Stochastic Models for Fractional Subdiffusion with Reactions and Forcing

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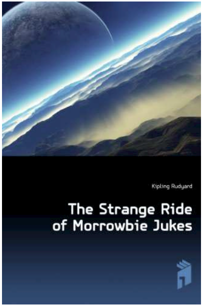
Preface

Rudyard Kipling (1885)

Four out from crow-clump: three left; nine out; two right; three back; two left; fourteen out; two left; seven out; one left; nine back; two right; six back; four right; seven back.



RANDOM WALKS - DIFFUSION

Uhlenbeck and Ornstein (Phys. Rev., 1930)

> *In the theory of Brownian motion the first concern has always been the calculation of the mean square displacement of the particle, because this could immediately be observed.*

$$\langle \Delta X^2(t) \rangle = \left\langle (X(t) - \langle X(t) \rangle)^2 \right\rangle \sim t$$

First Steps

Bachelier (*PhD, Theorie de la Speculation*,1900) first consideration of a stochastic process in continuous time $\int_0^\infty x\, p(x,t)\, dx = k\sqrt{t}$

Pearson (*Nature*, 1905): n steps, 2-dim off-lattice, probability to be between r and $r + dr$ from starting point

Rayleigh (*Nature*, 1905): $P = \frac{2}{n} e^{-\frac{r^2}{n}} r\, dr$ $\qquad \langle r^2 \rangle = n$

Einstein (*Ann. d. Phys.*, 1905):
$\frac{\partial f}{\partial t} = D \frac{\partial^2 f}{\partial x^2}, \quad \langle x^2(t) \rangle = 2Dt, \quad D = \left(\frac{RT}{6N\pi a\eta}\right) = \left(\frac{k_B T}{\gamma}\right)$

Langevin (*Comptes Rendues Acad. Sci.*,1908)
..a demonstration that is infinitely more simple ..$m\frac{d^2x}{dt^2} = F(t) - \gamma \frac{dx}{dt}$
$\langle F(t) \rangle = 0, \langle F(0)F(t) \rangle = D\delta(t), \langle x(t)F(t) \rangle = 0, \quad \langle x^2 \rangle \sim 2Dt, \qquad D = \frac{k_B T}{\gamma}$

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Diffusion with Reactions and Forcing

Diffusion with Reactions

Fisher (*Ann. Eug.*, 1937); Kolmogorov et al (*Moscow Math. Bull.*, 1937)

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} + \lambda n(1-n), \qquad \frac{\partial \mathbf{n}}{\partial t} = \underline{\underline{D}}\,\frac{\partial^2 \mathbf{n}}{\partial x^2} + \mathbf{f}(\mathbf{n}(x,t))$$

Diffusion with Forcing

Fokker (*Ann. Phys.*, (1914), Planck (1917), Kolmogorov (1931)

$$\frac{\partial \rho}{\partial t} = \frac{\partial^2}{\partial x^2}\left(D(x,t)\rho(x,t)\right) - \frac{\partial}{\partial x}\left(b(x,t)\rho(x,t)\right)$$

Smoluchowski (*Ann. Phys.*,1915)

$$\frac{\partial \rho}{\partial t} = D\frac{\partial^2 \rho}{\partial x^2} - \frac{\partial}{\partial x}\left(F(x,t)\rho(x,t)\right), \quad F(x,t) = -\frac{\partial V(x,t)}{\partial x}$$

Ito stochastic equation $dX_t = \mu(X_t,t)\,dt + \sigma\,dW_t$

ANOMALOUS DIFFUSION

Klafter (Physics World, 2005)

> *the clear picture that has emerged over the last few decades is that although these phenomena are called anomalous, they are abundant in everyday life: anomalous is normal!*

$$\langle \Delta X^2(t) \rangle = \left\langle (X(t) - \langle X(t) \rangle)^2 \right\rangle \not\propto t$$

Anomalous Diffusion

$\langle \Delta X^2 \rangle \sim t\,(\ln t)^\kappa$ $1 < \kappa < 4$	ultraslow diffusion	Sinai diffusion deterministic diffusion
$\langle \Delta X^2 \rangle \sim t^\alpha$ $0 < \alpha < 1$	subdiffusion	disordered solids biological media fractal media porous media
$\langle \Delta X^2 \rangle \sim \begin{cases} t^\alpha & t < \tau \\ t & t > \tau \end{cases}$	transient subdiffusion	biological media
$\langle \Delta X^2 \rangle \sim t$	standard diffusion	homogeneous media
$\langle \Delta X^2 \rangle \sim t^\beta \quad 1 < \beta < 2$	superdiffusion	turbulent plasmas Levy flights transport in polymers
$\langle \Delta X^2 \rangle \sim t^2$	ballistic diffusion	optical traps
$\langle \Delta \ell^2 \rangle \sim t^3$	Richardson diffusion	atmospheric turbulence

Subdiffusion

solute transport in porous media – Drazer and Zanette *Phys. Rev. E* (1999)

electrons in porous TiO_2 - Dittrich et al *Phys Rev E* (2006)

molecules in spiny nerve cells – Santamaria et al *Neuron* 2006

telomeres in mammalian cells – Bronstein et al *Phys Rev Letts* (2009)

lipid granules in yeast – Jeon et al *Phys Rev Letts* (2011)

lipid molecules in lipid bilayers – Akimoto et al *Phys Rev Letts* (2011)

