alpha/2}\left(\frac{\tau}{t^{2\beta/\alpha}}\right) \, d\tau = t^{-\beta/\alpha} K_{\alpha,\beta}^{0}\left(\frac{x}{t^{\beta/\alpha}}\right) . \tag{38}$$

Change of variable $\lambda = \tau \, t^{-2\beta/\alpha}$,

One-point one-time PDF:

$$\begin{aligned} f_{\alpha,\beta}(x;t) &= \int_0^\infty \frac{t^{-\beta/\alpha}}{\lambda^{1/2}} G\left(\frac{x\, t^{-\beta/\alpha}}{\lambda^{1/2}}\right) \, K_{\alpha/2,\beta}^{-\alpha/2}(\lambda) \, d\lambda \\ &= t^{-\beta/\alpha} K_{\alpha,\beta}^{0}(x\, t^{-\beta/\alpha}) \, , \end{aligned} \tag{39}$$

Stochastic Solution of Space-Time Fractional Diffusion

In terms of random variables it follows that

$$Z = X\, t^{-\beta/\alpha} \quad \text{and} \quad Z = Z_1 Z_2^{1/2}\,, \tag{40}$$

$$X = Z\, t^{\beta/\alpha} = \left(Z_1\, t^{\beta/\alpha} \right) Z_2^{1/2} = G_{2\beta/\alpha}(t)\, \sqrt{\Lambda_{\alpha/2,\beta}}\,. \tag{41}$$

Z_1: Gaussian random variable, i.e. $p_1 \equiv G$, with anomalous scaling

Natural choice: **standard fBm** with Hurst exponent H=$\beta/\alpha < 1$ for $G_{2\beta/\alpha}(t) = Z_1 t^{\beta/\alpha}$

$\Lambda_{\alpha/2,\beta} = Z_2$ distributed according to $p_2 \equiv K_{\alpha/2,\beta}^{-\alpha/2}$.

H-sssi Processes and fBm

Same constructive approach adopted by Mura (PhD, 2008) $\Rightarrow$ *generalized grey Brownian motion* (*Mura and Pagnini, J. Phys. A, 2008*).

Let $X_{\alpha,\beta}(t)$, $t \geq 0$, *be an H-sssi defined as*

$$X_{\alpha,\beta}(t) \stackrel{d}{=} \sqrt{\Lambda_{\alpha/2,\beta}}\; G_{2\beta/\alpha}(t)\,, \tag{42}$$

$$0 < \beta \leq 1\,, \quad 0 < \beta < \alpha \leq 2\,, \tag{43}$$

$\stackrel{d}{=}$ *denotes the equality of the finite-dimensional distribution, the stochastic process* $G_{2\beta/\alpha}(t)$ *is a standard fBm with Hurst exponent* $H = \beta/\alpha < 1$ *and* $\Lambda_{\alpha/2,\beta}$ *is an independent non-negative random variable with PDF* $K_{\alpha/2,\beta}^{-\alpha/2}(\lambda)$, $\lambda \geq 0$, *then the marginal PDF of* $X_{\alpha,\beta}(t)$ *is* $K_{\alpha,\beta}^{0}(x;t)$.

Special Cases: $\alpha = 2$ (grey Brownian motion)

Let $X_\beta(t)$, $t \geq 0$, be an H-sssi defined as

$$X_\beta(t) \stackrel{d}{=} \sqrt{\Lambda_\beta}\; G_\beta(t)\,, \tag{44}$$

$$0 < \beta \leq 1\,, \tag{45}$$

$\stackrel{d}{=}$ denotes the equality of the finite-dimensional distribution, the stochastic process $G_\beta(t)$ is a standard fBm with Hurst exponent $H = \beta/2 < 1$ and Λ_β is an independent non-negative random variable with PDF $K_{1,\beta}^{-1}(\lambda) = M_\beta(\lambda)$, $\lambda \geq 0$, then the marginal PDF of $X_\beta(t)$ is $K_{2,\beta}^{0}(x;t) = \dfrac{1}{2} M_{\beta/2}(x;t)$.

Special Cases: $\beta = 1$

Let $X_\alpha(t)$, $t \geq 0$, be an H-sssi defined as

$$X_\alpha(t) \stackrel{d}{=} \sqrt{\Lambda_{\alpha/2}}\, G_{2/\alpha}(t)\,, \tag{46}$$

$$1 < \alpha \leq 2\,, \tag{47}$$

$\stackrel{d}{=}$ denotes the equality of the finite-dimensional distribution, the stochastic process $G_{2/\alpha}(t)$ is a standard fBm with Hurst exponent $H = 1/\alpha < 1$ and $\Lambda_{\alpha/2}$ is an independent non-negative random variable with PDF $K^{-\alpha/2}_{\alpha/2,1}(\lambda) = L^{-\alpha/2}_{\alpha/2}(\lambda)$, $\lambda \geq 0$, then the marginal PDF of $X_\alpha(t)$ is $K^0_{\alpha,1}(x;t) = L^0_\alpha(x;t)$.

H-sssi Processes and fBm

The finite-dimensional distribution of $X_{\alpha,\beta}(t)$ is obtained from (33) according to

$$f_{\alpha,\beta}(x_1, x_2, \ldots, x_n; \gamma_{\alpha,\beta}) = \frac{(2\pi)^{-\frac{n-1}{2}}}{\sqrt{\det \gamma_{\alpha,\beta}}} \times \int_0^\infty \frac{1}{\lambda^{n/2}} G\left(\frac{z_n}{\lambda^{1/2}}\right) K_{\alpha/2,\beta}^{-\alpha/2}(\lambda)\, d\lambda\,, \qquad (48)$$

where z_n is the n-dimensional particle position vector

$$z_n = \left(\sum_{i,j=1}^{n} x_i \, {\gamma_{\alpha,\beta}}^{-1}(t_i, t_j)\, x_j \right)^{1/2} ,$$

and $\gamma_{\alpha,\beta}(t_i, t_j)$ is the covariance matrix (**fBm**)

$$\gamma_{\alpha,\beta}(t_i, t_j) = \frac{1}{2}(t_i^{2\beta/\alpha} + t_j^{2\beta/\alpha} - |t_i - t_j|^{2\beta/\alpha})\,, \quad i, j = 1, \ldots, n\,.$$

Stochastic Process Generation

From (14) it follows that

$$K^{-\alpha/2}_{\alpha/2,\beta}(\xi;t) = \int_0^\infty L^{-\alpha/2}_{\alpha/2}(\xi;\tau)\, M_\beta(\tau;t)\, d\tau\,, \quad 0 < \beta \le 1\,, \quad (49)$$

and by using the self-similarity properties and the changes of variable $\xi = t^{2\beta/\alpha}\lambda$ and $\tau = t^\beta y$ it holds

$$K^{-\alpha/2}_{\alpha/2,\beta}(\lambda) = \int_0^\infty L^{-\alpha/2}_{\alpha/2}\left(\frac{\lambda}{y^{2/\alpha}}\right) M_\beta(y)\, \frac{dy}{y^{2/\alpha}}\,, \quad 0 < \beta \le 1\,. \quad (50)$$

Stochastic Process Generation

Integral (50) suggests to obtain $\Lambda_{\alpha/2,\beta}$ again by means of the product of two independent random variables, i.e.

$$\Lambda_{\alpha/2,\beta} = \Lambda_1 \cdot \Lambda_2^{2/\alpha} = \mathcal{L}_{\alpha/2}^{ext} \cdot \mathcal{M}_\beta^{2/\alpha}\,, \tag{51}$$

where $\Lambda_1 = \mathcal{L}_{\alpha/2}^{ext}$ and $\Lambda_2 = \mathcal{M}_\beta$ are distributed according to the extremal stable density $L_{\alpha/2}^{-\alpha/2}(\lambda_1)$ and $M_\beta(\lambda_2)$, respectively, so that $\lambda = \lambda_1\,\lambda_2^{2/\alpha}$.

Stochastic Process Generation

Moreover, from (16) and setting $t = 1$, the random variable $\mathcal{M}_\beta$ can be determined by an extremal stable random variable according to

$$\mathcal{M}_\beta = \left[\mathcal{L}_\beta^{ext}\right]^{-\beta}, \qquad (52)$$

so that the random variable $\Lambda_{\alpha/2,\beta}$ is computed by the product

$$\Lambda_{\alpha/2,\beta} = \mathcal{L}_{\alpha/2}^{ext} \cdot \left[\mathcal{L}_\beta^{ext}\right]^{-2\beta/\alpha}. \qquad (53)$$

Finally, the desired H-sssi processes are established as follows

$$X_{\alpha,\beta}(t) = \sqrt{\mathcal{L}_{\alpha/2}^{ext}} \cdot \left[\mathcal{L}_\beta^{ext}\right]^{-\beta/\alpha} G_{2\beta/\alpha}(t). \qquad (54)$$

Numerical Generation

Computer generation of extremal stable random variables of order $0 < \mu < 1$ is obtained by using the method by Chambers, Mallows and Stuck

$$\mathcal{L}_\mu^{ext} = \frac{\sin[\mu(r_1 + \pi/2)]}{(\cos r_1)^{1/\mu}} \left\{ \frac{\cos[r_1 - \mu(r_1 + \pi/2)]}{-\ln r_2} \right\}^{(1-\mu)/\mu} , \quad (55)$$

where r_1 and r_2 are random variables uniformly distributed in $(-\pi/2, \pi/2)$ and $(0, 1)$, respectively.

Chambers, Mallows, Stuck J. Amer. Statist. Assoc. 1976
Weron Statist. Probab. Lett. 1996

Numerical Generation

The Hosking direct method is applied for generating the fBm $G_{2H}(t)$, $0 < H < 1$. In particular, first the so-called fractional Gaussian noise Y_{2H} is generated over the set of integer numbers with autocorrelation function

$$\langle Y_{2H}(k) Y_{2H}(k+n) \rangle = \frac{1}{2} \left[|n-1|^{2H} - |n|^{2H} + |n+1|^{2H} \right] . \quad (56)$$

Finally, the fBm is then generated as a sum of stationary increments, i.e. $Y_{2H}(n) = G_{2H}(n+1) - G_{2H}(n)$

$$G_{2H}(n+1) = G_{2H}(n) + Y_{2H}(n) . \quad (57)$$

Hosking Water Resour. Res. 1984
Dieker PhD Thesis Univ. of Twente, The Netherlands, 2004

Numerical Simulations

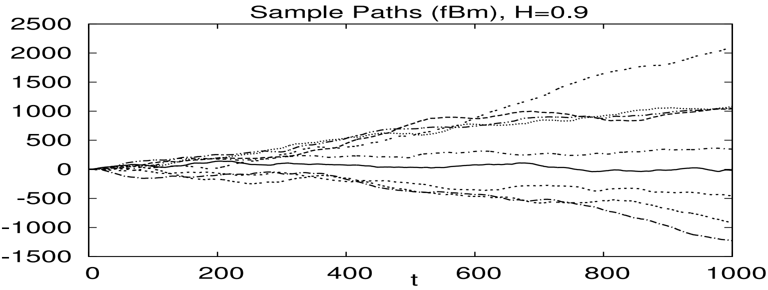
For a given set of parameter values (α,β),
10^4 trajectories generated for 10^3 time steps.
Time step: $\Delta t = 1$ (see formula (57))
For generic Δt use self-similarity.

