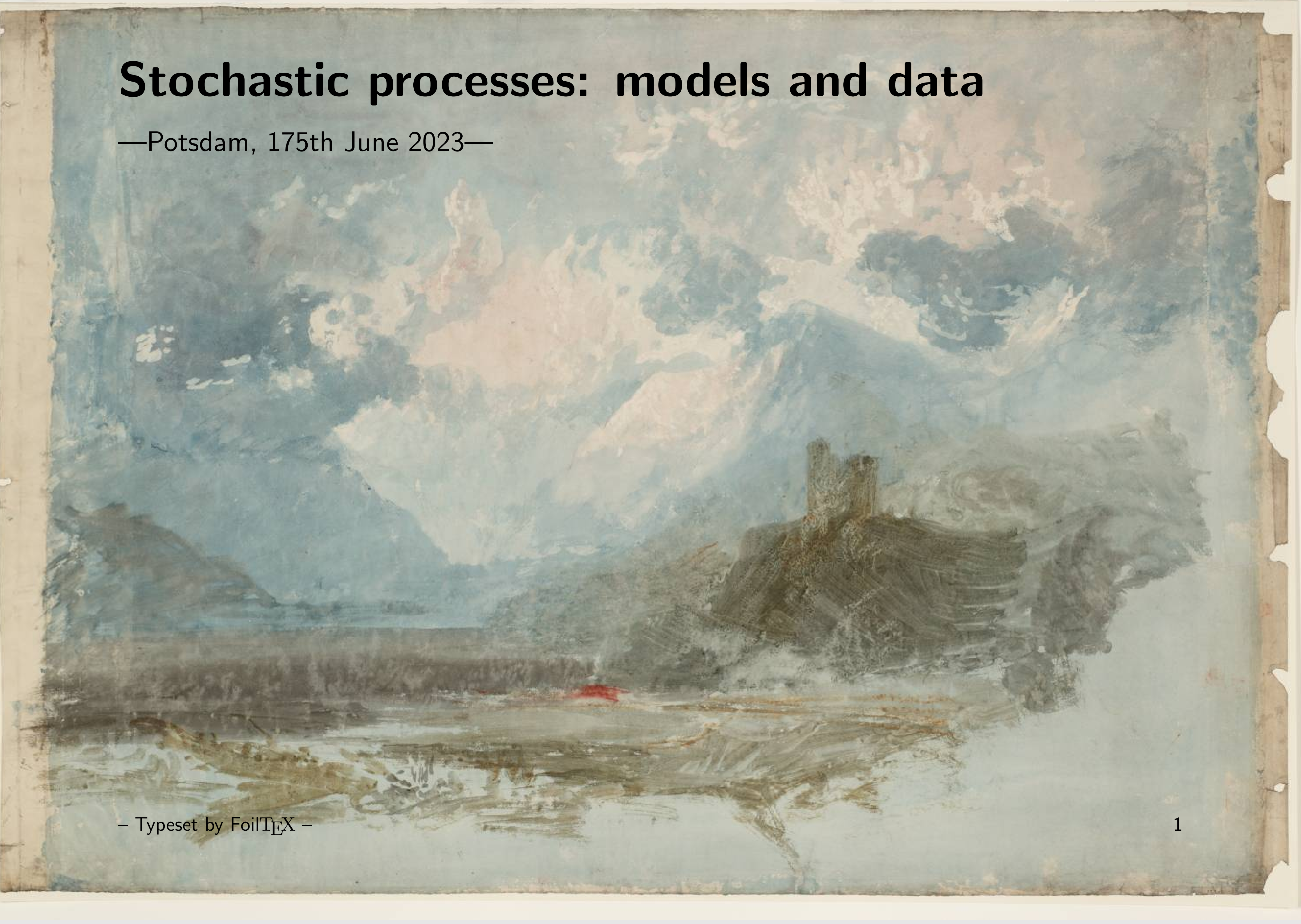


Stochastic processes: models and data

—Potsdam, 175th June 2023—

The founding fathers of diffusion theory: $\langle \mathbf{r}^2(t) \rangle \propto Kt$

Paul Langevin (1872-1946)
Albert Einstein (1879-1955)

Marian Smoluchowski
(1872-1917)

William Sutherland
(1859-1911)

Deterministic & stochastic equations

Continuity equation:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} S(x,t)$$

Constitutive equation (Fick's 1st law):

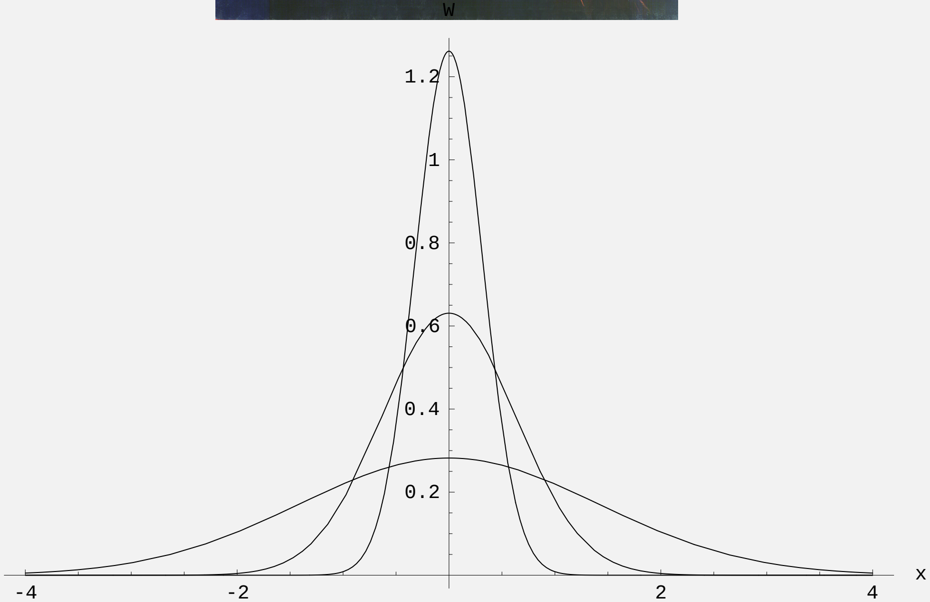
$$S(x,t) = -K \frac{\partial}{\partial x} P(x,t)$$

Diffusion equation (Fick's 2nd law):

$$\frac{\partial P(x,t)}{\partial t} = K \frac{\partial^2}{\partial x^2} P(x,t)$$

Gaussian solution for $P(x,0) = \delta(x)$:

$$P(x,t) = \frac{1}{\sqrt{4\pi K t}} \exp\left(-\frac{x^2}{4Kt}\right)$$



A. Fick, Poggendorff's Annal. Physik. **94** 59 (1855); Phil. Mag. **10**, 30 (1855)

Deterministic & stochastic equations II

Fokker-Planck equation in an external potential $V(x)$ & Boltzmann distribution:

$$\frac{\partial P(x,t)}{\partial t} = \left(\frac{\partial}{\partial x} \frac{V'(x)}{m\eta} + K \frac{\partial^2}{\partial x^2} \right) P(x,t) \quad \rightsquigarrow \quad P_{\mathrm{st}}(x) = \mathscr{N}_{V(x)} \exp\left(-\frac{V(x)}{k_B T} \right)$$

Einstein-Smoluchowski-Sutherland relation: $K = k_B T/(m\eta)$

Newton's second law for particle with Stokes friction $F = -m\eta v$:

$$m\dot{v}(t) + m\eta v(t) = 0 \quad \rightsquigarrow \quad v(t) = v(0) e^{-\eta t} \quad \text{Stat Phys: } \frac{1}{2} m \langle v^2 \rangle = \frac{1}{2} k_B T$$

Stochastic differential (Langevin) equation with fluctuating force $F_f(t)$:

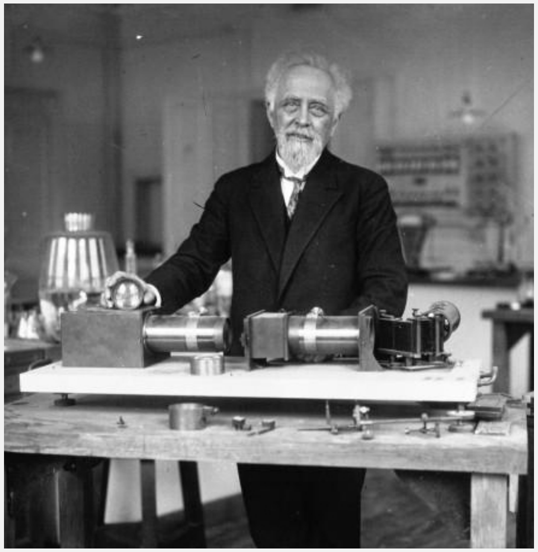
$$m\dot{v}(t) + m\eta v(t) = F_f(t) \quad \therefore \quad \langle F_f(t) \rangle = 0, \quad \langle F_f(t) F_f(t') \rangle = 2m\eta k_B T \delta(t - t')$$

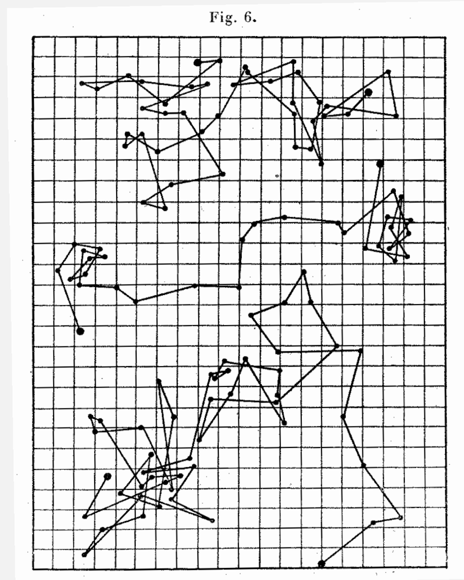
Mean squared displacement:

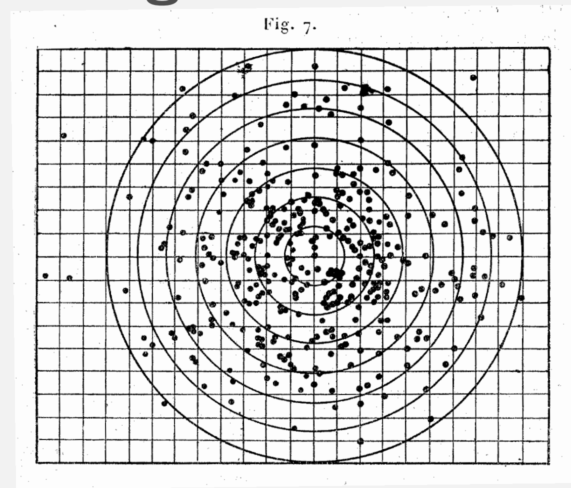
$$\langle x(t) \rangle \sim \begin{cases} v(0)^2 t^2, & t \ll 1/\eta \\ 2Kt, & t \gg 1/\eta \end{cases}$$

N van Kampen, Stochastic processes in physics & chemistry

Les atomes: Brownian motion and Avogadro’s number

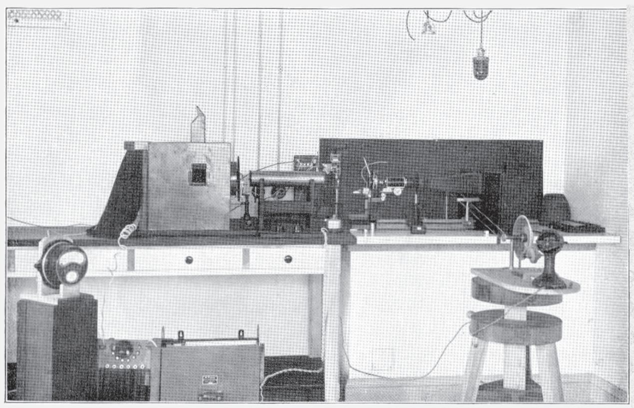


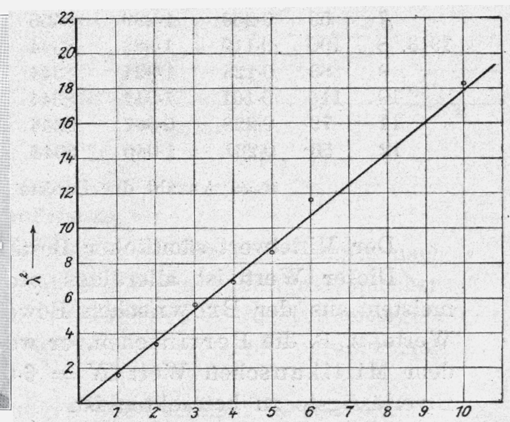


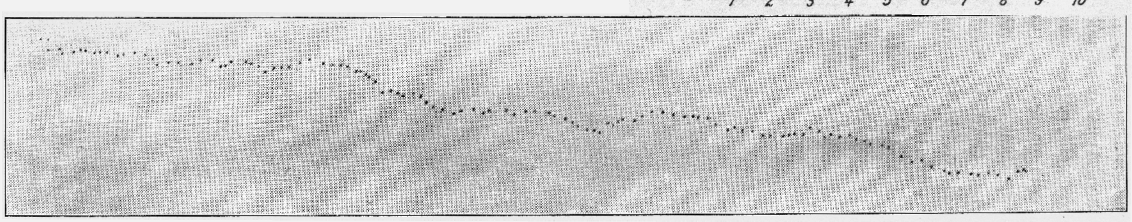


Δt=30 sec

$$K = \frac{k_B T}{m\eta} = \frac{(R/N_A)T}{m\eta}$$





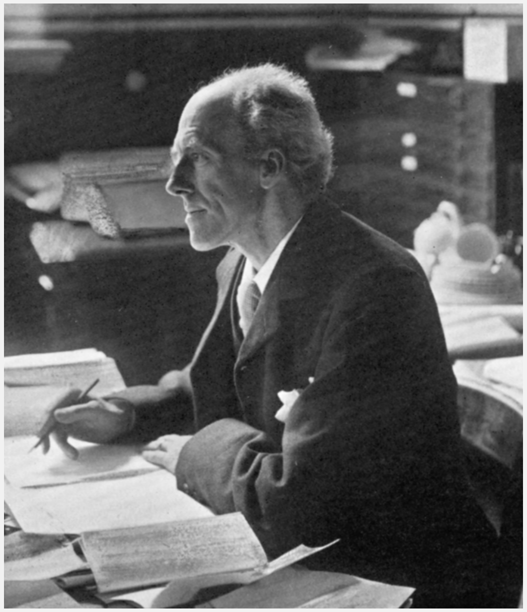


J Perrin, Comptes Rendus (Paris) 146 (1908) 967: $N_A = 70.5 \times 10^{22}$; I Nordlund, Z Physik (1914): $N_A = 5.91 \times 10^{23}$