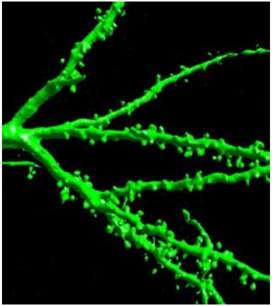
water in heterogeneous colloidal systems – Palombo et al *J Chem Phys* (2011)

proteins in cells – Roosen-Runge et al *PNAS* (2011)

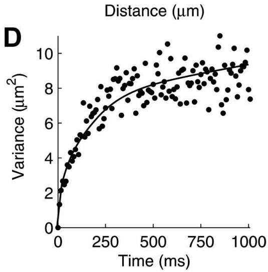
potassium channels in the brain – Weigel et al *PNAS* (2011)

Subdiffusion in Nerve Cells

Spiny dendrites, Computational Neurobiology and Imaging Centre, Mount Sinai School of Medicine, New York



FRAP experiments on spiny dendrites, (Santamaria, Wils, De Schutter, Augustine, *Neuron* 2006, *Eur. J. Neuorsci.* 2011)



Scaled Brownian Motion Diffusion Equation

Wang, Dong, Wu, Zhu, Ko (*Physica A*, 1994), Lutz (*Phys. Rev. E*, 2001)

- Time dependent diffusion coefficient $D(t) = \alpha t^{\alpha-1} D_0, \quad 0 < \alpha < 1$

$$\frac{\partial \rho}{\partial t} = \alpha t^{\alpha-1} D_0 \frac{\partial^2 \rho}{\partial x^2}$$

- Non-Markovian probability density function

$$\rho(x,t) = \frac{1}{\sqrt{4\pi D_0 t^\alpha}} \exp\left(-\frac{x^2}{4D_0 t^\alpha}\right)$$ Rescaled Gaussian

- Anomalous subdiffision

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 \rho(x,t)\, dx = 2D_0 t^\alpha = 2D_0 t^{2H}$$ H Hurst exponent

- Note $D(t) = {}_0\mathcal{D}_t^{1-\alpha}\left(\Gamma(\alpha+1) D_0\right) \quad {}_0\mathcal{D}_t^{1-\alpha} y(t) = \frac{d}{dt}\, {}_0\mathcal{I}_t^{\alpha} y(t)$

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Fractional Langevin Equation

- Dissipative memory kernel

$$m\frac{dv}{dt} = F(t) - m\int_0^t \gamma(t-t')v(t')\,dt'$$

$\langle F(t)\rangle = 0 \quad \langle F(0)F(t)\rangle = D_\alpha t^{-\alpha}$ coloured noise

- Equilibrium fluctuation-dissipation theorem

$\langle F(t)F(0)\rangle = mk_B T\gamma(t) \quad \Rightarrow \quad \gamma(t) = \frac{D_\alpha}{mk_b T} t^{-\alpha}$

$$\Rightarrow m\frac{dv}{dt} = F(t) - \frac{D_\alpha}{k_B T}\, {}_0\mathcal{D}_t^{\alpha-1} v(t) \quad 0 < \alpha < 1$$

- The probability density function for trajectories satisfies the fractional Brownian motion diffusion equation.

Fractional Diffusion – fBm

- Rescaled Gaussian

$$\rho(x,t) = \frac{1}{\sqrt{4\pi D_0 t^\alpha}} \exp\left(-\frac{x^2}{4D_0 t^\alpha}\right)$$

- Non-Markovian

$$P(T > t + s | T > s) > P(T > t)$$

- Ergodic

$$\langle x^2(t)\rangle_E = \langle x^2(t)\rangle_T = 2D_0 t^\alpha$$

  - Ensemble Average

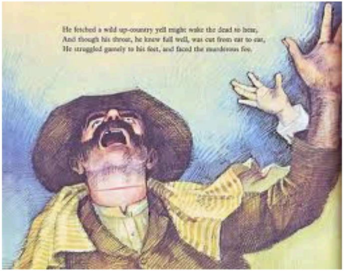
$$\langle x^2(t)\rangle_E = \langle (x(t) - x(0))^2\rangle$$

  - Moving Time Average

$$\langle x^2(t)\rangle_T = \frac{1}{T-t}\int_0^{T-t} (x(t+t') - x(t'))^2\, dt'$$

Banjo Patterson (The Bulletin, 1892)

It was the man from Ironbark
who struck the Sydney town,
he wandered over street and park,
he wandered up and down.
He loitered here, he loitered there,
till he was like to drop,
until at last in shear despair,
he sought a barbers shop.



Continuous Time Random Walks – CTRWs

Standard Random Walk

The step length is a fixed distance Δx

Steps occur at discrete times separated by a fixed time interval Δt

Continuous Time Random Walk

Montroll & Weiss, 1965; Scher & Lax, 1973

The step length is selected at random from a step length probability density $\lambda(x)$

Steps occur after a waiting time selected at random from a waiting time probability density $\psi(t)$

Standard Diffusion or Fractional Subdiffusion

Hilfer, Anton *Phys Rev E*, 1995; Compte (*Phys. Rev. E.*,1996)

Assume $\lambda(x) = \lambda(-x)$ with finite variance $\sigma^2 = \int x^2 \lambda(x)\, dx$

Gaussian $\lambda(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right)$ or n.n. $\lambda(x) = \delta(x \pm \Delta x)$.