(1) Generate trajectories for FBM with $H = \beta/\alpha$.

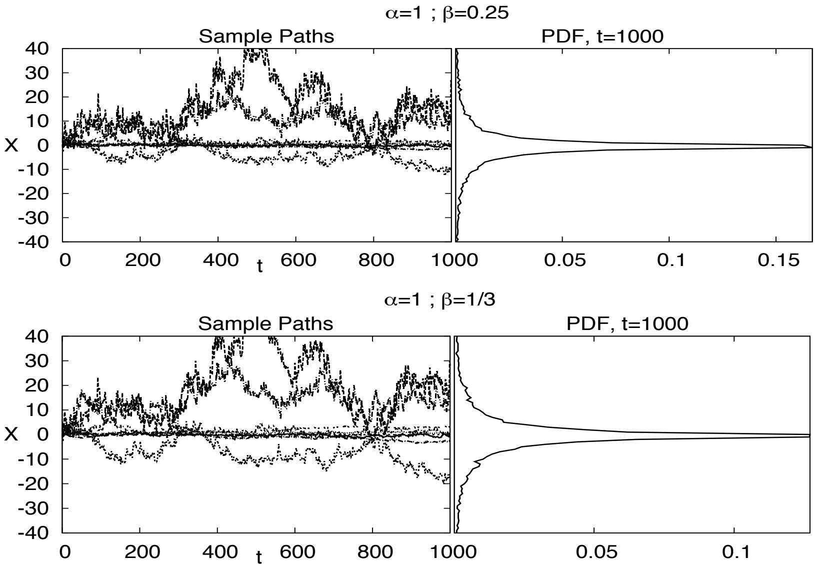
(2) For each trajectory draw random number from the Lévy density $\Rightarrow$ change amplitude of the trajectory randomly

NOTE:
Time averages depend on the fBm
(no effect of the random amplitude)
Ensemble averages affected by random amplitude
Non-ergodicity

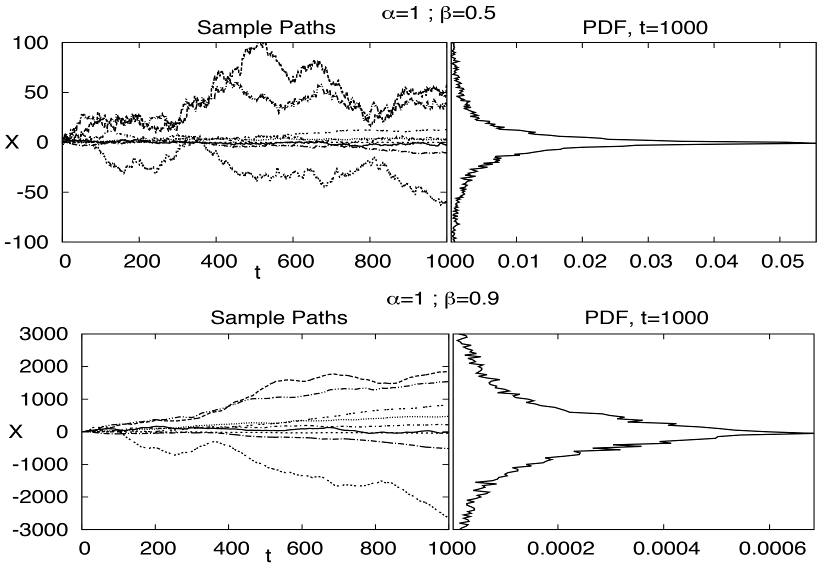
Numerical Simulations, $H = \beta/\alpha$



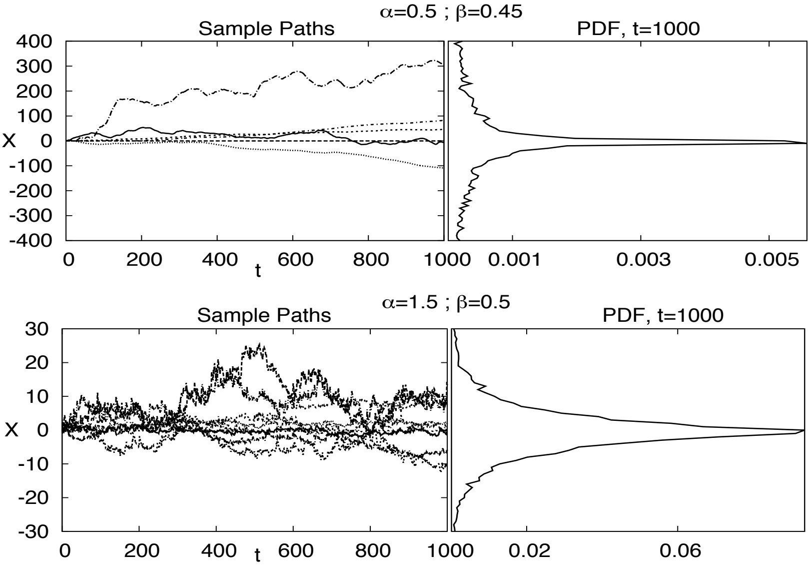
Numerical Simulations, $H = \beta/\alpha$



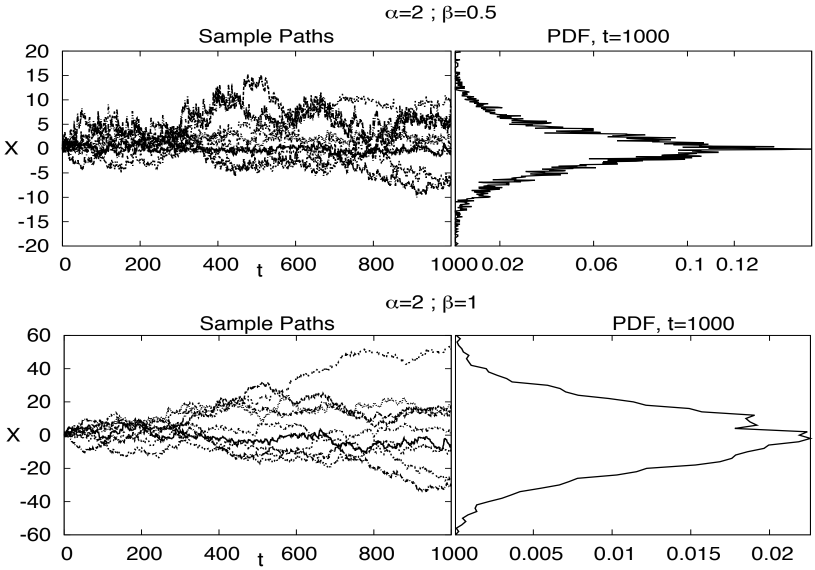
Numerical Simulations, $H = \beta/\alpha$



Numerical Simulations, $H = \beta/\alpha$

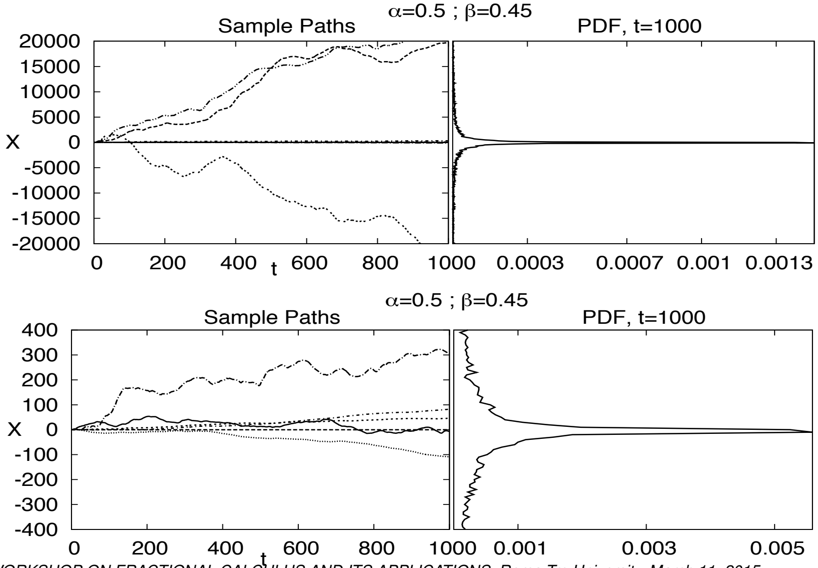


Numerical Simulations, $H = \beta/\alpha$

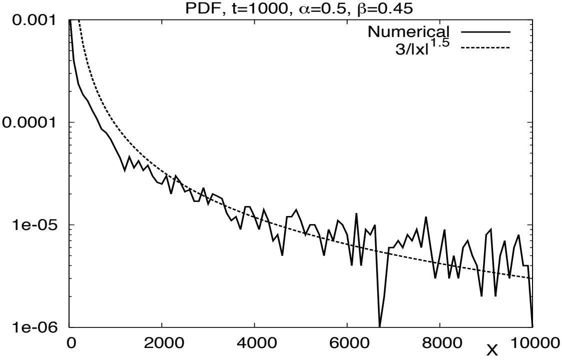


Numerical Simulations, $H = \beta/\alpha$

Self-similarity and large amplitudes



Numerical Simulations, $H = \beta/\alpha$



Power-law decay of PDF tail (large x) according to $\sim 1/|x|^{\alpha+1}$.

Generalized Grey Brownian Motion (ggBm)

Mura (PhD, 2008); Mura and Pagnini (J. Phys. A, 2008)

Let $X_{H,\beta}(t)$, $t \geq 0$, be an H-sssi defined as

$$X_{H,\beta}(t) \stackrel{d}{=} \sqrt{\Lambda_\beta}\; G_{2H}(t)\,, \tag{58}$$

$$0 < \beta \leq 1\,, \tag{59}$$

$\stackrel{d}{=}$ denotes the equality of the finite-dimensional distribution, the stochastic process $G_{2H}(t)$ is a standard fBm with Hurst exponent $H < 1$ and Λ_β is an independent non-negative random variable with PDF $M_\beta(\lambda)$, $\lambda \geq 0$, then the marginal PDF of $X_{H,\beta}(t)$ is $\frac{1}{2}M_{\beta/2}(x; t^{2H/\beta}) = \frac{1}{2}t^{-H}M_{\beta/2}(|x|t^{-H})$.

Time stretching

$$t \to t^{2H/\beta}\,.$$

Generalized Grey Brownian Motion (ggBm)

Master equation ($0 < \beta < 1$, $0 < H < 1$):

$$\frac{\partial \mathcal{P}}{\partial t} = \frac{2H}{\beta} t^{2H-1} D_{2H/\beta}^{\beta-1,1-\beta} \frac{\partial^2 \mathcal{P}}{\partial x^2}, \tag{60}$$

where $D_\eta^{\gamma,\mu}$ is the Erdélyi–Kober fractional derivative

Fundamental solution: $\mathcal{P}(x;t) = \frac{1}{2} t^{-H} M_{\beta/2}(|x| t^{-H})$,

Variance: $\langle x^2 \rangle = \frac{2}{\Gamma(1+\beta)} t^{2H}$.

