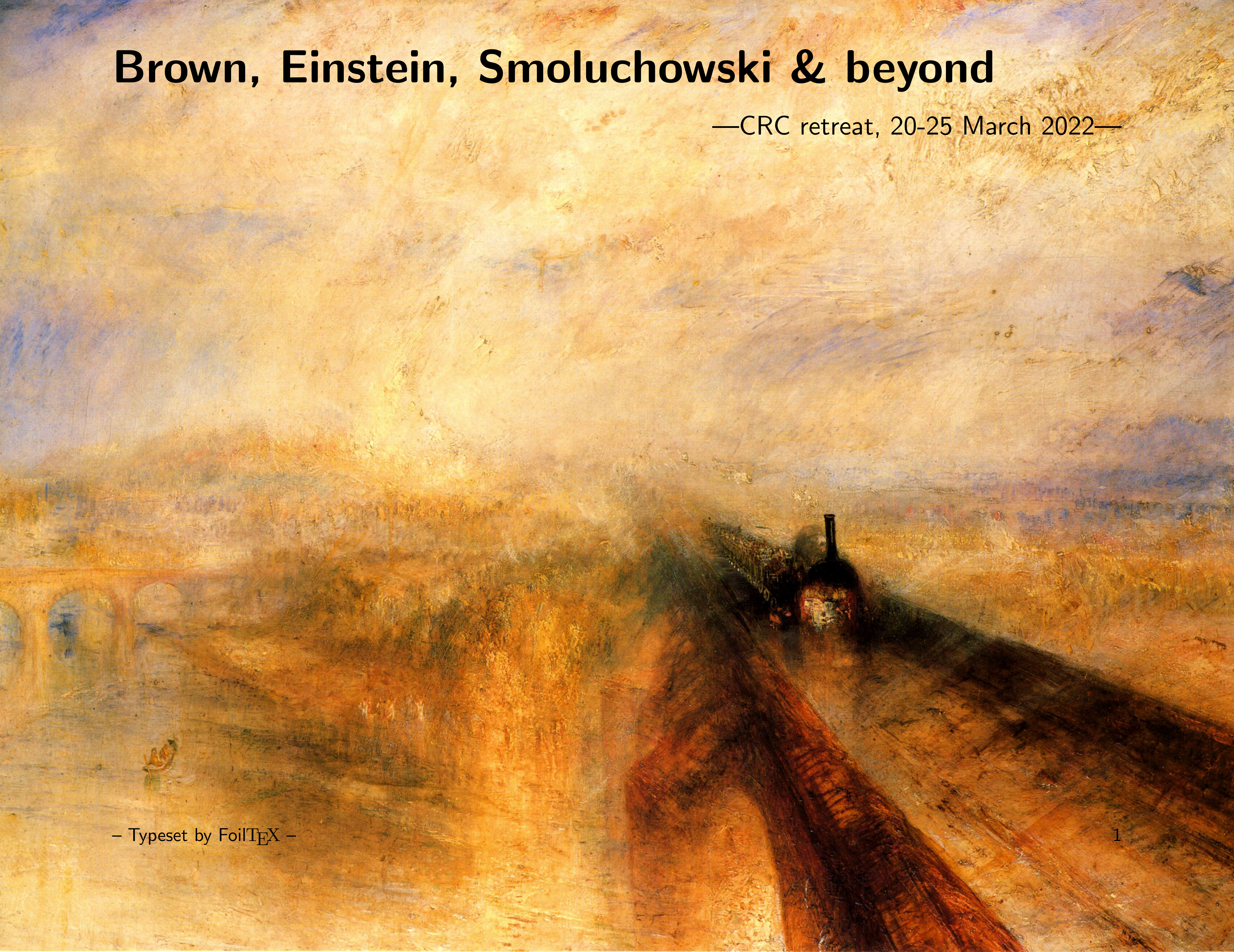
Brown, Einstein, Smoluchowski & beyond

—CRC retreat, 20-25 March 2022—



Tentative outline

1. General introduction to diffusion & some history
2. Anomalous diffusion, general observables ("features")
3. Reaction time distributions & mean vs typical
4. Non-Gaussianity
5. Ageing, (non-)ergodicity
6. Bayesian & deep learning approaches

Data from experiments & simulations are guiding examples throughout

THE

PHILOSOPHICAL MAGAZINE

AND

ANNALS OF PHILOSOPHY.

[NEW SERIES.]

SEPTEMBER 1828.

XXVII. *A brief Account of Microscopical Observations made in the Months of June, July, and August,* 1827, *on the Particles contained in the Pollen of Plants; and on the general Existence of active Molecules in Organic and Inorganic Bodies. By* ROBERT BROWN, *F.R.S., Hon. M.R.S.E. & R.I. Acad., V.P.L.S., Corresponding Member of the Royal Institutes of France and of the Netherlands, &c. &c.*

[We have been favoured by the Author with permission to insert the following paper, which has just been printed for private distribution.—ED.]

My inquiry on this point was commenced in June 1827, and the first plant examined proved in some respects remarkably well adapted to the object in view.

This plant was *Clarckia pulchella*, of which the grains of pollen, taken from antheræ full grown, but before bursting, were filled with particles or granules of unusually large size, varying from nearly $\frac{1}{4000}$th to about $\frac{1}{5000}$th of an inch in length, and of a figure between cylindrical and oblong, perhaps slightly flattened, and having rounded and equal extremities. While examining the form of these particles immersed in water, I observed many of them very evidently in motion; their motion consisting not only of a change of place in the fluid, manifested by alterations in their relative positions, but also not unfrequently of a change of form in the particle itself; a contraction or curvature taking place repeatedly about the middle of one side, accompanied by a corresponding swelling or convexity on the opposite side of the particle. In a few instances the particle was seen to turn on its longer axis. These motions were such as to satisfy me, after frequently repeated observation, that they arose neither from currents in the fluid, nor from its gradual evaporation, but belonged to the particle itself.

Rocks of all ages, including those in which organic remains have never been found, yielded the molecules in abundance. Their existence was ascertained in each of the constituent minerals of granite, a fragment of the Sphinx being one of the specimens examined.

Fluxes, random walks, & fluctuating forces . . .

Paul Langevin (1872-1946)

Albert Einstein (1879-1955)

Marian Smoluchowski (1872-1917)

William Sutherland (1859-1911)

Einstein's conditions on Brownian motion

Paul Lévy [Processus stochastiques & mouvement brownien (1948, 1965)]: ≪The stochastic process, that we will call linear Brownian motion, is a schematisation that well represents the properties of real Brownian motion, observable on a sufficiently small but not infinitely small scale, and which assumes that the same properties exist across the scales.≫

Einstein's postulate: a stochastic process describes normal diffusion if

(i) ∃ finite correlation time beyond which displacements are independent

(ii) displacements are identically distributed

(iii) displacements have a finite second moment

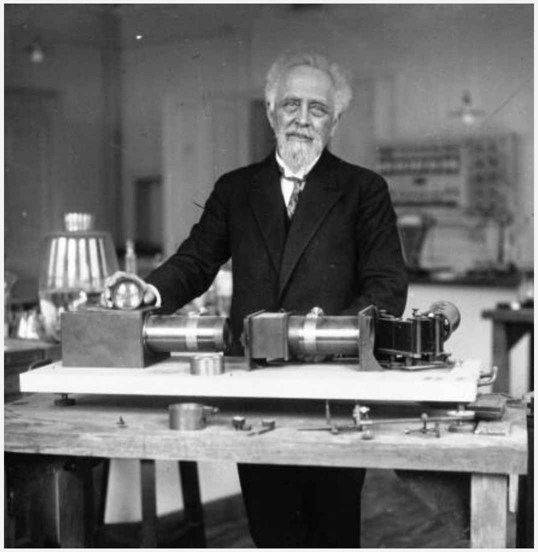
Main characteristics: linear mean squared displacement & Gaussian probability density

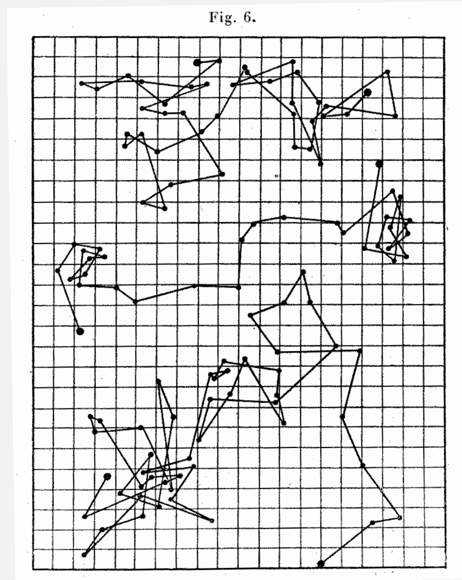
$$\langle \mathbf{r}^2(t)\rangle = 2dK_1t, \quad P(\mathbf{r},t) = (4\pi K_1 t)^{-d/2}\exp\left(-\frac{\mathbf{r}^2}{4K_1t}\right)$$

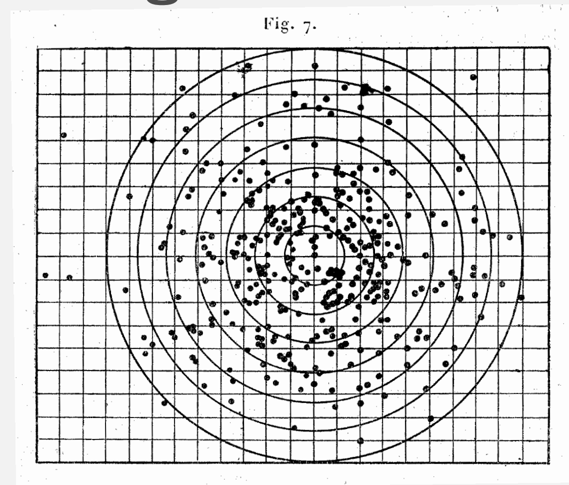
Violation of these conditions leads to anomalous diffusion with MSD $\langle \mathbf{r}^2(t)\rangle \simeq K_\alpha t^\alpha$ and/or non-Gaussian PDF

