Open Issues in Boundary Conditions of FPDEs and the Generalized Feynman-Kac Equation

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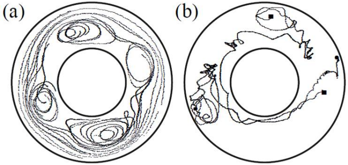

Outline

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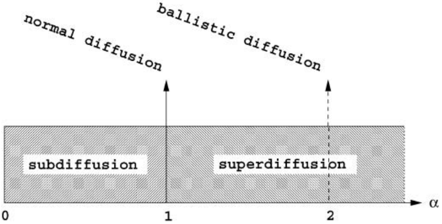
The types of diffusion are usually classified according to the relation of the mean squared displacement (MSD) of a particle to the time t.

- Subdiffusion, $\langle x^2(t) \rangle \sim t^\alpha$ with $0 < \alpha < 1$;
- Normal diffusion (Brownian motion), $\langle x^2(t) \rangle \sim t$;
- Superdiffusion, $\langle x^2(t) \rangle \sim t^\alpha$ with $\alpha > 1$.



When $\alpha \neq 1$, the corresponding diffusion is called anomalous diffusion.

Subdiffusion can be found in various natural phenomena, such as motion of labelled messenger RNA molecules in a living coli cell.

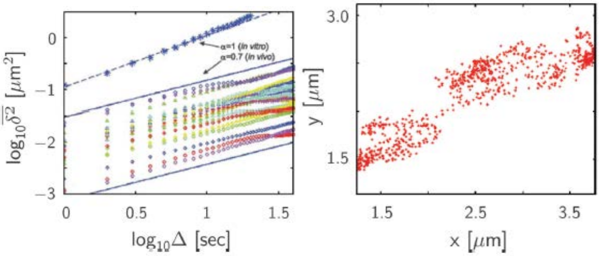


Figure: Motion of labelled messenger RNA molecules. Left: time averaged MSD of individual trajectories plotted as a function of the lag time Δ shows pronounced trajectory-to-trajectory scatter. All exhibit approximately the same anomalous diffusion exponent $\alpha \approx 0.7$ with some local variations. Right: points of the trajectory of an individual messenger RNA in the coli cell, showing that the molecule explores a major fraction of the bacterium's volume.

The other applications of anomalous diffusion:

- Subdiffusion can also be found in the following systems: charge carrier transport in amorphous semiconductors, nuclear magnetic resonance (NMR) diffusometry in percolative, Rouse or reptation dynamics in polymeric systems, transport on fractal geometries, the diffusion of a scalar tracer in an array of convection rolls, the dynamics of a bead in a polymeric network, etc.

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- Specially, a particle moving in porous systems also belongs to the subdiffusion region. Thus we can connect the problem of mould growing in barn which is a specific model of porous system with subdiffusion.
- Superdiffusion can model the food searching strategies of seagulls. It can also be used to determine the positions of locating N radar stations to optimize the searching for M targets. Superdiffusion is also observed in special domains of rotating flows, in collective slip diffusion on solid surfaces, in layered velocity fields, etc.

Brownian Motion (Normal Diffusion)

$W(x, t)$ – The probability density function (PDF) to find the particle under observation at position x at time t.
The classical Fokker-Planck equation.

$$\boxed{\frac{\partial W(x,t)}{\partial t} = K_1 \frac{\partial^2 W(x,t)}{\partial x^2}}$$

- K_1 – Coefficient of diffusion with the dimension of $[K_1] = cm^2/s$.
- If the particle is released at the origin at time $t = 0$ in an unbounded space, the solution is $W(x,t) = \frac{1}{\sqrt{4\pi K_1 t}} \exp\left(-\frac{x^2}{4K_1 t}\right)$.
- The variance $\langle x^2(t) \rangle = 2K_1 t$.

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This equation is indeed equivalent to Fick's second law for the concentration of a chemical substance originally presented by Adolf Fick from a combination of the continuity equation and the constitutive equation (Fick's first law). Using Taylor expansion can also obtain the master equation for Brownian motion instead of Fick's first law.

Another derivation of Brownian motion was published in 1980 by Paul Langevin using the concept of a stochastic force.

$$\boxed{m\frac{dv}{dt} = -\zeta v + F(t)}$$

- m and v are the mass and velocity of Brownian particle respectively.
- ζ – The frictional constant.
- $F(t)$ – The white Gaussian noise: $\langle F(t)\rangle = 0$ and $\langle F(t)F(t')\rangle = 2\zeta k_B T\delta(t-t')$, where k_B is the Boltzman constant and T is absolute temperature.
- $\langle x^2(t)\rangle = (2k_B T/\zeta)t$.
- The Langevin equation is actually obtained from Newton's second law.