Mura (PhD, 2008)
Mura and Pagnini (J. Phys. A, 2008)
Garra, Orsingher, Polito (arXiv:1501.04806 [math.PR], 2015)

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ikerbasque Basque Foundation for Science

(bcam) basque center for applied mathematics

EXCELENCIA SEVERO OCHOA

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Numerical solution of two-dimensional fractional diffusion equations by a high-order ADI method

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Workshop on Fractional Calculus and its Applications

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Rome

Overview

Introduction

Fractional partial **diffusion** or **reaction-diffusion** differential equations in **several space dimensions** can be used to model several phenomena in many fields of Science, and in particular in **Meteorology**. In case of **anomalous diffusion**, generalized models using fractional derivatives, thus leading to fractional partial diffusion equations have indeed been proposed, especially to describe diffusion and transport dynamics in complex systems [Baumer02, Chen12, Gorenflo00, Mainardi97].

Introduction

In fact, such equations may describe **fluid flow through porous media** better than classical diffusion equations. For instance, fractional time-derivatives may account for (time) **delays**, while fractional space-derivatives may explain a **nonlocal** behavior, typically characterized by power law (rather than exponential law) decay. Equations like these are also used in **groundwater hydrology** to model the transport of passive tracers carried by fluid flows in porous media and seepage [Benson00, Benson&Wheatcraft00, Benson01]

High-order approximations for Riemann-Liouville fractional derivatives

In this section, we recall some known results concerning fractional derivatives. We begin with the definition of the Riemann-Liouville (RL)

Definition

[Podlubny99] If $n-1 < \alpha \leq n$ for some $n \in \mathbf{N}$, the RL fractional left and right derivative of order α of the function $u(x)$, whose domain is $[a, b]$, at the point $x \in [a, b]$, are defined as follows.

- *left* Riemann-Liouville fractional derivative:

$$ {}_aD_x^\alpha u(x) := \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x \frac{u(\xi)}{(x-\xi)^{\alpha-n+1}}\, d\xi; $$

High-order approximations for Riemann-Liouville fractional derivatives

Definition

- *right* Riemann-Liouville fractional derivative:

$$ {}_xD_b^{\alpha} u(x) := \frac{-1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_x^b \frac{u(\xi)}{(\xi - x)^{\alpha - n + 1}} \, d\xi, $$

  where $\Gamma(\cdot)$ denotes the Gamma function.

When $\alpha = n$, ${}_aD_x^{\alpha} = \frac{d^n}{dx^n}$ and ${}_xD_b^{\alpha} = (-1)^n \frac{d^n}{dx^n}$.

High-order approximations for Riemann-Liouville fractional derivatives

In [Meerschaert06], it was shown that the **shifted Grünwald difference operator**, defined as

$$A_{h,p}^{\alpha}u(x) := \frac{1}{h^{\alpha}} \sum_{k=0}^{\infty} g_k^{(\alpha)}\, u(x-(k-p)h), \tag{1}$$

where p is an integer, and $g_k^{(\alpha)} := (-1)^k \binom{\alpha}{k}$, approximates the *left* RL fractional derivative of order α, uniformly, with first-order accuracy, i.e.,

$$A_{h,p}^{\alpha}u(x) = {}_{-\infty}D_x^{\alpha}u(x) + O(h). \tag{2}$$

High-order approximations for Riemann-Liouville fractional derivatives

Theorem

Let be $u \in L^1(\mathbf{R})$, and hence (as is known), ${}_{-\infty}D_x^{\alpha+2}u$ and its Fourier transform also belong to $L^1(\mathbf{R})$, and define the "weighted and shifted" Grünwald difference (WSGD) operator ${}_L\mathcal{D}_{h,p,q}^{\alpha}$ by

$$ {}_L\mathcal{D}_{h,p,q}^{\alpha}u(x) := \frac{\alpha - 2q}{2(p-q)} A_{h,p}^{\alpha}u(x) + \frac{2p-\alpha}{2(p-q)} A_{h,q}^{\alpha}u(x). \tag{3} $$

Then, we have

$$ {}_L\mathcal{D}_{h,p,q}^{\alpha}u(x) = {}_{-\infty}\mathcal{D}_x^{\alpha}u(x) + O(h^2) \tag{4} $$

uniformly for $x \in \mathbf{R}$, where $p,q \in \{-1,0,1\}$, with $p \neq q$.

Fractional diffusion equations in two space dimensions

Consider the following fPDE (*fractional partial differential equation*) in two space dimensions,

$$\begin{cases} \frac{\partial u}{\partial t} = \left(K_1^+ \, {}_aD_x^\alpha u + K_2^+ \, {}_xD_b^\alpha u\right) + \left(K_1^- \, {}_cD_y^\beta u + K_2^- \, {}_yD_d^\beta u\right) & \\ \qquad +f(x,y,t), & (x,y,t) \in \Omega \times [0,T], \\ u(x,y,0) = u_0(x,y), & (x,y,t) \in \Omega, \\ u(x,y,0) = \varphi(x,y,t), & (x,y,t) \in \partial\Omega \times [0,T], \end{cases} \tag{5}$$

where $u \equiv u(x,y,t)$, $\Omega := (a,b) \times (c,d)$, $K_i^\pm \geq 0$ for $i = 1,2$, ${}_aD_x^\alpha, {}_xD_b^\alpha$, and ${}_cD_y^\beta$, ${}_yD_d^\beta$ are RL fractional operators with $1 < \alpha, \beta \leq 2$, $T > 0$, u_0 and φ are the initial and boundary values. We assume that the problem in (5) has a unique sufficiently smooth solution.

The CN-WSGD scheme

In this section we derive a **Crank-Nicolson** difference scheme. We make a partition of the domain Ω by a uniform mesh with space steps $h_x := (b-a)/N_x$, $h_y := (d-c)/N_y$, and time step $\tau := T/M$, where N_x, N_y, and M are positive integers. Then, the grid points will be $x_i := ih_x$, $y_j := jh_y$, and $t_n := n\tau$, for $1 \leq i \leq N_x$, $1 \leq j \leq N_y$, and $0 \leq n \leq M$. Let define $t_{n+1/2} := (t_n + t_{n+1})/2$ for $0 \leq n \leq M-1$, and use the following notation

$$u_{i,j}^n := u(x_i, y_j, t_n), \quad f_{i,j}^{n+1/2} := f(x_i, y_j, t_{n+1/2}),$$

$$\delta_t u_{i,j}^n := \frac{u_{i,j}^{n+1} - u_{i,j}^n}{\tau}.$$

The CN-WSGD scheme

Time discretization of (5) leads to the definition of the operator

$$\delta_t u_{i,j}^n = \frac{1}{2}[K_+^1 \left({}_aD_x^\alpha u\right)_{i,j}^{n+1} + K_+^2 \left({}_xD_b^\alpha u\right)_{i,j}^{n+1} + \tag{6}$$

$$+K_-^1 \left({}_cD_y^\beta u\right)_{i,j}^{n+1} + K_-^2 \left({}_yD_d^\beta u\right)_{i,j}^{n+1} + K_+^1 \left({}_aD_x^\alpha u\right)_{i,j}^{n} + K_+^2 \left({}_xD_b^\alpha u\right)_{i,j}^{n} +$$

$$+K_-^1 \left({}_cD_y^\beta u\right)_{i,j}^{n} + K_-^2 \left({}_yD_d^\beta u\right)_{i,j}^{n})]f_{i,j}^{n+1/2} + O(\tau^2).$$

After a little algebra, and factoring the equation before, denoting with $U_{i,j}^n$ the numerical approximation to $u_{i,j}^n$, we obtain the finite difference approximation for problem (5),

$$\left(1 - \frac{\tau^2}{2}\delta_x^\alpha\right)\left(1 - \frac{\tau^2}{2}\delta_y^\beta\right) U_{i,j}^{n+1} = \left(1 + \frac{\tau^2}{2}\delta_x^\alpha\right)\left(1 + \frac{\tau^2}{2}\delta_y^\beta\right) U_{i,j}^{n}$$

$$+\tau f_{i,j}^{n+1/2}. \tag{7}$$

The CN-WSGD scheme

A simple calculation shows that

$$\frac{\tau^3}{2}\delta_x^\alpha\delta_x^\beta f_{i,j}^{n+1/2} = \frac{\tau^3}{2}\left(K_+^1\,{}_aD_x^\alpha + K_+^2\,{}_xD_b^\alpha\right)\left(K_-^1\,{}_cD_y^\beta + K_-^2\,{}_yD_d^\beta\right)f_{i,j}^{n+1/2}, \tag{8}$$
$$+O(\tau^3h^2).$$

so eliminating the truncating error and introducing the intermediate variable $V_{i,j}^n$, we obtain the locally one-dimensional (LOD) scheme mentioned in [Qin11, Wang06]

$$\left(1-\frac{\tau^2}{2}\delta_x^\alpha\right)V_{i,j}^n = \left(1+\frac{\tau^2}{2}\delta_x^\alpha\right)U_{i,j}^n + \frac{\tau}{2}\left(1+\frac{\tau^2}{2}\delta_x^\alpha\right)f_{i,j}^{n+1/2}, \tag{9a}$$

$$\left(1-\frac{\tau^2}{2}\delta_y^\beta\right)U_{i,j}^{n+1} = \left(1+\frac{\tau^2}{2}\delta_y^\beta\right)V_{i,j}^n + \frac{\tau}{2}\left(1+\frac{\tau^2}{2}\delta_y^\beta\right)f_{i,j}^{n+1/2}, \tag{9b}$$

A third-order CN-WSGD scheme

In the space discretization, we choose the so-called 3-WSGD operators, i.e., the weighted and shifted Grünwald difference operators, defined as

$$\mathcal{G}^{\alpha}_{h,p,q,r} u(x) := \lambda_1 \, A^{\alpha}_{h,p} u(x) + \lambda_2 \, A^{\alpha}_{h,q} u(x) + \lambda_3 \, A^{\alpha}_{h,r} u(x), \qquad (10)$$

where the $\lambda_i' s$ coefficients depend on p, q, r. The operator (10) is third-order accurate in time [Qin11].

