Anomalous diffusion equations

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Outline

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2. Standard diffusion model
3. Finite difference schemes
4. Convergence of the finite difference scheme
5. What is fractional diffusion ?
6. Fractional diffusion model
7. Grunwald-Letnikov formula
8. Discretization of the fractional derivative
9. Riemann-Liouville formula
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1. What is diffusion?

Diffusion is one of the fundamental processes by which material moves

Diffusion is a consequence of the constant motion of atoms, molecules, and particles, and results in material moving from areas of high to low concentration

Classical diffusion $\longrightarrow$ Particle motion described by Brownian motion

Brownian motion $\longrightarrow$ Gaussian distribution increments

2. Standard diffusion model

$$\frac{\partial u}{\partial t}(x,t) = D\frac{\partial^2 u}{\partial x^2}(x,t)$$

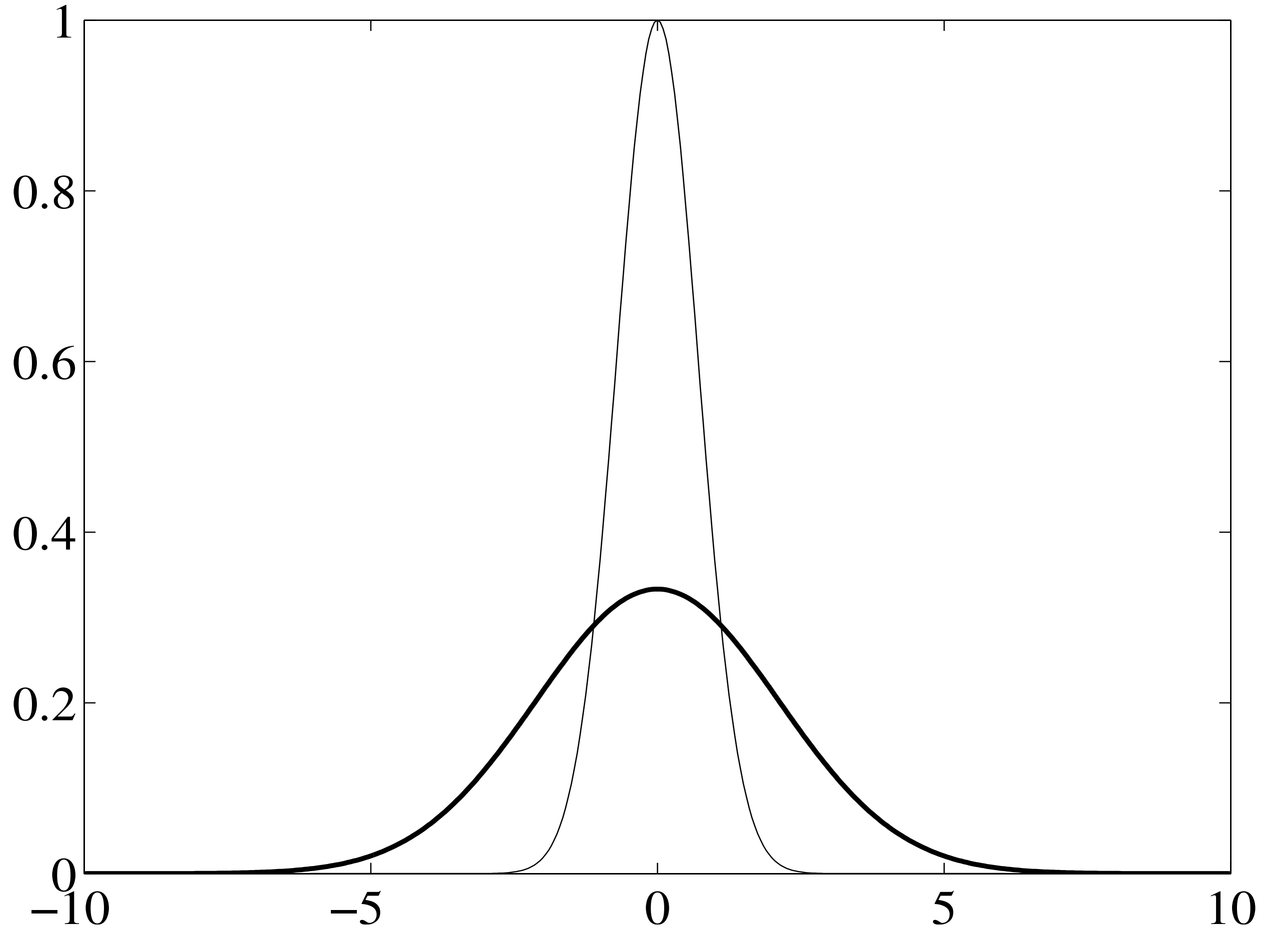
$$a < x < b, \quad D > 0$$

Initial condition : $\quad u(x,0) = f(x),\ a < x < b$

Dirichlet boundary conditions:

$$u(a,t) = g_a(t) \quad \text{and} \quad u(b,t) = g_b(t)$$

The effect of diffusion



3. Finite difference schemes

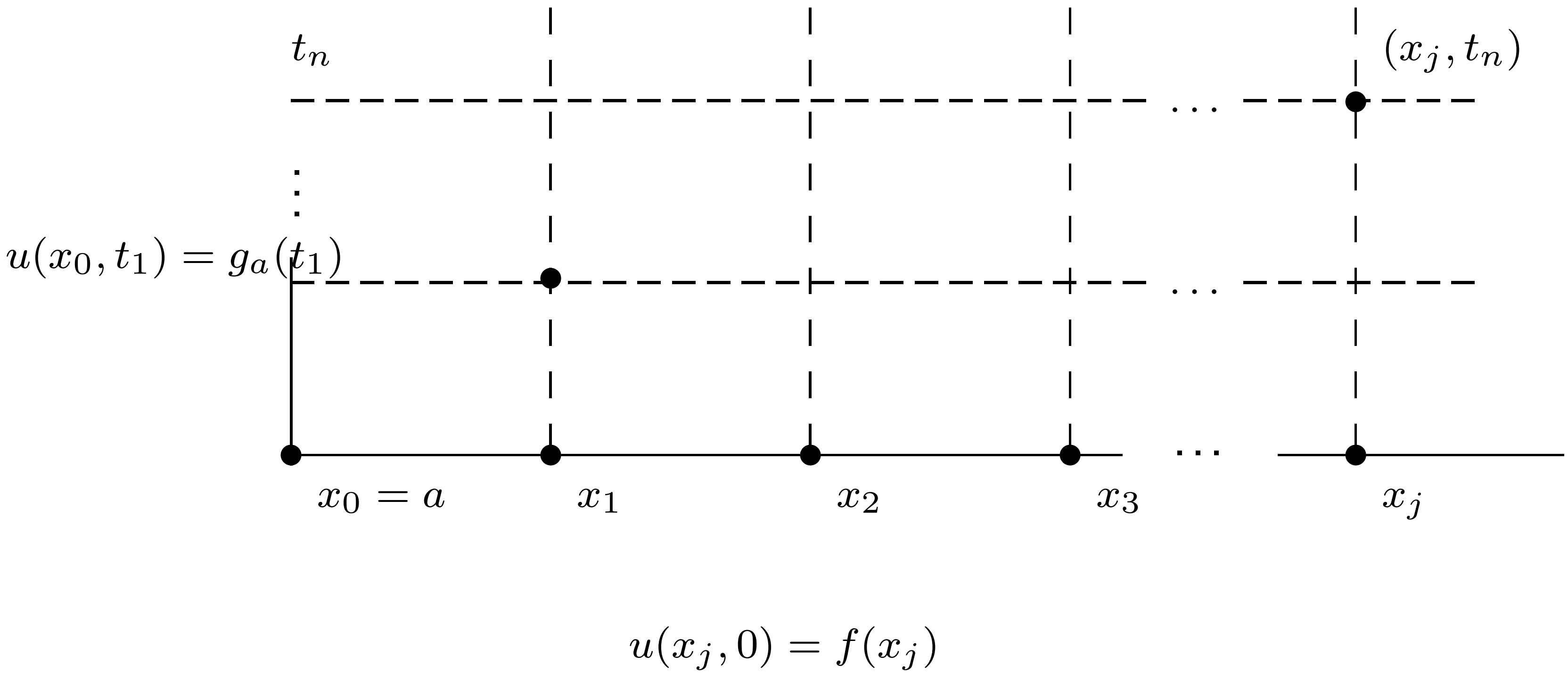
Suppose there are approximations $\mathbf{U}^n := \{U_j^n\}$ to the values $u(x_j, t_n)$ at the mesh points