- Markovian exponential waiting time density
  $\psi(t) = \frac{1}{\tau} \exp\left(-\frac{t}{\tau}\right)$

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}, \qquad D = \frac{\sigma^2}{2\tau}$$

- Non Markovian power law tail waiting time density
  Pareto $\psi(t) \sim \frac{\alpha \tau^\alpha}{t^{1+\alpha}} \quad t \in [\tau, \infty], \quad 0 < \alpha < 1$
  Mittag-Leffler $\psi(t) = -\frac{d}{dt} E_\alpha(-\frac{t^\alpha}{\tau^\alpha}) \quad E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}$
  Scalas, Gorenflo, Mainardi (2004)

$$\frac{\partial \rho}{\partial t} = {}_0\mathcal{D}_t^{1-\alpha} D_\alpha \frac{\partial^2 \rho}{\partial x^2}, \quad D_\alpha = \frac{\sigma^2}{2\tau^\alpha \Gamma(1-\alpha)} \quad 0 < \alpha < 1$$

Fractional Subdiffusion as Subordinated Diffusion

- Subordinated probability density function
  $G(x,t)$ – Green's solution time fractional subdiffusion
  $G^\star(x,t)$ – Green's solution standard diffusion

$$G(x,t) = \int_0^\infty G^\star(x,\tau)T(\tau,t)\,d\tau$$

$\mathcal{L}\left(T(\tau,t)\right) = \hat{T}(\tau,u) = u^{\alpha-1}e^{-\tau u^\alpha}$ t – physical time, τ – operational time scales as number of steps

- Subordinated stochastic process
  (Magdziarz, Weron, Weron, *Phys. Rev. E.*, 2007)

$$X(t) = Y(S_t) \qquad dY(\tau) = (2D_\alpha)^{\frac{1}{2}}dB(\tau)$$

S_t inverse-time α-stable subordinator $S_t = \inf\{\tau : U(\tau) > t)$
random time the process $U(\tau)$ exceeds t
$U(\tau)$ α-strictly increasing α-stable Levy process with p.d.f. $g(t,\tau)$
$\mathcal{L}[g(t,\tau)] = e^{-\tau u^\alpha}$ $\quad g(t,\tau) = \frac{1}{\tau^{1/\alpha}}g\left(\frac{t}{\tau^{1/\alpha}}\right)$ self-similar

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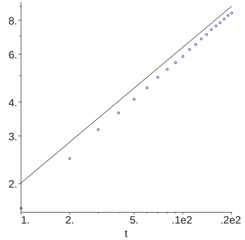
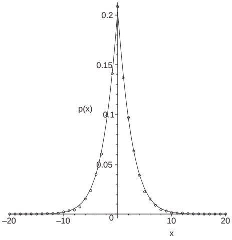
Fractional Diffusion – CTRW





- Non-Gaussian
- Non-Markovian

$$P(T > t + s | T > s) > P(T > t)$$

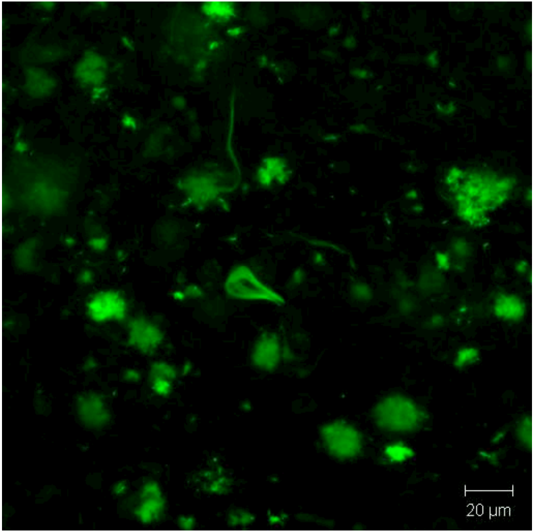
- Non-Ergodic

$$\langle x^2(t)\rangle_E \neq \langle x^2(t)\rangle_T$$

- Subdiffusive

$$\langle x^2(t)\rangle = \frac{2D_\alpha}{\Gamma(1+\alpha)} t^\alpha$$

SUBDIFFUSION WITH REACTIONS AND FORCING



Subdiffusion and Reaction Terms are not Simply Additive

Linear reaction kinetics

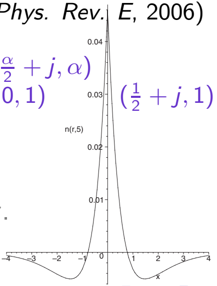
$$\frac{dn}{dt} = -kn \qquad \Rightarrow \qquad n(x,t) = n(x,0)e^{-\int_0^t k\,dt'}$$

Straightforward generalization A.

$$\frac{\partial n}{\partial t} = D_\alpha \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(\frac{\partial^2 n}{\partial x^2}\right) - kn$$

Infinite domain solution, (Henry, Langlands, Wearne, *Phys. Rev. E*, 2006)

$$n(x,t) = \frac{1}{\sqrt{4\pi D_\alpha t^\alpha}} \sum_{j=0}^{\infty} \frac{(-kt)^j}{j!} H^{2,0}_{1,2}\left[\frac{x^2}{4D_\alpha t^\alpha}\Big| \begin{matrix} (1-\frac{\alpha}{2}+j,\alpha) \\ (0,1) \quad (\frac{1}{2}+j,1) \end{matrix}\right]$$



The solution is not strictly positive for all x and t.

