Subdiffusion and nonlinear reaction-transport equations

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Fluid-Kinetic Modelling, Cambridge, 2010

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   - Fractional PDE's and continuous time random walk (CTRW)

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Reaction-Advection-Diffusion Equation for Density ρ

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• Probabilistic "solution" (path-integral) of the (macroscopic) initial-value problem is given by the Feynman-Kac formula

$$\rho(x,t) = \mathbb{E}_x \rho_0(X(t)) \exp\left(\int_0^t r(\rho(X(s), t-s))ds\right),$$

where $X(s)$ is a solution of (microscopic) SDE:

$$dX = -v(X(s), t-s)\, ds + (2D)^{1/2} dW(s), \; X(0) = x.$$

Fractional Reaction-Transport Equation for Density ρ

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$$D_t^{\gamma} \rho = -D_{\alpha} \left(-\Delta\right)^{\frac{\alpha}{2}} \rho$$

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Waiting time pdf $\phi(t) \sim \frac{\tau_0^\gamma}{t^{1+\gamma}}$ with $0 < \gamma < 1$ as $t \to \infty$. The mean waiting time is infinite. Example: heavy tails in human dynamic (Barabasi, Nature 435 (2005).

Biological Invasions and Compound Poisson Process

Kolmogorov-Feller equation for the mesoscopic mean-field density:

$$\frac{\partial \rho(x,t)}{\partial t} = \lambda \int \rho(x-z,t) w(z) dz - \lambda \rho(x,t) \tag{1}$$

where $w(z)$ is the jumps pdf (the dispersal kernel).

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$$\rho\left(x,t\right) = \mathbb{E}_x \rho_0\left(X\left(t\right)\right),$$

where $X(t)$ is the position of a particle at time t (Compound Poisson process)

$$X\left(t\right) = \sum_{i=1}^{N(t)} Z_i, \tag{2}$$

where $N(t)$ is a *Poisson process* (the random number of jumps up to time t) and jumps Z_i are IID random variables with pdf $w(z)$.

Continuous time random walk (CTRW)

Let $X(t)$ denote the position of a particle:

$$X(t) = \sum_{i=1}^{N(t)} Z_i, \tag{3}$$

where $N(t)$ is a *renewal* or *counting process*. $X(t)$ is called a continuous time random walk (CTRW).

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Jumps occur at random times $T_1,\ T_2, \ldots$ so that the intervals between jumps $\Theta_n = T_n - T_{n-1}$ are also IID variables. Statistical characteristics are completely determined by the joint pdf $\psi(z,t)$. The spatial jump length pdf is given by $w(z) = \int_0^\infty \psi(z,t)dt$ and the waiting time pdf by $\phi(t) = \int_{R^3} \psi(z,t)dz$.

R. Metzler and J. Klafter, Phys. Rep. **339**, 1 (2000).

Parabolic scaling vs anomalous scaling

Generalized Master equation for the mean-field density $\rho(x,t)$:

$$\frac{\partial \rho(x,t)}{\partial t} = \int_0^t K(t-s) \left[\int \rho(x-z,s) w(z) dz - \rho(x,s) \right] ds \qquad (4)$$

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If we apply the parabolic scaling (long-time large-scale limit) $x \longrightarrow \frac{x}{\varepsilon}, \quad t \longrightarrow \frac{t}{\varepsilon^2}$ then the density

$$\rho(x,t) = \lim_{\varepsilon \to 0} \rho^{\varepsilon}(x,t) = \lim_{\varepsilon \to 0} \rho\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2}\right)$$

obeys the macroscopic diffusion equation

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Probabilistic explanation: $X(t) \xrightarrow{d} B(t)$.

Anomalous diffusion

Assume that the pdf of the waiting time $\phi(\tau)$ decreases like $\tau^{-\gamma-1}$ as $\tau \to \infty$ (infinite mean waiting time) and the dispersal kernel $w(z)$ has heavy tails $|z|^{-1-\alpha}$ (infinite variance).