CTRW Model.

Considering a particle, which starts at the origin. It has to wait for a random waiting (trapping) time τ drawn from the waiting time PDF $\phi(\tau)$, before it makes a jump to left or right. The length of the jump can also be chosen to be a random variable, δx, distributed in terms of the PDF $\lambda(\delta x)$. After the jump, a new pair of waiting time and jump length are drawn from the PDFs $\phi(\tau)$ and $\lambda(\delta x)$.

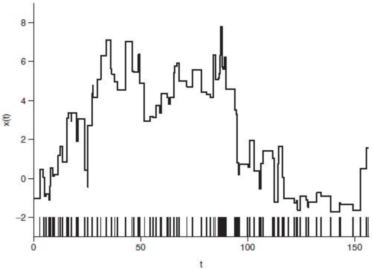

Figure: A trajectory of a CTRW with exponential distribution of waiting times ($\lambda = 1$) and Gaussian distribution of step lengths (with zero mean and unit dispersion).

For the space-time decoupled case, the PDF $W(x,t)$ obeys the algebraic relation in Fourier-Laplace space

$$W(k,s) = \frac{1-\phi(s)}{s}\frac{W_0(k)}{1-\lambda(k)\phi(s)}.$$

- $W_0(k)$ – The Fourier transform of the initial condition $W(x,t=0)$.

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- $W_0(k)$ – The Fourier transform of the initial condition $W(x, t = 0)$.
- The way of diffusion (sub-, normal or super diffusion) is determined by
    1. First moment of waiting time $\langle\tau\rangle = \int_0^\infty \tau\phi(\tau)d\tau$,
    2. Second moment of jump length $\langle(\delta x)^2\rangle = \int_{-\infty}^{\infty}(\delta x)^2\lambda(\delta x)d(\delta x)$.

Quantities/PDFs	Normal Diffusion	Subdiffusion	Lévy flight
$\langle\tau\rangle$	Finite	Infinite	Finite
$\langle(\delta x)^2\rangle$	Finite	Finite	Infinite
$\phi(\tau)$	Exponential	Power-law	Exponential
$\lambda(\delta x)$	Normal	Normal	Lévy distribution
Equation of $W(x,t)$	Classical	Time fractional	Space fractional
MSD $\langle x^2(t)\rangle$	$2K_1 t$	$\frac{2K_\alpha}{\Gamma(1+\alpha)}t^\alpha, 0<\alpha<1$	$t^{2/\mu}, 0<\mu<2$

Distributions in the table

- Exponential distribution: $\phi(\tau)=\gamma^{-1}\exp(-\tau/T)$ with $\langle\tau\rangle=\gamma$.
- Power-law distribution: $\phi(\tau)\sim(\gamma/\tau)^{1+\alpha}, 0<\alpha<1$ with Laplace transform $\phi(s)\sim 1-(\gamma s)^\alpha$.
- Normal distribution: $\lambda(\delta x)=(4\pi\sigma^2)^{-1/2}\exp(-(\delta x)^2/(4\sigma^2))$.
- Lévy distribution: the definition is given through its Fourier transform, $\lambda(k)=\exp(-\sigma^\mu|k|^\mu)\sim 1-\sigma^\mu|k|^\mu$ for $0<\mu<2$. The asymptotic behaviour is $\lambda(\delta x)\sim\sigma^{-\mu}|(\delta x)|^{-1-\mu}$ for $|(\delta x)|\gg\sigma$.

Equations for anomalous diffusion in the above table ($0 < \alpha < 1$, $0 < \mu < 2$)

- Time fractional Fokker-Planck equation (subdiffusion):

$$\boxed{\frac{\partial}{\partial t} W(x,t) = {}_{\mathrm{RL}}\mathrm{D}_t^{1-\alpha} K_\alpha \frac{\partial^2}{\partial x^2} W(x,t), \;\; K_\alpha \equiv \sigma^2/\gamma^\alpha.}$$

The fractional operator of the Riemann-Liouville form is defined as [1]

$$ {}_{\mathrm{RL}}\mathrm{D}_t^{1-\alpha} W(x,t) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{W(x,t')}{(t-t')^{1-\alpha}} dt'.$$

[1] M. M. Meerschaert and A. Sikorskii, Stochastic Models for Fractional Calculus (Walter de Gruyter, Berlin, 2012).

