From normal to anomalous deterministic diffusion
Part 3: Anomalous diffusion

Rainer Klages

Queen Mary University of London, School of Mathematical Sciences

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Outline

yesterday:

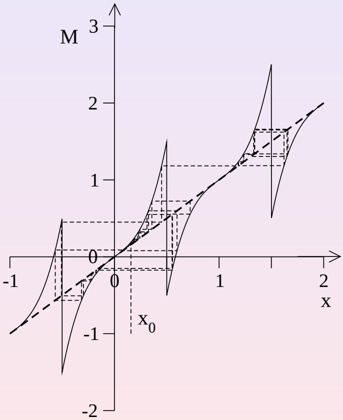
2. **From normal to anomalous deterministic diffusion:** normal diffusion in particle billiards and anomalous diffusion in intermittent maps

note: work by T.Akimoto

today:

3. **Anomalous diffusion:** generalized diffusion and Langevin equations, biological cell migration and fluctuation relations

Reminder: Intermittent map and CTRW theory



subdiffusion coefficient calculated from CTRW theory

key: solve Montroll-Weiss equation in Fourier-Laplace space,

$$\hat{\tilde{\varrho}}(k,s) = \frac{1-\tilde{w}(s)}{s} \frac{1}{1-\hat{\lambda}(k)\tilde{w}(s)}$$

Time-fractional equation for subdiffusion

For the lifted **PM map** $M(x) = x + ax^z \mod 1$, the MW equation in long-time and large-space asymptotic form reads

$$s^\gamma \hat{\tilde{\varrho}} - s^{\gamma-1} = -\frac{p\ell^2 a^\gamma}{2\Gamma(1-\gamma)\gamma^\gamma} k^2 \hat{\tilde{\varrho}} \, , \; \gamma := 1/(z-1)$$

LHS is the Laplace transform of the Caputo fractional derivative

$$\frac{\partial^\gamma \varrho}{\partial t^\gamma} := \begin{cases} \frac{\partial \varrho}{\partial t} & \gamma = 1 \\ \frac{1}{\Gamma(1-\gamma)} \int_0^t dt' (t-t')^{-\gamma} \frac{\partial \varrho}{\partial t'} & 0 < \gamma < 1 \end{cases}$$

transforming the Montroll-Weiss eq. back to real space yields the time-fractional (sub)diffusion equation

$$\boxed{\frac{\partial^\gamma \varrho(x,t)}{\partial t^\gamma} = K \frac{\Gamma(1+\alpha)}{2} \frac{\partial^2 \varrho(x,t)}{\partial x^2}}$$

Interlude: What is a fractional derivative?

letter from Leibniz to L'Hôpital (1695): $\frac{d^{1/2}}{dx^{1/2}} = ?$

one way to proceed: we know that for integer m, n

$$\frac{d^m}{dx^m}x^n = \frac{n!}{(n-m)!}x^{n-m} = \frac{\Gamma(n+1)}{\Gamma(n-m+1)}x^{n-m};$$

assume that this also holds for $m = 1/2$, $n = 1$

$$\Rightarrow \quad \boxed{\frac{d^{1/2}}{dx^{1/2}}x = \frac{2}{\sqrt{\pi}}x^{1/2}}$$

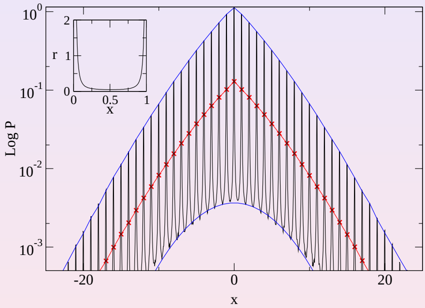
fractional derivatives are defined via power law memory kernels, which yield power laws in Fourier (Laplace) space:

$$\frac{d^\gamma}{dx^\gamma}F(x) \leftrightarrow (ik)^\gamma \tilde{F}(k)$$

$\exists$ well-developed mathematical theory of **fractional calculus**; see Sokolov, Klafter, Blumen, Phys. Today 2002 for a short intro

Deterministic vs. stochastic density

initial value problem for fractional diffusion equation can be solved exactly; compare with simulation results for $P = \varrho_n(x)$:



- Gaussian and non-Gaussian envelopes (blue) reflect intermittency
- fine structure due to density on the unit interval $r = \varrho_n(x)$ $(n \gg 1)$ (see inset)

Escape rate theory for anomalous diffusion?

recall the escape rate theory of Lecture 1 expressing the (normal) diffusion coefficient in terms of chaos quantities:

$$D = \lim_{L\to\infty} \left(\frac{L}{\pi}\right)^2 [\lambda(\mathcal{R}_L) - h_{KS}(\mathcal{R}_L)]$$

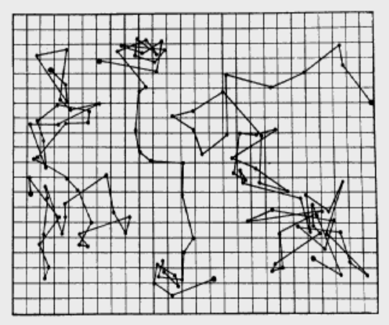
Q: Can this also be worked out for the subdiffusive PM map?