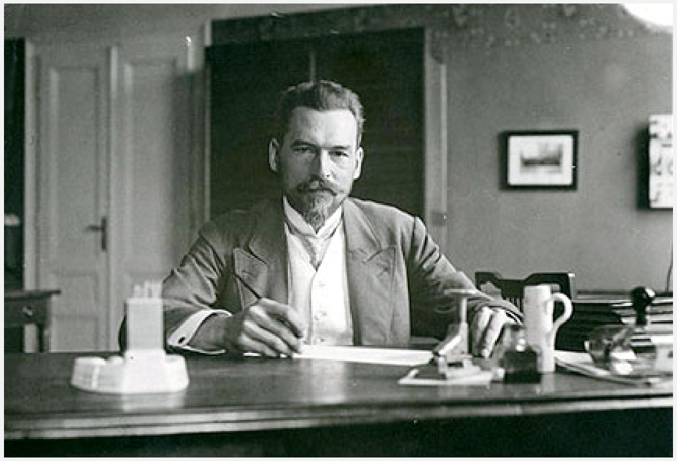
Brownian motion & random walks applied . . .

Louis Bachelier, 1900:
Brownian motion of
financial markets

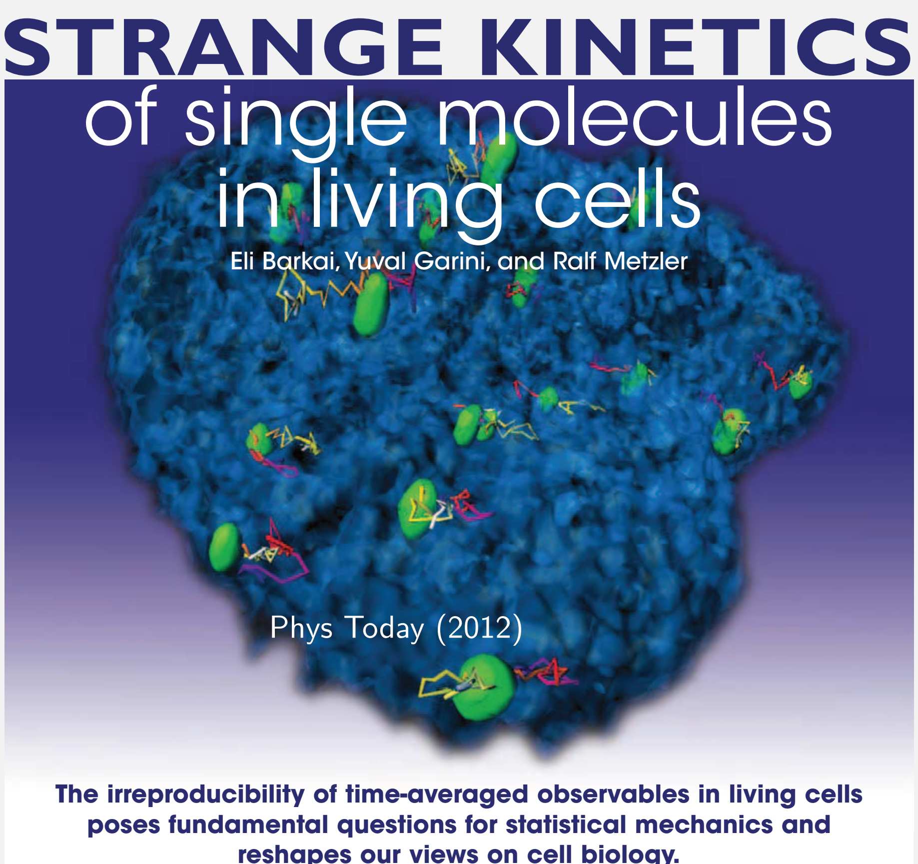
Karl Pearson, 1905:
Spreading of mosquitoes
in rain forests



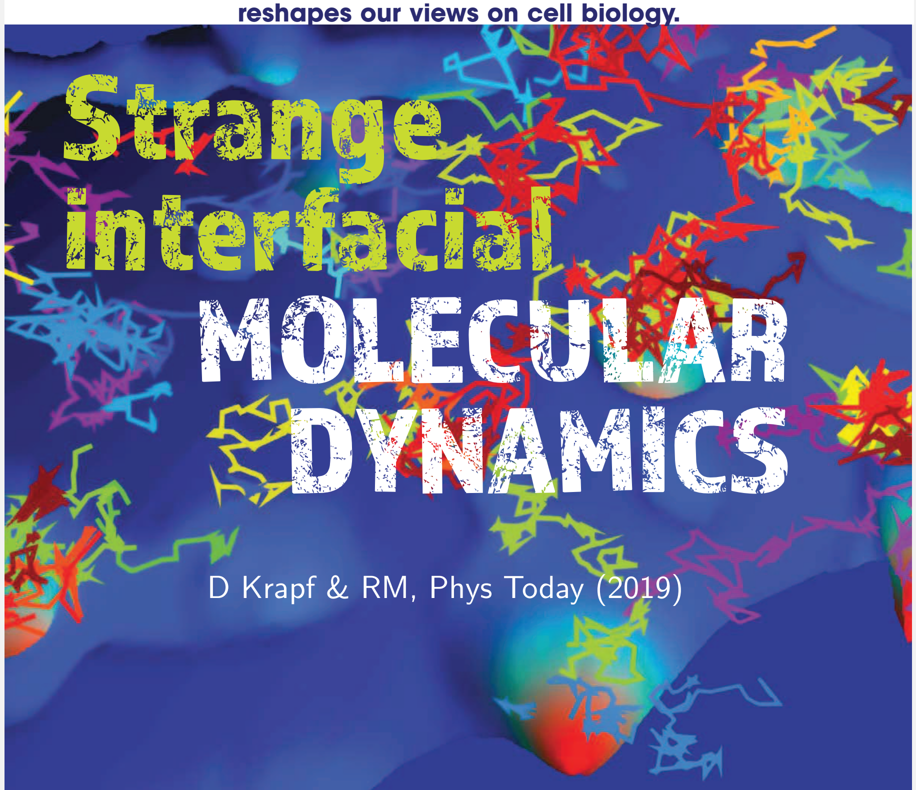
Marian v Smoluchowski, 1916:
Molecular reaction kinetics



Elliott Montroll, 1943:
Manhattan project,
chain reaction of
neutrons



Phys Today (2012)



D Krapf & RM, Phys Today (2019)

Stochastic processes: models $\longleftrightarrow$ data

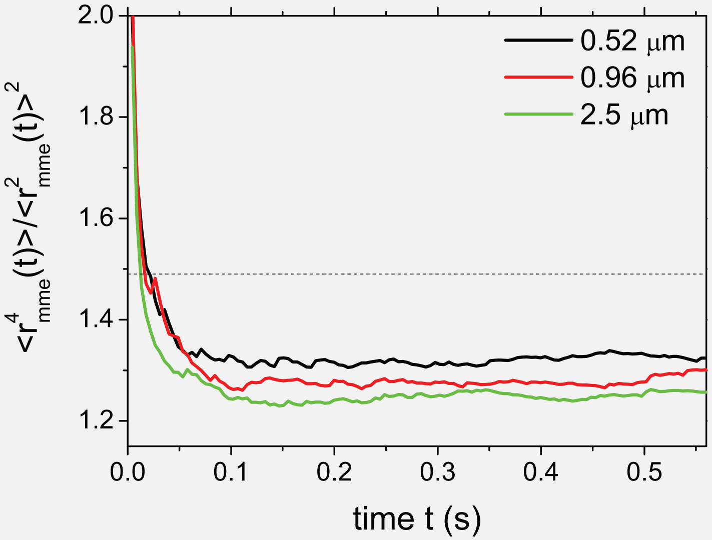
Anomalous diffusion: $\langle \mathrm{r}^2(t)\rangle \simeq t^\alpha$; $\quad H = \frac{\alpha}{2}$

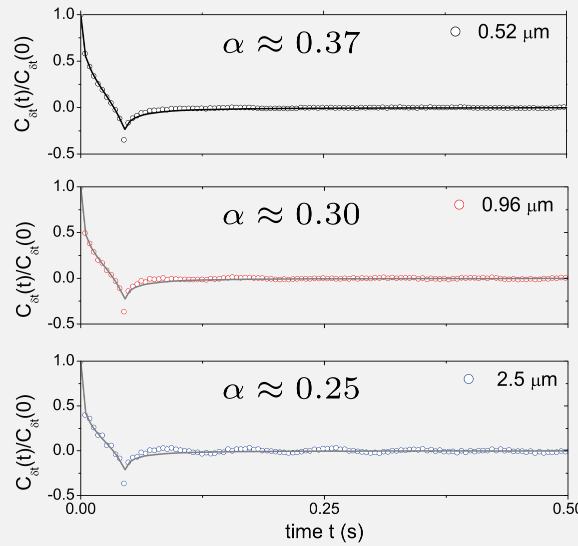
Disorder, ergodicity, Gaussianity, ageing . . .

data set	H measured	H prediction
Rhodamine 100%	$0.38 \pm 0.\ 02$	0.42 ± 0.04
Rhodamine 75%	0.18 ± 0.02	0.18 ± 0.01
Rhodamine 30%	0.07 ± 0.02	0.04 ± 0.03
Tracers in	0.31 ± 0.01	0.30 ± 0.02
treated cells	$0.44 \pm 0.\ 01$	0.44 ± 0.01
Tracers in	0.31 ± 0.01	0.33 ± 0.02
untreated cells	0.55 ± 0.01	0.57 ± 0.01
Amoeba	0.58 ± 0.01	0.55 ± 0.03
	0.42 ± 0.02	0.40 ± 0.02
Harvester ants	0.92 ± 0.12	0.95 ± 0.08
	0.47 ± 0.03	0.45 ± 0.03
Commuting kite	0.84 ± 0.02	0.86 ± 0.02
	0.76 ± 0.01	0.80 ± 0.02
Searching kite	0.06 ± 0.02	$0.\ 06 \pm 0.01$
Stork (Aug-Sep)	1.20 ± 0.03	1.08 ± 0.02
	1.03 ± 0.01	1.04 ± 0.06
Stork (Oct-Jan)	0.74 ± 0.02	$0.\ 68 \pm 0.03$
	0.80 ± 0.02	0.73 ± 0.10
Stork (Mar-Apr)	1.08 ± 0.02	1.04 ± 0.02
Vulture	0.82 ± 0.02	0.84 ± 0.02
	0.76 ± 0.02	0.70 ± 0.04

RM et al, PCCP (2014); O Vilk et al, PRR (2022)

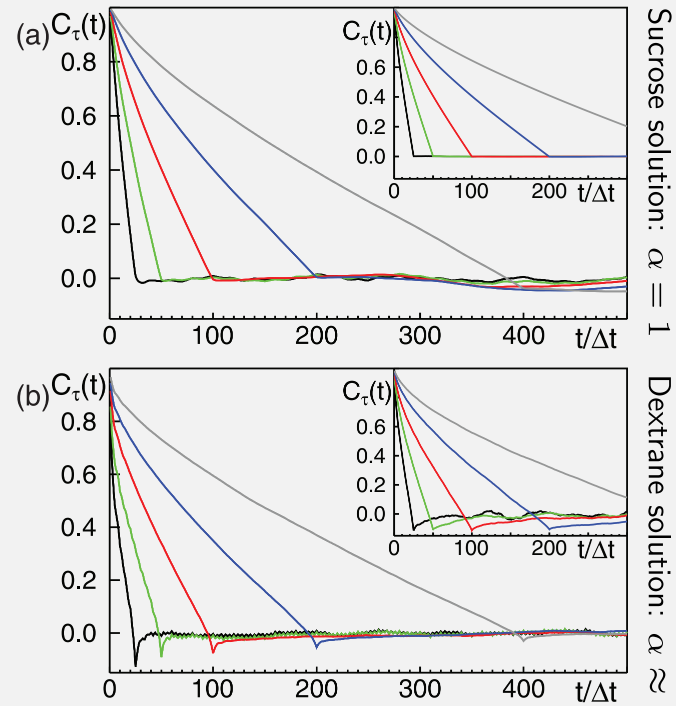
Passive motion of submicron tracers in cells is viscoelastic I