N van Kampen, Stochastic processes in physics & chemistry

Les atomes: Brownian motion and Avogadro's number

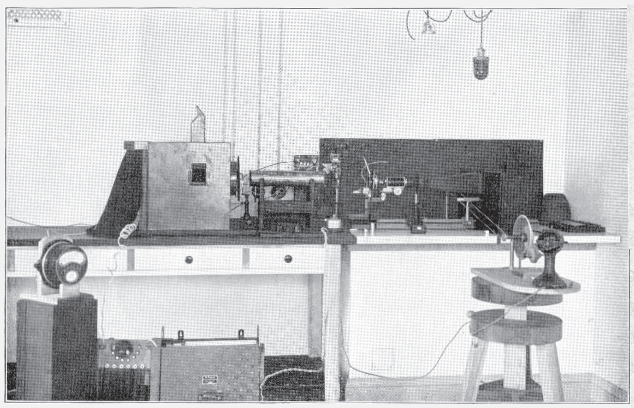


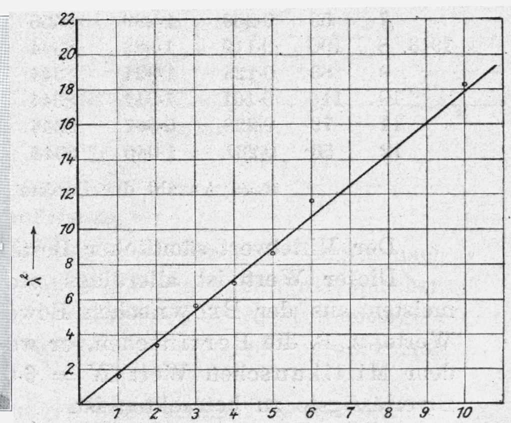


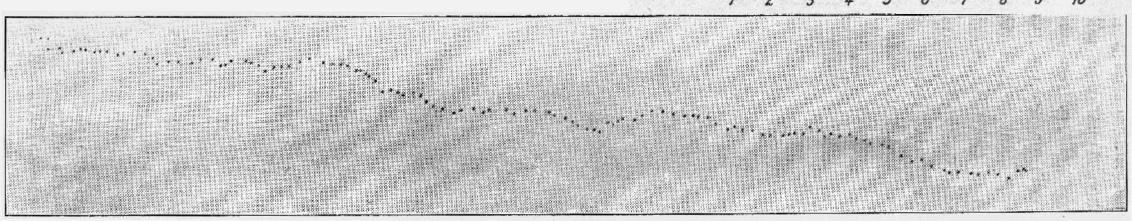


Δt=30 sec

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







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

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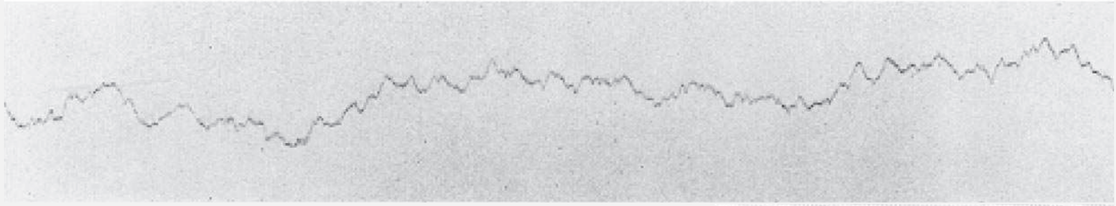
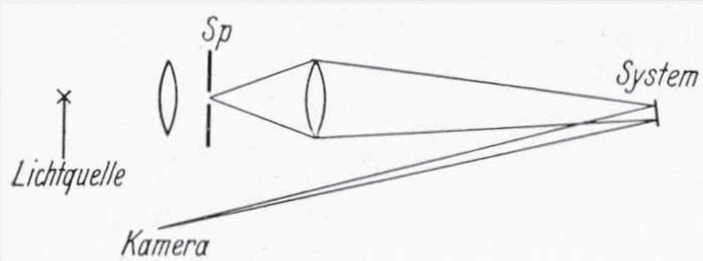
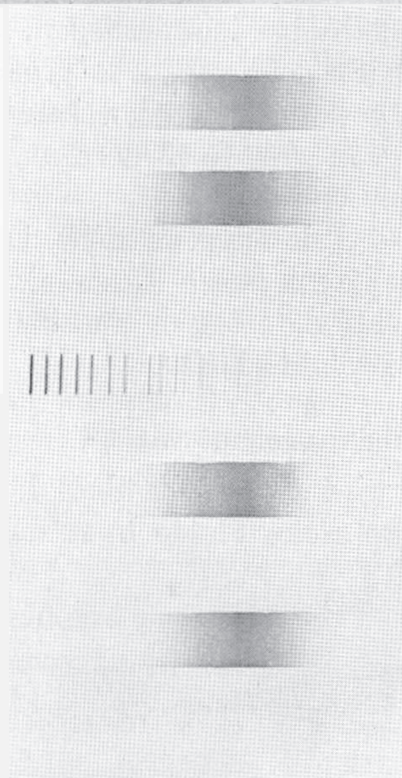
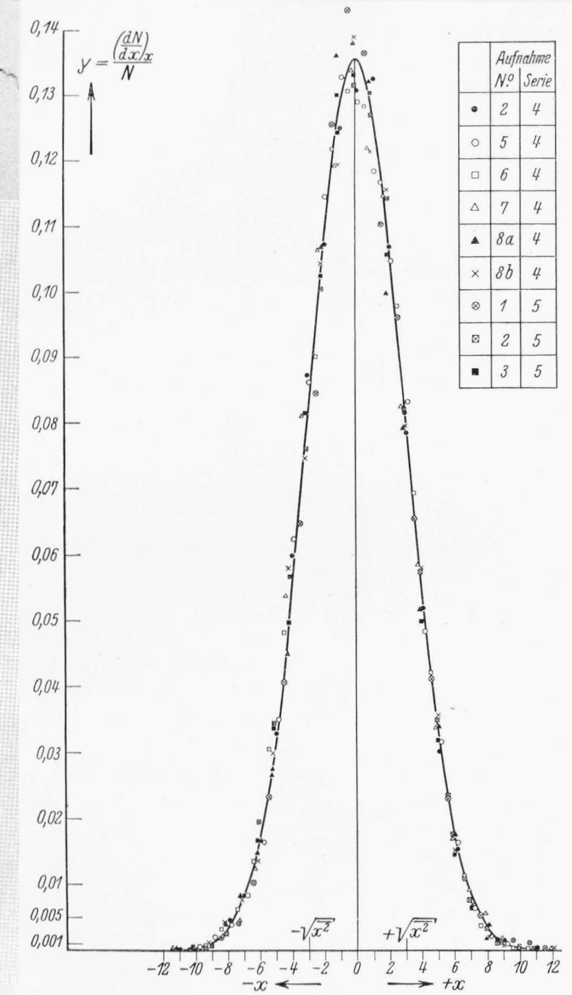
Kappler's diffusion measurements: mapping Boltzmann





Schema der Meßanordnung
Fig. 1

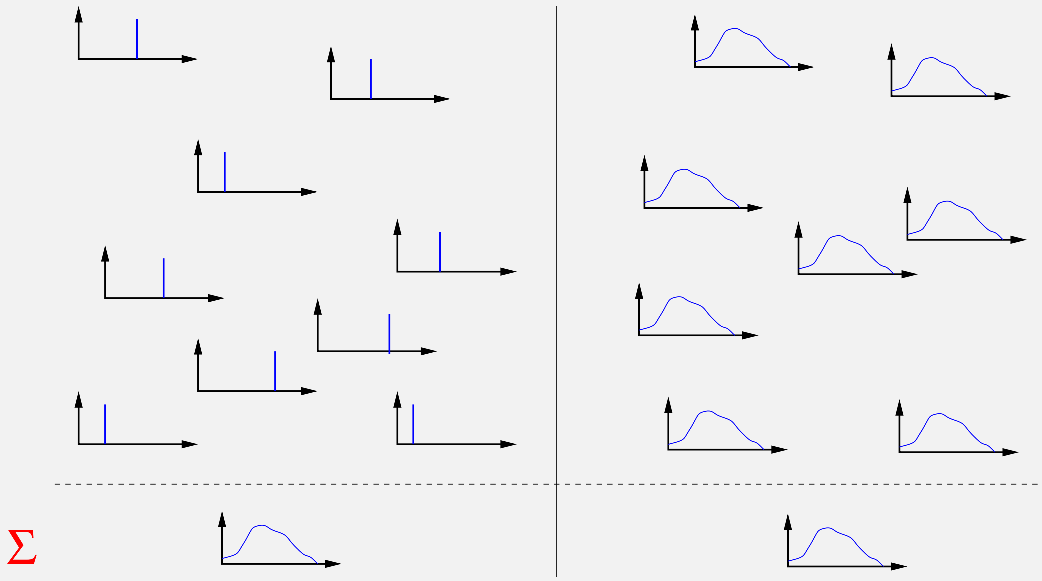


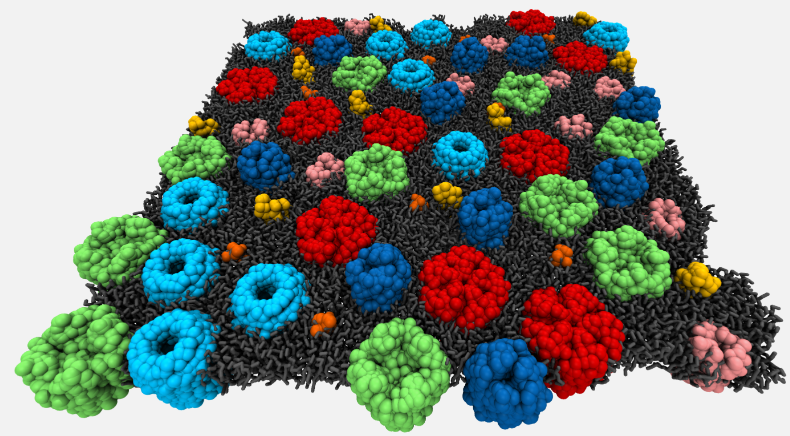


$$P_{\mathrm{eq}}(x) = \mathscr{N} \exp\left(-\frac{\theta x^2}{k_B T}\right)$$

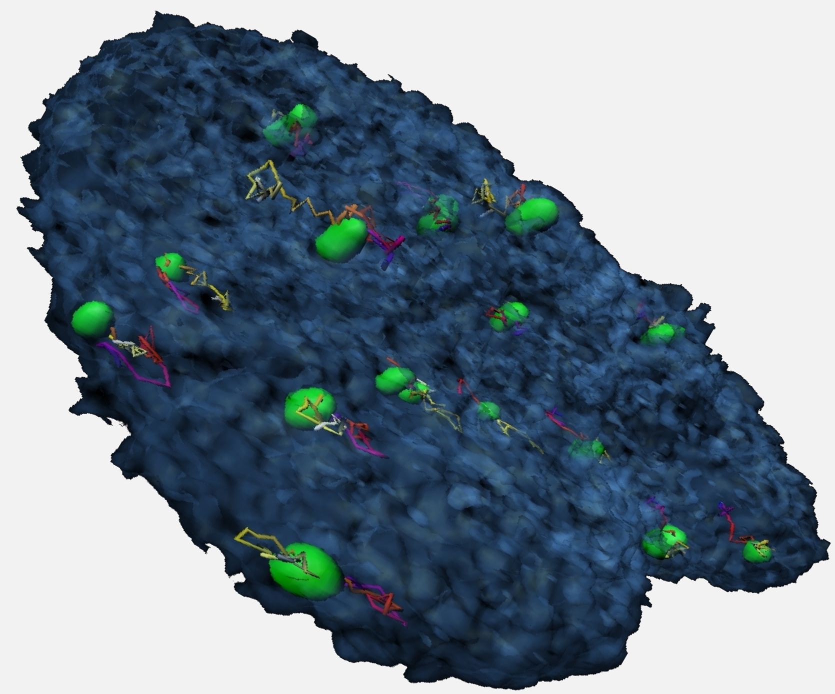
E Kappler, Ann d Physik (1931): $N_A = 60.59 \times 10^{22} \pm 1\%$