A third-order CN-WSGD scheme

We define ${}_L\mathcal{G}^{\alpha}_{h_x,p,q,r}u$, ${}_R\mathcal{G}^{\alpha}_{h_y,p,q,r}u$, and ${}_L\mathcal{G}^{\beta}_{h_y,p,q}u$, ${}_R\mathcal{G}^{\beta}_{h_y,p,q}u$, to approximate the fractional diffusion terms ${}_aD^{\alpha}_x u$, ${}_xD^{\alpha}_b u$, and ${}_cD^{\beta}_y u$, ${}_yD^{\beta}_d u$, respectively, see [Tadjeran06]. Multiplying both sides of (6) by τ, and separating the terms containing u^n and u^{n+1}, we have

$$\left(1 - \frac{K^1_+\tau}{2}\,{}_L\mathcal{G}^{\alpha}_{h_x,p,q} - \frac{K^2_+\tau}{2}\,{}_R\mathcal{G}^{\alpha}_{h_x,p,q} - \frac{K^1_-\tau}{2}\,{}_L\mathcal{G}^{\beta}_{h_y,p,q} - \frac{K^2_-\tau}{2}\,{}_R\mathcal{G}^{\beta}_{h_y,p,q}\right)u^{n+1}_{i,j} = \left(1 + \frac{K^1_+\tau}{2}\,{}_L\mathcal{G}^{\alpha}_{h_x,p,q} + \frac{K^2_+\tau}{2}\,{}_R\mathcal{G}^{\alpha}_{h_x,p,q} + \frac{K^1_-\tau}{2}\,{}_L\mathcal{G}^{\beta}_{h_y,p,q} + \frac{K^2_-\tau}{2}\,{}_R\mathcal{G}^{\beta}_{h_y,p,q}\right)u^{n}_{i,j} + \tau\, f^{n+1/2}_{i,j} + \tau\,\varepsilon^n_{i,j}, \quad (11)$$

where $\varepsilon_{i,j}^n$ denotes the (local) truncation error, and we have $|\varepsilon_{i,j}^n| \leq \tilde{c}\,(\tau^2 + h^3)$. We also write

$$\delta_x^\alpha = K_1^+ \, {}_L\mathcal{G}_{h_x,p,q}^\alpha + K_2^+ \, {}_R\mathcal{G}_{h_x,p,q}^\alpha, \qquad \delta_y^\beta = K_1^- \, {}_L\mathcal{G}_{h_y,p,q}^\beta + K_2^- \, {}_R\mathcal{G}_{h_y,p,q}^\beta.$$

We chose the same step sizes, $h_x = h_y = h$. A Taylor expansion yields

$$\frac{\tau^2}{4}\delta_x^\alpha \delta_y^\beta \left(u_{i,j}^{n+1} - u_{i,j}^n\right) =$$

$$= \frac{\tau^3}{4}\left[\left(K_+^1 \, {}_aD_x^\alpha + K_2^+ \, {}_xD_b^\alpha\right)\left(K_1^- \, {}_cD_y^\beta + K_2^- \, {}_yD_d^\beta\right) u_t\right]_{i,j}^{n+1/2}$$

$$+ O(\tau^5 + \tau^2 h^3). \qquad (12)$$

A new numerical method with examples: theoretical considerations

A considerable amount of computing time can be saved just resorting to an *extrapolation* technique. This procedure may also increase the accuracy of the method up to the third order in time [Marchuk83]. Let describe such a technique.

Step 1. Compute the numbers ζ_1, ζ_2, and ζ_3, solving the three linear algebraic equations

$$\begin{cases} \zeta_1 + \zeta_2 + \zeta_3 = 1 \\ \zeta_1 + \frac{1}{2}\zeta_2 + \frac{1}{4}\zeta_3 = 0 \\ \zeta_1 + \frac{1}{3}\zeta_2 - \frac{1}{9}\zeta_3 = 0. \end{cases}$$

An *extrapolated solution*, depending on U^n, is then used to solve the problem. The quantity U^n requires evaluating certain coefficients, which can be obtained by the "*PageRank* accelerating method" [Golub03]. The previous algebraic system yields the optimal coefficients $\zeta_1, \zeta_2, \zeta_3$.

A new numerical method with examples: theoretical considerations

Step 2. Compute the solution U^n of a *compact difference scheme* [Deng10, Spotz95, Tolstykh94, Zhuang08] (see below, at step 3), with the three time step sizes τ, $\frac{2}{3}\tau$, and $\frac{\tau}{3}$ [Tolstykh94]. This kind of methods is usually adopted for steady convection-diffusion numerical problems on uniform grids [Spotz95], rather than for time-dependent problems.

Step 3. Evaluate the *extrapolated solution*, $W^n(\tau)$, by

$$W^n(\tau) = \zeta_1\, U^n(\tau) + \zeta_2\, U^n\left(\frac{2}{3}\tau\right) + \zeta_3\, U^n\left(\frac{\tau}{3}\right),$$

where we have displayed the precise dependence of U^n on τ.

Example 1: Let be the FDE

$$ {}_0D_t^{\gamma} u = {}_0D_x^{\alpha} u + {}_xD_1^{\alpha} u + {}_0D_y^{\beta} u + {}_yD_1^{\beta} u + f(x,y,t) \qquad (13) $$

on the space domain $\Omega := (0,1) \times (0,1)$, for $t > 0$, subject to the boundary conditions

$$ u(x,y,t) = 0, \quad (x,y) \in \partial\Omega, \quad t \in [0,1], $$

with the initial value

$$ u(x,y,0) = x^3(1-x)^3 y^3 (1-y)^3 \quad (x,y) \in [0,1] \times [0,1]. $$

The analytical solution to this problem turns out to be known see [Deng12], and is

$$ u(x,y,t) = e^{-t} x^3 (1-x)^3 y^3 (1-y)^3, \qquad (14) $$

Numerical examples

if in (13), we choose the source term to be

$$
\begin{aligned}
f(x,y,t) = & - e^{-t}x^3(1-x)^3y^3(1-y)^3 \\
& + \Big(\frac{3!}{\Gamma(4-\alpha)}(x^{3-\alpha}+(1-x)^{3-\alpha}) - \frac{3\cdot 4!}{\Gamma(5-\alpha)}(x^{3-\alpha}+ \\
& + (1-x)^{3-\alpha}) + \frac{3\cdot 5!}{\Gamma(6-\alpha)}(x^{5-\alpha}+(1-x)^{5-\alpha}) - \\
& + \frac{6!}{\Gamma(7-\alpha)}(x^{6-\alpha}+(1-x)^{6-\alpha})\Big)y^3(1-y)^3 \\
& + \frac{3!}{\Gamma(4-\beta)}(y^{3-\beta}+(1-y)^{3-\beta}) - \frac{3\cdot 4!}{\Gamma(5-\beta)}(y^{4-\beta}+ \\
& + (1-y)^{4-\beta}) + \frac{3\cdot 5!}{\Gamma(6-\alpha)}(y^{5-\beta}+(1-y)^{5-\beta}) - \\
& + \frac{6!}{\Gamma(7-\beta)}(y^{6-\beta}+(1-y)^{6-\beta}))x^3(1-x)^3.
\end{aligned}
$$

This choice is useful to *validate* our algorithm and test its performance. Then, we will be confident that the code is as good as in this case also when **different sources**, possibly reflecting specific problems of practical interest replace the forcing term above.
In Fig. 2, the effect of replacing ordinary derivatives $(\alpha,\beta,\gamma) = (2,2,1)$ with fractional derivatives, in a given diffusion equation, e.g., with $(\alpha,\beta,\gamma) = (1.1, 1.7, 1)$, thus accounting for *anomalous* diffusion, is clear. In general, such a modification implies **new geometric patterns** in the solution, and a possibly **anisotropic behavior**. Even a different **speed of propagation**, depending on the order of the fractional derivatives can be reproduced in this way. Indeed, all these features are observed, e.g., in certain **porous media through which a fluid flows** [Crank47 ,Thambynayagam01].

Numerical examples

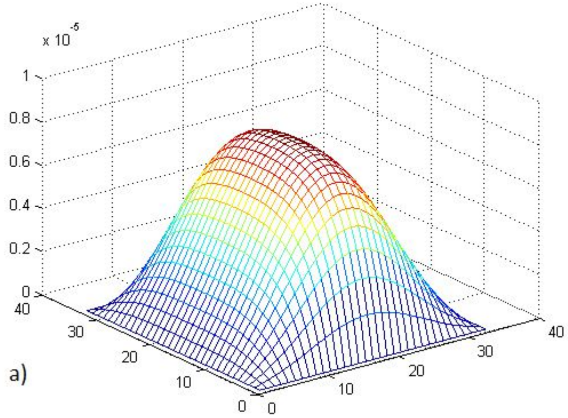

Figure: Classical solution (obtained by a fine grid numerical ADI method with $\tau = h/16$).

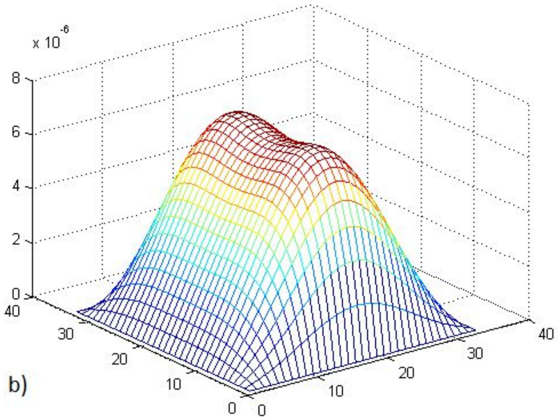

Figure: Exact (analytical) fractional diffusion solution with $(\alpha, \beta, \gamma) = (1.1, 1.7, 1)$.

Numerical examples

In Table 1, the absolute numerical errors $||u^n - W^n||_\infty$ and $\|u^n - W^n\|_2$, as well as the corresponding convergence rates achieved using different space step sizes, are shown.

(α, β)	N	$\|\|u^n - W^n\|\|_\infty$	time-rate	space-rate	$\|\|u^n - W^n\|\|_2$	time-rate	space-rate
$(1.1, 1.7)$	8	3.4852E-7	$--$	$--$	9.745252E-5	$--$	$--$
	16	2.4585E-8	2.95	1.92	7.7852E-5	2.93	1.87
	32	2.7852E-8	2.99	1.98	5.3255E-6	2.98	1.95
	64	4.8420E-9	3.00	1.99	4.7852E-6	2.99	1.98
	128	1.9651E-9	3.00	2.00	5.4525E-7	3.00	2.00
	256	4.4582E-11	3.00	2.00	3.6321E-10	3.00	2.00
	512	3.8512E-14	3.00	2.00	6.78521E-13	3.00	2.00

Table: L^∞ and L^2 norm errors, and convergence rates for Example 1, when the (LOD) CN-WSGD scheme, that is a FADI method, is used, at time $t = 5$, for several values of N, and $\tau = h$.

Figure 3 shows the infinity norm and the L^2 norm errors for Example 1, when the compact difference scheme is implemented, at times $t = 1$, for several values of N, and fixed α, β, and γ.

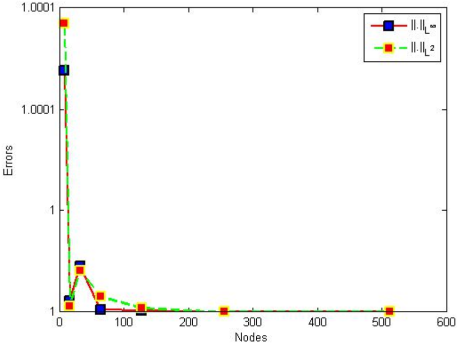

Figure: L^∞ and L^2 discrepancy between the numerical solution of the classical problem and that of the fractional problem with $(\alpha, \beta, \gamma) = (1.1, 1.7, 1)$, at $t = 1$.

Example 2: If one wants to predict the fluid motion for a concentrate introduced at the left side of a tank, which advects rightwards and diffuses in the y direction, the fractional evolutionary advection-diffusion equation

$$ {}_0D_t^{\gamma} u = K_1({}_0D_x^{\alpha} u + {}_xD_1^{\alpha} u) + K_2({}_0D_y^{\beta} u + {}_yD_1^{\beta} u) + a_1 \frac{\partial u}{\partial x} + a_2 \frac{\partial u}{\partial y}, \tag{15} $$

can be solved, for suitable values of the fractional orders, α, β, and γ.

Numerical examples

An example of a real case, where a dye is continuously introduced into a tank filled in with a fluid, is shown in Fig. 4. Here, the diffusion occurring in the direction of the y-axis is due to turbulence. Classical diffusion yields a parabolic profile, while in the picture the flow described by anomalous diffusion looks conic (in 3D) [Cushman06, Pritchard08].