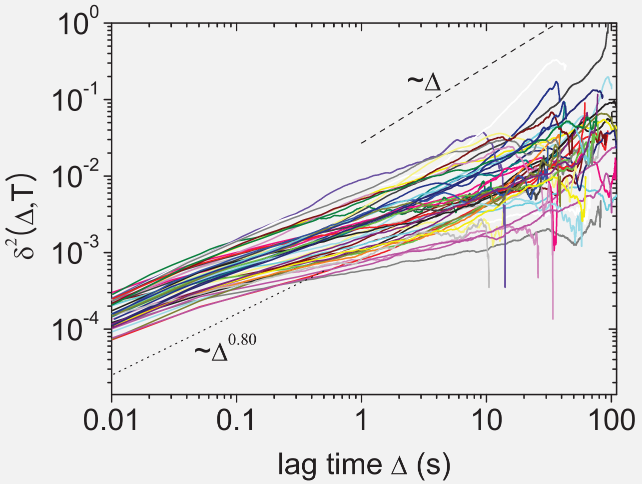


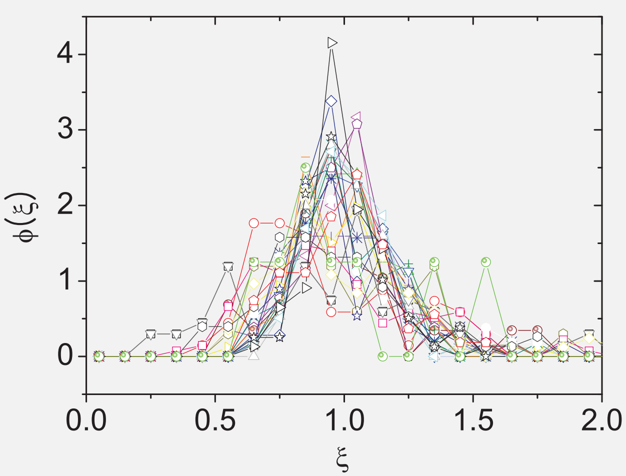
Beads in worm-like micellar solution

JH Jeon, N Leijnse, L Oddershede & RM, NJP (2013)



M Weiss, PRE (2013)





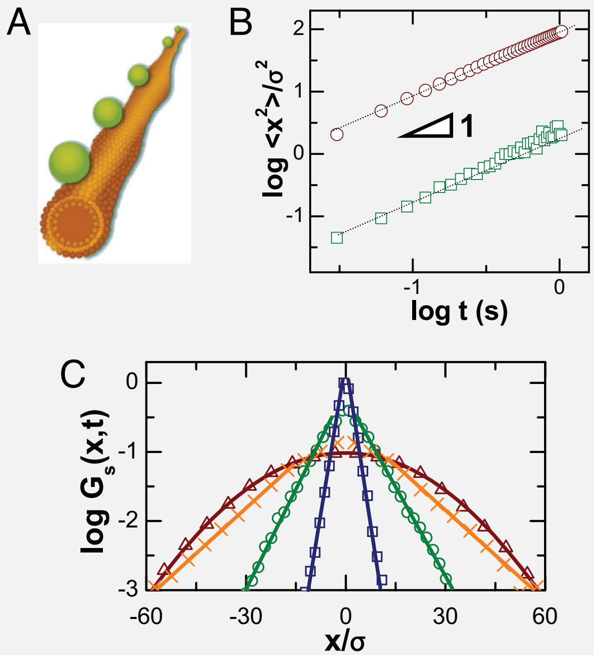
$$\overline{\delta^2(\Delta)} \simeq \Delta^\alpha$$

Endogeneous lipid granules

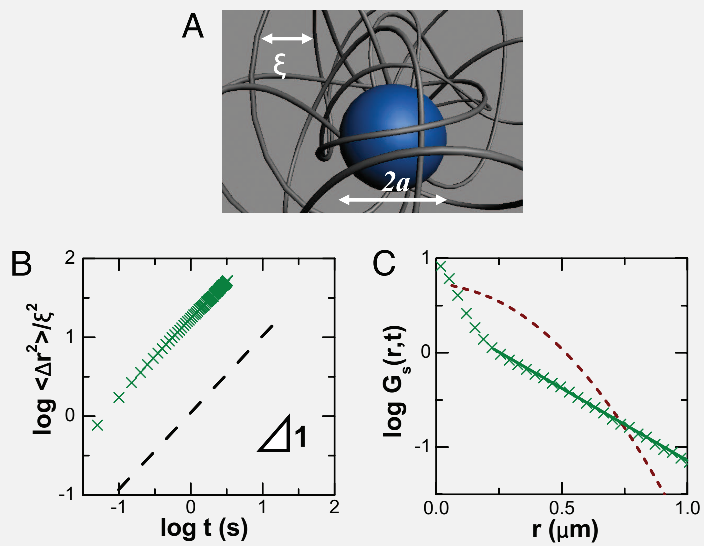
in living yeast cells

J-H Jeon, V Tejedor, S Burov, E Barkai, C Selhuber-Unkel, K Berg-Sørensen, L Oddershede & RM, PRL (2011)

Brownian yet non-Gaussian diffusion in soft & bio-matter

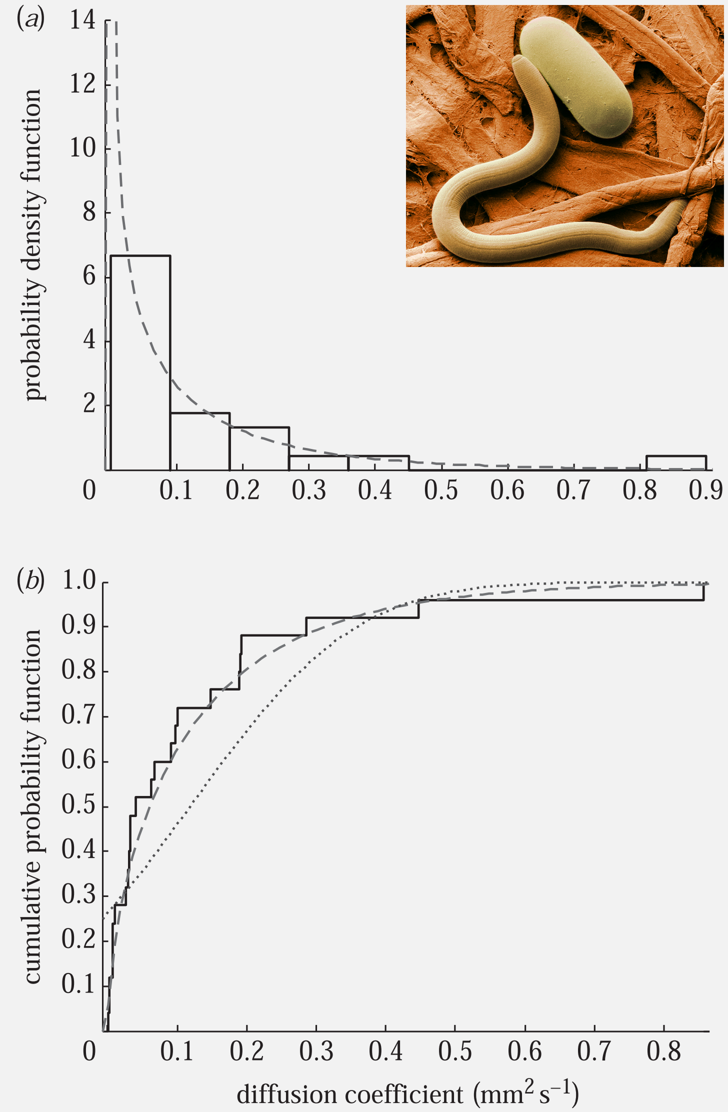


Colloidal beads on nanotubes



Nanospheres in entangled actin

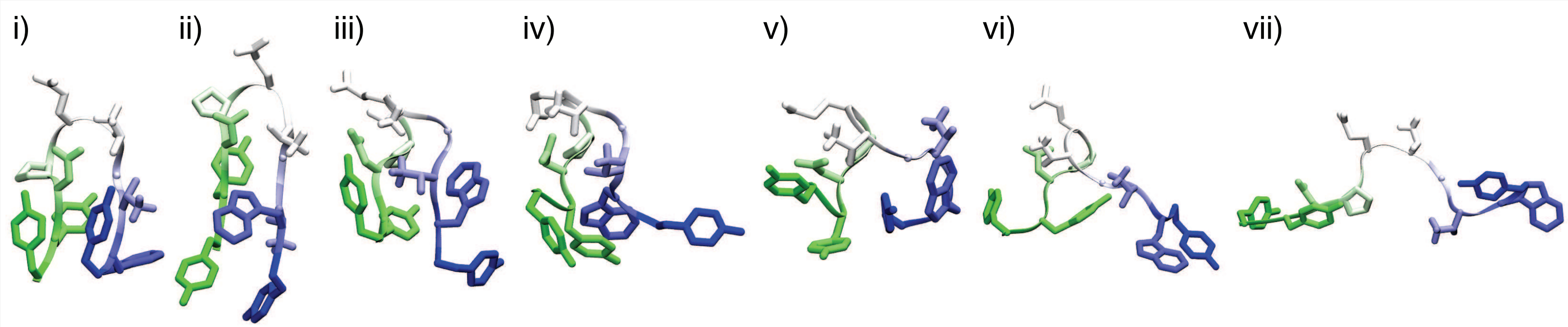
Motion of *Phasmarhabditis* nematodes



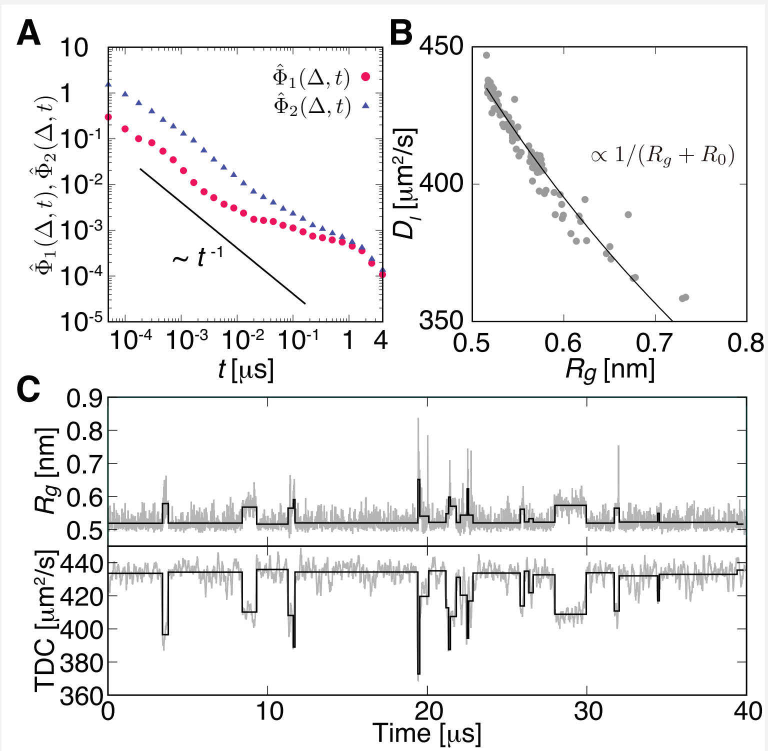
Wang et al, PNAS (2009); Nature Mat (2012)

S Hapca, JW Crawford & IM Young, Interface (2009)

Instantaneous diffusivity of shape-fluctuating proteins

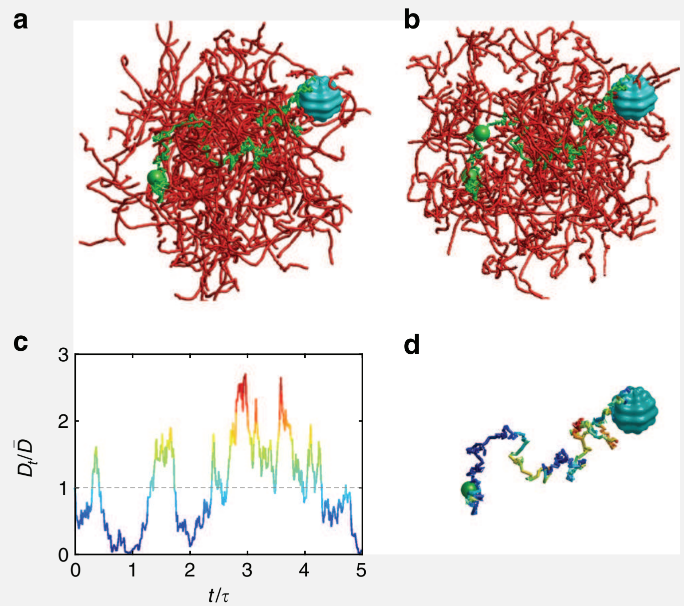


Chignolin ("miniprotein")



E Yamamoto, T Akimoto, A Mitsutake & RM, PRL (2021)