Single molecular insight & information from fluctuations





Courtesy Matti Javanainen



Courtesy Yuval Garini

Novel insights from single particle tracking (e.g., superresolution microscopy, supercomputing)

↷ Anomalous diffusion:

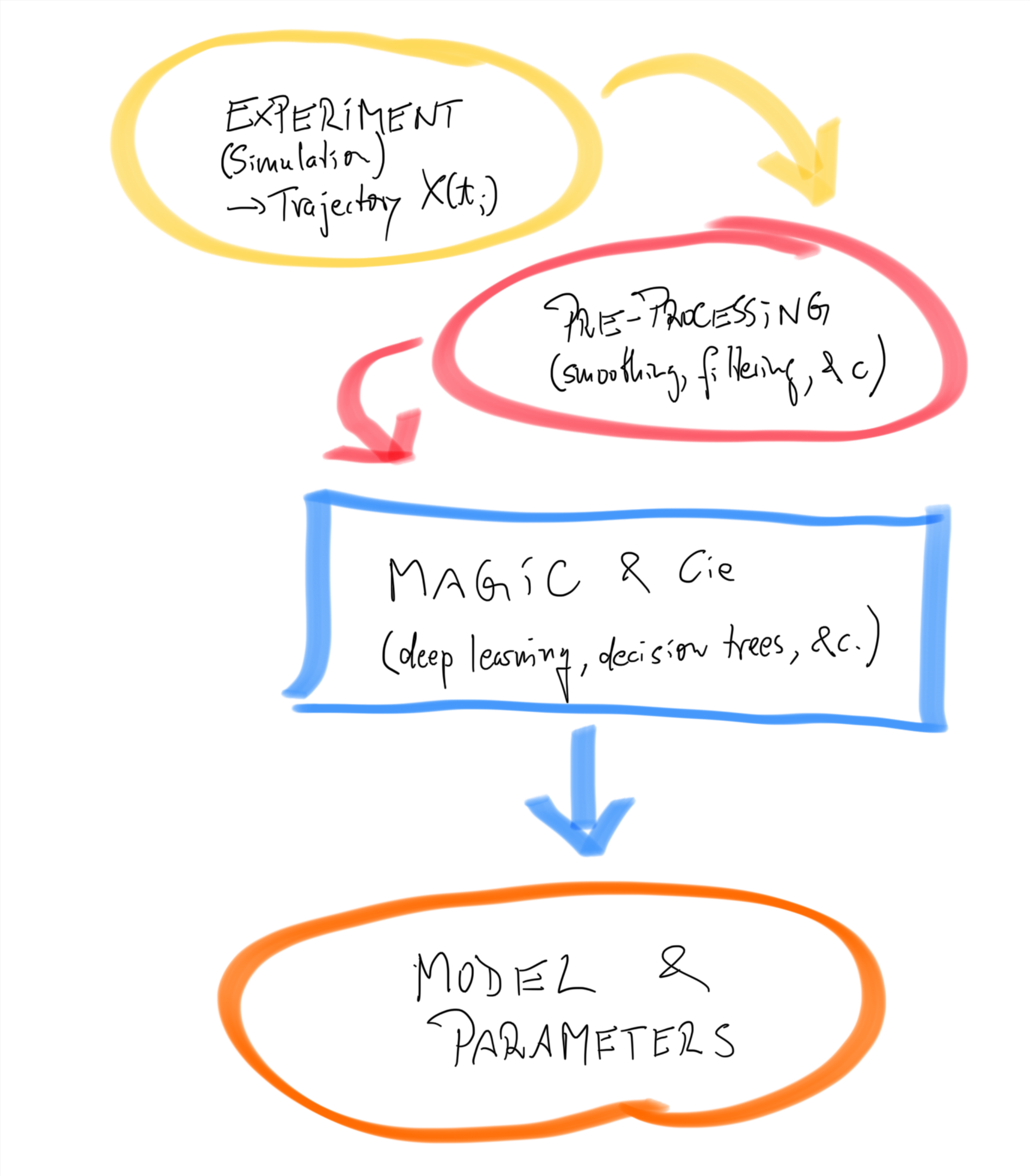
$$\langle \mathbf{r}^2(t) \rangle \simeq t^\alpha$$

(non)ergodicity, ageing, quenched/annealed disorder

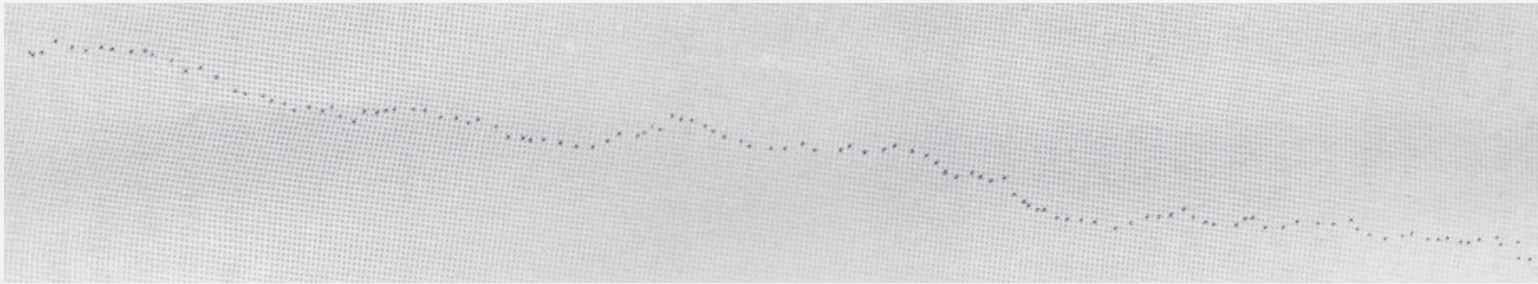
↷ Fluctuations are prominent:
– spatiotemporally fluctuating diffusivity
– strongly fluctuating reaction times

E Barkai, Y Garini & RM, Phys Today (2012)

How the data come in . . .



Extracting information from single Brownian trajectories



Ensemble averaged MSD for normal diffusion:

$$\left\langle \mathbf{r}^2(t) \right\rangle = \int \mathbf{r}^2 P(\mathbf{r}, t) d\mathbf{r} = 2dK_1 t$$

Single particle trajectory $\mathbf{r}(t)$, $t \in [0, T]$:

$$\overline{\delta^2(\Delta)} = \frac{1}{T-\Delta} \int_0^{T-\Delta} \left[\mathbf{r}(t' + \Delta) - \mathbf{r}(t') \right]^2 dt'$$

Brownian motion: on average # jumps $\sim$ elapsed time t:

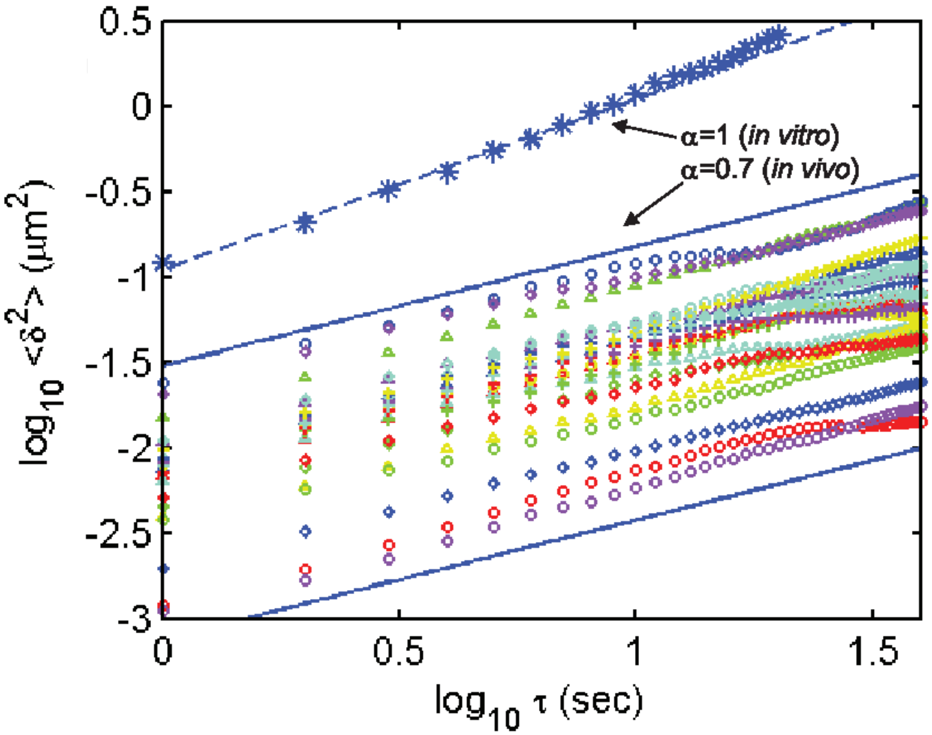
$$\left[\mathbf{r}(t' + \Delta) - \mathbf{r}(t') \right]^2 \sim \langle \delta \mathbf{r}^2 \rangle \frac{\Delta}{\tau}$$