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- Space fractional equation (superdiffusion):

$$\frac{\partial}{\partial t} W(x,t) = K^\mu \nabla_x^\mu W(x,t), \;\; K^\mu \equiv \sigma^\mu/\gamma.$$

The Fourier transform of the fractional operator is
$\mathcal{F}\left\{\nabla_x^\mu W(x,t)\right\} = -|k|^\mu W(k,t)$.

[1] M. M. Meerschaert and A. Sikorskii, Stochastic Models for Fractional Calculus (Walter de Gruyter, Berlin, 2012).

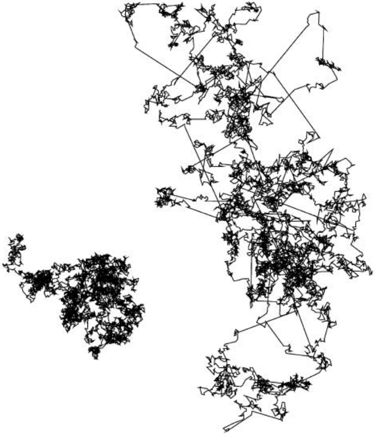


Figure: Comparison of the trajectories of a Brownian or subdiffusive random walk (left) and a Lévy flight (right)).

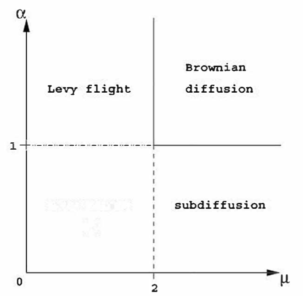
Continuous Time Random Walk Model (CTRW)

The composite between long rests and long jumps.

$$\frac{\partial}{\partial t} W(x,t) = {}_{\mathrm{RL}}\,\mathrm{D}_t^{1-\alpha} K_\alpha^\mu \frac{\partial^\mu}{\partial x^\mu} W(x,t), \;\; K_\alpha^\mu = \sigma^\mu / \gamma^\alpha .$$

$$\boxed{\left\langle |x|^2(t) \right\rangle \propto t^{2\alpha/\mu}}$$

According to the MSD, we have the following classification



Tempered Distribution.

Tempered power-law waiting time distribution:

$$\phi(\tau) \sim \frac{1}{-\Gamma(-\alpha)} \tau^{-(1+\alpha)} \exp(-\lambda\tau)$$

- The purpose of tempering: comparing with a sharp cutoff, the exponential tempering has both mathematical and practical advantages, i.e., the tempered process is still an infinitely divisible Lévy process.
- The process with tempered power-law waiting time distribution and normal jump length distribution become Brownian motion when time is sufficiently long. However, when time is short, subdiffusion is observed because the exponential tempering has little influence on the motion.
- Similarly, we can also define the tempered jump length distribution.

▲ Define the functional:

$$A = \int_0^t U[x(\tau)]d\tau$$

- $x(\tau)$ – Trajectory of a particle.
- $U(x)$ – A prescribed function.

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- $U(x)$ – A prescribed function.

▲ Applications:

- $U(x) = \begin{cases} 1, & \text{if } x > 0 \\ 0, & \text{otherwise.} \end{cases}$

  A means the occupation time in the positive half space.

- $U(x) = \begin{cases} 1, & \text{if } |x| \leq b \\ 0, & \text{otherwise.} \end{cases}$

  A means the total residence time of the particle in the interval $[-b, b]$.

- $U(x) = x$.

  A represents the total area under the random walk curve $x(t)$.

- Denoting $G(x, A, t)$ the joint pdf of x and A at time t.
- $G(x, p, t) = \int_0^\infty \exp(-pA) G(x, A, t) dA$ (Fourier transform w.r.t. A also makes sense).
- The classical Feynman-Kac equation [2]:

$$\boxed{\frac{\partial}{\partial t} G(x, p, t) = D \frac{\partial^2}{\partial x^2} G(x, p, t) - pU(x) G(x, p, t)}$$

D represents the diffusion coefficient.

Note: $p = 0 \Rightarrow$ The diffusion equation $\frac{\partial}{\partial t} G(x, t) = D \frac{\partial^2}{\partial x^2} G(x, t)$.

[2] M. Kac, On distributions of certain Wiener functionals. Trans. Am. Math. Soc. **65**, 1 (1949).