Annealed diffusing-diffusivity in rearranging heterogeneous environments

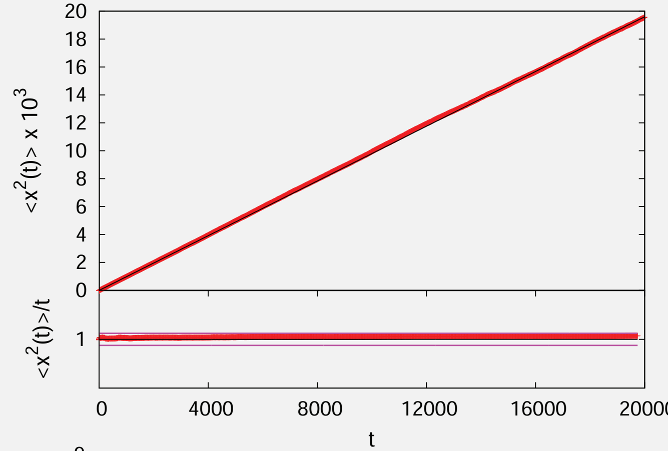


Y Lanoiselée, N Moutal, & D Grebenkov, Nat Comm (2018)

Fickian, non-Gaussian diffusion with diffusing diffusivity

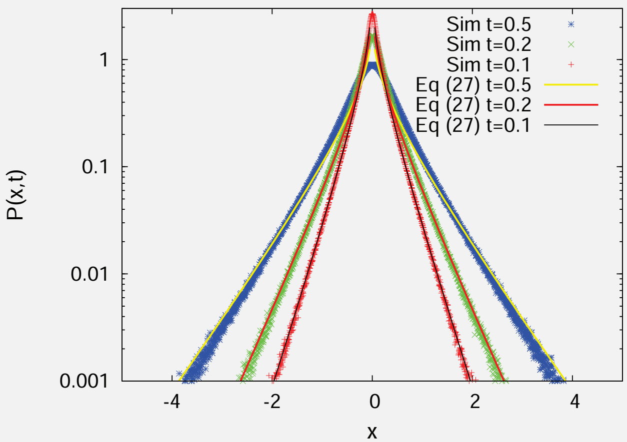
MV Chubinsky & G Slater, PRL (2014): diffusing diffusivity

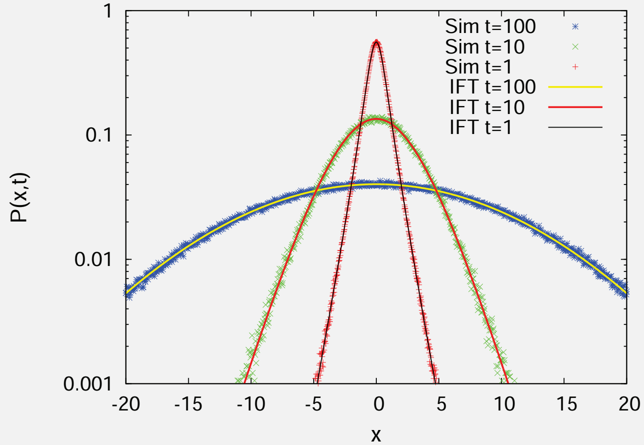
[see also R Jain & KL Sebastian, JPC B (2016)]

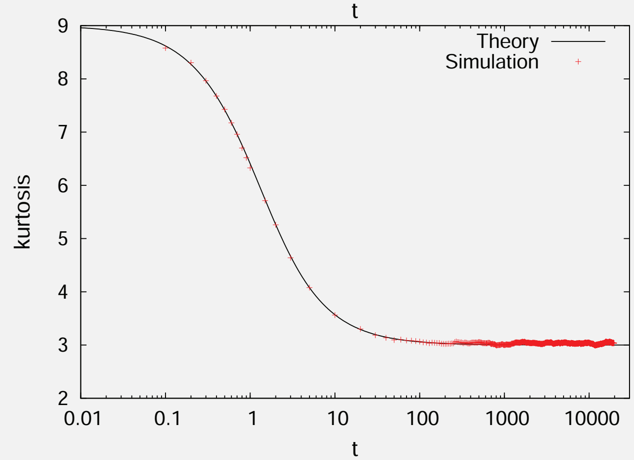


Our minimal model for diffusing diffusivity:

$$\dot{x}(t) = \sqrt{2D(t)}\xi(t)$$
$$D(t) = y^2(t)$$
$$\dot{y}(t) = -\tau^{-1}y + \sigma\eta(t)$$



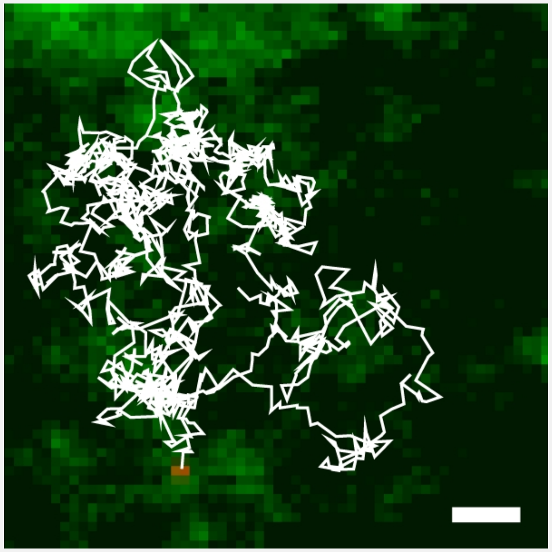


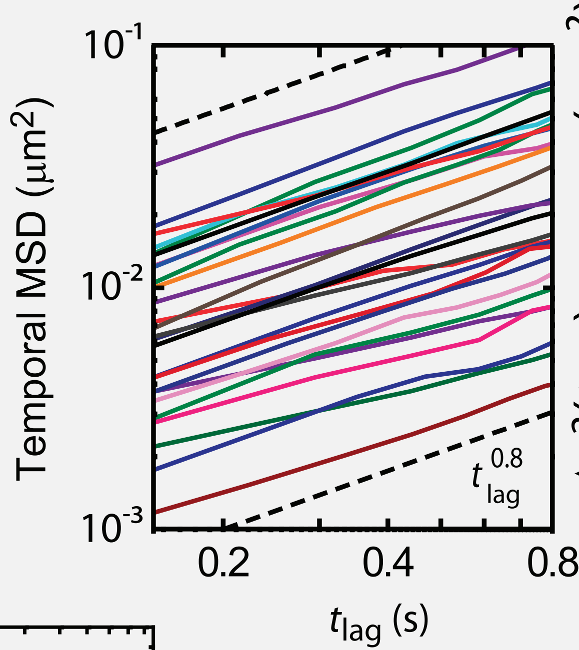


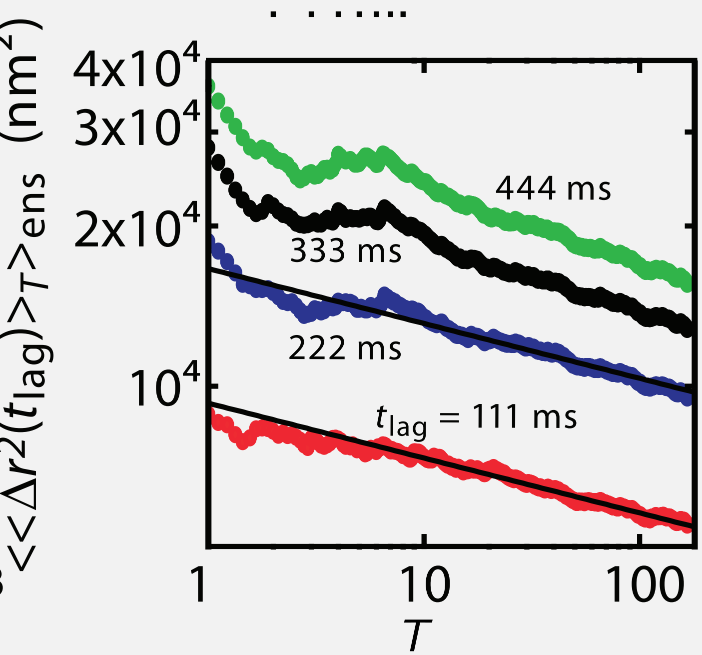
Generalised γ distribution & non-equilibrium diffusivity initial conditions: V Sposini, AV Chechkin, G Pagnini, F Seno & RM, NJP (2018)

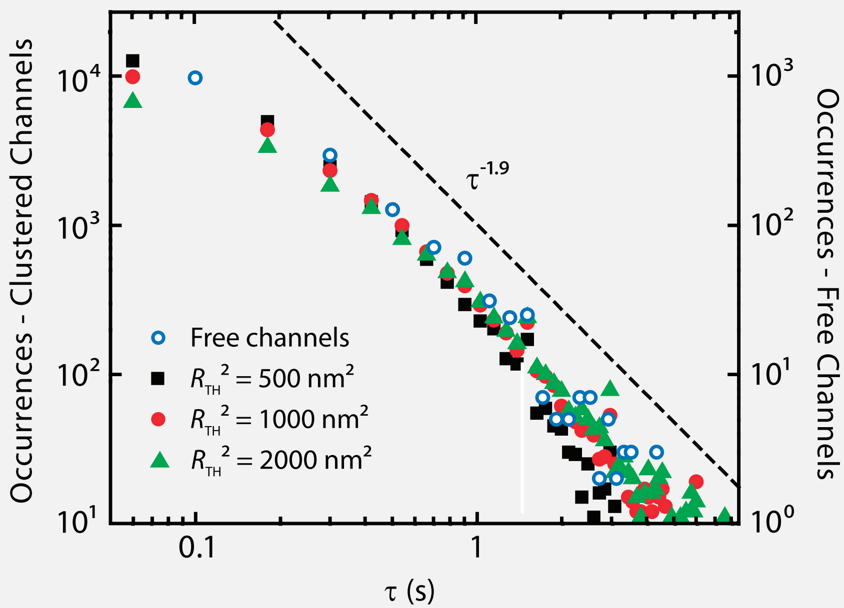
AV Chechkin, F Seno, RM & IM Sokolov, PRX (2017)

CTRW-like motion of Ka channels in plasma membrane









$\psi(\tau) \simeq \tau^{-1-\alpha}$ scale free

$\overline{\delta^2(\Delta)}$ apparently random

$\Delta/T^{1-\alpha} \simeq \overline{\delta^2(\Delta)} \neq \langle \mathbf{r}^2(\Delta) \rangle \simeq \Delta^\alpha$

$P(\mathbf{r}, t) \simeq \exp\left(-\beta r^{1/[1-\alpha/2]}\right)$

AV Weigel, B Simon, MM Tamkun & D Krapf, PNAS (2011); theory: Y He, S Burov, RM & E Barkai, PRL (2008)

Fractional Brownian motion

FLE: fluctuation-dissipation $\rightsquigarrow$ asymptotic thermal equilibrium [books by Zwanzig, Kubo]: Rouse chain, harmonically coupled passive particle, single-file diffusion

FBM: "external noise" for non-equilibrium systems or "open systems" [Klimontovich, Statistical physics of open systems] $\rightsquigarrow$ biological cells, animals, weather, finance

Mandelbrot-van Ness FBM [SIAM Rev (1968)]:

$$\frac{dx(t)}{dt} = \sqrt{2D_H}\xi_H(t) \quad \therefore \quad 0 < H < 1 : \quad \langle x^2(t)\rangle \simeq D_H t^{2H} \quad (\alpha = 2H)$$

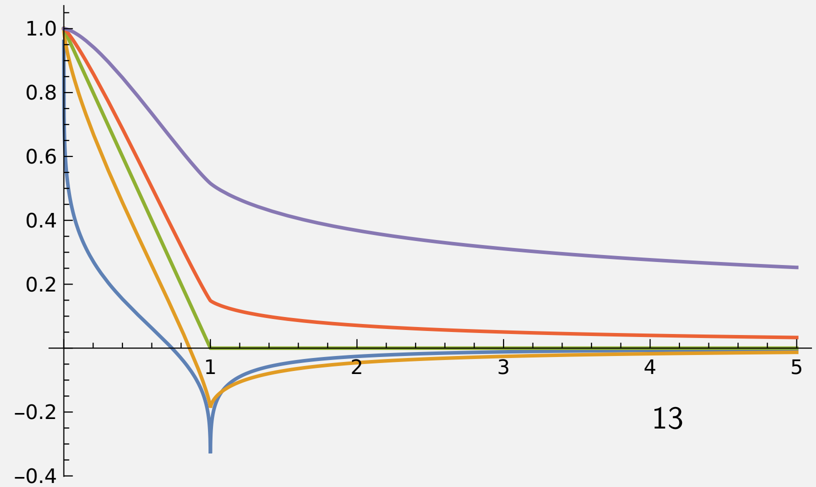
$\xi_H(t)$ is fractional Gaussian noise, understood as the derivative of smoothed FBM:

$$\langle \xi_H(t)\xi_H(t+\tau)\rangle = \frac{1}{2\delta}\left(|t+\delta|^{2H} - 2|\tau|^{2H} + |t-\delta|^{2H}\right) \sim H(2H-1)\tau^{2H-2}$$