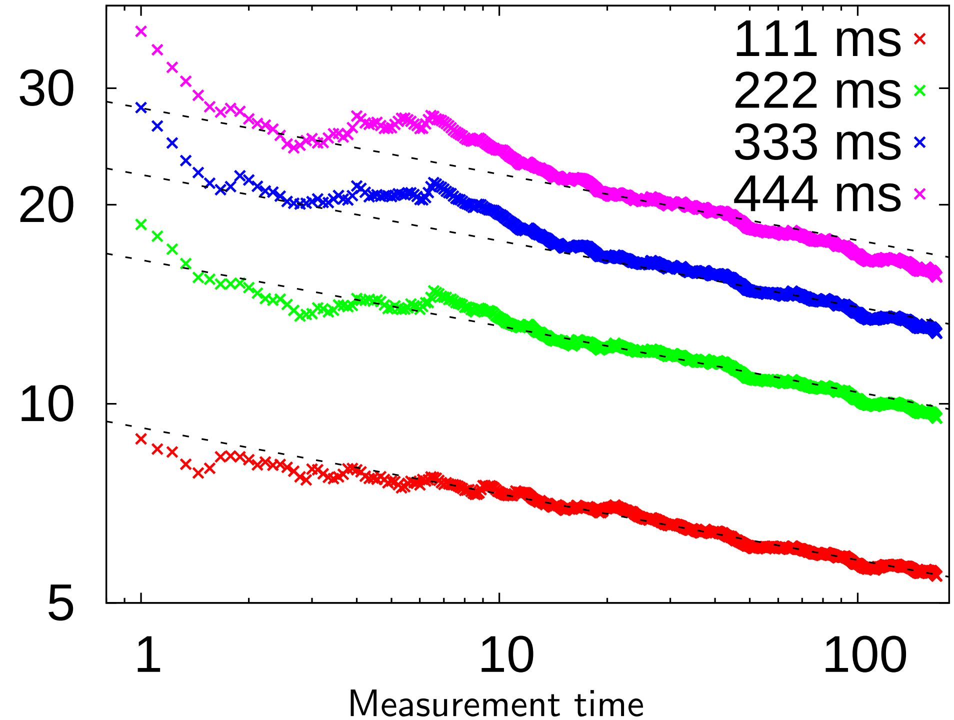
Single trajectory information equals ensemble information (*Boltzmann-Khinchin*):

$$\lim_{T\to\infty} \overline{\delta^2(\Delta)} = 2dK_1\Delta = \left\langle \mathbf{r}^2(\Delta) \right\rangle, \quad K_1 = \frac{\langle \delta \mathbf{r}^2 \rangle}{2d\tau}$$

E Barkai, Y Garini & RM, Phys Today (2012)

Challenges in single particle tracking in complex systems





I Anomalous diffusion: $\left\langle \mathbf{r}^2(t) \right\rangle \simeq K_\alpha t^\alpha$

II Weak ergodicity breaking: $\lim_{T\to\infty} \overline{\delta^2(\Delta)} \neq \left\langle \mathbf{r}^2(\Delta) \right\rangle$ (Boltzmann-Khinchin)

III Ageing: $\overline{\delta^2(\Delta)}$ depends on measurement time & initiation-measurement start time

IIII Amplitude scatter: $\phi(\xi)$ with $\xi = \overline{\delta^2(\Delta)} \Big/ \left\langle \overline{\delta^2(\Delta)} \right\rangle$

I Golding & EC Cox, PRL (2006); AV Weigel, B Simon, MM Tamkun & D Krapf, PNAS (2011)

Anomalous diffusion is non-universal & weakly non-ergodic

Montroll-Scher-Weiss CTRW:

$\psi(\tau) \simeq \tau^{-1-\alpha}$ & $\langle\tau\rangle = \infty$

$\left\langle\overline{\delta^2(\Delta)}\right\rangle \simeq K_\alpha \Delta / T^{1-\alpha}$

$\left\langle\overline{\delta_a^2(\Delta)}\right\rangle \sim \Lambda_\alpha(t_a/T)\left\langle\overline{\delta^2(\Delta)}\right\rangle$

$P(k,t) = E_\alpha(-ck^2t^\alpha) \simeq [k^2t^\alpha]^{-1}$

$\wp(t) \simeq t^{-1-\alpha}$

Mandelbrot-van Ness FBM:

$\langle\xi(t_1)\xi(t_2)\rangle \sim \alpha K_\alpha(\alpha-1)|t_1-t_2|^{\alpha-2}$

$\left\langle\overline{\delta^2(\Delta)}\right\rangle \simeq K_\alpha \Delta^\alpha$

$\left\langle\overline{\delta_a^2(\Delta)}\right\rangle \sim \left\langle\overline{\delta^2(\Delta)}\right\rangle$

$P(k,t) = \exp(-c_1k^2t^\alpha)$

$\wp(t) \simeq \exp(-c_2t)$

$$\langle\mathbf{r}^2\rangle \simeq K_\alpha t^\alpha$$

Scaled Brownian motion:

$K(t) \simeq K_\alpha t^{\alpha-1}$

$\left\langle\overline{\delta^2(\Delta)}\right\rangle \simeq K_\alpha \Delta / T^{1-\alpha}$

$\left\langle\overline{\delta_a^2(\Delta)}\right\rangle \sim \Lambda_\alpha(t_a/T)\left\langle\overline{\delta^2(\Delta)}\right\rangle$

$P(k,t) = \exp(-c_3k^2t^\alpha)$

$\wp(t) \simeq \ldots$

Heterogeneous diffusion process:

$K(x) \simeq K_\beta|x|^\beta$, $\alpha = 2/(2-\beta)$

$\left\langle\overline{\delta^2(\Delta)}\right\rangle \simeq K_\alpha \Delta / T^{1-\alpha}$

$\left\langle\overline{\delta_a^2(\Delta)}\right\rangle \sim \Lambda_\alpha(t_a/T)\left\langle\overline{\delta^2(\Delta)}\right\rangle$

$P(k,t) = L_{2/\alpha}(c_4|k|^2t^\alpha)$

$\wp(t) \simeq \ldots$

System specific dynamics (α, K_α) with vastly different secondary processes (FPT ...)

RM, J-H Jeon, AG Cherstvy & E Barkai, PCCP (2014)

Fitting power-laws & mean-maximal excursion method

(also studied by Erdös & Kac, Khinchine & Chung)

Maximal excursion in d dimensions: $M_t = \max\{||\mathbf{r}_u||_2, u \leq t\} \therefore ||\mathbf{r}_u||_2 = \sqrt{\sum_i r_i^2}$ is Euclidean distance

Limit distribution: $P_d(a,t) = \Pr\{M_t < a\}$ is the survival probability to remain in hypersphere with radius a up to t

In Laplace domain a closed form is known for $D = D_0 r^{-2+1/\nu}$:

$$P_{d,\nu}(a,s) = \frac{1}{s}\left(1 - \frac{2^{1-d\nu}}{\Gamma(d\nu)}\frac{\left(4\nu^2 D_0^{-1} a^{1/\nu} s\right)^{(d\nu-1)/2}}{I_{d\nu-1}\left(\sqrt{4\nu^2 D_0^{-1} a^{1/\nu} s}\right)}\right)$$

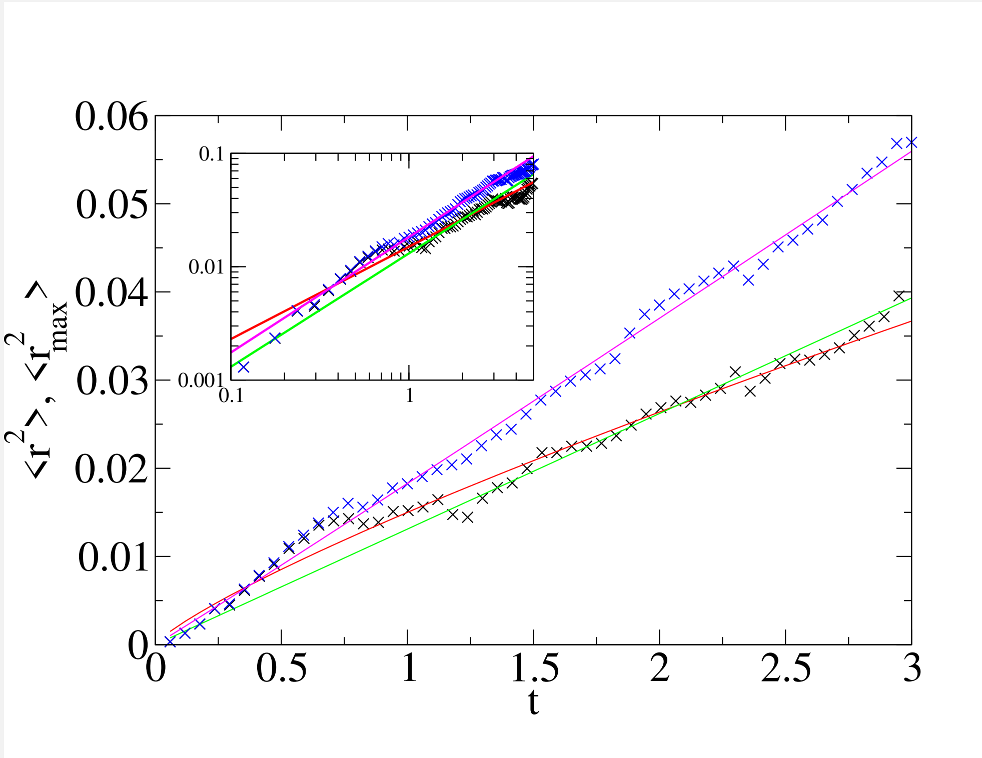
In $d \to \infty$ and $\nu = 1/2$ (Brownian case): $P_\infty(a,s) = \frac{1}{s}\Big(1 - \exp(-a^2 s)\Big)$ to leading order peaking at $a = \sqrt{t}$: $P_\infty(a,t) = 1 - \Theta(t - a^2)$ or $p_\infty(a,t) = \delta(t - a^2)$

Moments are known for certain processes or can be obtained numerically

R Bidaux, J Chave & R Vočka, JPA (1999)