1. solve the previous fractional subdiffusion equation for absorbing boundaries: can be done
2. solve the Frobenius-Perron equation of the subdiffusive PM map: **??** ($\exists$ methods by Tasaki, Gaspard (2004))
3. even if step 2 possible and modes can be matched: $\exists$ an anomalous escape rate formula **???**

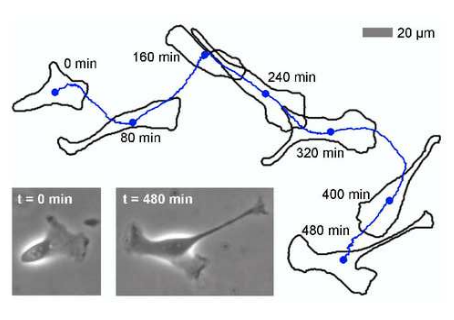
two big open questions...

Motivation: biological cell migration

Brownian motion



3 colloidal particles of radius 0.53μm; positions every 30 seconds, joined by straight lines (Perrin, 1913)



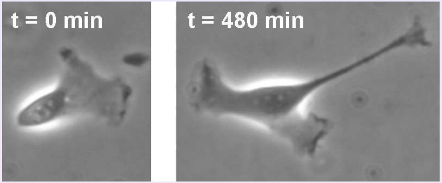
single biological cell crawling on a substrate (Dieterich, R.K. et al., PNAS, 2008)

Brownian motion?

Our cell types and how they migrate

MDCK-F (Madin-Darby canine kidney) cells

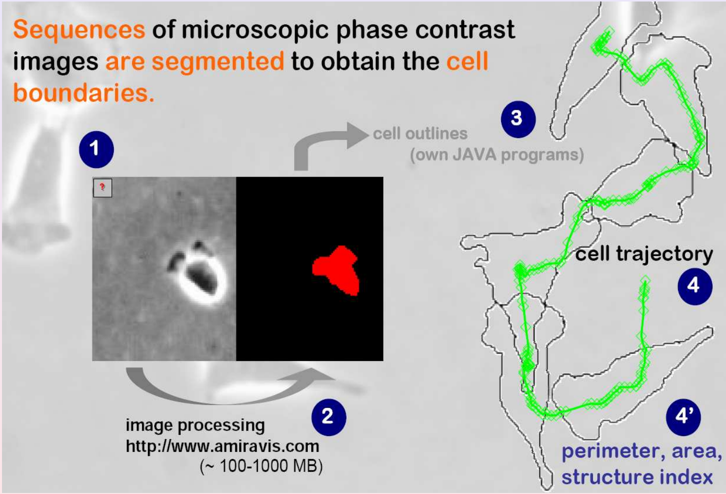
two types: wildtype (*NHE*$^+$) and NHE-deficient (*NHE*$^-$)



movie: NHE+: t=210min, dt=3min

note:
the *microscopic origin* of cell migration is a **highly complex process** involving a huge number of proteins and signaling mechanisms in the *cytoskeleton*, which is a complicated *biopolymer gel* – we do not consider this here!

Measuring cell migration

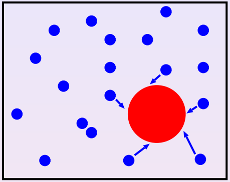


Theoretical modeling: the Langevin equation

Newton's law for a particle of mass m and velocity $\underline{v}$ immersed in a fluid

$$m\dot{\underline{v}} = \underline{F}_d(t) + \underline{F}_r(t)$$

with total force of surrounding particles decomposed into *viscous damping* $\underline{F}_d(t)$ and *random kicks* $\underline{F}_r(t)$



suppose $\underline{F}_d(t)/m = -\kappa\underline{v}$ and $\underline{F}_r(t)/m = \sqrt{\zeta}\,\underline{\xi}(t)$ as *Gaussian white noise* of strength $\sqrt{\zeta}$:

$$\boxed{\dot{\underline{v}} + \kappa\underline{v} = \sqrt{\zeta}\,\underline{\xi}(t)}$$ **Langevin equation** (1908)

'Newton's law of stochastic physics': apply to cell migration?

note: Brownian particles passively driven, whereas cells move actively by themselves!