$$x_j = a + j\Delta x,\ j = 0, \ldots, N$$

$$t_n = n\Delta t,\ n \geq 0$$

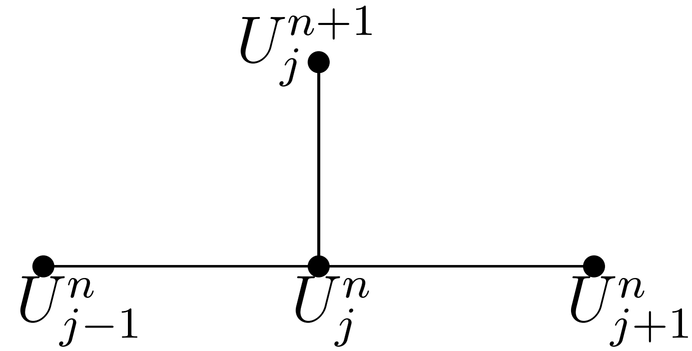
Δx space step; Δt time step

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


t_n
(x_j, t_n)
$\cdots$
$\vdots$
$u(x_0, t_1) = g_a(t_1)$
$x_0 = a$
x_1
x_2
x_3
x_j
$u(x_j, 0) = f(x_j)$

Discretization

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = D\frac{U_{j+1}^n - 2U_j^n + U_{j-1}^n}{\Delta x^2}$$



$$U_j^{n+1} = U_j^n + \mu \delta^2 U_j^n$$

$$\delta^2 U_j^n = U_{j+1}^n - 2U_j^n + U_{j-1}^n \qquad \mu = D \frac{\Delta t}{\Delta x^2}$$

Matricial form

$$\mathbf{U}^{n+1} = M\mathbf{U}^n + \mathbf{v}^n$$

$\mathbf{U}^n$ – vector with the spatial discrete points
$\mathbf{v}^n$ – vector with discrete boundary values

M is the matrix iteration

$$M = I + \mu B$$

B – diffusion discretisations

The matrix B is

$$B = \begin{bmatrix} -2 & 1 & 0 & \dots & & 0 \\ 1 & -2 & 1 & & & \\ & & & \ddots & & \vdots \\ \vdots & & \ddots & & & \\ & & & & & 1 \\ 0 & & \dots & & 1 & -2 \end{bmatrix}$$

4. Convergence of the numerical method

Assume that the initial value problem is approximated by

$$U_j^{n+1} = QU_j^n,$$

where $Q = \sum_{j=-r}^{p} a_j E^j$, $\quad EU_j^n = U_j^{n+1}$.