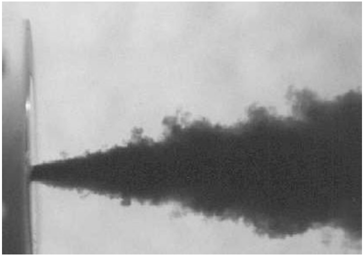

Figure: Example of an advecting plume, which is better described through anomalous rather than classical diffusion (from [Cushman06]).

Numerical examples

Let consider the space domain $\Omega := [0,10] \times [0,10]$, for $t \in [0,10]$. We impose the boundary condition

$$u(10,y,t) = u_y(x,0,t) = u_y(x,10,t) = 0, \tag{16}$$

and the initial condition

$$u(0,y,0) = \delta(y-5). \tag{17}$$

What we are doing is setting the boundary back to its initial value each time step. We do not want to allow to pass through the horizontal walls of the tank so the boundary conditions for both y axis are set to zero.
Setting then $K_1 = a_2 = 0$, we obtain

$${}_0D_t^{\gamma} u = K_2({}_0D_y^{\beta} u + {}_yD_1^{\beta} u) + a_1 \frac{\partial u}{\partial x}. \tag{18}$$

In Fig. 5, the numerical results are shown for the advection-diffusion plume, corresponding to the parameters $K_2 = 1$, $a_1 = 2$, $\Delta x = \Delta y = 1/20$, $\Delta t = 0.002$.

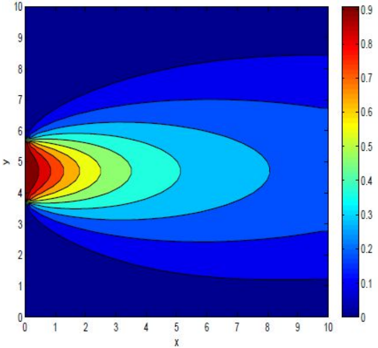

Figure: Numerical results for advection-diffusion plume, $\alpha = \beta = 1.6, \gamma = 0.6$ (from [Cushman06]).

Conclusions and future developments

We presented a **weighted and shifted Grünwald-Letnikov difference (WSGD)** operator is used to approximate RL fractional diffusion operators. It is shown that indeed **third-order accuracy in time** can be achieved solving numerically two-dimensional fPDEs by **ADI**-like methods. A new technique, designed to **accelerate** the algorithm, which is competitive with respect to the methods existing to date in the literature [Deng12], has also been developed. While the present method seems to outperform all the other existing algorithms, using very dense grids to attain low errors may require, however, as one may expect, a considerable computational time.

Confirming those models, it would be interesting to study the effects of **anisotropy** due to different fractional orders affecting different space directions.

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Thank you for interest.

SPECIAL POLYNOMIALS IN THE DESCRIPTION OF FRACTIONAL CALCULUS

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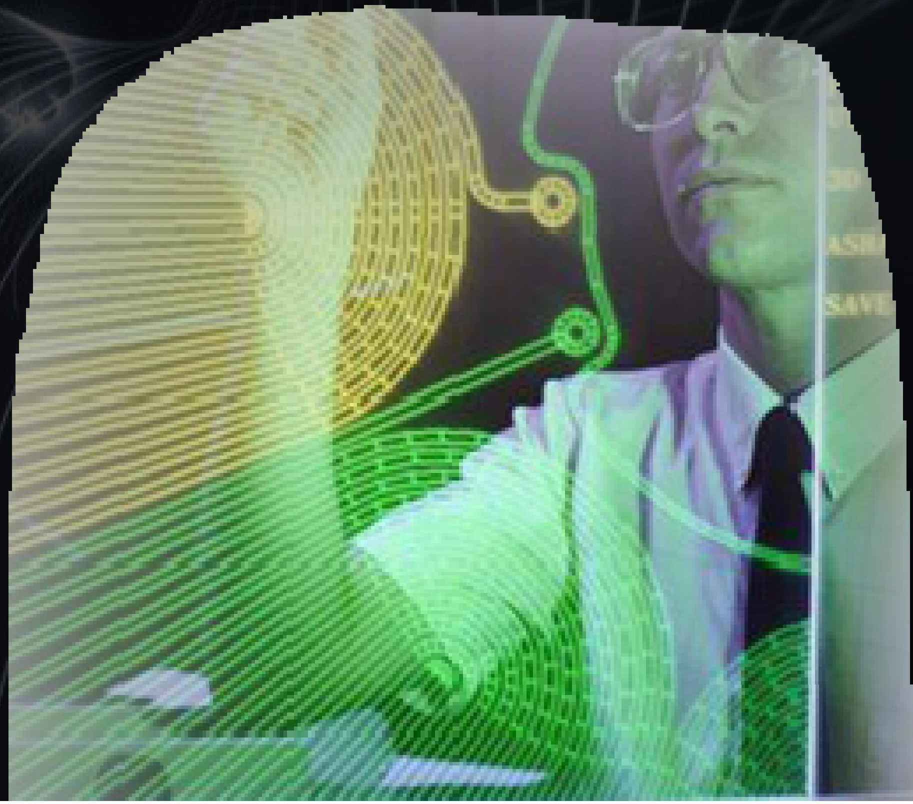
Topics

- Introduction
- Tanslation Operators and Integral Transforms
- Special Polynomials and Fractional Operators

Introduction



Fractional derivative

$$\frac{d^{\nu}}{dx^{\nu}} f(x), \qquad \nu \in \mathbb{R}$$

$f(x)$ real, $x \in \mathbb{R}$

we are looking for similar actions

$$\frac{d}{dx}\cdot\frac{d}{dx}=\frac{d^2}{dx^2}$$

$$\left(\frac{d}{dx}\right)^{-1}=\int^{x}dx$$

$$e^{\lambda\frac{d}{dx}}=\sum_{n=0}^{+\infty}\frac{\lambda^n}{n!}\frac{d^n}{dx^n},\qquad \lambda\in\mathbb{R}$$

and further more complicated forms, as:

$$e^{q(x)\frac{d}{dx}},\quad q(x)\ \text{real function with suitable conditions}$$

and, moreover

$$F\left(x, \frac{d}{dx}\right), \quad \sqrt{\frac{d}{dx}}, \quad \sqrt{\frac{d}{dx} + x}$$

explicative example

$$\begin{cases} \dfrac{\partial}{\partial t} f(x,t) = \alpha \dfrac{\partial}{\partial x} f(x,t) \\ f(x,0) = g(x) \end{cases}$$

$$\frac{\partial}{\partial t} f(x,t) = \hat{\Theta} f(x,t), \qquad \hat{\Theta} = \alpha \frac{\partial}{\partial x}$$

$$f(x,t) = e^{t\hat{\Theta}} g(x)$$

We will discuss how to represent the action of the operators involving fractional derivative, by using the concept and the related formalism of special classes of orthogonal polynomials

Translation Operators and Integral Transforms

we consider a real function which is analytic in a neighborhood of the origin

$$f(x+\lambda)=\sum_{n=0}^{+\infty}\frac{\lambda^n}{n!}f^{(n)}(x), \qquad \lambda\in\mathbb{R}$$

the so called *shift* or *translation* operator

$$e^{\lambda\frac{d}{dx}}$$

produces a shift of the variable

$$e^{\lambda\frac{d}{dx}}f(x)=\sum_{n=0}^{+\infty}\frac{\lambda^n}{n!}\frac{d^n}{dx^n}f(x)=\sum_{n=0}^{+\infty}\frac{\lambda^n}{n!}f^{(n)}(x)$$

$$e^{\lambda\frac{d}{dx}}f(x)=f(x+\lambda)$$

further identities

$$e^{\lambda x \frac{d}{dx}} f(x) = f\left(e^{\lambda} x\right), \qquad \lambda \in \mathbb{R}$$

$$e^{\lambda x^2 \frac{d}{dx}} f(x) = f\left(\frac{x}{1-\lambda x}\right), \qquad |x| < \frac{1}{|\lambda|}$$

$$e^{\lambda x^n \frac{d}{dx}} f(x) = f\left(\frac{x}{\sqrt[n-1]{1-(n-1)\lambda x^{n-1}}}\right),$$

$$|x| < \sqrt[n-1]{\frac{1}{(n-1)|\lambda|}}$$

generalized *translation* operators

$$e^{\lambda q(x)\frac{d}{dx}} f(x) = f\left(\varphi\left(\varphi^{-1}(x)+\lambda\right)\right), \qquad \lambda \in \mathbb{R}$$

where

$q(x), \quad \varphi(\theta)$ (invertible)

are real functions, such that

$$\varphi^{'}(\theta) = q(\varphi(\theta))$$

the Hausdorff identity and applications

$$e^{\lambda \hat{A}} \hat{B} e^{-\lambda \hat{A}} = \hat{B} + \lambda \left[\hat{A}, \hat{B} \right] + \frac{\lambda^2}{2!} \left[\hat{A}, \left[\hat{A}, \hat{B} \right] \right] + \ldots$$

where $\lambda \in \mathbb{R}$

$\hat{A}, \hat{B}$ generic operators, independent to λ

in general, $\forall m \in \mathbb{N}$

$$e^{\lambda \frac{d^m}{dx^m}}(1) = \sum_{n=0}^{+\infty} \frac{\lambda^n}{n!} \frac{d^{nm}}{dx^{nm}}(1) = 1, \quad \lambda \in \mathbb{R}$$

in the case $m = 2$

$$e^{\lambda \frac{d^2}{dx^2}} x = e^{\lambda \frac{d^2}{dx^2}} x e^{-\lambda \frac{d^2}{dx^2}}(1)$$

i.e.

$$e^{\lambda \frac{d^2}{dx^2}} x = \left(x + 2\lambda \frac{d}{dx} \right)(1) = x$$

which gives the generalization:

$$e^{\lambda \frac{d^2}{dx^2}} x^k = \left(x + 2\lambda \frac{d}{dx} \right)^k (1) = x^k, \quad k \in \mathbb{N}$$

and moreover, for an analytic function

$$e^{\lambda \frac{d^2}{dx^2}} f(x) = f\left(x + 2\lambda \frac{d}{dx} \right)(1)$$

in particular

$$e^{\lambda \frac{d^2}{dx^2}} e^x = e^{\lambda + x}$$

Integral representations

$$e^{b^2} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2+2bu}\,du, \qquad b \text{ constant}$$

$$e^{\lambda \frac{d^2}{dx^2}} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2+2\sqrt{2}u\frac{d}{dx}}\,du, \qquad \lambda \in \mathbb{R}$$

Integral transform

$$e^{\lambda \frac{d^2}{dx^2}} f(x) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2} f\left(x + 2\sqrt{2}u\right) du$$

The possibility of exploiting the integral transforms taking advantage from the definition of the Euler gamma function

$$\Gamma(x) = \int_0^{+\infty} e^{-t} t^{x-1} dt \qquad x, t \in \mathbb{R}$$

$$\left(\frac{d}{dx}\right)! f(x) = \int_0^{+\infty} e^{-t} t^{d/dx} f(x) dt$$

i.e.

