Subdiffusion and nonlinear reaction-transport equations

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Fluid-Kinetic Modelling, Cambridge, 2010
INTRODUCTION

- Reaction-advection-diffusion PDE’s and underlying random processes
- Fractional PDE’s and continuous time random walk (CTRW)
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NON-LOCAL IN SPACE AND TIME REACTION-TRANSPORT EQUATIONS

- Non-Markovian CTRW-models with nonlinear reactions
- Nonlinear Master equations for mean-field density
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TWO-STATE MODELS
- Examples: spiny dendrites of cerebellar cortex, colonization and human settlements along river valley
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- Advection-diffusion PDE:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (v(x, t) \rho) = D \Delta \rho$$
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- Advection-diffusion PDE:

$$\frac{\partial \rho}{\partial t} + v(x, t) \cdot \nabla \rho = D \Delta \rho + r(\rho) \rho, \quad \rho(x, 0) = \rho_0(x) \quad x \in \mathbb{R}^3$$

where $r(\rho)$ is the reaction rate.
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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:

$$dX = -v(X(s), t - s) ds + (2D)^{1/2} dW(s), \quad X(0) = x.$$
• **Fractional** PDE with anomalous transport (Levy flights, subdiffusion, etc.):

\[ D_t^{\gamma} \rho = -D_\alpha (-\Delta)^{\alpha/2} \rho \]
Fractional Reaction-Transport Equation for Density $\rho$

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  where $D_t^{\gamma} \rho$ is the **Caputo derivative** and the Laplacian $\Delta$ is replaced by a **Riesz fractional operator**: $-(-\Delta)^{\frac{\alpha}{2}}$.

  Is it a good model for reaction-transport?
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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)).
Kolmogorov-Feller equation for the mesoscopic mean-field density:

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

(1)

where $w(z)$ is the jumps pdf (the dispersal kernel).
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The solution is given by the formula

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Biological Invasions and Compound Poisson Process

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

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

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

(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:

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

where $N(t)$ is a renewal or counting process. $X(t)$ is called a continuous time random walk (CTRW).
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Let $X(t)$ denote the position of a particle:

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Jumps occur at random times $T_1, T_2, ...$ 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 $\phi(t) = \int_{R^3} \psi(z, t) dz$.

Parabolic scaling vs anomalous scaling

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

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

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Assume that the pdf $\phi(t)$ of the waiting time has a finite first moment and the dispersal kernel $w(z)$ has a finite variance.
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If we apply the parabolic scaling (long-time large-scale limit)

$x \to \frac{x}{\varepsilon}, \quad t \to \frac{t}{\varepsilon^2}$

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

$$\frac{\partial \rho}{\partial t} = D \frac{\partial^2 \rho}{\partial x^2}.$$
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Probabilistic explanation: $X(t) \overset{d}{\rightarrow} B(t).$
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^\gamma \rho}{\partial t^\gamma} = D^\alpha \frac{\partial^\alpha \rho}{\partial |x|^\alpha}, \quad 0 < \alpha < 2
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is the Caputo fractional derivative,

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

is the symmetric Riesz fractional derivative.
Generalized Master equation for the mean-field density:

\[
\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
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Can we add the non-linear kinetic term \( r(\rho)\rho \) to the RHS of non-Markovian transport equation?
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In general, the answer is NO!!
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.
The main challenge is to implement the non-linear kinetic term into non-Markovian transport equations involving CTRW.
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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)
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 $\rho(x, t)$:

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

and
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$$j(x, t) = \int_{\mathbb{R}} \rho_0(x - z) e^{\int_0^t r(\rho(x - z, u)) du} w(z) \phi(t) \, dz$$

$$+ \int_0^t \int_{\mathbb{R}} j(x - z, \tau) e^{\int_{\tau}^t r(\rho(x - z, u)) du} w(z) \phi(t - \tau) \, dz \, d\tau$$ \hspace{1cm} (7)

and

$$\rho(x, t) = \rho_0(x) e^{\int_0^t r(\rho(x, u)) du} \psi(t) + \int_0^t j(x, \tau) e^{\int_{\tau}^t r(\rho(x, u)) du} \psi(t - \tau) \, d\tau,$$ \hspace{1cm} (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

\[
\frac{\partial \rho}{\partial t} = \int_0^t K(t - \tau) \left( \int_{\mathbb{R}} \rho(x - z, \tau) e^{\int_{\tau}^t r(\rho(x-z,u))du} w(z) dz \right) d\tau + r(\rho) \rho.
\]

Transport and the reaction are not separable!
One can obtain nonlinear Master equation for the density $\rho(x,t)$ which is non-local in space and time

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

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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$$\frac{\partial \rho}{\partial t} = \int_0^t K(t - \tau) \left( \int_{\mathbb{R}} \rho(x - z, \tau) e^{-\int_\tau^t r^- (\rho(x - z, u))du} w(z) dz \right) d\tau \bigg) + r^+(\rho)\rho - r^-(\rho)\rho.$$
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$$-\rho (x, \tau) e^{-\int^t_\tau r^- (\rho (x, u)) du} d\tau + r^+ (\rho) \rho - r^- (\rho) \rho.$$  

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

$$\frac{\partial \rho}{\partial t} = \frac{\sigma^2}{2} \frac{\partial^2}{\partial x^2} \int^t_0 K (t - \tau) \rho (x, \tau) e^{-\int^t_\tau r^- (\rho (x, u)) du} d\tau$$

$$+ r^+ (\rho) \rho - r^- (\rho) \rho. \quad (9)$$

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

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:

\[ \mathbb{E}X^2(t) \sim t^{\gamma} \quad 0 < \gamma < 1 \]

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.)

![Image of tumor cell proliferation and migration](image-url)
Proliferation and migration of tumor cells are mutually exclusive: the spreading suppresses cell proliferation and visa versa (Giese et al.)


\[ n_1(x, t) \] - the density for the cells of migratory phenotype;

\[ n_2(x, t) \] - the density for the cells of proliferating phenotype.
Two-state Markovian random process: we assume that the transition probabilities $\gamma_1$ and $\gamma_2$ are constants.
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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

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

(10)

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

(11)

where the reaction rate $r_2(n_2)$ 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:

\[
\frac{\partial n_1}{\partial t} = L_x n_1 + j_1(x, t) - j_2(x, t),
\]

\[
\frac{\partial n_2}{\partial t} = r_2(n_2) n_2 + j_2(x, t) - j_1(x, t),
\]

where the densities \(j_1(x, t)\) and \(j_2(x, t)\) describe the exchange flux of particles:
Non-Markovian model for the transport and reactions of particles in two-state systems

Nonlinear Master equations:

\[ \frac{\partial n_1}{\partial t} = L_x n_1 + j_1(x, t) - j_2(x, t), \]  

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

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

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

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

Main Results

Numerical simulations reveal a very interesting dynamical behavior: the emergence of large-scale settlement pattern along a 3-branched river.
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Model provides an explanation for the formation of settlements as a dynamical phenomenon. The individual farmers have a tendency for aggregation and clustering as a result of non-linear random migration.
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Model provides an explanation for the formation of settlements as a dynamical phenomenon. The individual farmers have a tendency for aggregation and clustering as a result of non-linear random migration.

The model describes subsequent decay of these clusters (settlements) due to land degradation. The entire population decays over about 1000 yr.
Let me show the results of numerical simulations. We consider the river with three branches. Initial conditions are: the population is zero everywhere, except one point where the farmers arrive at time \( t = 0 \).
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This picture illustrates what happens after 500 years.
Conclusions

- The mesoscopic description of non-Markovian reaction-transport systems is still an open problem.
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