Subdiffusion and Reaction Terms are not Subordinated

$$\frac{dn}{dt} = -kn \qquad \Rightarrow \qquad n(x,t) = n(x,0)e^{-\int_0^t k\,dt'}$$

Straightforward generalization B.

$$\frac{\partial n}{\partial t} = \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\left(D_\gamma \frac{\partial^2 n}{\partial x^2} - kn\right)$$

This models the case when a fixed fraction of walkers is removed at the start of each waiting time (Henry, Langlands, Wearne, *Phys. Rev. E*, 2006)

$$n(x,t) = (1-k)\Phi(t)n(x,0) + \sum_{x'}\int_0^t n(x',t')(1-k)\psi(t-t')\lambda(x-x')\,dt'$$

Subdiffusion and Reaction Terms are Entwined

$$\frac{dn}{dt} = -kn \qquad \Rightarrow \qquad n(x,t) = n(x,0)e^{-\int_0^t k\,dt'}$$

Correct equations (Henry, Langlands, Wearne, *Phys. Rev. E*, 2006)

$$n(x,t) = e^{-kt}\Phi(t)n(x,0) + \sum_{x'} \int_0^t n(x',t')e^{-k(t-t')}\psi(t-t')\lambda(x-x')\,dt'$$

$$\frac{\partial n}{\partial t} = D_\gamma e^{-kt} \frac{\partial^{1-\gamma}}{\partial t^{1-\gamma}} \left(e^{kt} \frac{\partial^2 n}{\partial x^2} \right) - kn$$

Sokolov, Schmidt, Sagués *Phys. Rev. E* (2006)

$$\frac{\partial n}{\partial t} = \int_0^t K(t-t')e^{-k(t-t')} \frac{\partial^2 n}{\partial x^2} dt' - kn$$

Subdiffusion and Nonlinear Reactions

Fedotov (*Phys. Rev. E.*, 2010)

Nonlinear reaction kinetics

$$\frac{dn}{dt} = r(n)n \qquad \Rightarrow \qquad n(x,t) = n(x,0)e^{\int_0^t r(n(x,t'))\,dt'}$$

Master equation

$$\frac{\partial n}{\partial t} = \int_0^t K(t-t')\left(\int_{-\infty}^{+\infty} n(x',t')e^{\int_{t'}^t r(n(x',t''))\,dt''}\lambda(x-x')\,dx' - n(x,t')e^{\int_{t'}^t r(n(x,t''))\,dt''}\right)dt' + r(n)n, \quad K(t) = \mathcal{L}^{-1}\left[\frac{\mathcal{L}[\psi(t)]}{\mathcal{L}[\Phi(t)]}\right]$$

Abad, Yuste and Lindenberg (*Phys. Rev. E.*, 2010)

$$\frac{\partial n}{\partial t} = \phi(x,t)K_\gamma\, {}_0D_t^{1-\gamma}\frac{\partial^2}{\partial x^2}\left(\frac{n}{\phi(x,t)}\right) + \frac{1}{\phi(x,t)}\frac{d\phi}{dt}n$$

$\phi(x,t) = \exp\int_{t'}^t r(n(x,t''))\,dt''$

Subdiffusion and External Forces run on Different Clocks

Gorenflo and Mainardi, *Eur. Phys. J. Special Topics* (2011)

Space dependent force (Barkai, Metzler, Klafter, *Phys. Rev. Letts*, 2000)

$$\frac{\partial \rho(x,t)}{\partial t} = {}_0D_t^{1-\alpha}\left[\kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha}\frac{\partial}{\partial x}F(x)\right]\rho(x,t)$$

Magdziarz, Weron, Weron (*Phys. Rev. E.*, 2007)

$X(t) = Y(S_t) \quad dY(\tau) = \frac{1}{\eta}F(Y(\tau))\,d\tau + (2\kappa)^{\frac{1}{2}}\,dB(\tau)$

Simply time-subordinated to the solution of the standard Fokker-Planck equation.

Time dependent force (Sokolov & Klafter, *Phys. Rev. E*, 2006)

$$\frac{\partial \rho(x,t)}{\partial t} = \left[\kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha}F(t)\frac{\partial}{\partial x}\right]{}_0D_t^{1-\alpha}\rho(x,t)$$

Magdziarz, Weron, Klafter (*Phys. Rev. Letts.*, 2008)

$X(t) = Y(S_t) \quad dY(\tau) = \frac{1}{\eta}F(U(\tau))\,d\tau + (2\kappa)^{\frac{1}{2}}\,dB(\tau)$

Not simply time-subordinated to the solution of the standard Fokker-Planck equation.