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$$\frac{\partial^{\alpha}\rho}{\partial |x|^{\alpha}} := \Gamma(1+\alpha)\frac{\sin(\pi\alpha/2)}{\pi}\int_0^{\infty} \frac{\rho(x-z,t) - 2\rho(x,t) + \rho(x+z,t)}{z^{1+\alpha}}dz$$

is the symmetric Riesz fractional derivative.

Non-Markovian transport equation and non-linear kinetics

Generalized Master equation for the mean-field density:

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Non-Markovian behavior of particles performing CTRW occurs when particles are trapped during the random time with non-exponential distribution.

CTRW with reactions.

The main challenge is to implement the non-linear kinetic term into non-Markovian transport equations involving CTRW.

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The main challenge is to implement the non-linear kinetic term into non-Markovian transport equations involving CTRW.

We assume that the chemical reaction follows the mass action law and reaction term is of the form $r(\rho)\rho$. It is also convenient to represent the non-linear reaction rate $r(\rho)$ as the difference between the birth rate $r^{+}(\rho)$ and the death rate $r^{-}(\rho)$

$$r(\rho) = r^{+}(\rho) - r^{-}(\rho). \tag{6}$$

Now we consider two different models for reaction and transport process.
S. Fedotov, Phys. Rev. E 81, 011117 (2010)

Model A

We introduce the density of particles $j(x,t)$ arriving at point x exactly at time t. Let us now implement a nonlinear growth process into non-Markovian transport equations for the densities $j(x,t)$ and $\rho(x,t)$:

$$\begin{aligned} j(x,t) &= \int_{\mathbb{R}} \rho_0(x-z)\, e^{\int_0^t r(\rho(x-z,u))du} w(z)\phi(t)\, dz \\ &+ \int_0^t \int_{\mathbb{R}} j(x-z,\tau)\, e^{\int_\tau^t r(\rho(x-z,u))du} w(z)\phi(t-\tau)\, dz d\tau \quad (7) \end{aligned}$$

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and

$$\rho(x,t) = \rho_0(x)\, e^{\int_0^t r(\rho(x,u))du} \Psi(t) + \int_0^t j(x,\tau)\, e^{\int_\tau^t r(\rho(x,u))du} \Psi(t-\tau) d\tau, \quad (8)$$

where $\Psi(t) = 1 - \int_0^t \phi(s)ds$ is the survival probability.

Nonlinear Master equation

One can obtain nonlinear Master equation for the density $\rho(x,t)$ which is non-local in space and time

$$\frac{\partial \rho}{\partial t} = \int_0^t K(t-\tau)\Big(\int_{\mathbb{R}} \rho(x-z,\tau)\, e^{\int_\tau^t r(\rho(x-z,u))du} w(z)\, dz$$

$$-\rho(x,\tau)\, e^{\int_\tau^t r(\rho(x,u))du}\Big) d\tau + r(\rho)\,\rho.$$

Transport and the reaction are not separable!

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Transport and the reaction are not separable!

For the Markov processes, the kernel $K(t-\tau) = \lambda\delta(t-\tau)$ and, therefore, we have separation of transport and reactions.

In a linear case, this equation has been derived by *Sokolov, et al, PRE, 2006 and Henry, et al, PRE, 2006*

Model B: Reaction-transport Master equation

We assume that the particles created with the rate $r^{+}(\rho)\rho$ have zero age. We interpret the density $j(x,t)$ as a zero-age density of particles arriving at the point x exactly at time t.