$$\left(\frac{d}{dx}\right)! f(x) = \int_0^{+\infty} e^{-t} f(x + \log(t)) dt$$

by using the previous results, we deduced further integral transforms for more complicated operators

$$\left(x\frac{d}{dx}\right)! f(x) = \int_0^{+\infty} e^{-t} f(xt)dt$$

$$\left(\frac{d}{dx}\right)^{-\nu} f(x) = \frac{1}{\Gamma(\nu)} \int_0^{+\infty} t^{\nu-1} f(x-t)dt$$

furthermore, by noting that

$$a^{-\nu} = \frac{1}{\Gamma(\nu)} \int_0^{+\infty} t^{\nu-1} e^{-at} dt$$

the following expression

$$\left(x\frac{d}{dx}\right)^{-\nu} f(x) = \frac{1}{\Gamma(\nu)}\int_0^{+\infty} t^{\nu-1} f(e^{-t}x)\,dt$$

becomes more interesting, by noting that

$$\left(x\frac{d}{dx}\right)^{-\nu}\left[\frac{1}{1-x}-1\right] = \frac{1}{\Gamma(\nu)}\int_0^{+\infty}\frac{t^{\nu-1}x}{e^t-1}\,dt = \sum_{n=1}^{+\infty}\frac{x^n}{n^\nu}$$

Second-order derivatives

$$\left(\alpha - x\frac{d^2}{dx^2}\right)^{-\nu} f(x) = \frac{1}{\Gamma(\nu)}\int_0^{+\infty} e^{-\alpha t} t^{\nu-1} e^{t(d^2/dx^2)} f(x)\,dt$$

since

$$e^{t(d^2/dx^2)} f(x) = \frac{1}{2\sqrt{\pi t}}\int_{-\infty}^{+\infty} e^{-(x-\xi)^2/4t} f(\xi)\,d\xi$$

we get

$$\left(\alpha - x\frac{d^2}{dx^2}\right)^{-\nu} f(x) = \frac{1}{2\Gamma(\nu)}\int_0^{+\infty} \frac{e^{-\alpha t} t^{\nu-1}}{\sqrt{\pi t}}\,dt\left[\int_{-\infty}^{+\infty} e^{-(x-\xi)^2/4t} f(\xi)\,d\xi\right]$$

for example, if

$$f(x) = e^{-x^2}$$

the Gauss transform can be explicit worked out, to give

$$\left(\alpha - x\frac{d^2}{dx^2}\right)^{-\nu} e^{-x^2} = \frac{1}{\Gamma(\nu)} \int_0^{+\infty} \frac{e^{-\alpha t} t^{\nu-1}}{\sqrt{1+4t}} e^{-x^2/(1+4t)} dt$$

Special Polynomials and Fractional Operators

The generalized, two-variable Hermite polynomials (Kampé de Fériet)

$$H_n(x,y) = n! \sum_{s=0}^{[n/2]} \frac{x^{n-2s} y^s}{(n-2s)!s!}$$

can be viewed as the Gauss transform of the monomial x^n

$$H_n(x,y) = \frac{1}{2\sqrt{\pi y}} \int_{-\infty}^{+\infty} e^{-(x-\xi)^2/4y} \xi^n d\xi$$

fractional derivative acting on the monomial

$$\left(\alpha - x\frac{\partial^2}{\partial x^2}\right)^{-\nu} x^n = \frac{1}{\Gamma(\nu)}\int_0^{+\infty} e^{-\alpha t} t^{\nu-1} H_n(x, yt)\,dt$$

this integral transform defines a new family of polynomials, strictly related to Hermite polynomials, denoted by

$${}_{\nu}H_n(x, y;\alpha)$$

operational definition

$$ {}_{\nu}H_n(x,y;\alpha) = \left(\alpha - y\frac{\partial^2}{\partial x^2} \right)^{-\nu} x^n $$

helps us to write

$$ \sum_{n=0}^{+\infty} \frac{\xi^n}{n!}\, {}_{\nu}H_n(x,y;\alpha) = \left(\alpha - x\frac{\partial^2}{\partial x^2} \right)^{-\nu} e^{x\xi} $$

which gives the relevant generating function

$$ \sum_{n=0}^{+\infty} \frac{\xi^n}{n!}\, {}_{\nu}H_n(x,y;\alpha) = \frac{e^{x\xi}}{\left(\alpha - y\xi^2\right)^{\nu}}, \quad |\xi| < \left(\frac{\alpha}{y}\right)^{1/2} $$

There are many interesting relations satisfied by this family of Hermite-like polynomials, these can be derived by analogous properties of ordinary Hermite polynomials. We just observe that they solve the following partial differential equation

$$\frac{\partial}{\partial y}\,{}_{v}H_{n}(x,y;\alpha)=-\frac{\partial^{3}}{\partial x^{2}\partial\alpha}\,{}_{v}H_{n}(x,y;\alpha)$$

an interesting operational rule involving the fractional derivative

$$\left(\alpha - x\frac{\partial^2}{\partial x^2}\right)^{1-\nu} x^n = \alpha\,{}_{\nu}H_n(x,y;\alpha) - yn(n-1)\,{}_{\nu}H_{n-2}(x,y;\alpha)$$

and, finally it is worth stressing that

$$\left(\alpha - y\frac{\partial^2}{\partial x^2}\right)^{\nu} {}_{\nu}H_n(x,y;\alpha) = x^n$$

Expressions involving the first-order derivative can be obtained by noting the structure of the Hermite polynomials

$$e^{y\frac{\partial}{\partial x}} x^n = \left(x+y\right)^n, \quad e^{y\frac{\partial^2}{\partial x^2}} x^n = H_n(x,y)$$

which suggest an elementary form of Hermite polynomials

$$H_n^{(1)}(x,y) = \left(x+y\right)^n$$

then, the previous relation

$$\left(\alpha - x\frac{\partial^2}{\partial x^2}\right)^{-\nu} x^n = \frac{1}{\Gamma(\nu)}\int_0^{+\infty} e^{-\alpha t} t^{\nu-1} H_n(x, yt)\,dt$$

allows to write

$$\left(\alpha - x\frac{\partial}{\partial x}\right)^{-\nu} x^n = \frac{1}{\Gamma(\nu)}\int_0^{+\infty} e^{-\alpha t} t^{\nu-1} (x + yt)^n\,dt$$

so that we can introduce the following polynomials

$$ {}_{\nu}H_n^{(1)}(x,y;\alpha)=\frac{1}{\Gamma(\nu)}\int_0^{+\infty} e^{-\alpha t}t^{\nu-1}(x+yt)^n\,dt $$

and similarly, we obtain the operational relation

$$ \left(\alpha-y\frac{\partial}{\partial x}\right)^{\nu} {}_{\nu}H_n^{(1)}(x,y;\alpha)=x^n $$

The considerations we have seen offer the possibility of developing a different point of view regarding the fractional derivatives representations and allow to include, within a more general and wider context, families of apparently uncorrelated polynomials. For instance, an obvious generalization of the above discussed polynomials can be provide by the following identity:

$$\left(\alpha-\sum_{s=2}^{m} x_s \frac{\partial^s}{\partial x_1^s}\right)^{-\nu} x_1^n = \frac{1}{\Gamma(\nu)} \int_0^{+\infty} e^{-\alpha t} t^{\nu-1} H_n^{(m)}(x_1, x_2 t, \ldots, x_m t)\, dt$$

which defines the further generalized Hermite-like polynomials

$$\left(\alpha-\sum_{s=2}^{m} x_s \frac{\partial^s}{\partial x_1^s}\right)^{-\nu} x_1^n = {}_{\nu}H_n^{(1)}\left(\{x\}_1^m ;\alpha\right)$$

where

$$ {}_{\nu}H_n^{(1)}\left(\{x\}_1^m;\alpha\right)=n!\sum_{r=0}^{\left[n/m\right]}\frac{x_m^r H_{n-mr}^{(m-1)}\left(\{x\}_1^{m-1}\right)}{r!(n-mr)!} $$

$$ \{x\}_1^m = x_1, x_2, \ldots, x_m $$

the generating function is easily obtained

$$ \sum_{n=0}^{+\infty}\frac{\xi^n}{n!}\,{}_{\nu}H_n^{(1)}\left(\{x\}_1^m;\alpha\right)=\frac{e^{x_1\xi}}{\left(\alpha-\sum_{s=2}^{m}x_s\xi^s\right)^{\nu}} $$

The formalism and the polynomials we have proposed may offer significant advantages to compute the effect of fractional operators on a given function. For example, if we introduce the following Bessel-like functions

$$ {}_{v}J_{n}(x,y;\alpha)=\sum_{r=0}^{+\infty}\frac{(-1)^{r}\,{}_{v}H_{n}(x,y;\alpha)}{2^{n+2r}\,r!(n+r)!} $$

we can obtain

$$\frac{1}{\left(\alpha - y\frac{\partial^2}{\partial x^2}\right)^{\nu}} J_n(x) = {}_{\nu}J_n(x, y; \alpha)$$

$J_n(x)$ is a first kind Bessel function similarly, we can derive the related generating function for the Bessel-like function

$$\sum_{n=0}^{+\infty} e^{in\vartheta}\ {}_{\nu}J_{n}(x,y;\alpha)=\frac{e^{ix\sin\vartheta}}{\left(\alpha-y\sin\vartheta^{2}\right)^{\nu}}$$

In conclusion, the combined use of integral transforms and special polynomials provides a powerful tool to deal with fractional derivative and integrals.

Fractional diffusions with time-varying coefficients

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Outline

1. Diffusion equations with time-varying coefficients: probabilistic motivation and generalizations

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2. Fractional generalizations: the first approach

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See R.Garra, E.Orsingher, F.Polito, *Fractional diffusions with time-varying coefficients*, http://arxiv.org/pdf/1501.04806.pdf

Diffusion equations with time-varying coefficients: probabilistic motivation

The diffusion equation governing the one-dimensional marginal of the fractional Brownian motion $B_H(t)$, $t \geq 0$, $0 < H < 1$ is given by

$$\left(t^{1-2H} \frac{\partial}{\partial t} \right) u(x,t) = H \frac{\partial^2}{\partial x^2} u(x,t), \qquad H \in (0,1), \; x \in \mathbb{R}, \quad (1)$$

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Here we consider *bifractional* diffusion equations, involving the Hurst parameter linked to the fractional Brownian motion and the real order of the power of operators appearing in the governing equations.

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- The time-varying diffusion equation involving the fractional power of the operator $\left(t^{1-2H}\frac{\partial}{\partial t}\right)$

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- The time-varying diffusion equation involving the Caputo time-fractional derivative

Fractional generalizations: the first approach

We first consider the fractional diffusion equation with time-dependent coefficients

$$\left(t^{1-2H}\frac{\partial}{\partial t}\right)^{\alpha} u_{\alpha}(x,t) = H^{\alpha}\frac{\partial^2}{\partial x^2}u_{\alpha}(x,t), \tag{2}$$

where $H \in (0,1)$ is the Hurst parameter and $\alpha \in (0,1)$.

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McBride theory of fractional powers of hyper-Bessel operators

McBride considered the generalized hyper-Bessel operator

$$L = t^{a_1}\frac{\mathrm{d}}{\mathrm{d}t}t^{a_2}\dots t^{a_n}\frac{\mathrm{d}}{\mathrm{d}t}t^{a_{n+1}}, \qquad t > 0, \tag{3}$$

where n is an integer number and $a_1, \dots, a_{n+1}$ are real numbers.