Space and Time Dependent Forcing

Weron, Magdziarz, Weron, (*Phys. Rev. Letts*, 2008)

$$X(t) = Y(S_t) \quad \begin{pmatrix} dY(\tau) \\ dZ(\tau) \end{pmatrix} = \begin{pmatrix} F(Y(\tau), Z(\tau)) \\ 0 \end{pmatrix} d\tau + \begin{pmatrix} (2\kappa)^{\frac{1}{2}} dB(\tau) \\ dU(\tau) \end{pmatrix}$$

$S_t = \inf\{\tau : U(\tau) > t)$

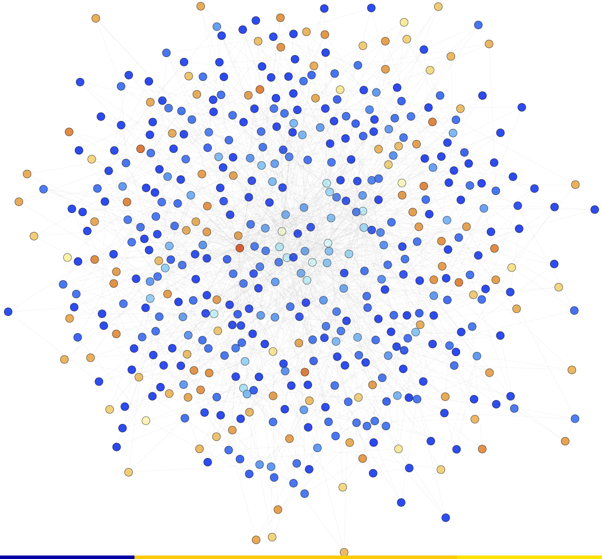
Henry, Langlands, Straka (*Phys. Rev. Letts.* 2010)

$$\frac{\partial \rho(x,t)}{\partial t} = \left[\kappa_\alpha \frac{\partial^2}{\partial x^2} - \frac{1}{\eta_\alpha} \frac{\partial}{\partial x} F(x,t) \right] {}_0D_t^{1-\alpha} \rho(x,t)$$

$\kappa_\alpha = A_\alpha \frac{\Delta x^2}{2\tau^\alpha} \qquad \eta_\alpha = (2\beta\kappa_\alpha)^{-1}$

GENERALIZED MASTER EQUATION DERIVATION

Angstmann, Donnelly, Henry *Mathematical Modelling of Natural Phenomenon* (2013)



Reactions: Birth and Death Processes

$\omega(x,t)\delta t + o(\delta t)$ probability of a particle dying in $(t, t+\delta t)$

$\eta(x,t)\delta t + o(\delta t)$ probability of a particle being created in $(t, t+\delta t)$

$\theta(x,t,s) = e^{-\int_s^t \omega(x,t')dt'}$ probability of particle surviving to time t

$\theta(x,t,s) = \theta(x,t',s)\theta(x,t,t')$ useful identity

Example

$A + B \rightleftharpoons_{k_{-1}}^{k_1} A + 2B, \quad B \rightharpoonup^{k_2} C$

$$\frac{dc_B}{dt} = k_1 c_A c_B - k_2 c_B - k_{-1} c_A c_B^2$$

$\omega_B(x,t)\delta t = (k_2 + k_{-1} c_A c_B)\delta t$

$\eta_B(x,t)\delta t = k_1 c_A c_B \delta t$

Forcing: Biased Jumps

$\Psi(x, x', t, t') = \lambda(x, x', t)\psi(x', t - t')$ transition probability for a particle at x' at time t' to jump to x at time t

$\lambda(x, x', t)$ jump density allowing for space and time dependent forcing

$$\sum_x \lambda(x, x', t) = 1 \qquad \text{for fixed } x' \text{ and } t$$

$\psi(x', t - t')$ waiting time density allowing for spatially dependent trapping

$$\int_{t'}^{\infty} \psi(x', t - t')\, dt = 1 \qquad \text{for fixed } x' \text{ and } t'.$$

Single Particle Master Equation

Probability per unit time for a walker **to arrive** at point x at time t given that it was at point x_0 at time 0

$$q(x,t|x_0,0) = \delta_{x,x_0}\delta(t-0^+) + \sum_{x'}\int_0^t \Psi(x,x',t,t')\theta(x',t',t)q(x',t'|x_0,0)dt$$

Probability per unit time for a walker **to leave** point x at time t given that it was at point x_0 at time 0

$$i(x,t|x_0,0) = \int_0^t \psi(x,t-t')\theta(x',t',t)q(x',t'|x_0,0)dt'$$

Probability of a particle **to be** at point x at time t

$$\rho(x,t|x_0,0) = \int_0^t \Phi(x,t-t')\theta(x,t,t')q(x,t'|x_0,0)dt'$$

Jump survival probability

$$\Phi(x,t-t') = 1 - \int_0^{t-t'} \psi(x,t'')dt''$$

Single Particle Master Equation

Useful separation

$$q(x,t|x_0,0) = \delta_{x,x_0}\delta(t-0^+) + q^+(x,t|x_0,0)$$

Differentiation of $\rho(x,t)$

$$\begin{aligned}\frac{\partial \rho(x,t|,x_0,0)}{\partial t} &= q^+(x,t|x_0,0) - \delta_{x,x_0}\theta(x,t,0)\psi(x,t) \\ &- \int_0^t q^+(x,t'|x_0,0)\theta(x,t,t')\psi(x,t-t')dt' \\ &-\omega(x,t)\rho(x,t|x_0,0)\end{aligned}$$

Formally equivalent to a flux balance

$$\frac{\partial \rho(x,t|,x_0,0)}{\partial t} = q^+(x,t|x_0,0) - i(x,t|x_0,0) - \omega(x,t)\rho(x,t|x_0,0)$$

Single Particle Master Equation

Useful identity

$$\frac{\rho(x,t|x_0,0)}{\theta(x,t,0)} = \int_0^t \frac{q(x,t'|x_0,0)}{\theta(x,t',0)}\Phi(x,t-t')dt'$$