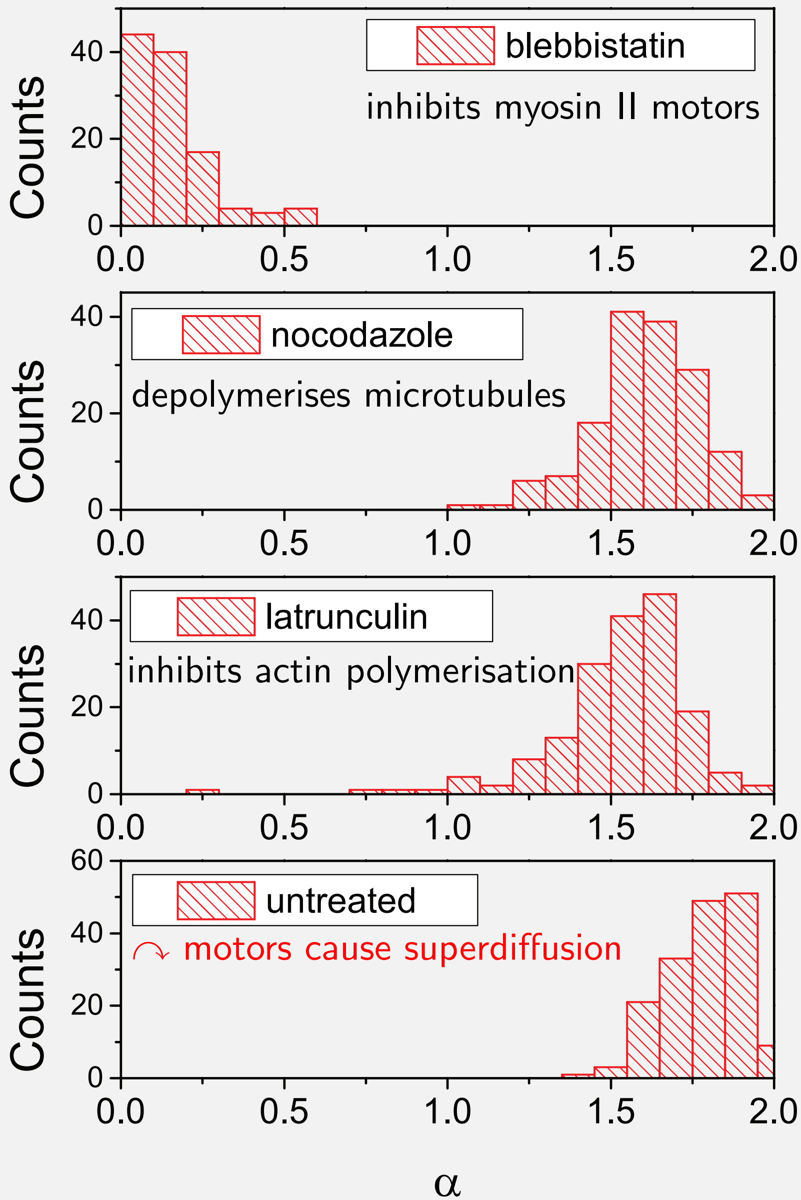
Displacement correlator:

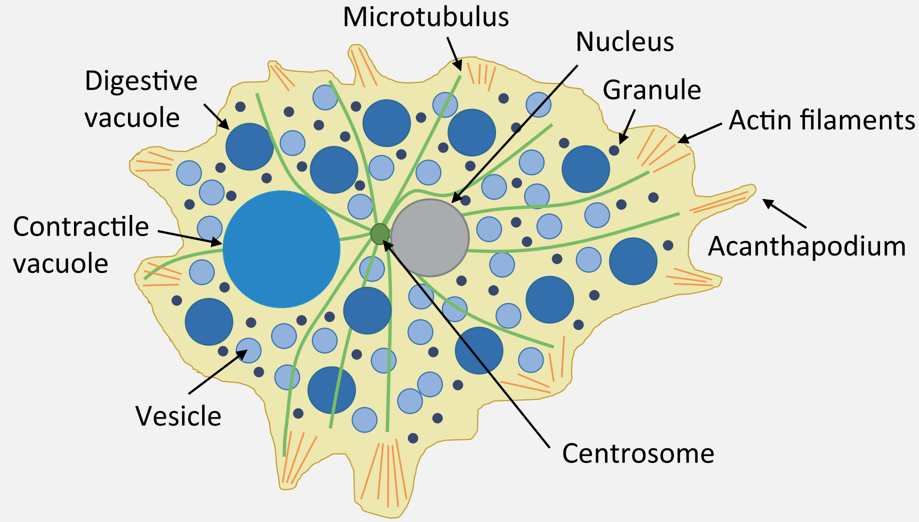
$$C_{\delta t}(t) = \frac{\langle[\mathbf{r}(t+\delta t) - \mathbf{r}(t)]\cdot[\mathbf{r}(\delta t) - \mathbf{r}(0)]\rangle}{\delta t^2}$$

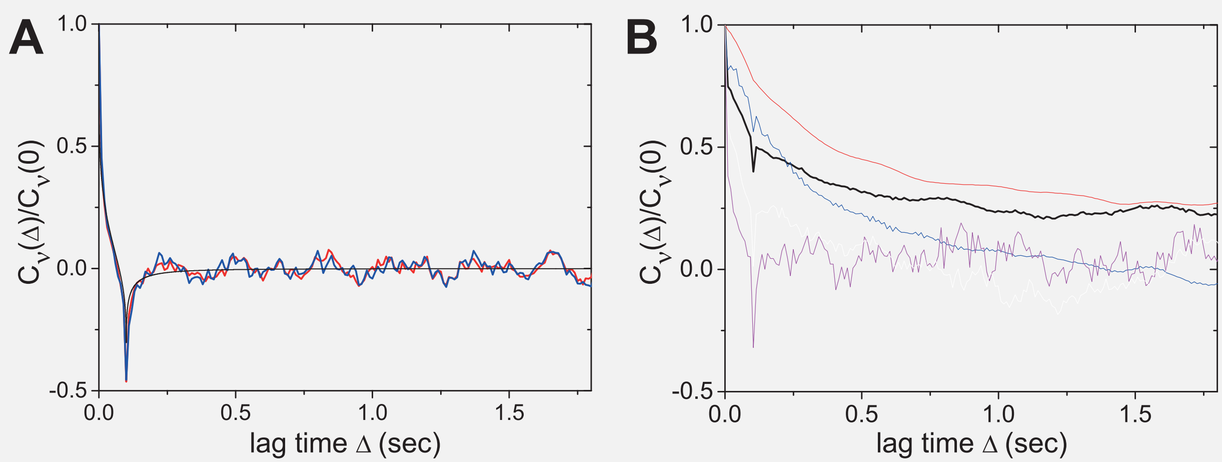
$$\frac{C_{\delta t}(t)}{C_{\delta t}(0)} = \frac{(t+\delta t)^{2H} - 2t^{2H} + |t-\delta t|^{2H}}{2\delta t^{2H}}$$



Superdiffusion in supercrowded Acanthamoeba castellani

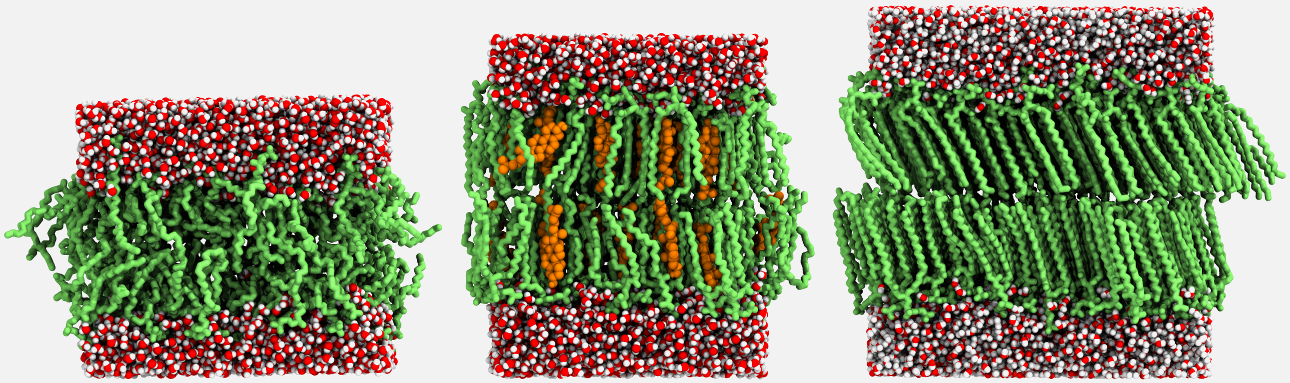


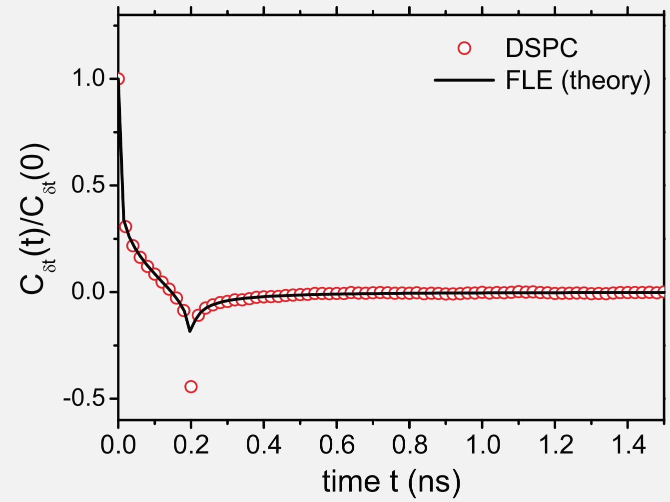


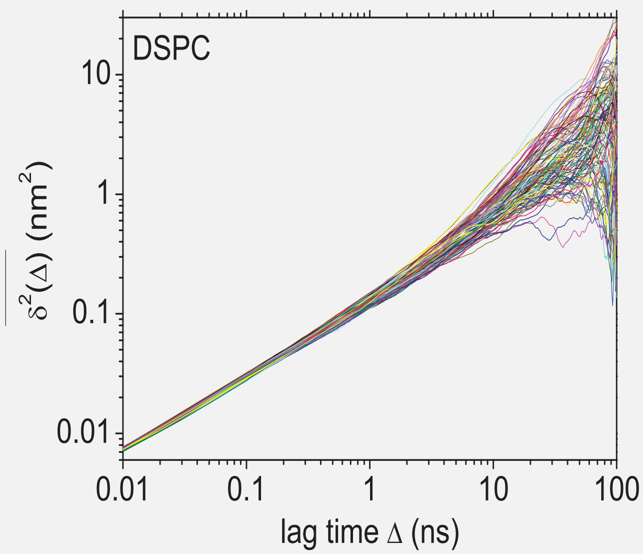


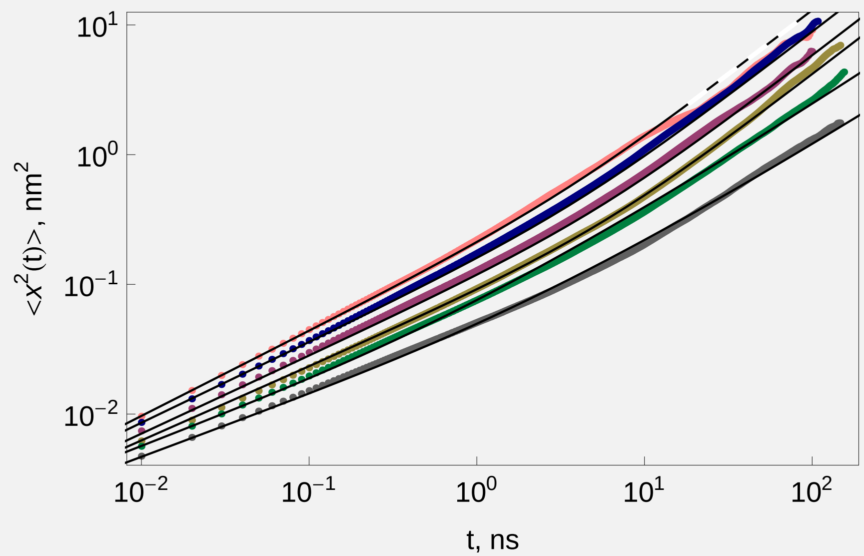
JF Reverey, J-H Jeon, H Bao, M Leippe, RM & C Selhuber-Unkel, Sci Rep (2015); S Thapa, N Lukat, C Selhuber-Unkel, A Cherstvy & RM, JCP (2019)

Single lipid motion in bilayer membranes: FBM, Gaussian









Pure bilayer:

$t^{2/3} \longrightarrow t^1$

/w cholesterol/gel:

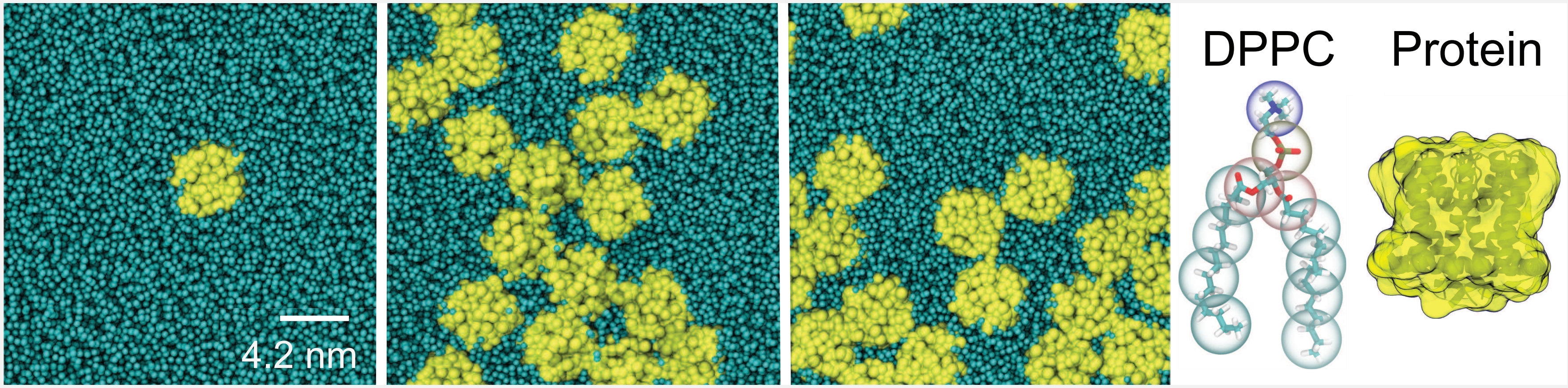
$t^{\alpha} \longrightarrow t^{\alpha'>\alpha}$