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$$-\rho(x,\tau)\, e^{-\int_\tau^t r^-(\rho(x,u))du}\Big) d\tau + r^+(\rho)\rho - r^-(\rho)\rho.$$

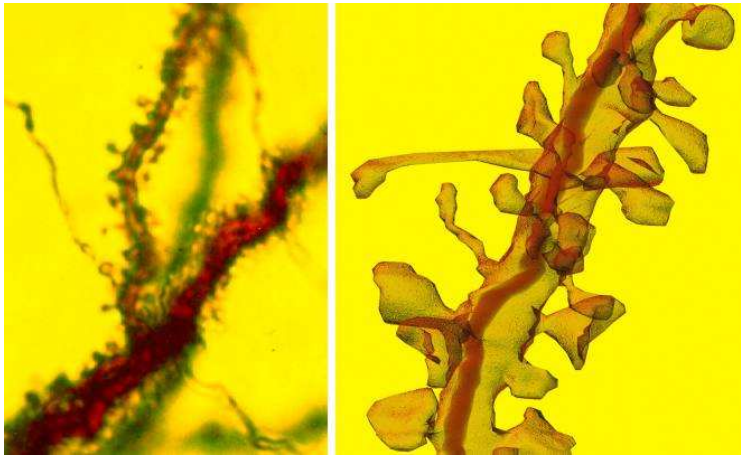
If we expand the expression in the brackets for small z, we obtain

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}\int_0^t K(t-\tau)\rho(x,\tau)\, e^{-\int_\tau^t r^-(\rho(x,u))du} d\tau \\ &\quad + r^+(\rho)\rho - r^-(\rho)\rho. \qquad (9)\end{aligned}$$

Model B describes the situation when newborn particles have been given new waiting time (Vlad, Ross (2002); Yadav, Horsthemke (2006).

Applications: subdiffusion in two-state model

Spiny Dendrites:



Dendritic spines are essential elements of most brain regions because they form a surface for receiving synaptic inputs.

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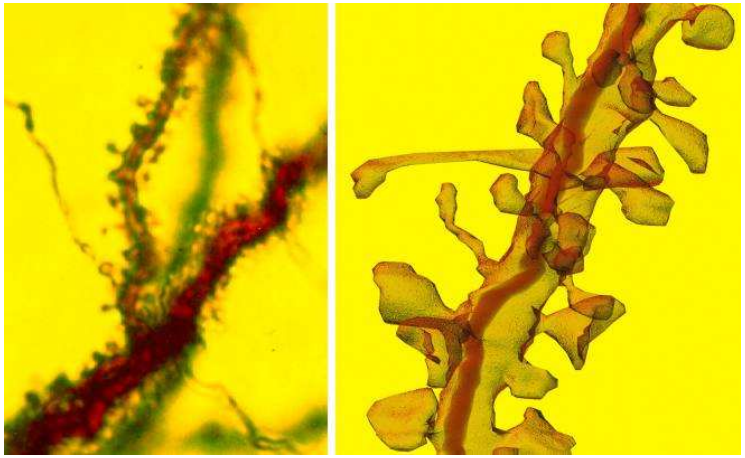

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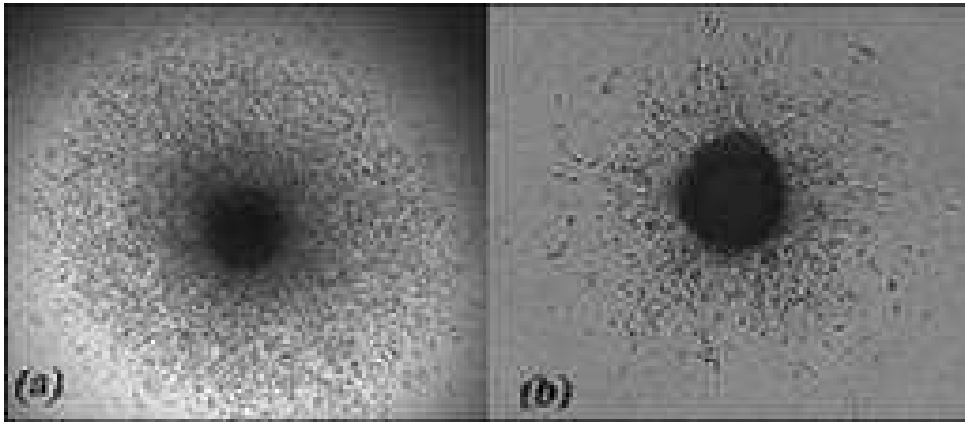
It has been found recently [Santamaria et al., Neuron 52, 635 (2006)] that the transport of biologically inert particles (fluorescein dextran) in spiny dendrites is subdiffusive:

$$\mathbb{E}X^2(t) \sim t^\gamma \qquad 0 < \gamma < 1$$

Two-state model: Fedotov, Mendez, PRL 101, 218102 (2008)

Migration and proliferation dichotomy in the tumor invasion

Proliferation and migration of tumor cells are mutually exclusive: the spreading suppresses cell proliferation and visa versa (Giese et al.)



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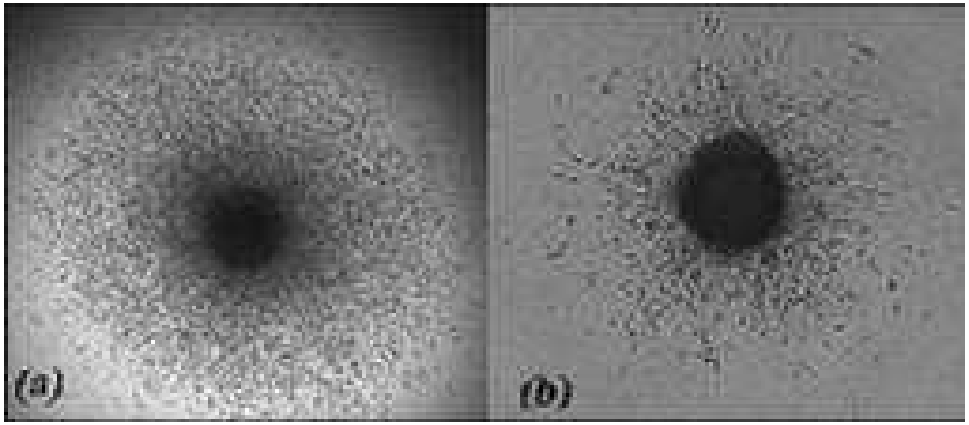

Two-state model: S. Fedotov and A. Iomin, Phys. Rev. Lett. **98**, 118101 (2007)

$n_1(x,t)$ - the density for the cells of migratory phenotype;

$n_2(x,t)$ - the density for the cells of proliferating phenotype.

Anomalous Transport and Nonlinear Reactions in Two-State Systems

Two-state Markovian random process: we assume that the transition probabilities γ_1 and γ_2 are constants.

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Two-state Markovian random process: we assume that the transition probabilities γ_1 and γ_2 are constants.
Master equations for the mean density of particles in state 1 (mobile), $n_1(x,t)$, and the density of particles in state 2 (immobile), $n_2(x,t)$, are

$$\frac{\partial n_1}{\partial t} = L_x n_1 - \gamma_1 n_1 + \gamma_2 n_2, \tag{10}$$

$$\frac{\partial n_2}{\partial t} = r_2\left(n_2\right) n_2 - \gamma_2 n_2 + \gamma_1 n_1, \tag{11}$$

where the reaction rate $r_2\left(n_2\right)$ depends on the local density of particles n_2. Here L_x is the transport operator acting on x-coordinate.