Simplification

$$\begin{aligned}\frac{\partial\rho(x,t|,x_0,0)}{\partial t} &= \sum_{x'}\lambda(x,x',t)\int_0^t K(x',t-t')\rho(x',t'|x_0,0)\theta(x',t,t')dt' \\ &\quad -\int_0^t K(x,t-t')\rho(x,t'|x_0,0)\theta(x,t,t')dt' \\ &\quad -\omega(x,t)\rho(x,t|x_0,0)\end{aligned}$$

Kernel

$$\hat{K}(x,s) = \frac{\hat{\psi}(x,s)}{\hat{\Phi}(x,s)}$$

Ensemble Master Equation

Ensemble of particles, created and destroyed by a reactions, subject to an external force field, newly created particles draw a new waiting time

Density of particles at x at time t

$$u(x,t) = \sum_{x_0} \int_0^t \rho(x,t|x_0,t_0)\eta(x_0,t_0)dt_0$$

Differentiation, using the single particle master equation,

$$\frac{\partial u(x,t)}{\partial t} = \sum_{x'} \lambda(x,x',t) \int_0^t K(x',t-t')\theta(x',t,t')u(x',t')dt' - \int_0^t K(x,t-t')\theta(x,t,t')u(x,t')dt' - \omega(x,t)u(x,t) + \eta(x,t)$$

Angstmann, Donnelly, Henry *Mathematical Modelling of Natural Phenomenon* (2013)

Special Cases

I) Reduction to Checkin, Gorenflo, Sokolov (2005)
$\psi(x, t-t')$ spatially inhomogeneous
$\lambda(x, x', t) = \frac{1}{2}(\delta(x, x-\Delta x) + \delta(x, x+\Delta x))$ no forcing
$\theta(x, t, t') = 0, \omega(x, t) = 0, \eta(x, t) = 0$ no reactions

$$\int_0^t K(x, t-t')\rho(x, t')\, dt' = \frac{d}{dt}\int_0^t M(x, t-t')\rho(x, t')\, dt', \quad \hat{M}(x, s) = \frac{\hat{\psi}(x, s)}{s\hat{\Phi}(x, s)}$$

II) Reduction to Henry, Langlands, Wearne (2006)
$\psi(x, t-t') = \psi(t-t')$ spatially homogeneous
$\lambda(x, x', t) = \frac{1}{2}(\delta(x, x-\Delta x) + \delta(x, x+\Delta x))$ no forcing
$\theta(x, t, t') = e^{-k(t-t')}$, $\omega(x, t) = k$, $\eta(x, t) = 0$ no births

III) Reduction to Fedotov (2010)
$\psi(x', t-t') = \psi(t-t')$ spatially homogeneous
$\lambda(x, x', t) = \frac{1}{2}(\delta(x, x-\Delta x) + \delta(x, x+\Delta x))$ no forcing
$\theta(x, t, t') = e^{-\int_{t'}^{t} r^-(u(x, t''))\, dt''}$, $\omega(x, t) = r^-(u(x, t))$, $\eta(x, t) = r^+(u(x, t))\, u(x, t)$

Generalized Master Equation - Nearest neighbour jumps

One dimensional lattice, biased nearest neighbour jumps

$\lambda(x_i, x_{i-1}, t) = p_r(x_{i-1}, t)$ probability to jump to the right from x_{i-1}

$\lambda(x_i, x_{i+1}, t) = p_\ell(x_{i+1}, t)$ probability to jump to the left from x_{i+1}

$$\begin{aligned}\frac{\partial u(x_i, t)}{\partial t} &= \int_0^t K(x_{i-1}, t - t')p_r(x_{i-1}, t)\theta(x_{i-1}, t, t')u(x_{i-1}, t')dt' \\ &+ \int_0^t K(x_{i+1}, t - t')p_\ell(x_{i+1}, t)\theta(x_{i+1}, t, t')u(x_{i+1}, t')dt' \\ &- \int_0^t K(x_i, t - t')\theta(x_i, t, t')u(x_i, t')dt' \\ &- \omega(x_i, t)u(x_i, t) + \eta(x_i, t)\end{aligned}$$

Biased Jumps

$F(x,t) = -\frac{\partial V(x,t)}{\partial x}$ near thermodynamic equilibrium, Boltzmann weights

$$
\begin{aligned}
p_r(x_i,t) &= \frac{e^{-\beta V(x_{i+1},t)}}{e^{-\beta V(x_{i+1},t)} + e^{-\beta V(x_{i-1},t)}}, \\
p_\ell(x_i,t) &= \frac{e^{-\beta V(x_{i-1},t)}}{e^{-\beta V(x_{i+1},t)} + e^{-\beta V(x_{i-1},t)}}
\end{aligned}
$$

Continuum limit, $x_i = x$, $x_{i\pm 1} = x \pm \Delta x$, Taylor series expansions in x, retaining leading order terms in Δx

$$
\begin{aligned}
\frac{\partial u(x,t)}{\partial t} &= \frac{\Delta x^2}{2}\frac{\partial^2}{\partial x^2}\int_0^t \theta(x,t,t')u(x,t')K(x,t-t')\,dt' \\
&\quad - \beta\Delta x^2 \frac{\partial}{\partial x}\left(F(x,t)\int_0^t \theta(x,t,t')u(x,t')K(x,t-t')\,dt'\right) \\
&\quad - \omega(x,t)u(x,t) + \eta(x,t) \qquad (2)
\end{aligned}
$$