Previous example:

$$U_j^{n+1} = QU_j^n \quad \text{where} \quad Q = 1 + \mu\delta^2$$

Discretization error – is the amount by which the continuous solution fails to satisfy the discrete formula. [Consistency]

Round off error – is due to the finite precision of computer. It is the amount by which the computer fails to solve the discrete formulas with infinite precision. [Stability]

Consistency

Definition: A finite difference scheme is consistent up to time T_0 in the norm $||\cdot||$ with the respective equation if the actual solution u to the initial value problem satisfies

$$u_j^{n+1} = Qu_j^n + \Delta t T^n,$$

where $u_j^n = u(j\Delta x, n\Delta t)$, $||T^n|| \leq \tau(\Delta x)$, $n\Delta t < T_0$ and $\tau(\Delta x) \to 0$ as $\Delta t \to 0$. Here is assumed that Δx is defined in terms of Δt and goes to zero with Δt.

Stability

Definition: The finite difference method is called stable in the norm $||\cdot||$ if there exist constants K and c such that

$$||U^n|| \leq K\mathrm{e}^{cn\Delta t}||U^0|| = K\mathrm{e}^{ct_n}||U^0||$$

where $t_n = n\Delta t$, and $K > 0$ and c are independent of the space steps and time step.

Lax Equivalence Theorem: Given a properly posed initial-value problem for a linear partial differential equation and a linear finite difference approximation to it that satisfies the consistency condition, stability is the necessary and sufficient condition for convergence.

Peter Lax (1926 –) ; Wolf prize 1987; Abel prize 2005

Convergence of the previous example

Consistency:

$$\Delta t T^n = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x^2)$$

Stability:

$$\mu \leq 1/2 \qquad \mu = D\frac{\Delta t}{\Delta x^2}$$

$$\Delta t \leq \frac{\Delta x^2}{2D}$$

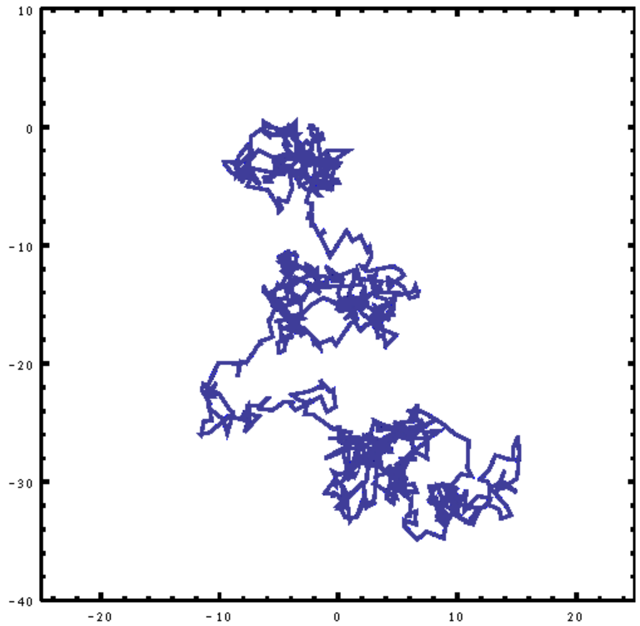
5. What is fractional diffusion?

Fractional diffusion $\longrightarrow$ Particle motion described by Lévy flights

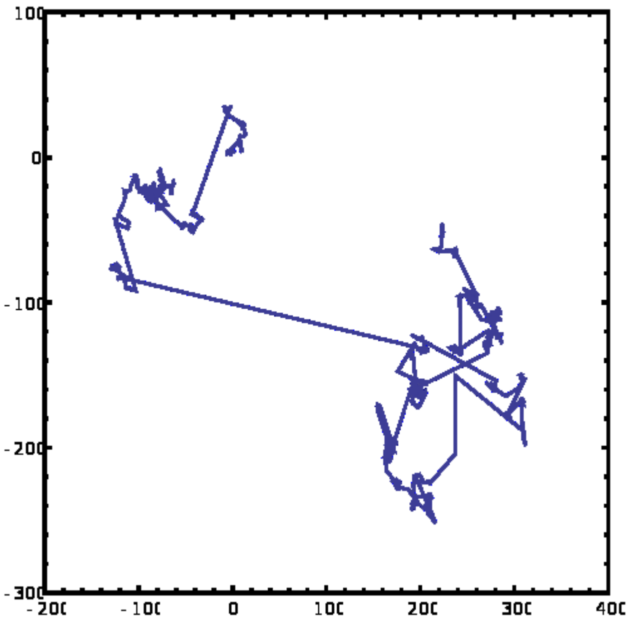
Lévy flights differ from Brownian motion in the probability distribution of the jumps