Tempered GLE

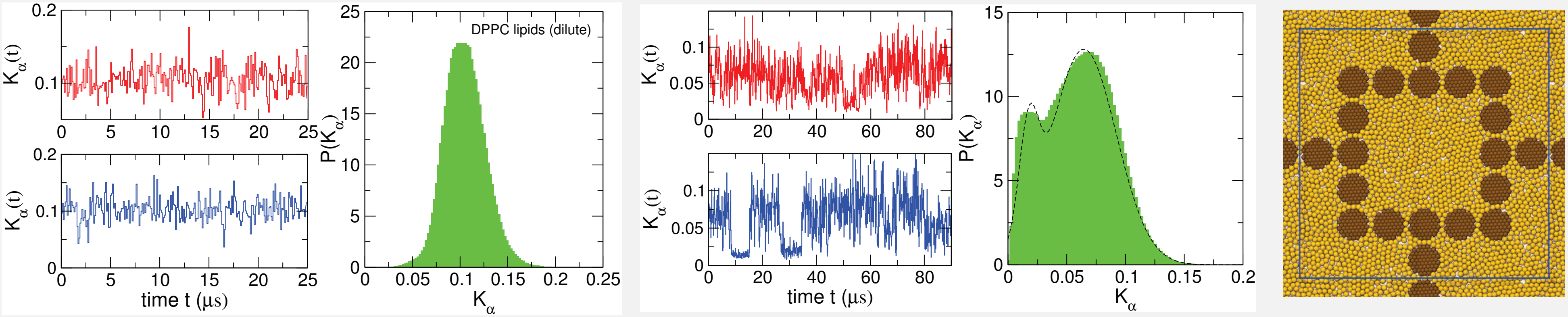
D Molina-Garcia, T Sandev, H Safdari, G Pagnini, AV Chechkin & RM, NJP (2018)

J-H Jeon, H Martinez-Seara Monne, M Javanainen & RM, PRL (2012)

Crowding in membranes: non-Gaussian lipid/protein diffusion



Observation: $P(r,t) \propto \exp\left(-\left[r/(ct^{\alpha/2})\right]^{\delta}\right)$, $\delta \approx 1.3 \ldots 1.7$



Single NaK channel

Protein-crowded

Argon gas

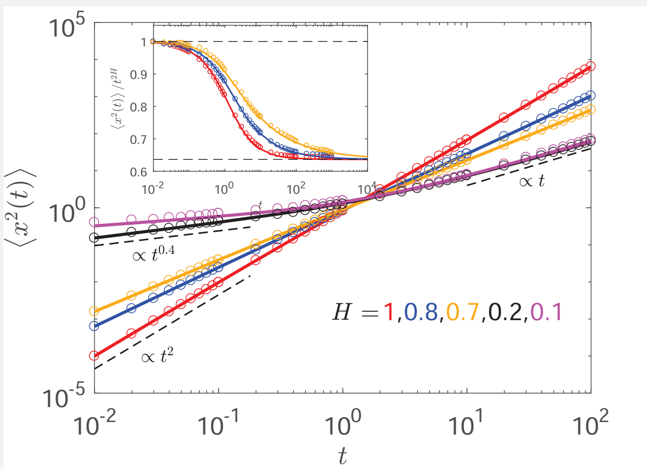
Viscoelastic diffusing-diffusivity model

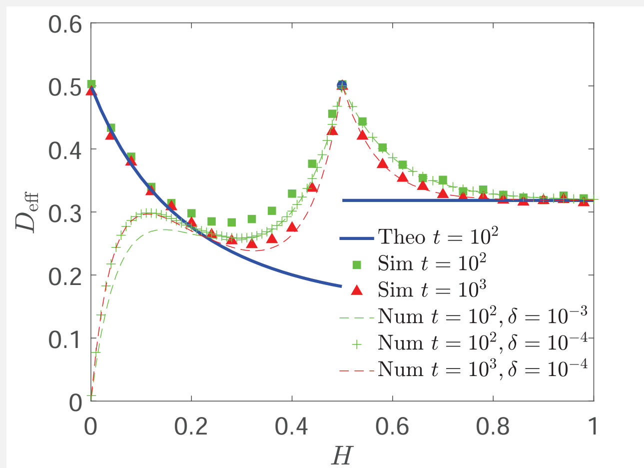
FBM-generalised diffusing-diffusivity model:

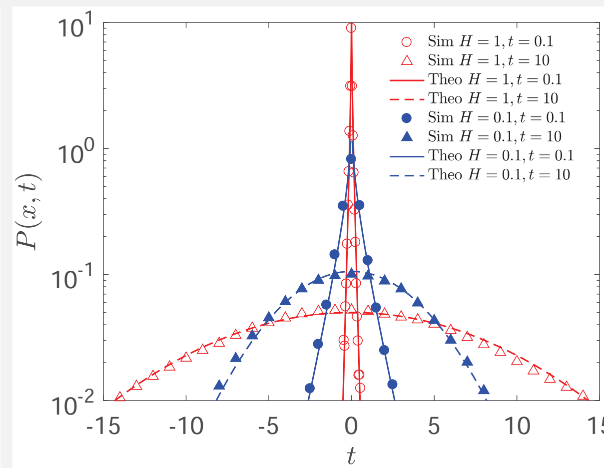
$$\frac{dx(t)}{dt} = \sqrt{2D(t)}\xi_H(t)$$

with $D(t)$ as squared Ornstein-Uhlenbeck process $Y(t)$:

$$D(t) = Y^2(t), \quad \frac{dY(t)}{dt} = -Y + \eta(t)$$

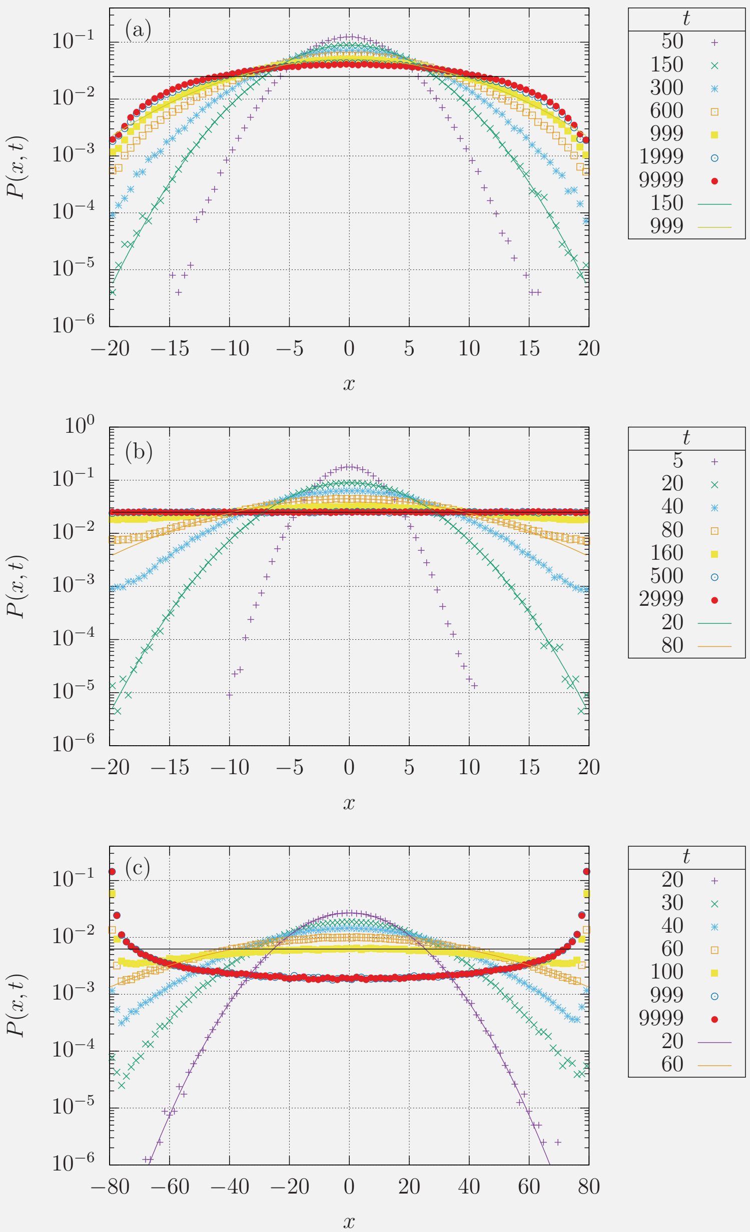


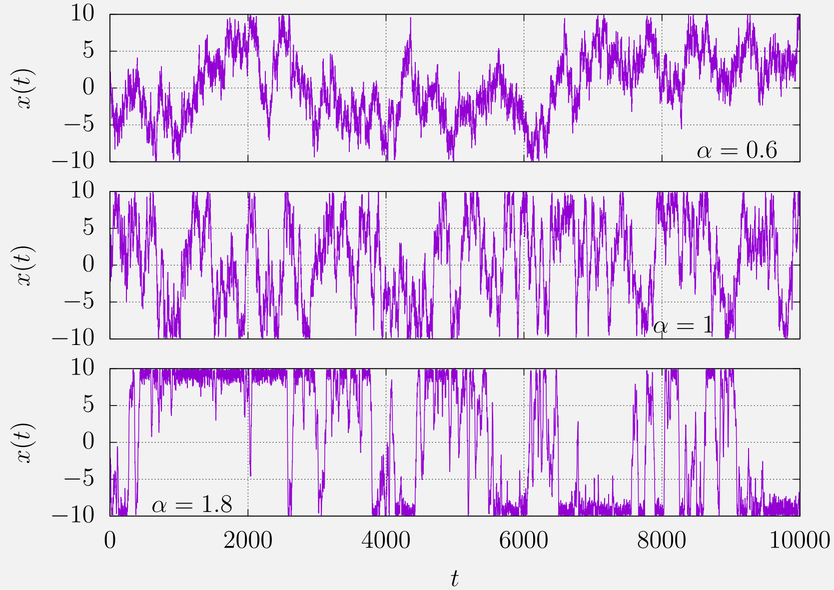


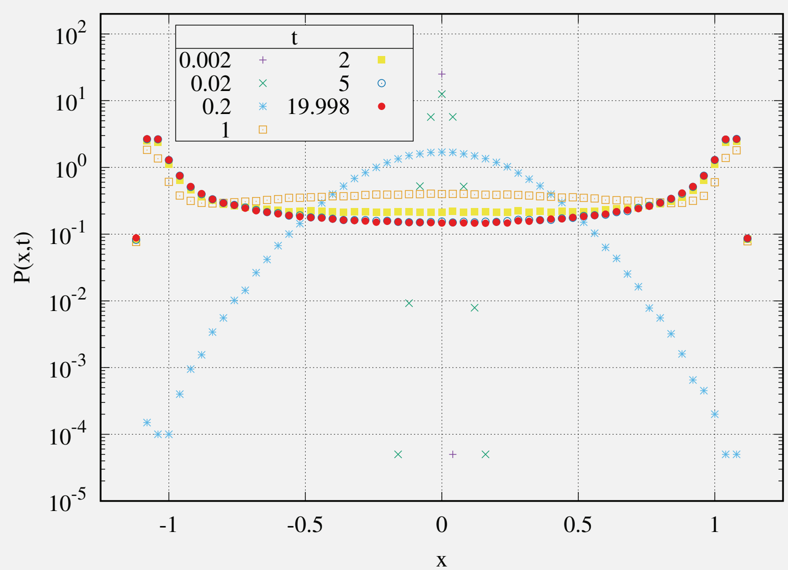


W Wang, AV Chechkin, F Seno, IM Sokolov & RM, NJP (2020); W Wang, AG Cherstvy, AV Chechkin, S Thapa, F Seno, X Liu & RM, JPA (2020)