The forward equation for Lévy flights (with power-law waiting time):

$$\frac{\partial}{\partial t} G(x,p,t) = K_\alpha^\mu \nabla_x^\mu \mathcal{D}_t^{1-\alpha} G(x,p,t) - pU(x)G(x,p,t)$$

- ∇_x^μ – Riesz spatial fractional derivative operator defined in Fourier space as $\nabla_x^\mu \to -|k|^\mu$ $(x \to k)$.
- $\mathcal{D}_t^{1-\alpha}$ – Substantial fractional derivative operator, defined as

$$\mathcal{D}_t^{1-\alpha} G(x,p,t) = \frac{1}{\Gamma(\alpha)} \left[\frac{\partial}{\partial t} + pU(x) \right] \int_0^t \frac{\exp[-(t-\tau)pU(x)]}{(t-\tau)^{1-\alpha}} G(x,p,\tau) d\tau.$$

- $\alpha = 1 \Rightarrow$ The classical Feynman-Kac equation.
- $p = 0 \Rightarrow$ The fractional Fokker-Planck equation.

Note: For the backward or tempered fractional Feynman-Kac equation please see [3] [4].

[3] S. Carmi, L. Turgeman, and E. Barkai, On Distributions of Functionals of Anomalous Diffusion Paths, J. Stat. Phys. **141**, 1071 (2010).

[4] X. C. Wu, W. H. Deng, and E. Barkai, Tempered fractional Feynman-Kac equation: Theory and examples, Phys. Rev. E **93**, 032151 (2016).

Summary of This Section

Brownian motion (normal diffusion) $\left\{ \begin{array}{l} \text{Classical Fokker-Planck equation} \\ \text{Classical Langevin equation} \end{array} \right.$

CTRW model (anomalous diffusion) $\left\{ \begin{array}{l} \text{Introduction of the model} \\ \text{Fractional Fokker-Planck equations} \\ \text{Tempered distribution} \\ \text{Fractional Feynman-Kac equation.} \end{array} \right.$

Outline

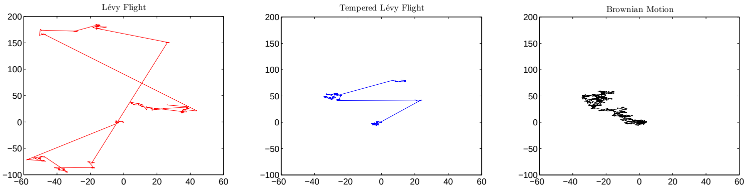


Figure: Random trajectories (1000 steps) of Lévy flight, tempered Lévy flight, and Brownian motion.

For Lévy processes, except Brownian motion, all others have discontinuous paths.

- Most of the research works on the mean first exit time or escape probability appear in the mathematical, physical, and engineering literatures, with the Langevin type dynamical system

$$\mathrm{d}X_t = F(X_t)\mathrm{d}t + \sigma(X_t)\mathrm{d}W_t.$$

- If W_t denotes a non-Gaussian $\beta-$stable type Lévy process whose trajectories are not continuous, escape probability in this case [5] represents the probability of a particle starting at a point $\mathbf{x}$ in D, first escaping a domain D and landing in a subset E of D^c (the complement of D).

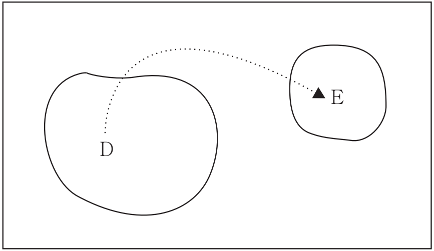
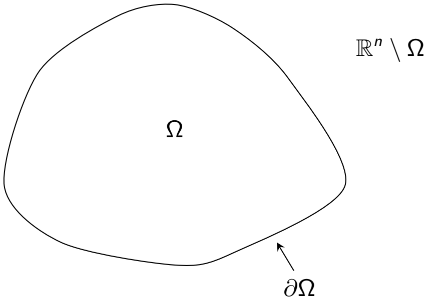


Figure: The exit phenomenon of Lévy flight with discontinuous paths.

[5] W. H. Deng, X. C. Wu, and W. L. Wang, Mean exit time and escape probability for the anomalous processes with the tempered power-law waiting times, EPL, 117 (2017), p. 10009.

Discontinuous Paths



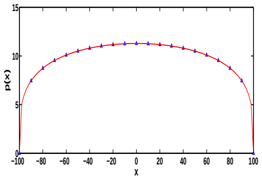
- The boundary $\partial\Omega$ itself can not be hit by the majority of discontinuous sample trajectories.
- The generalized boundary conditions must be introduced, which must contain the information on the domain $\mathbb{R}^n \backslash \Omega$.