Fitting power-laws & mean-maximal excursion method

Coefficient of variation is smaller for MME PDF than for regular PDF

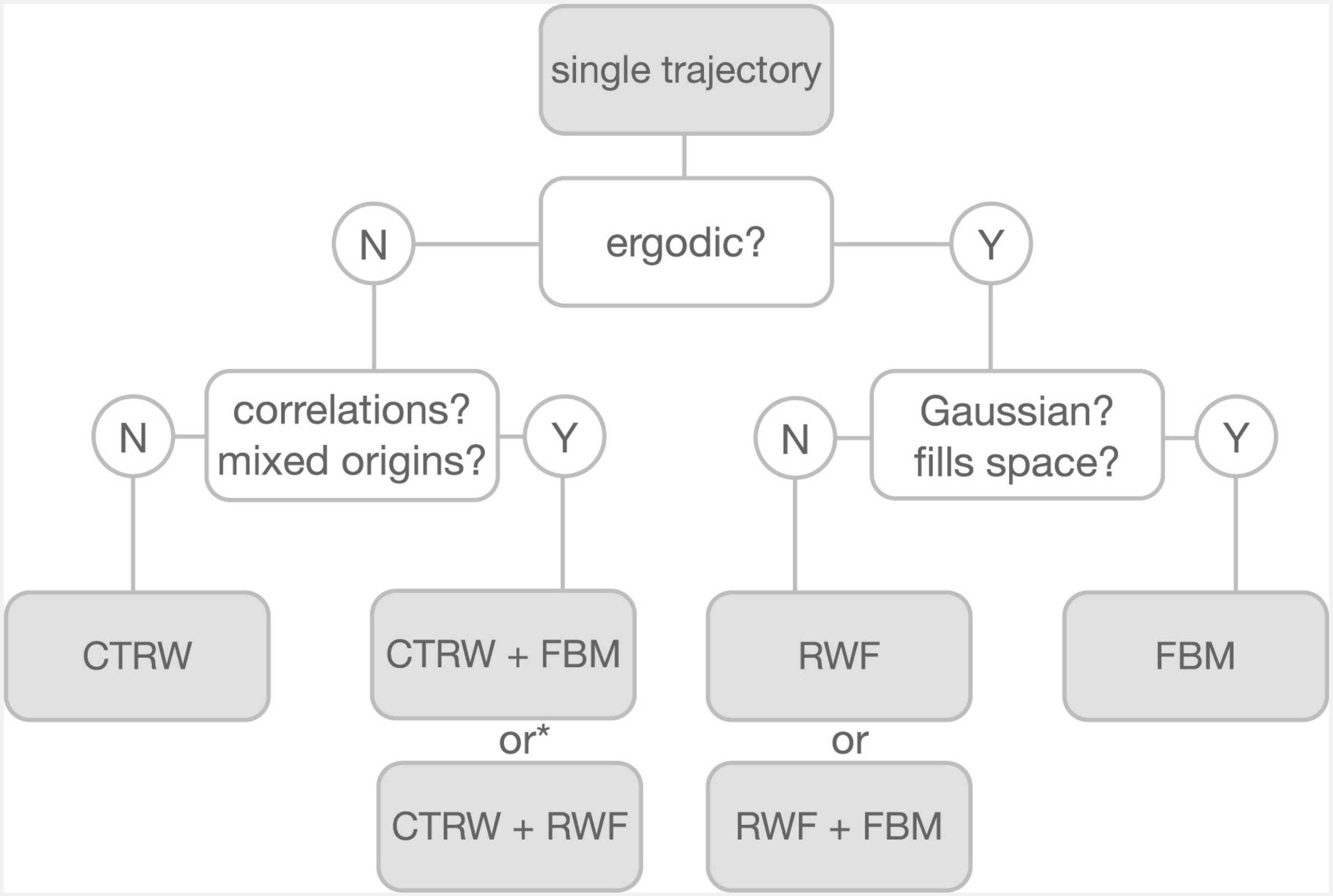


Analysis of an experimental set of 67 trajectories, the longest consisting of 210 points, for quantum dots freely diffusing in a solvent. MSD (black $\times$), fitted by a power law with exponents $\alpha = 0.81$ (red line). We also show a fit with fixed exponent $\alpha = 1$ (green line, expected behavior for Brownian motion). MME (blue $\times$), fitted by a power law (red line, $\alpha = 1.02$). Time is in seconds, distances are in $\mu\mathrm{m}^2$. Inset: double-logarithmic plot of the same data.

$$\gamma = \frac{\sqrt{\langle \mathbf{r}^2(t) \rangle - \langle \mathbf{r}(t) \rangle^2}}{\langle \mathbf{r}(t) \rangle} \rightsquigarrow \frac{\gamma(\text{MSD})}{\gamma(\text{MME})} = 1.61\ (\text{1D}),\ 1.44\ (\text{2D}),\ 1.34\ (\text{3D})$$

V Tejedor, O Bénichou, R Voituriez, R Jungmann, F Simmel, C Selhuber-Unkel, L Oddershede, BPJ (2010)

From classical statistical observables to decision tress . . .



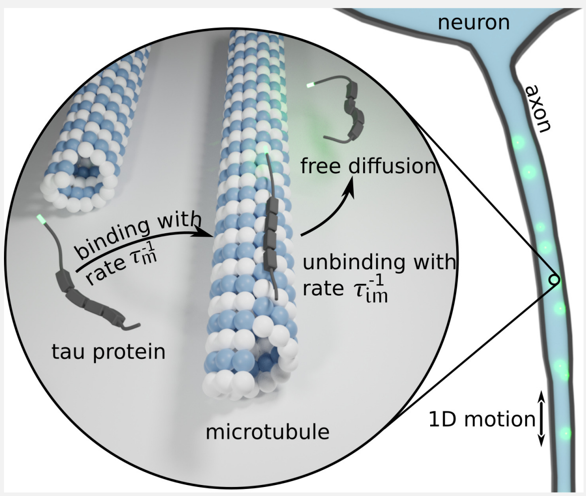
Y Meroz & IM Sokolov, Phys Rep (2015)

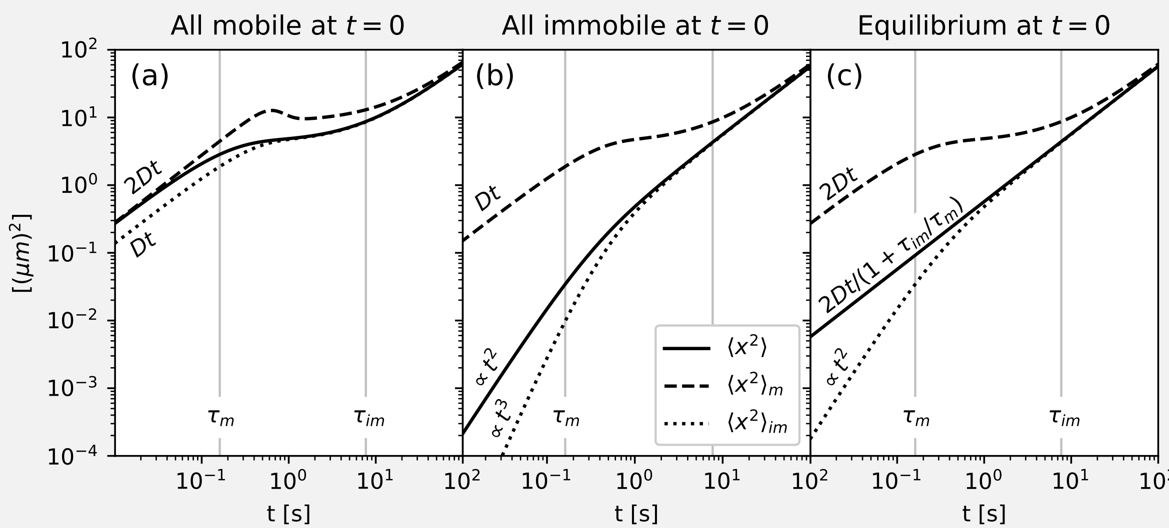
Apparent anomalous diffusion & non-Gaussianity

Anomalous diffusion in groundwater dispersal may persist over km-scales [N Goeppert, N Goldscheider & B Berkowitz, Wat Res Res (2020)]

Transient anomalous diffusion may occur in simple rate-exchange mobile-immobile models:

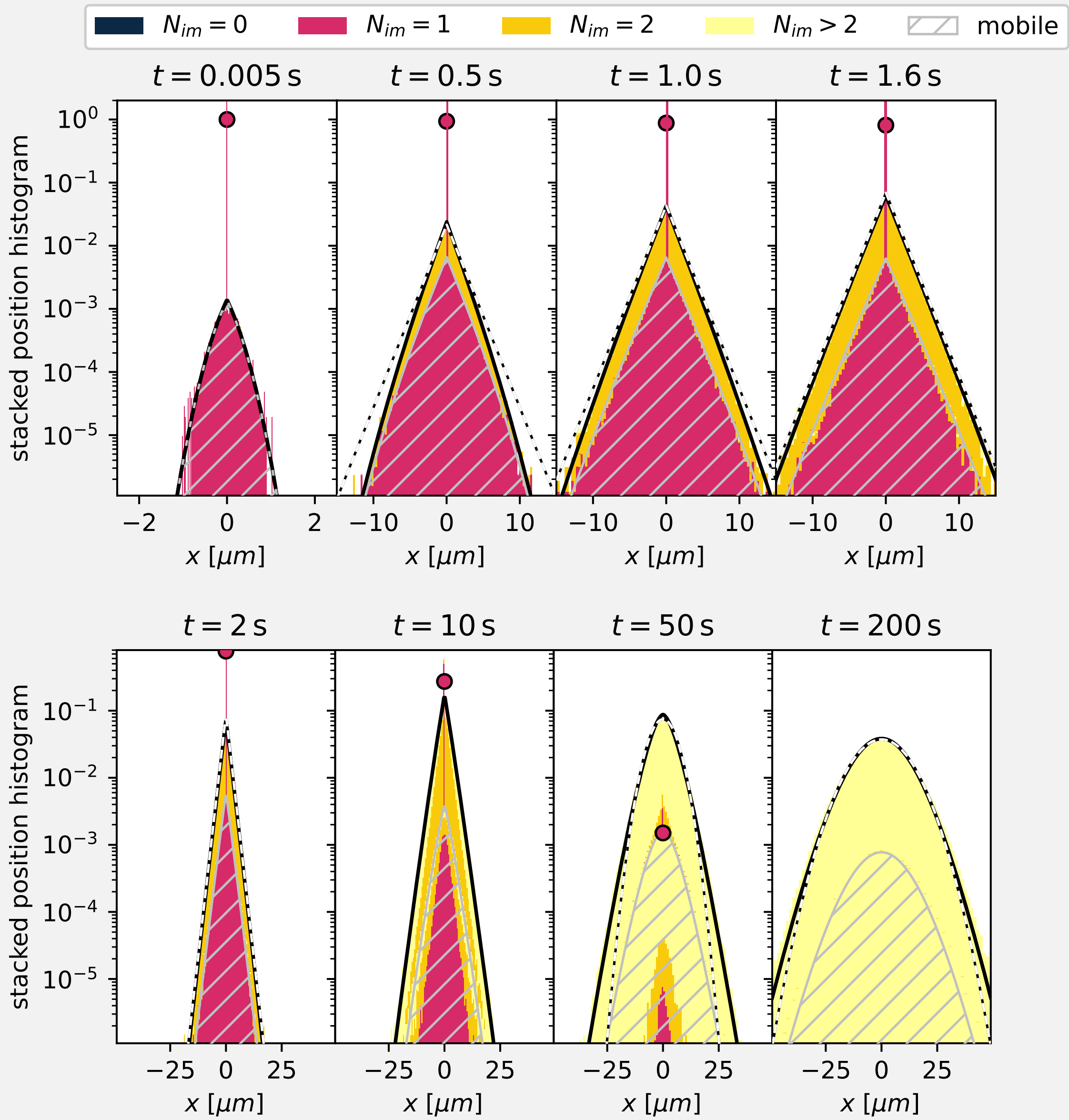
$$\begin{aligned} \frac{\partial}{\partial t} n_{\rm m}(x,t) &= -\frac{1}{\tau_{\rm m}} n_{\rm m}(x,t) + \frac{1}{\tau_{\rm im}} n_{\rm im}(x,t) + D\frac{\partial^2}{\partial x^2} n_{\rm m}(x,t) \\ \frac{\partial}{\partial t} n_{\rm im}(x,t) &= -\frac{1}{\tau_{\rm im}} n_{\rm im}(x,t) + \frac{1}{\tau_{\rm m}} n_{\rm m}(x,t) \end{aligned}$$





T Doerries, AV Chechkin & RM (2022)