Non-Markovian model for the transport and reactions of particles in two-state systems

Nonlinear Master equations:

$$\frac{\partial n_1}{\partial t} = L_x n_1 + j_1(x,t) - j_2(x,t), \tag{12}$$

$$\frac{\partial n_2}{\partial t} = r_2\left(n_2\right) n_2 + j_2(x,t) - j_1(x,t), \tag{13}$$

where the densities $j_1(x,t)$ and $j_2(x,t)$ describe the exchange flux of particles:

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where the densities $j_1(x,t)$ and $j_2(x,t)$ describe the exchange flux of particles:

$$j_1(x,t) = \int_0^t K_2(t-t') n_2(x,t') e^{\int_{t'}^{t} r_2(n_2(x,s))ds} dt', \tag{14}$$

$$j_2(x,t) = \int_0^t \int_{\mathbb{R}} K_1(t-t') p(x-z, t-t') n_1(z,t') dz dt', \tag{15}$$

where $K_i(t)$ is the memory kernel defined as $\tilde{K}_i(s) = \frac{\tilde{\psi}_i(s)}{\tilde{\Psi}_i(s)}$.

Human Settlements Along River Valley (Neolithic Age)

We split total population density as $n = n_1 + n_2$, where n_1 is the density of semi-sedentary farmers and n_2 is the density of sedentary farmers.

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We split total population density as $n = n_1 + n_2$, where n_1 is the density of semi-sedentary farmers and n_2 is the density of sedentary farmers. The main idea behind this splitting is to distinguish between mobile farmers (n_1) with very low growth rate and immobile farmers (n_2) with high growth rate around $1 - 3\%$ per year.

Human Settlements Along River Valley (Neolithic Age)

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Balance equations for $n_1(x,t)$ and $n_2(x,t)$:

$$\frac{\partial n_1}{\partial t} = \int \lambda(q(x-z,t))n_1(x-z,t)\rho(z)dz - \lambda(q)n_1 - \alpha_1(q)n_1 + \alpha_2(q)n_2$$

$$\frac{\partial n_2}{\partial t} = rn_2\left(1 - \frac{n}{K(q)}\right) + \alpha_1(q)n_1 + \alpha_2(q)n_2,$$

where $q(x,t)$ - the rate of crop production measured in kilograms per person per year.

Fedotov, Campos, Moss, Phys. Rev. E 78, 026107 (2008).

Main Results

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The model describes subsequent decay of these clusters (settlements) due to land degradation. The entire population decays over about 1000 yr.

Settlement pattern in $2 - D$

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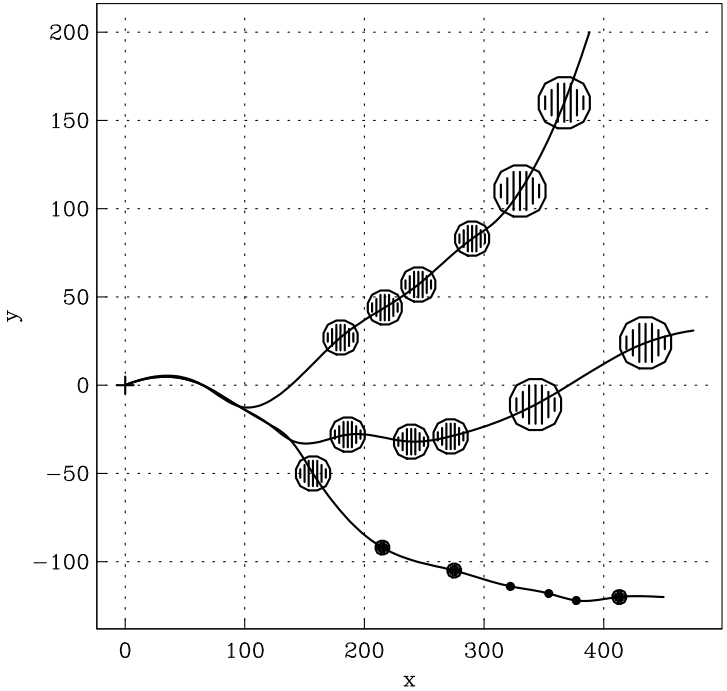
This picture illustrates what happens after 500 years.



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