Solving Langevin dynamics

calculate two important quantities (in one dimension):

1. the diffusion coefficient $D := \lim_{t\to\infty} \frac{msd(t)}{2t}$

with $msd(t) :=< [x(t) - x(0)]^2 >$; for Langevin eq. one obtains
$msd(t) = 2v_{th}^2 \left(t - \kappa^{-1}(1 - \exp(-\kappa t))\right)/\kappa$ with $v_{th}^2 = kT/m$
note that $msd(t) \sim t^2 \ (t \to 0)$ and $msd(t) \sim t \ (t \to \infty) \Rightarrow \exists D$

2. the probability distribution function $P(x, v, t)$:

• Langevin dynamics obeys (for $\kappa \gg 1$) the diffusion equation

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2}$$

solution for initial condition $P(x, 0) = \delta(x)$ yields *position distribution* $P(x, t) = \exp(-\frac{x^2}{4Dt})/\sqrt{4\pi Dt}$

Fokker-Planck equations

- for *velocity distribution* $P(v,t)$ of Langevin dynamics one can derive the Fokker-Planck equation

$$\frac{\partial P}{\partial t} = \kappa \left[\frac{\partial}{\partial v} v + v_{th}^2 \frac{\partial^2}{\partial v^2} \right] P$$

stationary solution is $P(v) = \exp(-\frac{v^2}{2v_{th}^2})/\sqrt{2\pi} v_{th}$

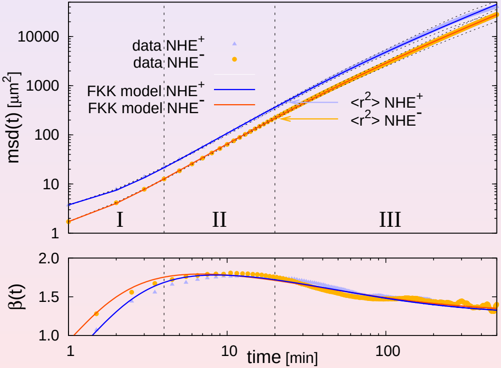
- Fokker-Planck equation for position *and* velocity distribution $P(x,v,t)$ of Langevin dynamics is the Klein-Kramers equation

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}[vP] + \kappa \left[\frac{\partial}{\partial v} v + v_{th}^2 \frac{\partial^2}{\partial v^2} \right] P$$

the above two eqns. can be derived from it as special cases

Experimental results I: mean square displacement

- $msd(t) := <[x(t) - x(0)]^2> \sim t^\beta$ with $\beta \to 2$ $(t \to 0)$ and $\beta \to 1$ $(t \to \infty)$ for Brownian motion; $\beta(t) = d \ln msd(t)/d \ln t$
- *solid lines:* (Bayes) fits from our model



anomalous diffusion if $\beta \neq 1$ $(t \to \infty)$: here superdiffusion

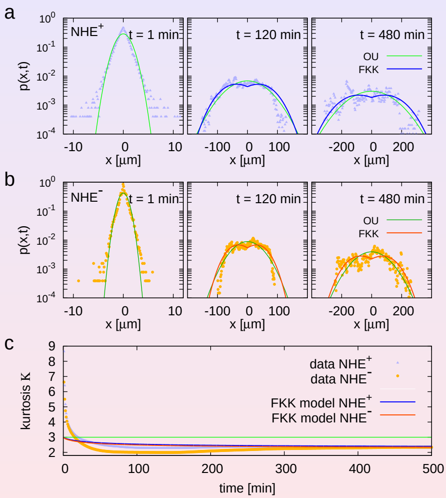
Experimental results II: position distribution function

- $P(x,t) \to$ Gaussian $(t \to \infty)$ and kurtosis

$$\kappa(t) := \frac{<x^4(t)>}{<x^2(t)>^2} \to 3 \ (t \to \infty)$$

for Brownian motion (green lines, in 1d)

- *other solid lines:* fits from our model; parameter values as before



⇒ crossover from peaked to broad non-Gaussian distributions

The generalized model

- **Fractional Klein-Kramers equation** (Barkai, Silbey, 2000)**:**

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}[vP] + \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\kappa\left[\frac{\partial}{\partial v}v + v_{th}^2\frac{\partial^2}{\partial v^2}\right]P$$

with probability distribution $P = P(x, v, t)$, damping term κ, thermal velocity $v_{th}^2 = kT/m$ and Riemann-Liouville fractional derivative of order $1 - \alpha$

for $\alpha = 1$ Langevin's theory of Brownian motion recovered

- **analytical solutions** for $msd(t)$ and $P(x, t)$ can be obtained in terms of special functions (Barkai, Silbey, 2000; Schneider, Wyss, 1989)