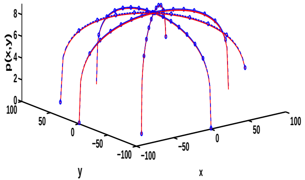
Consider the steady state fractional diffusion equation

$$\begin{cases} \Delta^{\beta/2} p(\mathbf{X}) = -1 & \text{in } \Omega, \\ p(\mathbf{X}) = 0 & \text{in } \mathbb{R}^n \backslash \Omega. \end{cases} \quad (1)$$

The meaning of the solution $p(\mathbf{X})$ is the mean first exit time of particles performing Lévy flights; if taking $\Omega = \{\mathbf{X} : |\mathbf{X}| < r\}$, then [6]

$$p(\mathbf{X}) = \frac{\Gamma(n/2)(r^2 - |\mathbf{x}|^2)^{\beta/2}}{2^\beta \Gamma(1+\beta/2)\Gamma(n/2+\beta/2)}. \quad (2)$$





[6] R. K. Getoor, First passage times for symmetric stable processes in space, Trans. Amer. Math. Soc., 101 (1961).

Another steady state fractional diffusion equation

$$\begin{cases} \Delta^{\beta/2} p(\mathbf{X}) = 0 & \text{in } \Omega, \\ p(\mathbf{X}) = g(\mathbf{X}) & \text{in } \mathbb{R}^n \backslash \Omega. \end{cases} \tag{3}$$

- Given a domain $E \subset \mathbb{R}^n \backslash \Omega$, if taking $g(\mathbf{X}) = 1$ for $\mathbf{X} \in E$ and 0 for $\mathbf{X} \in (\mathbb{R}^n \backslash \Omega) \backslash E$, then the solution $p(\mathbf{X})$ is the escape probability undergoing Lévy flights.
- If $g(\mathbf{X}) \equiv 1$ in $\mathbb{R}^n \backslash \Omega$, then $p(\mathbf{X})$ equals to 1 in Ω because of the probability interpretation.

- The initial and boundary value problem (anisotropy):

$$\begin{cases} \dfrac{\partial p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial t} = \dfrac{\partial^{\beta_1} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_1|^{\beta_1}} + \dfrac{\partial^{\beta_2} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_2|^{\beta_2}} \\ \qquad\qquad + \cdots + \dfrac{\partial^{\beta_n} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_n|^{\beta_n}} \quad \text{in } \Omega, \\ p(\mathbf{x}_1,\cdots,\mathbf{x}_n,0) = p_0(\mathbf{x}_1,\cdots,\mathbf{x}_n) \quad \text{in } \Omega, \\ p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t) = g(\mathbf{x}_1,\cdots,\mathbf{x}_n,t) \quad \text{in } \mathbb{R}^n \backslash \Omega. \end{cases}$$

- $g(\mathbf{x}_1,\cdots,\mathbf{x}_j,\cdots,\mathbf{x}_n,t)$ should satisfies that there exist positive M and C such that for $j=1,\cdots,n$, when $|\mathbf{x}_j|>M$,

$$\frac{|g(\mathbf{x}_1,\cdots,\mathbf{x}_j,\cdots,\mathbf{x}_n,t)|}{|\mathbf{x}_j|^{\beta_j-\varepsilon}} < C \quad \text{for positive small } \varepsilon.$$

- Another initial and boundary value problems (isotropic):

$$\begin{cases} \dfrac{\partial p(\mathbf{X},t)}{\partial t} = \Delta^{\beta/2} p(\mathbf{X},t) \\ p(\mathbf{X},0) = p_0(\mathbf{X}) \quad \text{in } \Omega, \\ p(\mathbf{X},t) = g(\mathbf{X},t) \quad \text{in } \mathbb{R}^n \backslash \Omega. \end{cases} \tag{4}$$

- $g(\mathbf{X},t)$ should satisfy that there exist positive M and C such that when $|\mathbf{X}| > M$,

$$\frac{|g(\mathbf{X},t)|}{|\mathbf{X}|^{\beta-\varepsilon}} < C \quad \text{for positive small } \varepsilon.$$

Absorbing boundary conditions correspond to $g(\mathbf{X},t) = 0$.

▲ Sending $\beta \to 2$ in Eq. (4), the classical Dirichlet boundary conditions is recovered.

Generalized Dirichlet type Boundary Conditions

▲ Sending $\beta \to 2$ in Eq. (4), the classical Dirichlet boundary conditions is recovered.

▲ The fractional laplacian operator in Eq. (4) reduces to classical laplacian operator. Thus only $g(\mathbf{X}, t)$ on $\partial\Omega$ will be used when solving this equation.