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where n is an integer number and $a_1, \dots, a_{n+1}$ are real numbers.
Lemma 1: The operator L in (3) can be written as

$$Lf = m^n t^{a-n}\prod_{k=1}^{n} t^{m-mb_k} D_m t^{mb_k} f, \tag{4}$$

where

$$D_m := \frac{d}{dt^m} = m^{-1}t^{1-m}\frac{d}{dt}.$$

The constants appearing in (4) are defined as

$$a = \sum_{k=1}^{n+1} a_k, \qquad m = |a-n|, \qquad b_k = \frac{1}{m}\left(\sum_{i=k+1}^{n+1} a_i + k - n\right).$$

Lemma 2: Let r be a positive integer, $a < n$. Then

$$L^r f = m^{nr} t^{-mr} \prod_{k=1}^{n} I_m^{b_k,-r} f, \tag{5}$$

where, for $\alpha > 0$

$$I_m^{\eta,\alpha} f = \frac{t^{-m\eta-m\alpha}}{\Gamma(\alpha)} \int_0^t (t^m - u^m)^{\alpha-1} u^{m\eta} f(u)\, d(u^m), \tag{6}$$

and for $\alpha \leq 0$

$$I_m^{\eta,\alpha} f = (\eta + \alpha + 1) I_m^{\eta,\alpha+1} f + \frac{1}{m} I_m^{\eta,\alpha+1} \left(t \frac{d}{dt} f \right). \tag{7}$$

The fractional integrals $I_m^{\eta,\alpha}$ are Erdélyi–Kober-type operators.

Definition 1: Let $m = n - a > 0$, η any real number. Then, for any $f(x) \in F_{p,\mu}$

$$L^{\eta} f = m^{n\eta} t^{-m\eta} \prod_{k=1}^{n} I_m^{b_k, -\eta} f, \tag{8}$$

In order to understand the key-role played by the operator D_m, we remark that the following equality holds

$$(D_m)^{\eta} f = \frac{m}{\Gamma(n-\eta)} (D_m)^n \int_0^t (t^m - u^m)^{n-\eta-1} u^{m-1} f(u)\, du. \tag{9}$$

Then it is possible to prove Lemma 2, considering the relation between negative powers of D_m and Erdélyi–Kober integrals.

Caputo-like counterpart of the operator (8)

In analogy with the classical theory of fractional operators, we introduce the following

Definition 2: Let α be a positive real number, $m = n - a > 0$, $f \in F_{p,\mu}$ is such that

$$L^{\alpha}\left(f(t) - \sum_{k=0}^{b-1} \frac{t^k}{k!} f^{(k)}(0^+)\right)$$

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$${}^{C}L^{\alpha} f(t) = L^{\alpha}\left(f(t) - \sum_{k=0}^{b-1} \frac{t^k}{k!} f^{(k)}(0^+)\right), \tag{10}$$

where $b = \lceil \alpha \rceil$.

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where $b = \lceil \alpha \rceil$.

The relevance of this definition for the applications is due to the fact that for physical reasons we are interested in solving fractional Cauchy problems involving initial conditions on the functions.

Fractional diffusions with time-varying coefficients: the first approach

Theorem
The solution to the Cauchy problem

$$\begin{cases} {}^C\left(t^{1-2H}\frac{\partial}{\partial t}\right)^{\alpha} u_\alpha(x,t) = H^{\alpha}\frac{\partial^2}{\partial x^2} u_\alpha(x,t), \quad \alpha \in (0,1),\ t>0 \\ u_\alpha(x,0) = \delta(x), \end{cases} \tag{11}$$

is given by

$$u_\alpha(x,t) = \frac{1}{2^{1-\alpha/2} t^{H\alpha}} W_{-\alpha/2, 1-\alpha/2}\left(-\frac{2^{\alpha/2}|x|}{t^{H\alpha}}\right). \tag{12}$$

In view of definitions 1 and 2 the regularized Caputo-like operator appearing in (11) reads

$$ {}^{C}\left(t^{1-2H}\frac{\partial}{\partial t}\right)^{\alpha} u_\alpha(x,t) = \left(t^{1-2H}\frac{\partial}{\partial t}\right)^{\alpha} u_\alpha(x,t) \qquad (13) $$

$$ - (2H)^{\alpha}\frac{t^{-2H\alpha}}{\Gamma(1-\alpha)} u_\alpha(x,0) $$

$$ = (2H)^{\alpha} t^{-2H\alpha} I_{2H}^{0,-\alpha} u_\alpha(x,t) - (2H)^{\alpha}\frac{t^{-2H\alpha}}{\Gamma(1-\alpha)} u_\alpha(x,0). $$

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Therefore the Fourier transform of (11) reads

$$(2H)^\alpha t^{-2H\alpha} I_{2H}^{0,-\alpha} \widehat{u}_\alpha(\beta,t) = -H^\alpha \beta^2 \widehat{u}_\alpha(\beta,t) + (2H)^\alpha \frac{t^{-2H\alpha}}{\Gamma(1-\alpha)}, \tag{14}$$

whose solution is

$$\widehat{u}_\alpha(\beta,t) = E_{\alpha,1}\left(-\frac{\beta^2 t^{2H\alpha}}{2^\alpha}\right). \tag{15}$$

Then, by inverting the Fourier transform we obtain the claimed result.

Relation with the generalized grey Brownian motion (ggBm)

The generalized grey Brownian motion (ggBm) was recently introduced and studied by A. Mura and coauthors in as a series of papers as a family of non-Markovian stochastic processes for anomalous fast or slow diffusions.

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In his PhD thesis A. Mura introduced the fractional equation governing the probability density of the ggBm, that is given by

$$P(x,t) = P(x,0) + \frac{1}{\Gamma(\delta)} \frac{\gamma}{\delta} \int_0^t \tau^{\frac{\gamma}{\delta}-1} (t^{\gamma/\delta} - \tau^{\gamma/\delta})^{\delta-1} \frac{\partial^2}{\partial x^2} P(x,\tau)\, \mathrm{d}\tau, \tag{16}$$

involving the Erdélyi–Kober integras.

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involving the Erdélyi–Kober integras.
We now discuss the equivalence between (16) and our master equation, in the case of $\delta = \alpha$ and $\gamma/2 = H\alpha$.

From Definitions 1 and 2, we recall that the diffusion equation (11) can be written as

$$
\begin{aligned}
{}^{C}\left(t^{1-2H}\frac{\partial}{\partial t}\right)^{\alpha} P(x,t) &= \left(t^{1-2H}\frac{\partial}{\partial t}\right)^{\alpha} \left(P(x,t) - P(x,0)\right) \qquad (17)\\
&= (2H)^{\alpha} t^{-2H\alpha} I_{2H}^{0,-\alpha} \left(P(x,t) - P(x,0)\right)\\
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\end{aligned}
$$

and therefore in the integro-differential form

$$
I_{2H}^{0,-\alpha} \left(P(x,t) - P(x,0)\right) = \frac{t^{2H\alpha}}{2^{\alpha}} \frac{\partial^2}{\partial x^2} P(x,t). \qquad (18)
$$

We now recall the following property of the Erdélyi–Kober integral (see McBride (1982), Theorem 2.7, page 523)

$$(I_m^{\eta,\alpha})^{-1} = I_m^{\eta+\alpha,-\alpha}. \tag{19}$$

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In our case, the inverse of the operator appearing in the left hand side of (18) is given by

$$\left(I_{2H}^{0,-\alpha}\right)^{-1} = I_{2H}^{-\alpha,\alpha}. \tag{20}$$

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By applying the inverse operator (20) to both sides of (18), we arrive at

$$\begin{aligned} P(x,t) - P(x,0) &= \frac{I_{2H}^{-\alpha,\alpha}}{2^\alpha}\left(t^{2H\alpha}\frac{\partial^2}{\partial x^2}P(x,t)\right) \qquad (21) \\ &= \frac{2^{1-\alpha}H}{\Gamma(\alpha)}\int_0^t \tau^{2H-1}\left(t^{2H}-\tau^{2H}\right)^{\alpha-1}\frac{\partial^2}{\partial x^2}P(x,t)\,\mathrm{d}\tau, \end{aligned}$$

which coincides with (16) for $\delta = \alpha$ and $\gamma = 2H\alpha$, up to a multiplicative constant.

Other results

- We prove that $u_\alpha(x,t)$ is the law of the r.v. $X_{\alpha,H}(t)$ which is connected to the fractional Brownian motion by means of the relation

$$X_{\alpha,H}(t) \stackrel{d}{=} X_{2\alpha,H}\left(|B_H(t)|^{\frac{1}{2H}}\right), \quad 0<\alpha<\frac{1}{2} \tag{22}$$

and has variance

$$\mathbb{V}\mathrm{ar}\, X_{2\alpha,H}(t) = \frac{t^{2H\alpha}}{2^{\alpha-1}\Gamma(\alpha+1)}. \tag{23}$$

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- We establish a relationship between solutions of equation (2) and solutions of higher order diffusion equations

$$t^{1-2H}\frac{\partial u}{\partial t} = (-1)^k H \frac{\partial^k u}{\partial x^k}, \qquad k>2. \tag{24}$$

Fractional generalizations: the second approach

The second fractional generalization of equation (1) is given by

$$ {}^{C}D^{\nu}_{0^+} u\left(x,t\right) = Ht^{2H-1}\frac{\partial^2}{\partial x^2}u\left(x,t\right), \qquad \nu \in (0,1),\ x\in\mathbb{R},\ t>0, \tag{25}$$

involving Caputo time-fractional derivatives of order ν.

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- M. Bologna, A. Svenkeson, B.J. West, P. Grigolini, Diffusion in heterogeneous media: An iterative scheme for finding approximate solutions to fractional differential equations with time-dependent coefficients. *Journal of Computational Physics*, in press, (2014)

Analytical results

Theorem. The fundamental solution $u(x, t)$ to (25) can be written as

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-i\beta x} E_{\nu,1+\frac{2H-1}{\nu},\frac{2H-1}{\nu}} \left(-H\beta^2 t^{\nu+2H-1}\right) \mathrm{d}\beta, \tag{26}$$

where

$$E_{\nu,1+\frac{2H-1}{\nu},\frac{2H-1}{\nu}} \left(-H\beta^2 t^{\nu+2H-1}\right)$$

is the Saigo-Kilbas generalized Mittag-Leffler function.

The proof is simply based on the fact that the Fourier transform of the Cauchy problem reads

$$\begin{cases} {}^C D^{\nu}_{0^+} U(\beta, t) = -Ht^{2H-1}\beta^2 U(\beta, t), & t > 0,\ \nu \in (0,1], \\ U(\beta, 0) = 1, \end{cases} \tag{27}$$

whose solution is given by

$$E_{\nu, 1+\frac{2H-1}{\nu}, \frac{2H-1}{\nu}} \left(-H\beta^2 t^{\nu+2H-1} \right).$$

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We underline that the Cauchy problem (27) has been firstly considered by Kilbas and Saigo in a series of papers and recently studied by E. Capelas de Oliveira, F. Mainardi and J. Vaz Jr. (2014) in the framework of fractional relaxation models. In this paper complete monoticity of Kilbas and Saigo function has been considered.

Probabilistic results

From the probabilistic point of view an interesting result comes from the special choice $H = 1/4$, $\nu = 3/4$.