Brownian motion $\longrightarrow$ Gaussian distribution increments

Lévy flights $\longrightarrow$ Power law distribution increments



Brownian motion



Lévy flights

Note the presence of large jumps compared to Brownian motion

6. Fractional diffusion equation

Fractional diffusion equation describing superdiffusion

$$\frac{\partial u}{\partial t}(x,t) = D\frac{\partial^\alpha u}{\partial x^\alpha}(x,t)$$

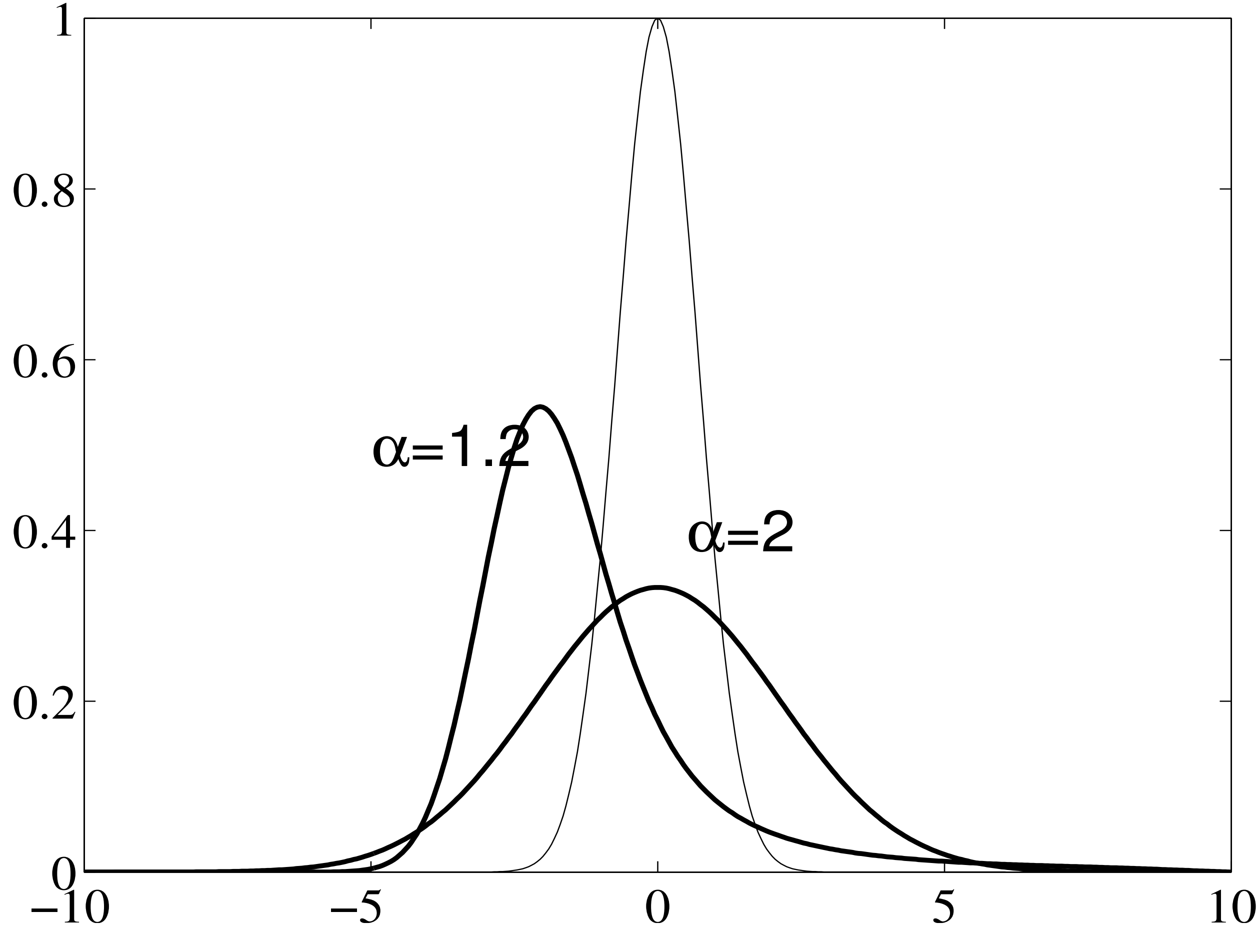
$$a < x < b, \quad 1 < \alpha \leq 2, \quad D > 0$$