Consider the time-dependent problem:

$$\begin{cases} \dfrac{\partial p}{\partial t} - \Delta^{\frac{\beta}{2}} p = f & \text{in } \Omega, \\ p(\cdot, 0) = p_0 & \text{in } \Omega, \\ p = g & \text{in } \mathbb{R}^n \backslash \Omega. \end{cases} \tag{5}$$

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$$\begin{cases} \dfrac{\partial p}{\partial t} - \Delta^{\frac{\beta}{2}} p = f & \text{in } \Omega, \\ p(\cdot, 0) = p_0 & \text{in } \Omega, \\ p = g & \text{in } \mathbb{R}^n \backslash \Omega. \end{cases} \quad (5)$$

The weak formulation of (5) is to find $p = g + \phi$ such that

$$\phi \in L^2(0, T; H_0^{\frac{\beta}{2}}(\Omega)) \cap H^1(0, T; H^{-\frac{\beta}{2}}(\Omega)) \hookrightarrow C([0, T]; L^2(\Omega))$$

and $\forall\ q \in L^2(0, T; H_0^{\frac{\beta}{2}}(\Omega))$

$$\boxed{\int_0^T \int_\Omega \partial_t \phi\, q\, d\mathbf{X} dt + \int_0^T \int_{\mathbb{R}^n} \Delta^{\frac{\beta}{4}} \phi\, \Delta^{\frac{\beta}{4}} q\, d\mathbf{X} dt = \int_0^T \int_\Omega (f + \Delta^{\frac{\beta}{2}} g - \partial_t g) q\, d\mathbf{X} dt.} \quad (6)$$

- $a(\phi, q) := \int_{\mathbb{R}^n} \Delta^{\frac{\beta}{4}} \phi \, \Delta^{\frac{\beta}{4}} q \, d\mathbf{X}$ is a coercive bilinear form on $H_0^{\frac{\beta}{2}}(\Omega) \times H_0^{\frac{\beta}{2}}(\Omega)$,
- $\ell(q) := \int_\Omega (f + \Delta^{\frac{\beta}{2}} g - \partial_t g) q \, d\mathbf{X}$ is a continuous linear functional on $L^2(0, T; H_0^{\frac{\beta}{2}}(\Omega))$.

Such a problem as (6) has a unique weak solution [7].

[7] E. Zeidler, Nonlinear Functional Analysis and its Applications II/B: Nonlinear Monotone Operators, Springer Science+Business Media, LLC, 1990.

- Consider the classical diffusion equation:

$$\begin{cases} \frac{\partial p(\mathbf{X},t)}{\partial t} = \Delta p(\mathbf{X},t) \quad \text{in } \Omega, \\ p(\mathbf{X},0) = p_0(\mathbf{X}) \quad \text{in } \Omega, \\ \nabla p(\mathbf{X},t) = g(\mathbf{X},t) \quad \text{in } \partial\Omega. \end{cases} \tag{7}$$

- This equation can be derived by:
  1. mass conservation: $\frac{\partial p(\mathbf{X},t)}{\partial t} = -\nabla \cdot \mathbf{j}$,
  2. Fick's law: $\mathbf{j} = -\nabla p(\mathbf{X},t)$.

- The reflecting boundary condition $g = 0$ corresponds to $\mathbf{j} = 0$, which means that the particles will reflect once they hit the boundary $\partial\Omega$.

- Consider the anomalous diffusion equation:

$$\begin{cases} \dfrac{\partial p(\mathbf{X},t)}{\partial t} = \Delta^{\beta/2} p(\mathbf{X},t) \quad \text{in } \Omega, \\ p(\mathbf{X},0) = p_0(\mathbf{X}) \quad \text{in } \Omega, \\ \text{Neumann type boundary conditions.} \end{cases} \tag{8}$$

- We can
  1. maintain mass conservation: $\frac{\partial p(\mathbf{X},t)}{\partial t} = -\nabla \cdot \mathbf{j}$,
  2. generalize Fick's law: $\mathbf{j} =$ something, such that $\Delta^{\frac{\beta}{2}} p(\mathbf{X},t) = -\nabla \cdot \mathbf{j}$.

  Thus Eq. (8) is established.

▲ The reflecting boundary condition $\mathbf{j} = 0$ here means differently with the classical case.

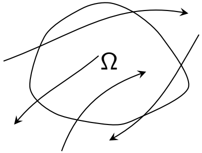

Figure: Sketch map of particles jumping into, or jumping out of, or passing through the domain Ω. But the number of particles inside Ω is conservative.