- **4 fit parameters** v_{th}, α, κ (plus another one for short-time dynamics)

Possible physical interpretation

- **physical meaning of the fractional derivative?**

fractional Klein-Kramers equation can *approximately* be related to generalized Langevin equation of the type

$$\dot{v} + \int_0^t dt'\, \kappa(t-t')v(t') = \sqrt{\zeta}\,\xi(t)$$

e.g., Mori, Kubo, 1965/66

with time-dependent friction coefficient $\kappa(t) \sim t^{-\alpha}$

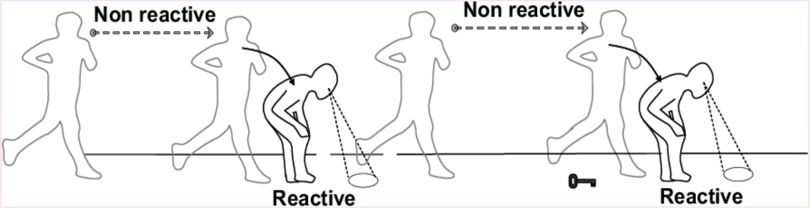
cell anomalies might originate from soft glassy behavior of the cytoskeleton gel, where power law exponents are conjectured to be universal (Fabry et al., 2003; Kroy et al., 2008)

Possible biological interpretation

- **biological meaning of anomalous cell migration?**

experimental data and theoretical modeling suggest *slower diffusion for small times* while *long-time motion is faster*

compare with intermittent optimal search strategies of foraging animals (Bénichou et al., 2006)



note: ∃ current controversy about **Lévy hypothesis** for optimal foraging of organisms (albatross, fruitflies, bumblebees,...)

Fluctuation relations

system evolving from an initial state into a nonequilibrium state; measure pdf $\rho(W_t)$ of entropy production W_t during time t:

$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = W_t$$ **transient fluctuation relation** (TFR)

Evans, Cohen, Morriss (1993); Gallavotti, Cohen (1995)

1. generalizes the Second Law to small noneq. systems
2. yields nonlinear response relations
3. connection with fluctuation dissipation relations (FDR)

example: check the above TFR for Langevin dynamics with constant field F; $W_t = Fx(t)$, $\rho(W_t) \sim \rho(x,t)$ is Gaussian

TFR holds if $< W_t > = < \sigma^2_{W_t} > /2$ (FDR1)

for Gaussian stochastic process: **FDR2 $\Rightarrow$ FDR1 $\Rightarrow$ TFR**

An anomalous fluctuation relation

check TFR for the overdamped generalized Langevin equation

$$\dot{x} = F + \xi(t)$$

with $< \xi(t)\xi(t') > \sim |t-t'|^{-\beta}$, $0 < \beta < 1$: **no FDT2**

$\rho(W_t)$ is Gaussian with $< W_t > \sim t$, $< \sigma^2_{W_t} > \sim t^{2-\beta}$: **no FDT1**

and superdiffusion

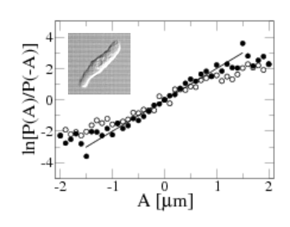
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = \mathbf{C}_\beta \mathbf{t}^{\beta-1} W_t$$

$(0 < \beta < 1)$

anomalous TFR

Chechkin, R.K. (2009)

experiments on slime mold:



Hayashi, Takagi (2007)

note: we see this aTFR in experiments on cell migration

Dieterich, Chechkin, Schwab, R.K., tbp

Summary

nonequilibrium conditions →

		equilibrium	nonequilibrium steady states	nonequilibrium non-steady states
microscopic	dynamical systems	ergodic hypothesis	**microscopic chaos**: strong	weak
↓	statistical mechanics	Gibbs ensembles	**complexity**: fractal SRB measures	infinite measures
macroscopic	thermodynamics	thermodynamic properties	**deterministic transport**: normal	anomalous

⇒ general theory of nonequilibrium statistical physics starting from **weak** microscopic chaos?

Acknowledgements and literature

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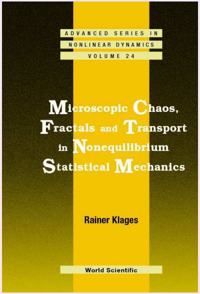
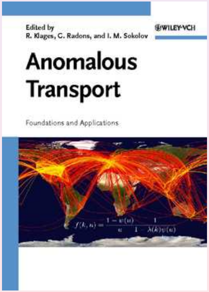
background information to:

Part 1,2



Part 2,3



and for cell migration: Dieterich et al., PNAS **105**, 459 (2008)