Apparent anomalous diffusion & non-Gaussianity



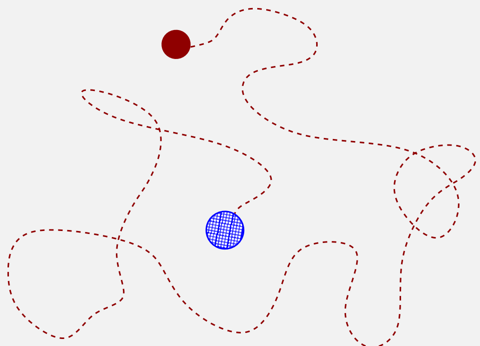
T Doerries, AV Chechkin & RM (2022)

& now it's time for something completely different

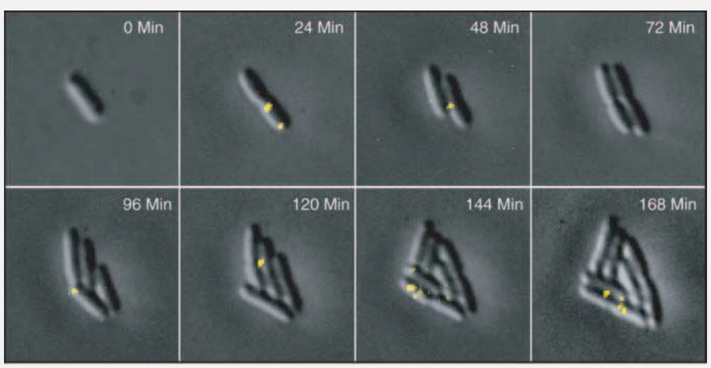
Molecular reaction times: macro vs micro

Search rate for particle with diffusivity D_{3d} to find an immobile target of radius a (assuming immediate binding):

$$k_{on} = 4\pi D_{3d} a$$



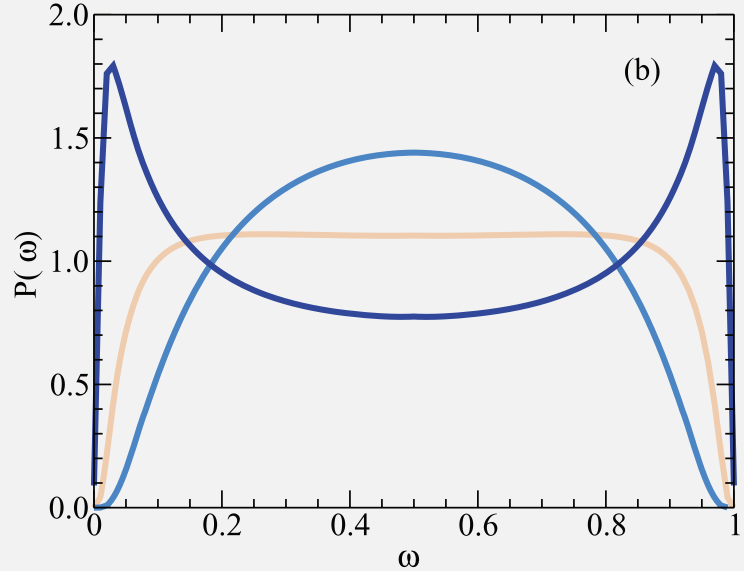
Yu et al, Science (2006)



Uniformity index for two independent first-passage times τ_1, τ_2:

$$\omega = \frac{\tau_1}{\tau_1 + \tau_2}$$

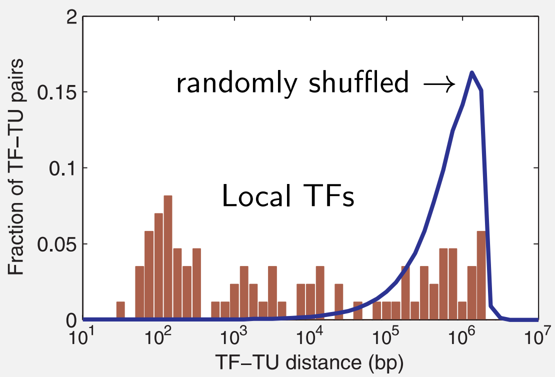
$\curvearrowright$ $\omega = 1/2$ means good reproducibility ↯ many processes

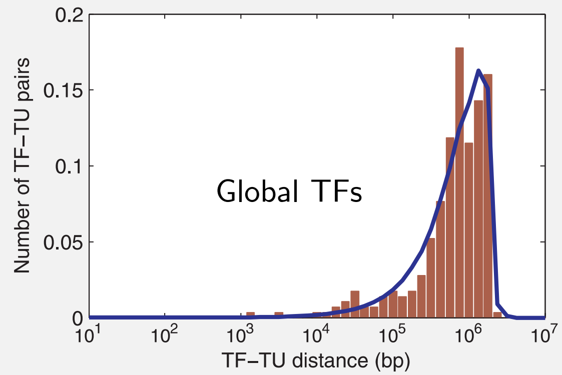


M v Smoluchowski, Physikal Zeitschr (1916)

T Mattos, C Mejía-Monasterio, RM & G Oshanin, PRE (2012)

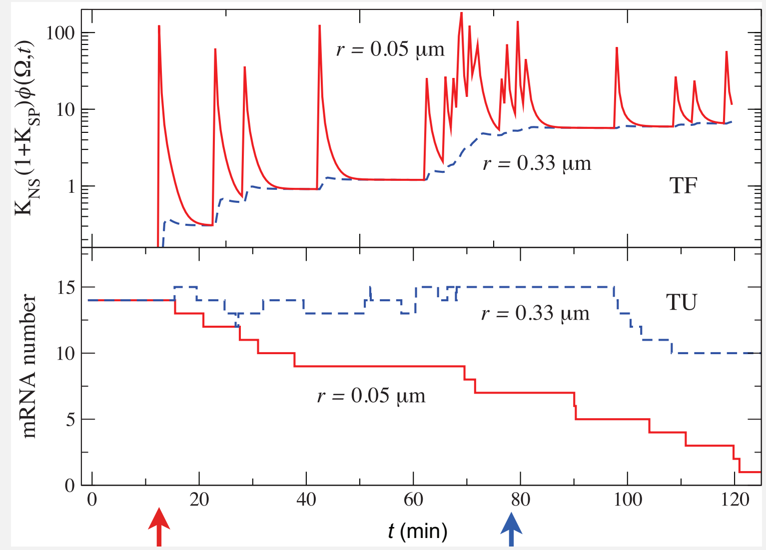
Transient intracellular signalling is geometry-controlled

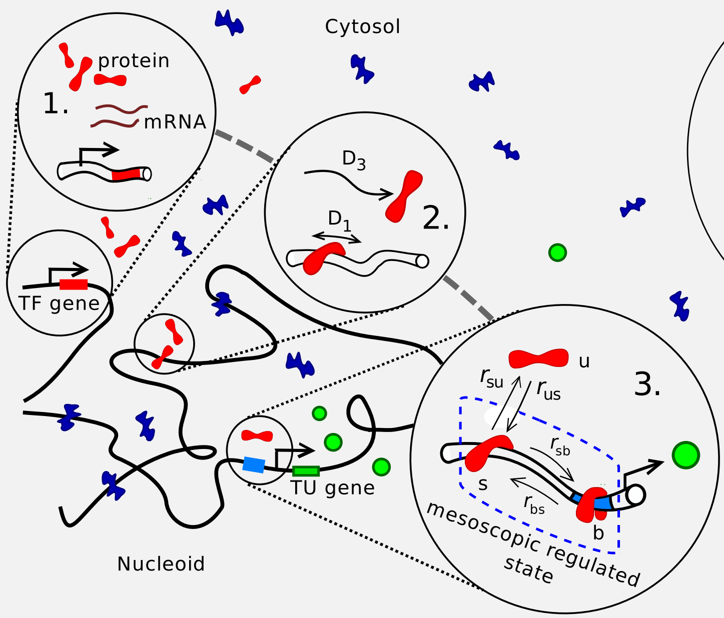


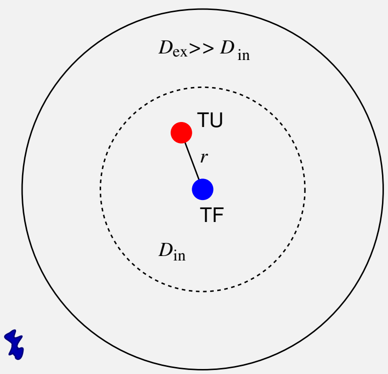


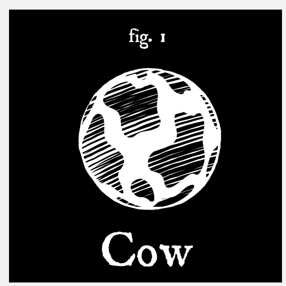
TF-TU gene-gene distance [G Kolesov . . . LA Mirny, PNAS (2007)]

TF concentration @ TU (long time)