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In this case, we have that the Fourier transform of the fundamental solution of (25) reads

$$U(\beta, t) = E_{\frac{3}{4},\frac{1}{3},-\frac{2}{3}}\left(-\frac{1}{4}\beta^2 t^{1/4}\right) = 1 + \sum_{k=1}^{\infty}\left(-\frac{\beta^2 t^{1/4}}{2^2}\right)^k \prod_{j=0}^{k-1}\frac{\Gamma(\frac{j}{4}+\frac{1}{2})}{\Gamma(\frac{j}{4}+\frac{5}{4})}.$$

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Since

$$\prod_{j=0}^{k-1}\frac{\Gamma(\frac{j}{4}+\frac{1}{2})}{\Gamma(\frac{j}{4}+\frac{5}{4})} = \frac{\Gamma(1/2)\Gamma(3/4)}{\Gamma(\frac{k+2}{4})\Gamma(\frac{k+3}{4})\Gamma(\frac{k+4}{4})} \tag{28}$$

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and using the multiplication formula for the Gamma function we have that

$$\prod_{j=0}^{k-1}\frac{\Gamma(\frac{j}{4}+\frac{1}{2})}{\Gamma(\frac{j}{4}+\frac{5}{4})} = \frac{\Gamma(\frac{k+1}{4})\Gamma(3/4)}{\pi\ 2^{-2k+\frac{1}{2}}\,k!}. \tag{29}$$

Therefore,

$$
\begin{aligned}
U(\beta, t) &= E_{\frac{3}{4},\frac{1}{3},-\frac{2}{3}}\left(-\frac{1}{4}\beta^2 t^{1/4}\right) = 1 + \frac{\Gamma(3/4)}{\pi\sqrt{2}} \sum_{k=1}^{\infty} \left(-\beta^2 t^{1/4}\right)^k \frac{\Gamma\left(\frac{k+1}{4}\right)}{k!} \\
&= 1 + \frac{\Gamma(3/4)}{\pi\sqrt{2}} \int_0^{\infty} e^{-w} w^{-3/4} \sum_{k=1}^{\infty} \frac{\left(-\beta^2 w^{1/4} t^{1/4}\right)^k}{k!} \mathrm{d}w \\
&= \frac{\Gamma(3/4)}{\pi\sqrt{2}} \int_0^{\infty} e^{-w} w^{-3/4} e^{-\beta^2 \sqrt[4]{tw}} \mathrm{d}w.
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
U(\beta,t) &= E_{\frac{3}{4},\frac{1}{3},-\frac{2}{3}}\left(-\frac{1}{4}\beta^2 t^{1/4}\right) = 1+\frac{\Gamma(3/4)}{\pi\sqrt{2}}\sum_{k=1}^{\infty}\left(-\beta^2 t^{1/4}\right)^k \frac{\Gamma\left(\frac{k+1}{4}\right)}{k!} \\
&= 1+\frac{\Gamma(3/4)}{\pi\sqrt{2}}\int_0^\infty e^{-w}w^{-3/4}\sum_{k=1}^{\infty}\frac{\left(-\beta^2 w^{1/4}t^{1/4}\right)^k}{k!}\mathrm{d}w \\
&= \frac{\Gamma(3/4)}{\pi\sqrt{2}}\int_0^\infty e^{-w}w^{-3/4}e^{-\beta^2\sqrt[4]{tw}}\mathrm{d}w.
\end{aligned}
$$

Finally, we have

$$
\begin{aligned}
u(x,t) &= \frac{\Gamma(3/4)}{\pi\sqrt{2}}\int_0^\infty e^{-w}w^{-3/4}\frac{e^{-\frac{x^2}{4\sqrt[4]{tw}}}}{\sqrt{4\pi\sqrt[4]{tw}}}\mathrm{d}w \qquad (30) \\
&= \frac{\sqrt{2}\Gamma(3/4)}{\pi\sqrt[4]{t}}\int_0^\infty \frac{e^{-\frac{x^2}{2w}}}{\sqrt{2\pi w}}\cdot e^{-\frac{w^4}{2^4 t}}\mathrm{d}w,
\end{aligned}
$$

The solution (30) is the probability law of the time-changed Brownian motion $B(W_t)$, where

$$\mathbb{P}\{W_t \in \mathrm{d}z\}/\mathrm{d}z = \frac{\sqrt{2}\Gamma(3/4)e^{-\frac{z^4}{2^4 t}}}{\pi\sqrt[4]{t}}, \qquad z > 0,$$

and B is a standard Brownian motion.

Conclusions and remarks

- The McBride theory for fractional powers of hyper-Bessel-type operators represents a convenient framework to derive the governing equation of the ggBm

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- The McBride theory for fractional powers of hyper-Bessel-type operators represents a convenient framework to derive the governing equation of the ggBm
- The analysis of fractional PDEs with variable coefficients is a developing field both from the mathematical and applied point of view
- Applications of the discussed results in other problems of mathematical-physics and probability where the governing equations involve operators with variable coefficients will be object of further research. For example time-fractional Poisson process where state probabilities are governed by

$$\left(t^{1-2H}\frac{d}{dt}\right)^{\nu} p_k(t) = -\lambda\left(p_k(t) - p_{k-1}(t)\right), \quad k \geq 1 \quad (31)$$

leads to homogeneous Poisson process with a random time related to ggBm?

Overview of the Fractional Calculus of variations and its application to non-standard Lagrangians

Giorgio S. Taverna

University of Leeds

Workshop on Fractional Calculus
11th March 2015
Università di Roma Tre, Italy

Outline

- Background

  → FALVA

  → Generalized Fractional Action Principle

- Methodology and results

  → Bauer's theorem?

  → Non Standard Lagrangians+ Generalized Fractional Action Principle

- Conclusions and future works

- The fractional variational principle (FVP) is a promising topic and several applications given (*El Nabulsi and Torres*, *2008 ; Malinskowa and Torres 2012*).

- In 2005, El Nabulsi introduced the Fractional Action-Like Variational (FALVA) Action $A_F(x)$:

$$A_F(x)=\frac{1}{\Gamma(\alpha)}\int_a^b L(x,\dot{x},\tau)(t-\tau)^{(\alpha-1)}d\tau$$

$$\Downarrow$$

$$\frac{\partial L}{\partial x}-\frac{d}{d\tau}\left(\frac{\partial L}{\partial \dot{x}}\right)=\frac{1-\alpha}{1-\tau}\frac{\partial L}{\partial \dot{x}}$$

with

$\cdot\ 0<\alpha<1$
$\cdot\ t\in[a,b]$
$\cdot\ \tau\in(a,t)$

El Nabulsi, 2005

Generalized Fractional Action Principle

- A generalization of the FALVA is an action involving a generalized kernel.

$$A(x)=\int_a^b k_\alpha(b,\tau)L(x,\dot{x},\tau)d\tau$$

- Theorem: *Let x be a solution to the problem of finding a function x that minimizes the functional A subject to boundary conditions* $x(a)=x_a$, $x(b)=x_b$. *Also, if*

  - $L\in C^1([a,b]\times\mathbb{R}^2;\mathbb{R})$
  - $k_\alpha(t,\tau)$ is square-integrable in $\Delta=[a,b]\times[a,b]$
  - $k_\alpha(t,\tau)=k_\alpha(t-\tau)$
  - $k_\alpha(b,\tau),\partial_{\dot{x}}L\in AC[a,b]$
  - $k_\alpha(b,\tau),\partial_x L\in C[a,b]$

then,

$$\frac{\partial L}{\partial x}-\frac{d}{d\tau}\left(\frac{\partial L}{\partial \dot{x}}\right)=\frac{1}{k_\alpha(b,\tau)}\frac{dk_\alpha(b,\tau)}{d\tau}\frac{\partial L}{\partial \dot{x}}$$

$\forall\tau\in[a,b]$

Odzijewick et al., 2012

ound: Non Standard Lagrangians

- A linear dissipative dynamical system can be described as :

$$\ddot{x} + A(\tau)\dot{x} + B(\tau)x = 0$$

This equation of motion can be derived from the non standard Lagrangian

$$L(x, \dot{x}, \tau) = \frac{1}{r(\tau)\dot{x} + s(\tau)x},$$

if A(τ), B(τ),r(τ) and s(τ) are continuous, differentiable and integrable functions and if they are a solution of a proper Riccati equation.

Musielak, 2008

dard Lagrangians+ Generalized Fractional Action Principle

- Let us consider the Non Standard Lagrangian, with r and s constant in time and insert in the Generalized Euler-Lagrange equation. We obtain the equation of motion

$$\ddot{x}+\frac{\dot{x}}{2}+\left[\frac{3s}{r}-\frac{\dot{k}_\alpha}{k_\alpha}\right]+x\left[\frac{s^2}{2r^2}-\frac{s}{2r}\frac{\dot{k}_\alpha}{k_\alpha}\right]=0$$

- In order to get physical solutions, it is easy to show that the following condition must hold

$$\begin{cases}\dfrac{s}{r}>0\\[2ex]\dfrac{\dot{k}_\alpha}{k_\alpha}<\dfrac{s}{r}\end{cases}$$

$$\forall\tau\in[a,b]$$

- Let us consider the Hamiltonian formalism for the non nonstandard Lagrangian

$$L(x,\dot{x},\tau)=\frac{1}{r(\tau)\dot{x}+s(\tau)x},$$

It is easy to show that

$$\begin{cases} p=\dfrac{-\partial L}{\partial \dot{x}}=\dfrac{-r}{(r\dot{x}+sx)^2} \\ H=\dfrac{-spx}{r} \end{cases}.$$

Also,

$$\begin{cases} \dot{p}=\dfrac{-\partial H}{\partial x}-\dfrac{p\dot{k}_\alpha}{k_\alpha}=\dfrac{sp}{r}-\dfrac{p\dot{k}_\alpha}{k_\alpha} \\ \dot{x}=\dfrac{-\partial H}{\partial p}=\dfrac{-sx}{r} \end{cases}.$$

with r,s constant in time and $\dfrac{s}{r}>0,\quad \forall\tau\in[a,b].$

Taverna and Torres, 2014

ology and results: Bauer's theorem

- In 1931 Bauer proved the following corollary

"The equations of motion of a dissipative linear dynamical system with constant coefficients are not given by a variational principle".

- Let's consider the Lagrangian of simple harmonic oscillator :

$$L(x,\dot{x})=\frac{m\dot{x}^2}{2}-\frac{cx^2}{2}$$

$$m\ddot{x}=-cx$$

- If we apply the Generalized Euler-Lagrange equation we get :

$$m\ddot{x}=-cx-m\dot{x}\frac{\dot{k}_\alpha}{k_\alpha}$$

..which becomes the equation of a damped harmonic oscillator if $k_\alpha(b,\tau)=e^{\alpha\tau}, \alpha>0$

$$m\ddot{x}=-cx-m\dot{x}\alpha.$$

Conclusions and future works

- In this talk we analyzed the impact of the Generalized Fractional Variational principle on dynamical systems.
- We found out that the Bauer's theorem can be easily overcome with this approach and interesting results about damped systems have been shown.
- In case of non-standard Lagrangians, this approach constrains the freedom in choosing the kernel.
- Future works could focus on choosing appropriate kernel to model realistic physical phenomena.

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