FBM: accretion & depletion effects near hard boundaries



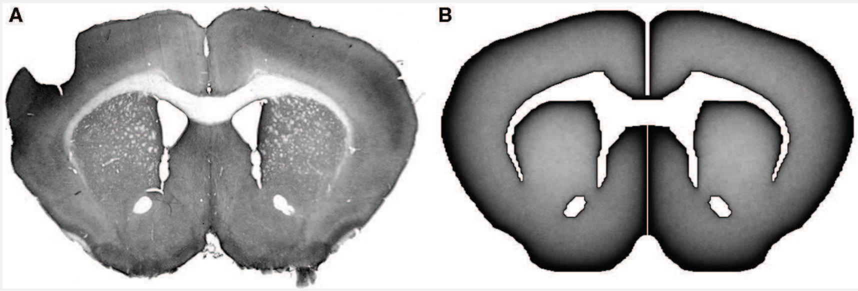


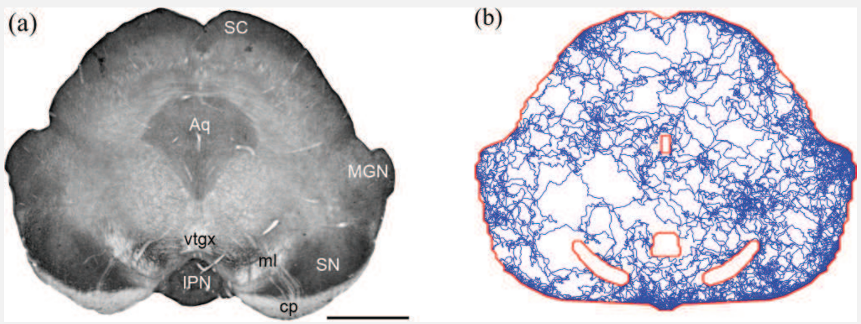


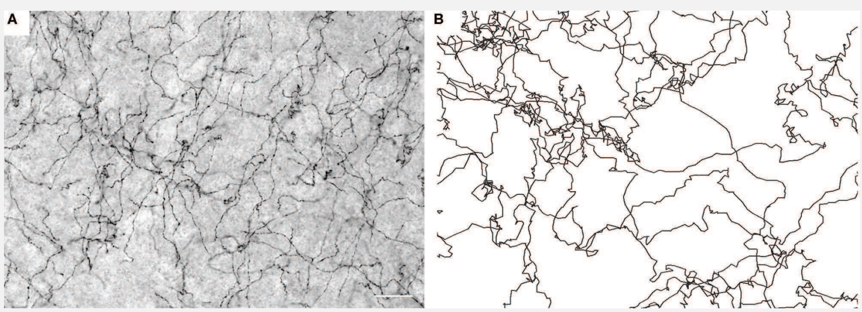
T Guggenberger, G Pagnini, T Vojta & RM, NJP (2019); AHO Wada & T Vojta, PRE (2018); T Vojta, S Skinner & RM, PRE (2019)

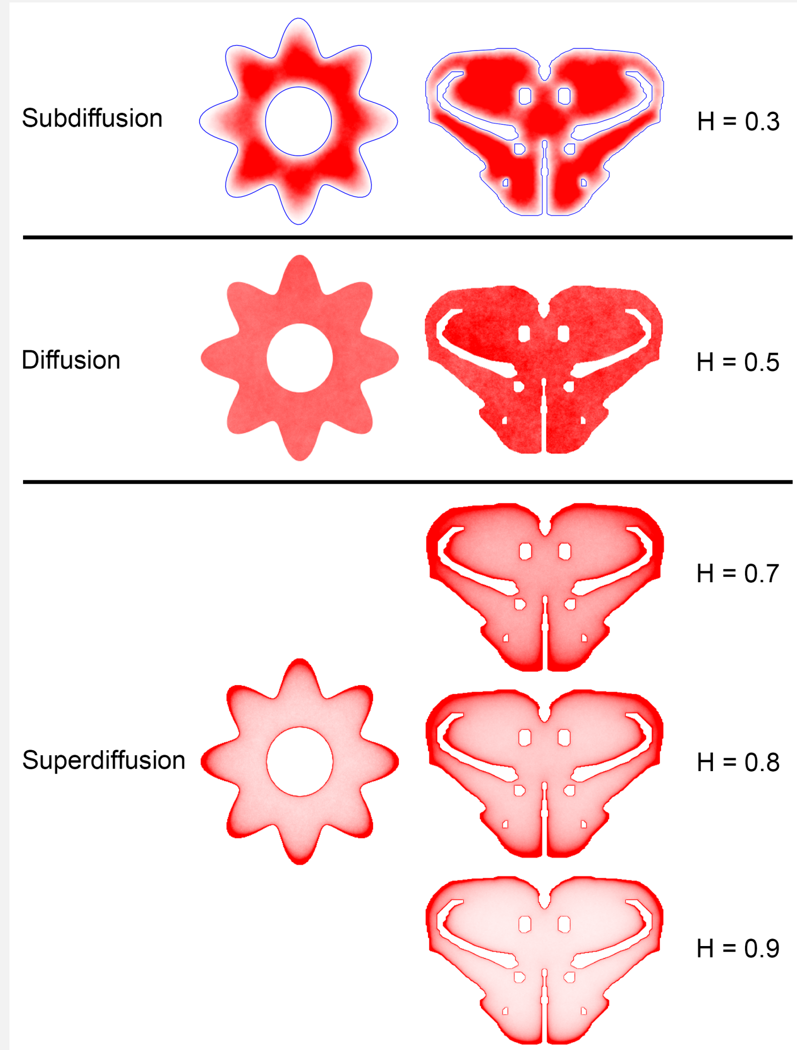
Brain serotonergic axons as FBM paths

Correlated fluctuations effect non-flat profile









S Janušonis, N Detering, RM & T Vojta, Front Comp Neurosc (2020); T Guggenberger, T Vojta & RM, NJP (2019)

The case $H(t)$

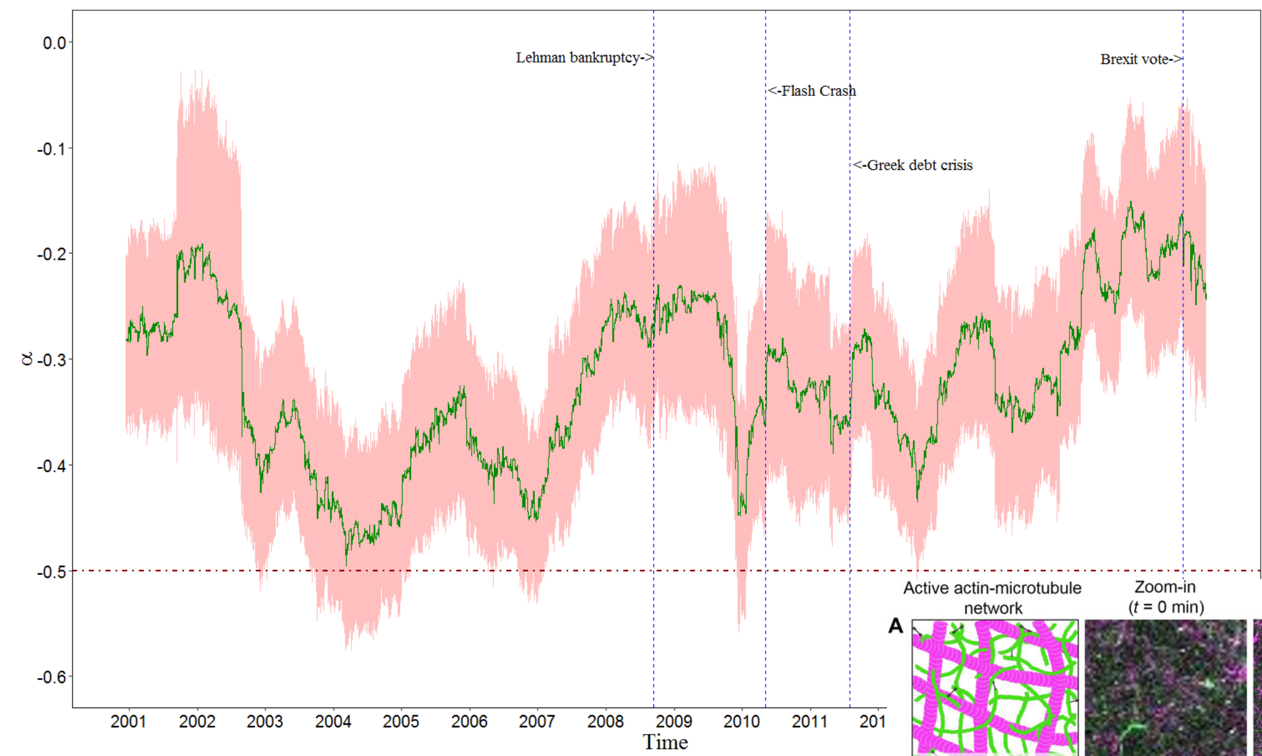
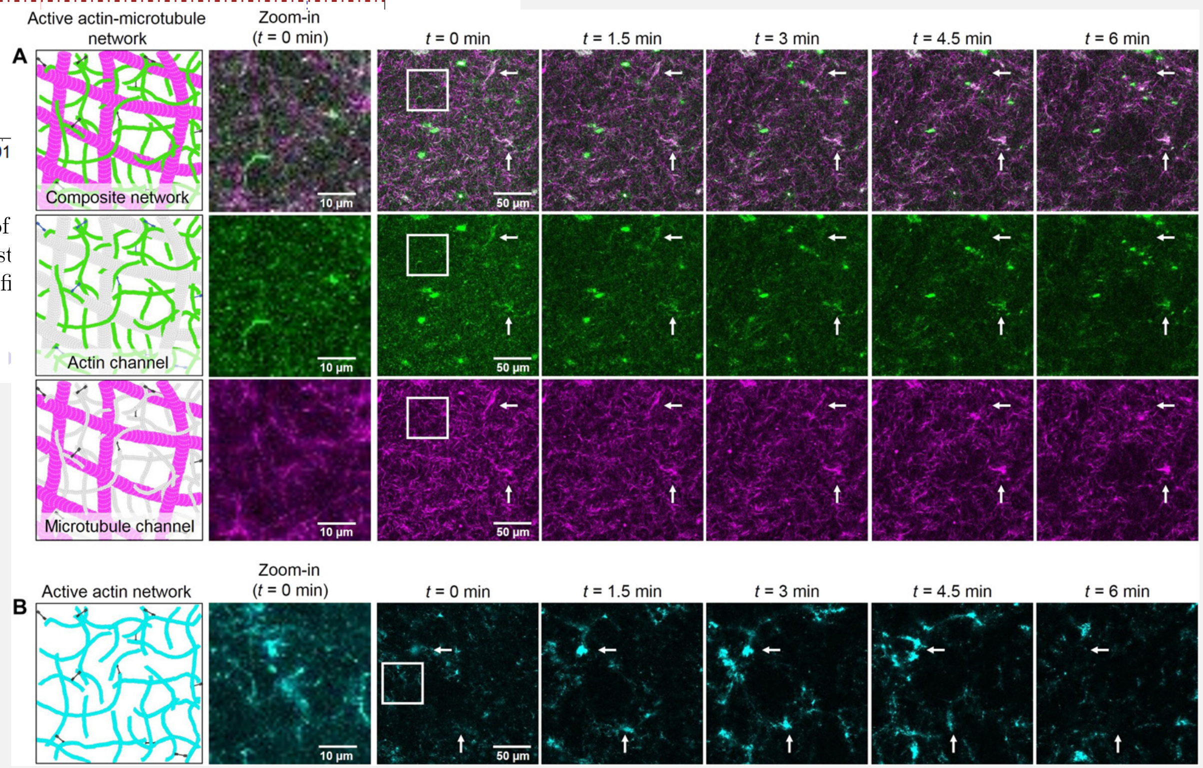
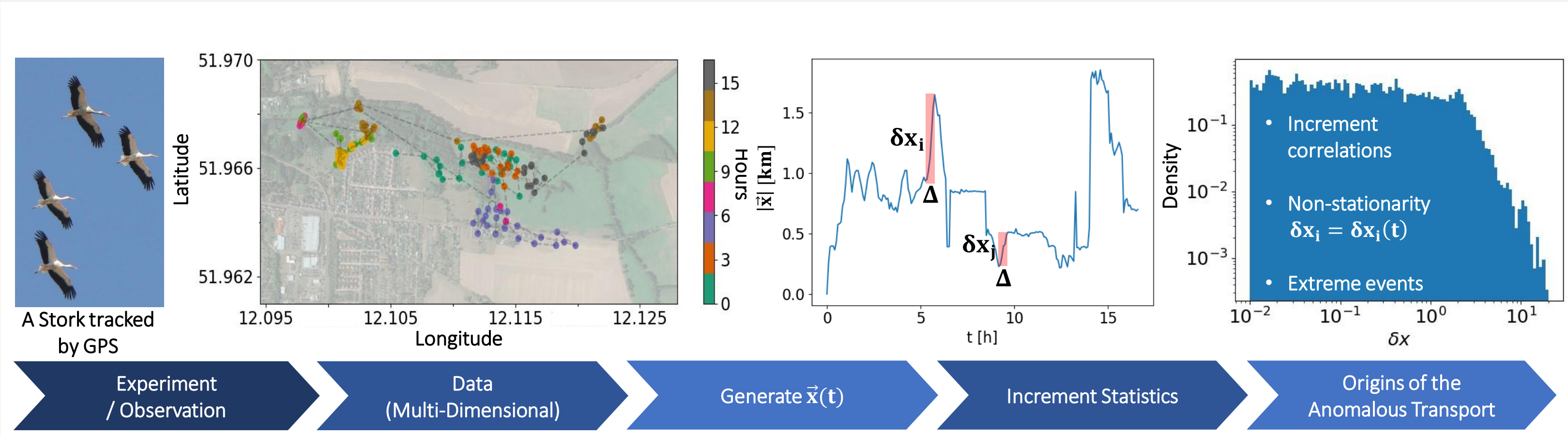