Special Case - Fractional Dispersion

Reduction to Sokolov, Klafter (2006)
Field-Induced Dispersion in Subdiffusion

$\psi(x,t-t') = \psi(t-t')$ spatially homogeneous

$F(x,t) = F(t)$ time dependent forcing

$\theta(x,t,t') = 0, \omega(x,t) = 0, \eta(x,t) = 0$ no reactions

$$\int_0^t K(x,t-t')\rho(x,t')\,dt' = \frac{d}{dt}\int_0^t M(x,t-t')\rho(x,t')\,dt', \quad \hat{M}(x,s) = \frac{\hat{\psi}(x,s)}{s\hat{\Phi}(x,s)}$$

Fokker-Planck Equation with Reactions

$\psi(x,t) = \gamma(x)e^{-\gamma(x)t}$ exponential waiting time density $K(x,t) = \gamma(x)\delta(t)$

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left(D(x)u(x,t)\right) - \frac{\partial}{\partial x}\left(\frac{1}{\zeta(x)}F(x,t)u(x,t)\right) - \omega(x,t)u(x,t) + \eta(x,t)$$

$$D(x) = \lim_{\Delta x, \langle\tau(x)\rangle \to 0} \frac{\Delta x^2}{2\langle\tau(x)\rangle}, \qquad \zeta(x) = \lim_{\Delta x, \langle\tau(x)\rangle \to 0} \frac{2\langle\tau(x)\rangle}{\beta \Delta x^2}$$

$D(x)$ and $\zeta(x)$ finite and differentiable w.r.t. x

Fractional Fokker-Planck Equation with Reactions

Angstmann, Donnelly, Henry *Mathematical Modelling of Natural Phenomenon* (2013)
Spatially dependent Pareto waiting time density

$$\psi(x,t) = \begin{cases} \frac{\alpha(x)\tau^{\alpha(x)}}{t^{1+\alpha(x)}} & t \in [\tau, \infty], \\ 0 & t \in [0, \tau) \end{cases} \qquad \text{for } 0 < \alpha(x) < 1$$

$$\int_0^t K(x, t-t')y(x,t')\,dt' \approx \frac{1}{\tau^{\alpha(x)}\Gamma(1-\alpha(x))} D_t^{1-\alpha(x)} y(x,t), \quad \theta(x,t,t') = \frac{\theta(x,t,0)}{\theta(x,t',0)}$$

$$\frac{\partial u(x,t)}{\partial t} = \frac{\partial^2}{\partial x^2}\left(D_{\alpha(x)}\theta(x,t,0)D_t^{1-\alpha(x)}\left[\frac{u(x,t)}{\theta(x,t,0)}\right]\right) - \frac{\partial}{\partial x}\left(\frac{1}{\zeta_{\alpha(x)}}F(x,t)\theta(x,t,0)D_t^{1-\alpha(x)}\left[\frac{u(x,t)}{\theta(x,t,0)}\right]\right) - \omega(x,t)u(x,t) + \eta(x,t)$$

$$D_{\alpha(x)} = \lim_{\Delta x^2,\ \tau\to 0} \frac{\Delta x^2}{2\tau^{\alpha(x)}\Gamma(1-\alpha(x))}, \qquad \zeta_{\alpha(x)} = \lim_{\Delta x^2,\ \tau\to 0} \frac{\tau^{\alpha(x)}\Gamma(1-\alpha(x))}{\beta\Delta x^2}$$

Special Cases - Fractional Fokker-Planck Equation

No reactions $\theta(x,t,t') = 0, \omega(x,t) = 0, \eta(x,t) = 0$

I) Reduction to Barkai, Klafter, Metzler (2000)

From continuous time random walks to the fractional Fokker-Planck equation

$F(x,t) = F(x), \quad \alpha(x) = \alpha$

II) Reduction to Sokolov, Klafter (2006)

Field-Induced Dispersion in Subdiffusion

$F(x,t) = F(t), \quad \alpha(x) = \alpha$

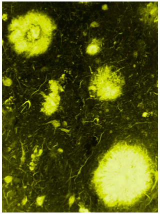
III) Reduction to Henry, Langlands, Straka (2010)

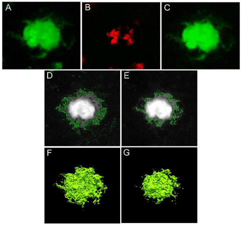
Fractional Fokker-Planck Equations for Subdiffusion with Space- and Time-Dependent Forces

$F(x,t) = F(x,t), \quad \alpha(x) = \alpha$

Fractional subdiffusion with chemotaxis and reactions

Collaboration – CNIC Mount Sinai School of Medicine New York





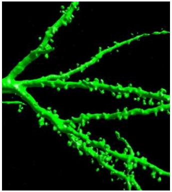
- Subdiffusion from macromolecular crowding in amyloid beta plaques associated with Alzheimer's disease, (Mueggler, Meyer-Luehmann, Rausch, Staufenbiel, Jucker, Rudin, *Eur. J. Neur.* 2004)
- Fractional chemotaxis with linear reactions, (Langlands, Henry, Phys. Rev. E., 2010)