Initial condition : $u(x,0) = f(x),\ a < x < b$

Dirichlet boundary conditions:

$$u(a,t) = g_a(t) \quad \text{and} \quad u(b,t) = g_b(t)$$

The effect of fractional diffusion



Evidence of fractional diffusion models

Numerical results are in agreement with experimental results

- Benson et al, 2000 $\longrightarrow$ Transport processes with heavy tailed plumes
- Pachepsky et al, 2000 $\longrightarrow$ Solute transport in soils
- Zhou and Selin, 2003 $\longrightarrow$ Porous media
- Huang et al , 2006 $\longrightarrow$ Solute transport in soils

7. Grünwald-Letnikov formula, $\alpha > 0$

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \lim_{\Delta x \to 0} \frac{1}{\Delta x^\alpha} \sum_{k=0}^{\left[\frac{x-a}{\Delta x}\right]} (-1)^k \begin{pmatrix} \alpha \\ k \end{pmatrix} u(x - k\Delta x, t)$$

$$\begin{aligned} g_k &= (-1)^k \begin{pmatrix} \alpha \\ k \end{pmatrix} \\ &= (-1)^k \frac{\alpha(\alpha-1)\ldots(\alpha-k+1)}{k!} = \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} \end{aligned}$$

This is a non-local property

$$\alpha = 1$$

$$g_0 = 1 \qquad g_1 = -\alpha = -1 \qquad g_k = 0,\ k \geq 2$$

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \lim_{\Delta x \to 0} \frac{1}{\Delta x}\left(u(x) - u(x - \Delta x)\right)$$

$$\alpha = 2$$

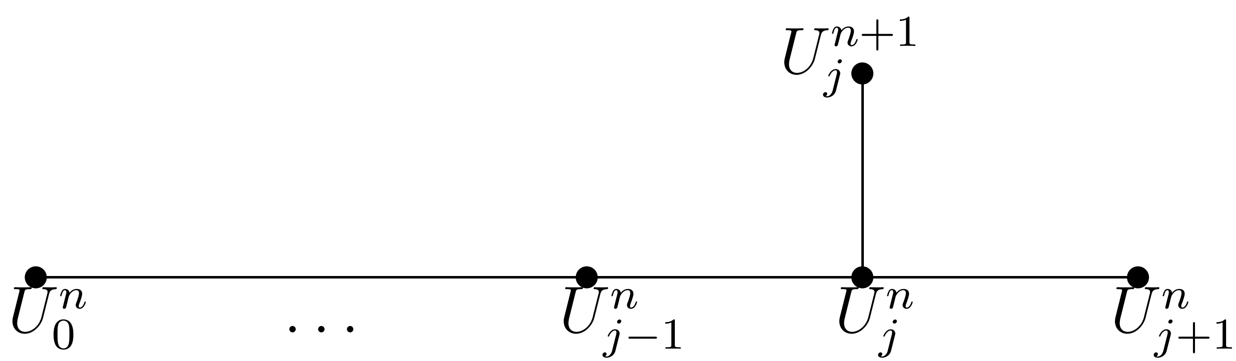
$$g_0 = 1 \qquad g_1 = -\alpha = -2 \qquad g_2 = 1 \quad g_k = 0, k \geq 3$$