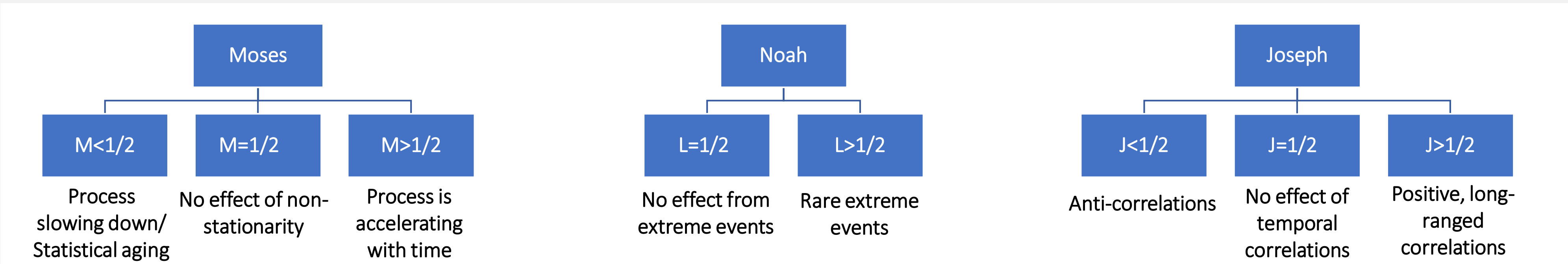
Figure 10: Half year rolling-window estimates of α on the realized variance measures of regression (3.10) with $m = 3$. The pink area is the 95% confidence interval by bootst vertical dashed blue lines indicate four periods of market turmoil: Lehman Brothers fi the first bailout during Greek debt crisis and the Brexit referendum.

$$\longleftarrow \alpha = H - 1/2$$



Scaling analysis of anomalous diffusion: molecules $\to$ animals

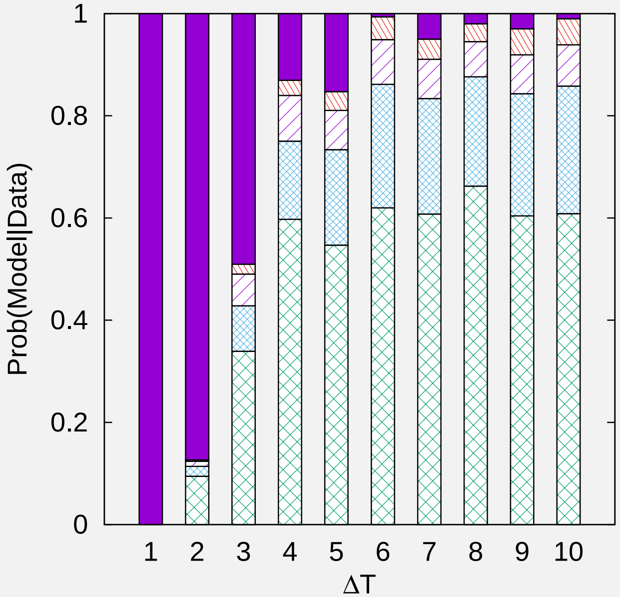


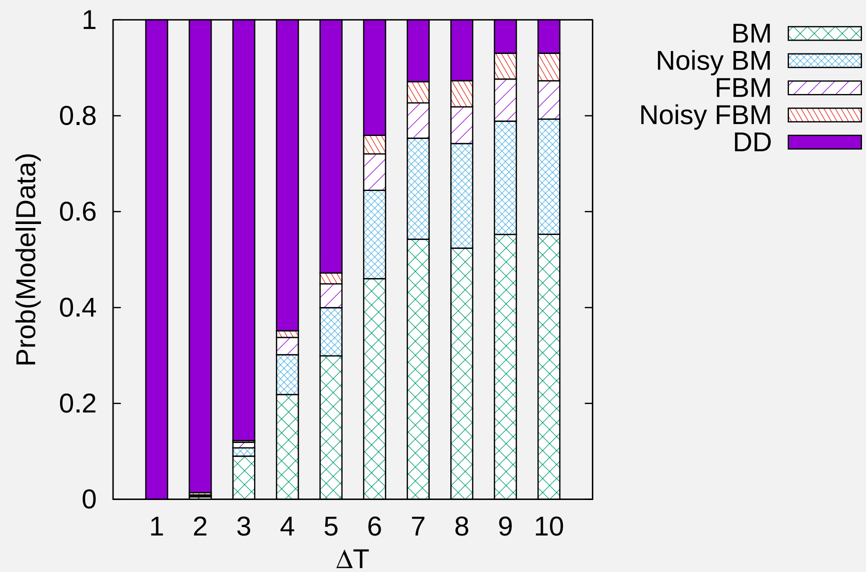


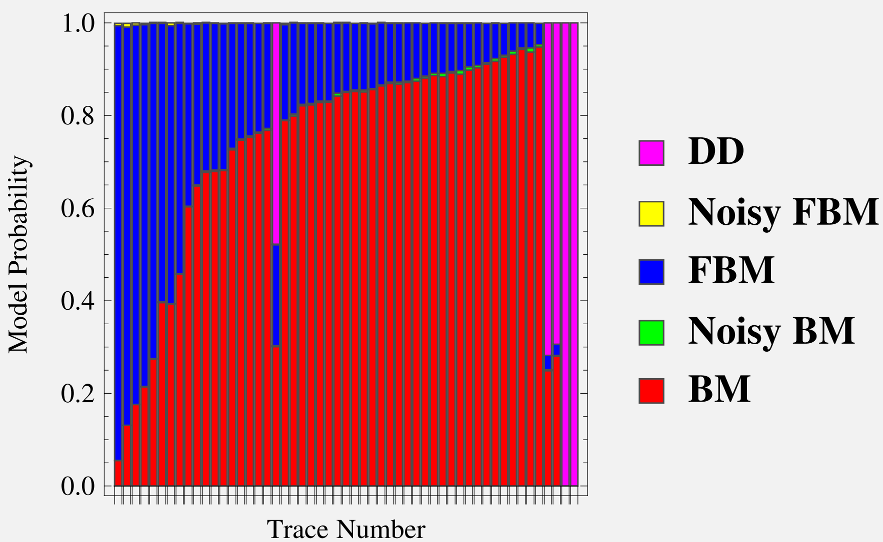
Persistent FBM identified for the flights of larger birds

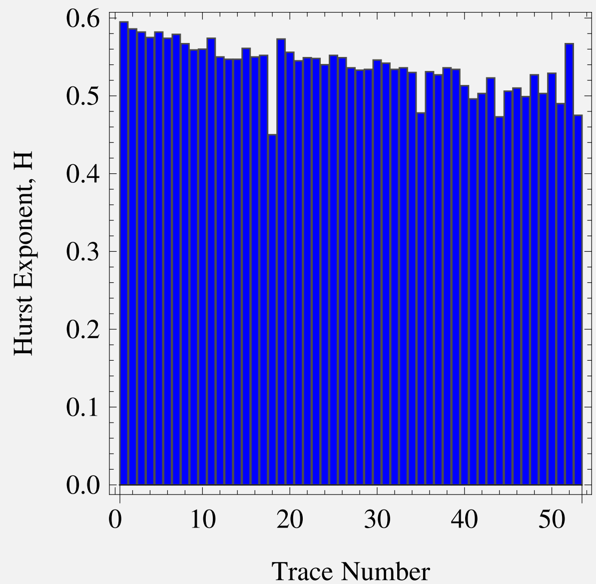
O Vilk, E Aghion, T Avgar, C Beta, O Nagel, M Weiss, A Sabri, D Krapf, R Sarfati, DK Schwartz, RM, R Nathan & M Assaf, PRR (2022)

Maximum likelihood Bayesian data analyses









S Thapa, AG Cherstvy & RM (2018); AG Cherstvy, S Thapa, CE Wagner & RM, Soft Matter (2019)

nature COMMUNICATIONS

ARTICLE

https://doi.org/10.1038/s41467-021-26320-w OPEN

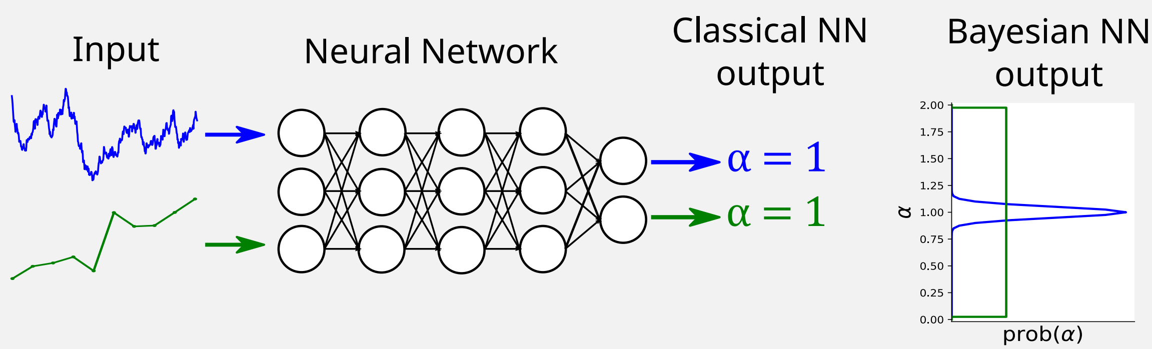
Check for updates

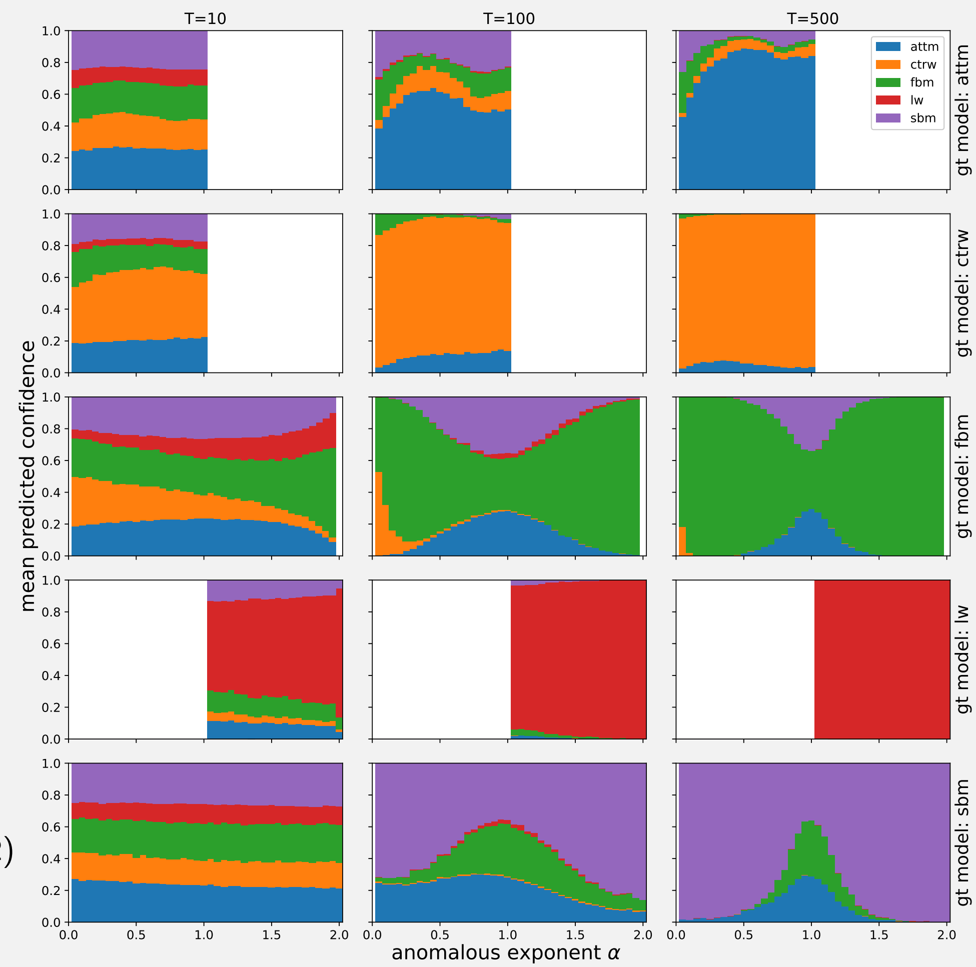
Objective comparison of methods to decode anomalous diffusion

Gorka Muñoz-Gil[1], Giovanni Volpe[2✉], Miguel Angel Garcia-March[3], Erez Aghion[4], Aykut Argun[2], Chang Beom Hong[5], Tom Bland[6], Stefano Bo[4], J. Alberto Conejero[3], Nicolás Firbas[3], Òscar Garibo i Orts[3], Alessia Gentili[7], Zihan Huang[8], Jae-Hyung Jeon[5], Hélène Kabbech[9], Yeongjin Kim[5], Patrycja Kowalek[10], Diego Krapf[11], Hanna Loch-Olszewska[10], Michael A. Lomholt[12], Jean-Baptiste Masson[13], Philipp G. Meyer[4], Seongyu Park[5], Borja Requena[1], Ihor Smal[9], Taegeun Song[5,14,15], Janusz Szwabiński[10], Samudrajit Thapa[16,17,18], Hippolyte Verdier[13], Giorgio Volpe[7], Artur Widera[19], Maciej Lewenstein[1,20], Ralf Metzler[16] & Carlo Manzo[1,21✉]

Bayesian-weighted deep learning model selection

“Beyond the Black Box problem”





Bayesian-weighted deep learning model selection