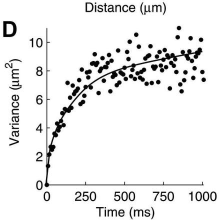
$$\frac{\partial n}{\partial t} = e^{kt}\,{}_0D_t^{1-\alpha}\left(e^{-kt}\kappa_\alpha \frac{\partial^2 n}{\partial x^2}\right) - \chi_\alpha \frac{\partial}{\partial x}\left(\frac{\partial c}{\partial x} e^{kt}\,{}_0D_t^{1-\alpha}(e^{-kt}n)\right) + kn$$

- In progress, nonlinear reaction diffusion equations with chemotaxis and anomalous diffusion

Fractional electro-diffusion

Collaboration – CNIC Mount Sinai School of Medicine New York





- Subdiffusion from trapping by spines on dendrites, (Santamaria, Wils, De Schutter, Augustine, *Neuron* 2006, *Eur. J. Neuorsci* 2011)
- Fractional cable equation
  Henry, Langlands, Wearne (*Phys. Rev. Letts*, 2008), Langlands, Henry, Wearne (*SIAM J. Appl. Math*, 2011)

$$\frac{\partial V}{\partial T} = {}_0D_T^{1-\gamma}\frac{\partial^2 V}{\partial X^2} - \mu^2\, {}_0D_T^{1-\kappa}(V - i_e r_m)$$

- In progress, fractional compartmental models for whole neurons

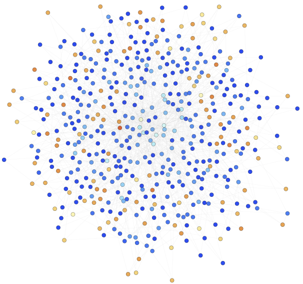
CTRW with Reactions on Networks

Angstmann, Donnelly, Henry *Phys. Rev. E* (2012)

$$\frac{du(w_j,t)}{dt} = \int_0^t \left[\sum_{i=1}^{J} K(w_i, t-t')\lambda(w_i,w_j)\theta(w_i,t,t')u(w_i,t') - K(w_j,t-t')\theta(w_j,t,t')u(w_j,t') \right] dt' - \beta(w_j,t)u(w_j,t) + \eta(w_j,t).$$

Reaction survival function
$\theta(w_i,t,t') = e^{-\int_{t'}^{t} \beta(w_i,t'')dt''}$

Standard diffusion
$\psi(w_j,t) = \alpha(w_j)e^{-\alpha(w_j)t}$
$\Rightarrow \quad K(w_j,t) = \alpha(w_j)\delta(t)$
$\lambda(w_i,w_j) = \frac{A_{ij}}{k_i}$

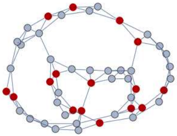


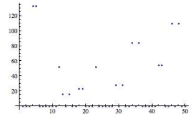
CTRW with Forcing on Networks

$$\frac{du(v_i,t)}{dt} = \sum_{j=1}^{J} \lambda(v_i|t,v_j) \int_{t_0}^{t} K(t-t'|v_j)u(v_j,t')\,dt' - \int_{t_0}^{t} K(t-t'|v_i)u(v_i,t')\,dt'$$

Self-chemotactic like forcing

Bias in the jump density dependent on the concentration of particles on neighbouring vertices





$$\lambda(v_i|t,v_j) = \frac{A_{j,i}e^{\beta u(v_i,t)}}{\sum_{k=1}^{J} A_{j,k}e^{\beta u(v_k,t)}}$$

Steady state pairing patterns, concentration localized in distinct pairs of adjacent vertices

Thank You

Appendix: Stochastic Subdiffusion Process

Conjecture (Weron, Magdziarz, Weron, Phys. Rev.Letts, 2008), Proof (HLS, *Phys. Rev. Letts.* 2010)

$$X(t) = Y(S_t) \quad \begin{pmatrix} dY(\tau) \\ dZ(\tau) \end{pmatrix} = \begin{pmatrix} F(Y(\tau), Z(\tau)) \\ 0 \end{pmatrix} d\tau + \begin{pmatrix} (2\kappa)^{\frac{1}{2}} dB(\tau) \\ dU(\tau) \end{pmatrix}$$

$S_t = \inf\{\tau : U(\tau) > t\}$
$q_t(y, z)$ p.d.f. of (Y_t, Z_t) – generalized stochastic process, Levy noise

$$\frac{\partial}{\partial t} q_t(y, z) = \kappa \frac{\partial^2}{\partial y^2} q_t(y, z) - \frac{\partial}{\partial y} \left(\frac{F(y, z)}{\eta} q_t(y, z) \right) - {}_0D_z^{\alpha} q_t(y, z)$$

ρ_t p.d.f. of $X(t)$ – compensation formula
$\int_I p_t(x)\, dx = \int_0^\infty dt' \int_I dy \int_0^t dz\, q_{t'}(y, z) \frac{(t-z)^{-\alpha}}{\Gamma(1-\alpha)}$
$p_t(x) = \int_0^\infty dt'\, {}_0I_t^{1-\alpha}\, q_{t'}(x, t)$

$$\frac{\partial}{\partial t} p_t(x) = \kappa \frac{\partial^2}{\partial x^2}\, {}_0D_t^{1-\alpha}\, p_t(x) - \frac{\partial}{\partial x} \left(\frac{F(x, t)}{\eta}\, {}_0D_t^{1-\alpha}\, p_t(x) \right)$$

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