▲ If $\mathbf{j}\,|_{\mathbb{R}^n\backslash\Omega}$=0, then $\Delta^{\frac{\beta}{2}} p(\mathbf{X}, t) = -\nabla \cdot \mathbf{j} = 0$ in $\mathbb{R}^n\backslash\Omega$. The Neumann type boundary condition in (8) can be, heuristically, defined as

$$\boxed{\Delta^{\frac{\beta}{2}} p(\mathbf{X}, t) = g(\mathbf{X}) \;\text{ in }\; \mathbb{R}^n\backslash\Omega.}$$

- Another initial and boundary value problem (anisotropy):

$$
\begin{cases}
\dfrac{\partial p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial t} = \dfrac{\partial^{\beta_1} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_1|^{\beta_1}} + \dfrac{\partial^{\beta_2} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_2|^{\beta_2}} \\
\qquad\qquad + \cdots + \dfrac{\partial^{\beta_n} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_n|^{\beta_n}} \quad \text{in } \Omega, \\
p(\mathbf{x}_1,\cdots,\mathbf{x}_n,0) = p_0(\mathbf{x}_1,\cdots,\mathbf{x}_n) \quad \text{in } \Omega, \\
\dfrac{\partial^{\beta_1} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_1|^{\beta_1}} + \dfrac{\partial^{\beta_2} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_2|^{\beta_2}} \\
\qquad\qquad + \cdots + \dfrac{\partial^{\beta_n} p(\mathbf{x}_1,\cdots,\mathbf{x}_n,t)}{\partial |\mathbf{x}_n|^{\beta_n}} = g(\mathbf{X},t) \quad \text{in } \mathbb{R}^n \backslash \Omega.
\end{cases}
$$

▲ Sending $\beta \to 2$ in Eq. (8), the classical Neumann boundary condition is recovered.

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▲ The weak solution $p : [0, +\infty) \to H^{\beta/2}(\mathbb{R}^n)$ of Eq. (8) satisfies

$$\int_\Omega p_t q d\mathbf{X} + \int_{\mathbb{R}^n} \Delta^{\beta/4} p \Delta^{\beta/4} q d\mathbf{X} = -\int_{\mathbb{R}^n \backslash \Omega} g q d\mathbf{X} \quad \forall q \in H^{\beta/2}(\mathbb{R}^n).$$

Taking $\beta \to 2$,

$$\boxed{\int_\Omega p_t q d\mathbf{X} + \int_\Omega \nabla p \cdot \nabla q d\mathbf{X} = \int_{\partial\Omega} \frac{\partial p}{\partial n} q ds,}$$

since

$$\int_{\mathbb{R}^n \backslash \Omega} g q d\mathbf{X} = \int_{\mathbb{R}^n \backslash \Omega} (\Delta p) q d\mathbf{X} = -\int_{\partial\Omega} \frac{\partial p}{\partial n} q ds - \int_{\mathbb{R}^n \backslash \Omega} \nabla p \cdot \nabla q d\mathbf{X}$$

and

$$\int_{\mathbb{R}^n} \Delta^{1/2} p \Delta^{1/2} q d\mathbf{X} = \int_{\mathbb{R}^n} \nabla p \cdot \nabla q d\mathbf{X}.$$

Consider the problem:

$$\begin{cases} \dfrac{\partial p}{\partial t} - \Delta^{\frac{\beta}{2}} p = f & \text{in } \Omega, \\ \Delta^{\frac{\beta}{2}} p = g & \text{in } \mathbb{R}^n \backslash \Omega, \\ p(\cdot, 0) = p_0 & \text{in } \Omega. \end{cases} \tag{9}$$

Definition (Weak solutions)

The weak formulation of (9) is to find $p \in L^2(0, T; H^{\frac{\beta}{2}}(\mathbb{R}^n)) \cap C([0, T]; L^2(\Omega))$ such that

$$\partial_t p \in L^2(0, T; H^{\frac{\beta}{2}}(\Omega)') \text{ and } p(\cdot, 0) = p_0,$$

satisfying the following equation: $\forall\, q \in L^2(0, T; H^{\frac{\beta}{2}}(\mathbb{R}^n))$

$$\begin{aligned} &\int_0^T \int_\Omega \partial_t p(\mathbf{X}, t) q(\mathbf{X}, t) d\mathbf{X} dt + \int_0^T \int_{\mathbb{R}^n} \Delta^{\frac{\beta}{4}} p(\mathbf{X}, t) \Delta^{\frac{\beta}{4}} q(\mathbf{X}, t) d\mathbf{X} dt \\ = &\int_0^T \int_\Omega f(\mathbf{X}, t) q(\mathbf{X}, t) d\mathbf{X} dt - \int_0^T \int_{\mathbb{R}^n \backslash \Omega} g(\mathbf{X}, t) q(\mathbf{X}, t) d\mathbf{X} dt. \end{aligned} \tag{10}$$