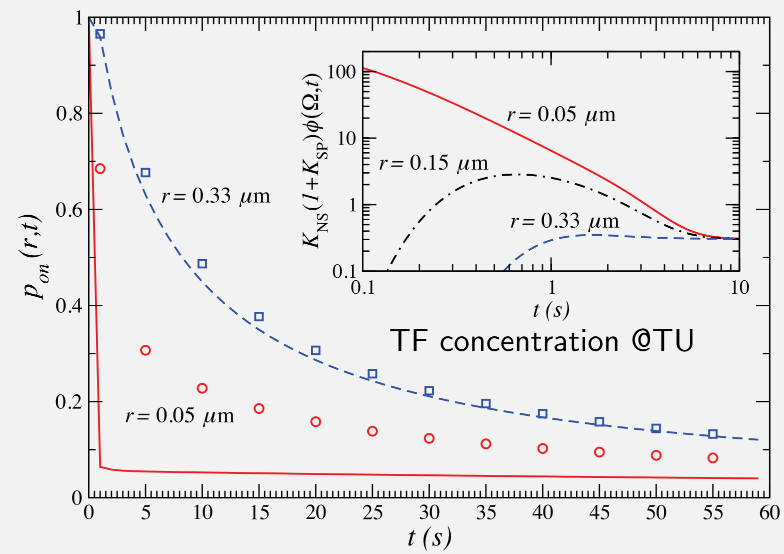








Probability that target gene TU is active



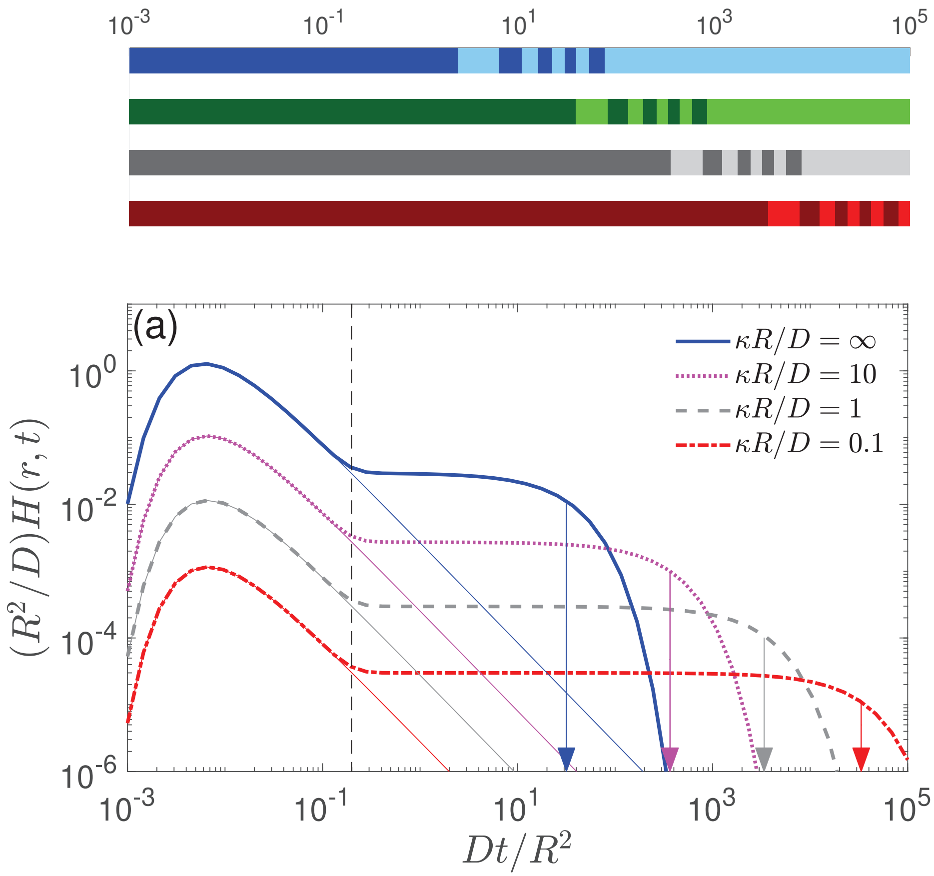
O Pulkkinen & RM, PRL (2013)

Strongly defocused (fluctuating) reaction times

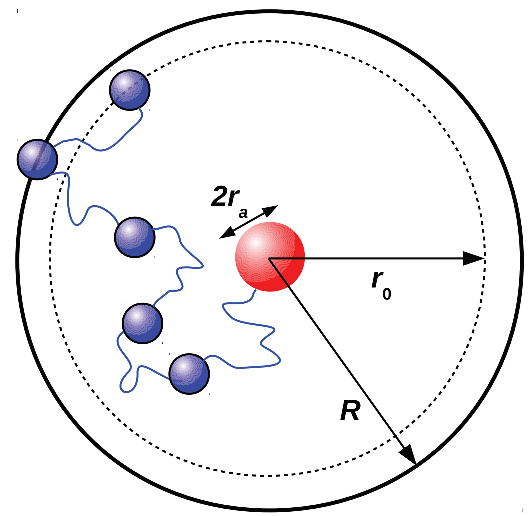
Geometry control: direct trajectories independent of outer boundary

Reaction control: finite reactivity requires multiple collisions

Full first passage time density:



Direct vs indirect trajectories:



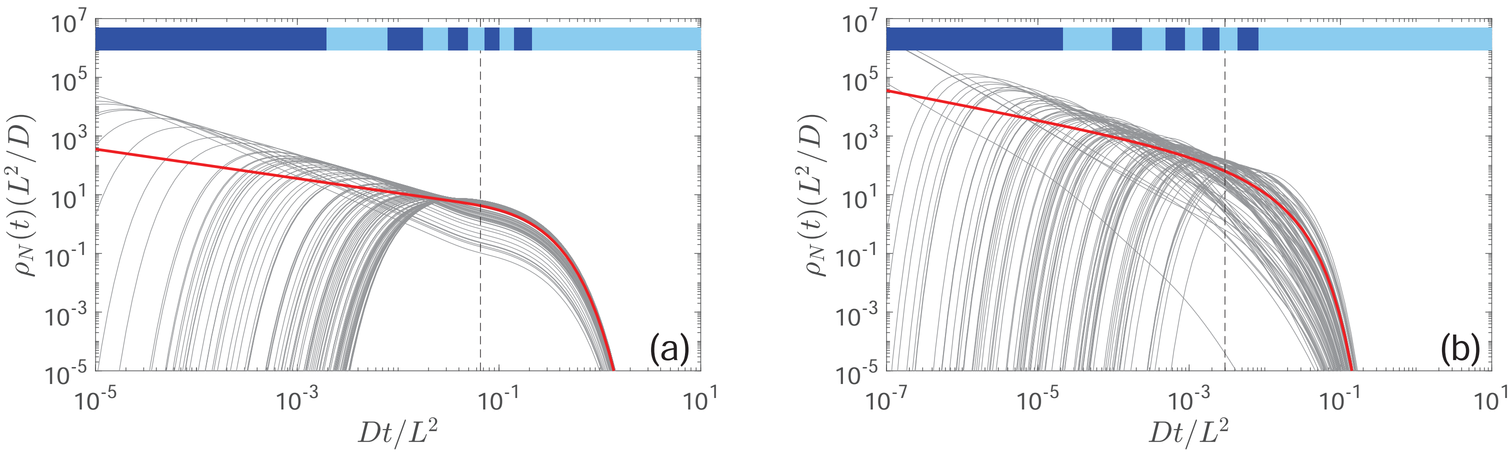
$$\langle t \rangle = \frac{(r_0 - r_a)(2R^3 - r_0 r_a [r_0 + r_a])}{6 D r_0 r_a} + \frac{R^3 - r_a^3}{3 \kappa r_a}$$

D Grebenkov, RM & G Oshanin, Comm Chem (2019), PCCP (2018), NJP (2019); A Godec & RM, PRX (2016), Sci Rep (2016)

Reaction/search speedup for N "molecules" in parallel

Fixed starting point: fastest FPT $\langle t \rangle \simeq 1/\ln N$

Uniformly distributed initial conditions: $\langle t \rangle \simeq \begin{cases} 1/N^2, & \text{perfect reactivity} \\ 1/N, & \text{partial reactivity} \end{cases}$



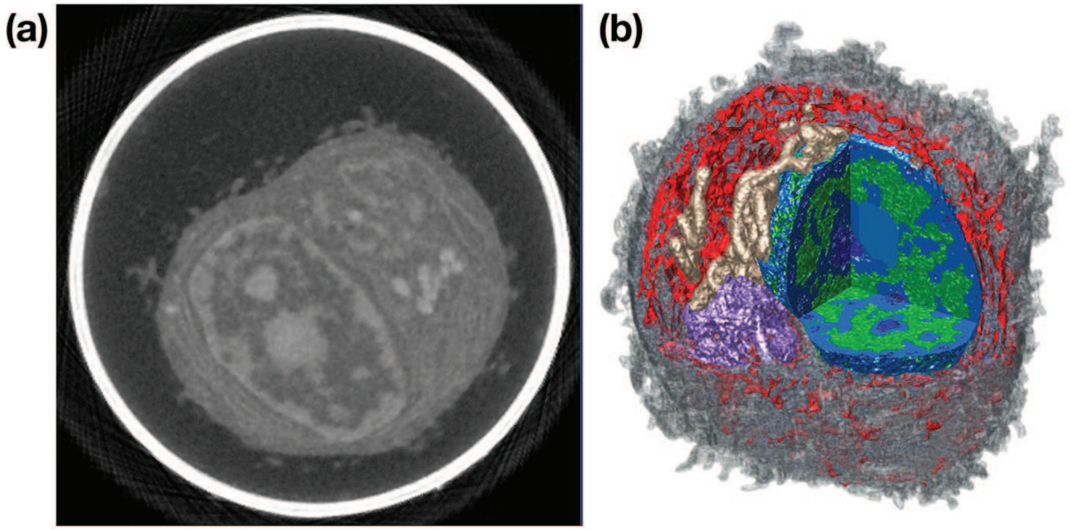
Grey lines: 100 random initial positions

$\rightsquigarrow$ Particles initially located close to target are purely reaction controlled

$\rightsquigarrow$ Initial conditions matter significantly & chemical rate approach requires sufficiently high concentrations

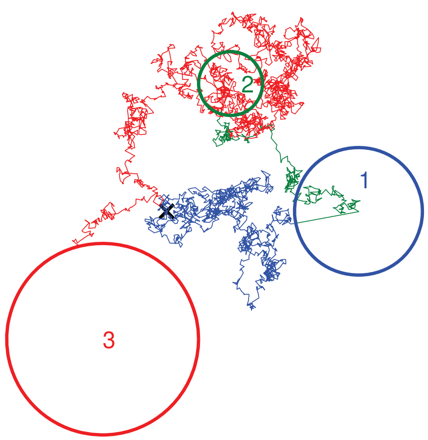
D Grebenkov, RM & G Oshanin, NJP (2020)

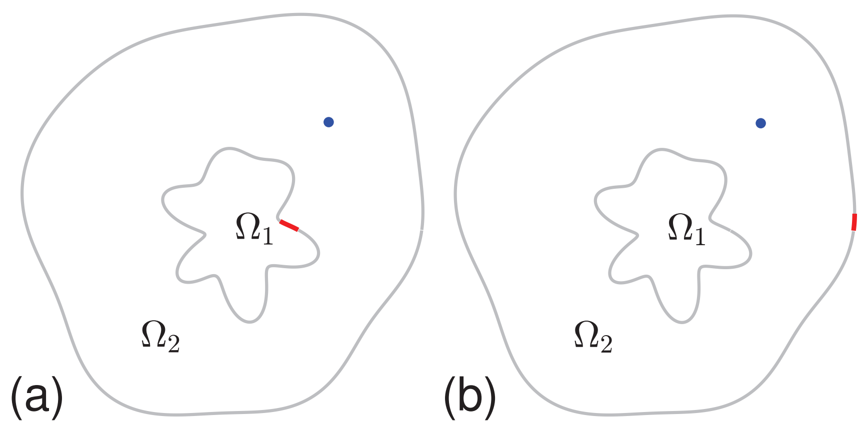
Computational models for intracellular signalling



[J Ma . . . SA Isaacson, PLoS Comp Biol (2021)]

Reaction cascades & reaction in onion-like shell regions





DS Grebenkov, RM & G Oshanin, NJP (2021); E-print (2021)

Typical versus mean, a lesson from disordered systems

N searchers with initial position $\mathbf{r}_i$ & single-searcher survival probability $Q_i(\mathbf{r}_i, t)$:

$$\mathscr{S}(t) = \prod_{i=1}^{N} Q_i(\mathbf{r}_i, t)$$

$\mathscr{S}(t)$ is random variable, mean:

$$\langle \mathscr{S} \rangle_{\mathbf{r}_i}$$

Typical $\mathscr{S}(t)$:

$$\mathscr{S}_{\text{typ}}(t) = \exp\Big(\langle \ln \mathscr{S}(t) \rangle_{\mathbf{r}_i} \Big)$$