$$\begin{aligned}
\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) &= \lim_{\Delta x \to 0} \frac{1}{\Delta x^2}(u(x) - 2u(x-\Delta x) + u(x - 2\Delta x)) \\
&= \lim_{\Delta x \to 0} \frac{1}{\Delta x}\left(u'(x) - u'(x - \Delta x)\right)
\end{aligned}$$

8. Discretization of the fractional derivative

$$\left(\frac{\partial^\alpha u}{\partial x^\alpha}\right)_j^n \quad \simeq \quad \frac{1}{\Delta x^\alpha} \sum_{k=0}^{j+1} g_k U_{j+1-k}^n$$

$$g_k = (-1)^k \begin{pmatrix} \alpha \\ k \end{pmatrix} = \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)}$$



Classical scheme

$$U_j^{n+1} = U_j^n + \mu\delta^2 U_j^n$$

Fractional scheme

$$U_j^{n+1} = U_j^n + \mu_\alpha \delta^\alpha U_j^n$$

$$\delta^\alpha U_j^n = \sum_{k=0}^{j+1} g_k U_{j+1-k}^n \qquad \mu_\alpha = D\frac{\Delta t}{\Delta x^\alpha}$$

Matricial form

$$\mathbf{U}^{n+1} = M\mathbf{U}^n + \mathbf{v}^n$$

$\mathbf{U}^n$ – vector with the spatial discrete points
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M is the matrix iteration

$$M = I + \mu_\alpha B$$

B – diffusion discretisations

The matrix B is

$$B = \begin{bmatrix} g_1 & g_0 & 0 & \cdots & & 0 \\ g_2 & & & & & \\ & & & \ddots & & \vdots \\ \vdots & & \ddots & & & 0 \\ & & & & & g_0 \\ g_{2N-1} & & \cdots & & g_2 & g_1 \end{bmatrix}$$

Consistency and Stability

This approximation of the fractional derivative, for $1 < \alpha < 2$, is first order accurate

$$\frac{\delta^\alpha u_j^n}{\Delta x^\alpha} = \left(\frac{\partial^\alpha u}{\partial x^\alpha}\right)_j^n + \mathcal{O}(\Delta x)$$ (Meerschaert and Tadjeran, JCP, 2004)

Consistency: $\Delta t T^n = \mathcal{O}(\Delta t) + \mathcal{O}(\Delta x)$

Stability condition:

$$2^{\alpha-1}\mu_\alpha \leq 1 \qquad \Delta t \leq \frac{\Delta x^\alpha}{2^{\alpha-1}D}$$ (Sousa, JCP, 2009)

Some comments

- Although the standard operator is second order accurate, the fractional operator is only first order

- Being first order is the main disadvantage of using this definition of the fractional derivative

- We need new numerical methods based on the integral formulas of the fractional derivative

9. Riemann-Liouville formula

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) \quad = \quad \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_a^x \frac{u(\xi,t)}{(x-\xi)^{\alpha-n+1}}d\xi$$

$$a < x < b, \quad n = [\alpha] + 1$$

For $1 < \alpha < 2$,

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) \quad = \quad \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_a^x \frac{u(\xi,t)}{(x-\xi)^{\alpha-1}}d\xi$$

Why is difficult to handle the integral form?

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_a^x \frac{u(\xi,t)}{(x-\xi)^{\alpha-1}}d\xi$$

10. Final Remarks

- We have a non-local derivative

- The definition using the limit only allows first order accuracy. Not enough for many problems

- The integral definition has an improper integral, which is difficult to handle.

- Many physical models involving fractional derivatives are waiting to be solved with high accuracy.