Let $t_k = k\tau$, $k = 0, 1, \dots, N$, be a partition of the time interval $[0, T]$, and define

$$f_k(\mathbf{X}) := \frac{1}{\tau}\int_{t_{k-1}}^{t_k} f(\mathbf{X}, t)dt, \quad k = 0, 1, \dots, N,$$
$$g_k(\mathbf{X}) := \frac{1}{\tau}\int_{t_{k-1}}^{t_k} g(\mathbf{X}, t)dt, \quad k = 0, 1, \dots, N.$$

Consider the time-discrete problem: for a given $p_{k-1} \in L^2(\mathbb{R}^n)$, find $p_k \in H^{\frac{\beta}{2}}(\mathbb{R}^n)$ such that the following equation holds:

$$\frac{1}{\tau}\int_\Omega p_k(\mathbf{X})q(\mathbf{X})d\mathbf{X} + \int_{\mathbb{R}^n} \Delta^{\frac{\beta}{4}} p_k(\mathbf{X})\Delta^{\frac{\beta}{4}} q(\mathbf{X})d\mathbf{X}$$
$$= \frac{1}{\tau}\int_\Omega p_{k-1}(\mathbf{X})q(\mathbf{X})d\mathbf{X} + \int_\Omega f_k(\mathbf{X})q(\mathbf{X})d\mathbf{X} - \int_{\mathbb{R}^n\setminus\Omega} g_k(\mathbf{X})q(\mathbf{X})d\mathbf{X} \quad \forall\, q \in H^{\frac{\beta}{2}}(\mathbb{R}^n). \tag{11}$$

If we define the piecewise constant functions

$$f^{(\tau)}(\mathbf{X},t) := f_k(\mathbf{X}) = \frac{1}{\tau}\int_{t_{k-1}}^{t_k} f(\mathbf{X},t)dt \qquad \text{for} \ \ t \in (t_{k-1},t_k], \ \ k = 0,1,\ldots,N,$$

$$g^{(\tau)}(\mathbf{X},t) := g_k(\mathbf{X}) = \frac{1}{\tau}\int_{t_{k-1}}^{t_k} g(\mathbf{X},t)dt \qquad \text{for} \ \ t \in (t_{k-1},t_k], \ \ k = 0,1,\ldots,N,$$

$$p_+^{(\tau)}(\mathbf{X},t) := p_k(\mathbf{X}) \qquad \text{for} \ \ t \in (t_{k-1},t_k], \ \ k = 0,1,\ldots,N,$$

and the piecewise linear function

$$p^{(\tau)}(\mathbf{X},t) := \frac{t_k - t}{\tau}p_{k-1}(\mathbf{X}) + \frac{t-t_{k-1}}{\tau}p_k(\mathbf{X}) \quad \text{for} \ \ t \in [t_{k-1},t_k], \ \ k = 0,1,\ldots,N,$$

[8] P. L. Lions, Mathematical Topics in Fluid Mechanics: Volume 1: Incompressible Models, Clarendon Press, Oxford, USA., 1996.

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then (11) implies

$$\begin{aligned}&\int_0^T\int_\Omega \partial_t p^{(\tau)}(\mathbf{X},t)q(\mathbf{X},t)d\mathbf{X}dt + \int_0^T\int_{\mathbb{R}^n} \Delta^{\frac{\beta}{4}} p_+^{(\tau)}(\mathbf{X},t)\Delta^{\frac{\beta}{4}} q(\mathbf{X},t)d\mathbf{X}dt \\ &= \int_0^T\int_\Omega f^{(\tau)}(\mathbf{X},t)q(\mathbf{X},t)d\mathbf{X}dt - \int_0^T\int_{\mathbb{R}^n\setminus\Omega} g^{(\tau)}(\mathbf{X},t)q(\mathbf{X},t)d\mathbf{X}dt.\end{aligned} \tag{12}$$

By taking $\tau=\tau_j\to 0$ [8]. in (12), we obtain (10).

[8] P. L. Lions, Mathematical Topics in Fluid Mechanics: Volume 1: Incompressible Models, Clarendon Press, Oxford, USA., 1996.

Thanks for Your Attention!

Main References:

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