In language of disordered systems $\mathscr{S}(t)$ is the partition function, $\mathbf{r}_i$ are disorder variables. Average: annealed limit, i.e., average over partition function $\mathscr{Z}$. Typical: quenched, i.e., average over free energy $\ln \mathscr{Z}$

MR Evans & SN Majumdar, PRL (2011)

Application to maximum of random diffusivity processes

Maximal positive displacement $M_T = \max_{0\leq t\leq T}\{x_t\} \geq 0$ of random process x_t

As shown by Paul Lévy [Processus stochastiques et mouvement brownien (Paris: Gauthier-Villars. 1948)], the PDF of M_T is

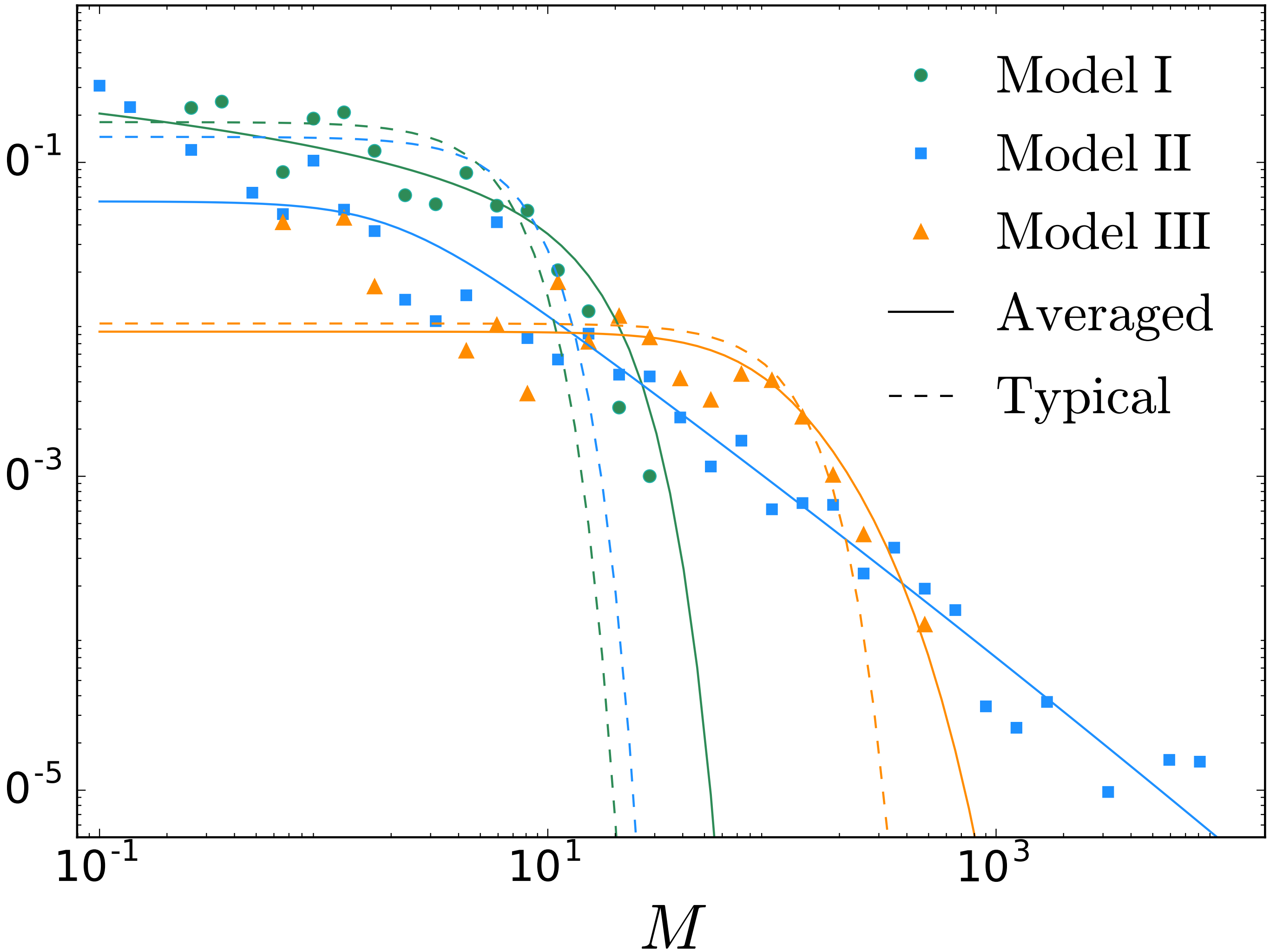
$$P_T(M_T) = \frac{1}{\sqrt{\pi DT}} \exp\left(-\frac{M_T^2}{4DT}\right)$$

Analogous typical PDF (p auxiliary parameter to fix dimensions, normalisation $\mathscr{N}_M$):

$$P_T^{(\mathrm{typ})}(M_T) = p\mathscr{N}_M \exp\left(\left\langle \ln \frac{\mathscr{P}(M_T)}{p} \right\rangle\right),$$

where $\mathscr{P}(M_T)$ is the PDF of a single realisation

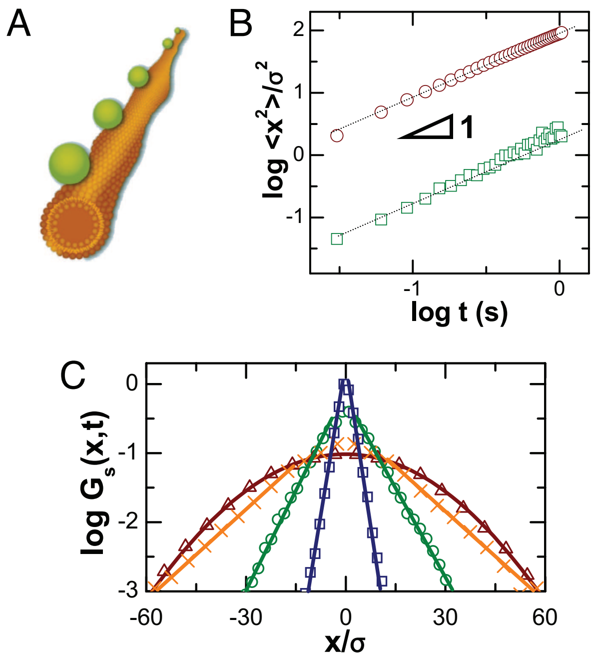
Application to maximum of random diffusivity processes



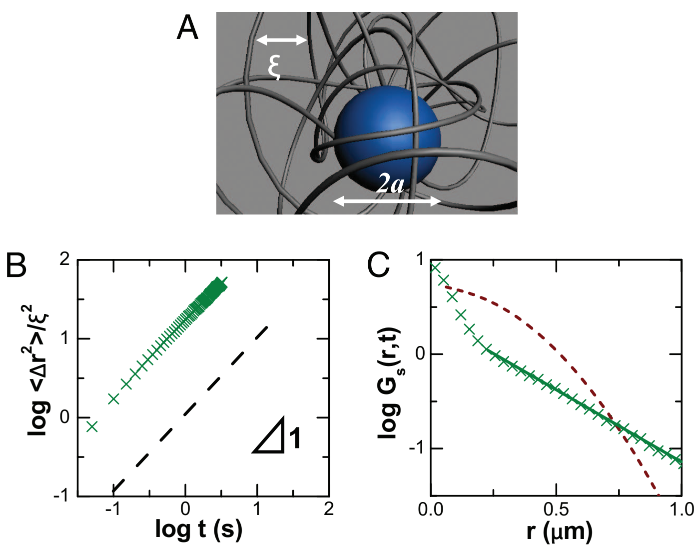
DS Grebenkov, V Sposini, RM, G Oshanin & F Seno, NJP (2020)


THE FOLLY OF CALLING IN
A THEORETICAL PLUMBER
The most radical solution would be
an instant drought or other drastic reduction
in water pressure. A sudden fall in temperature
causing all water to freeze would be another
solution...
Harris

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

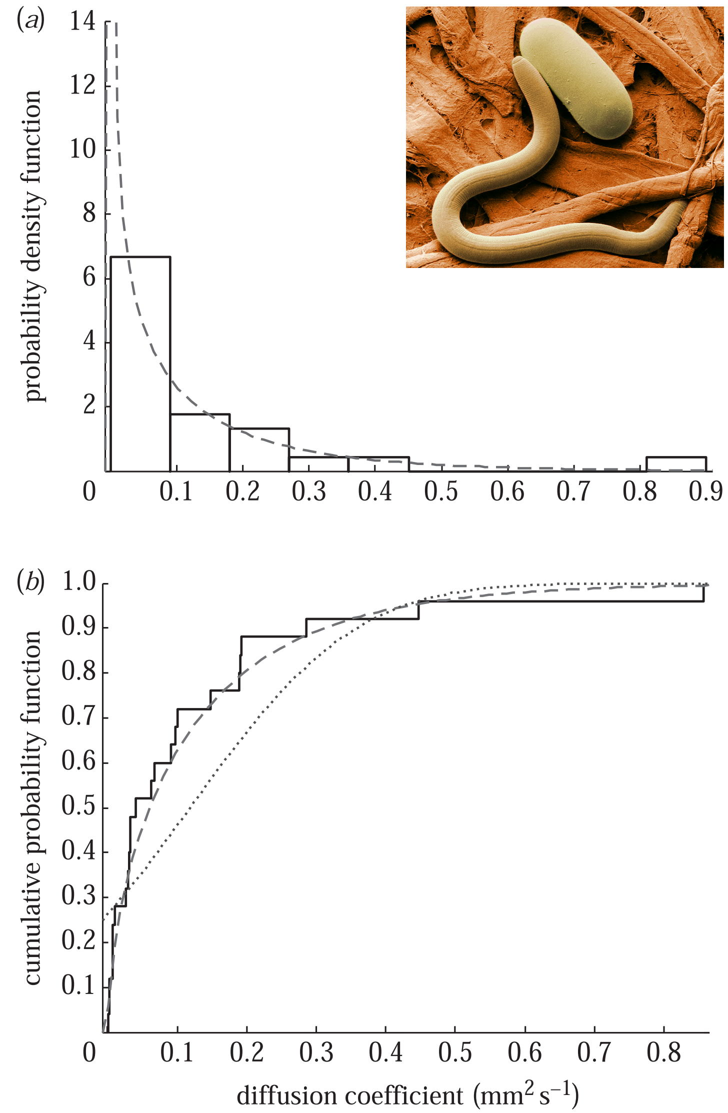


Colloidal beads on nanotubes



Nanospheres in entangled actin

Motion of *Phasmarhabditis* nematodes

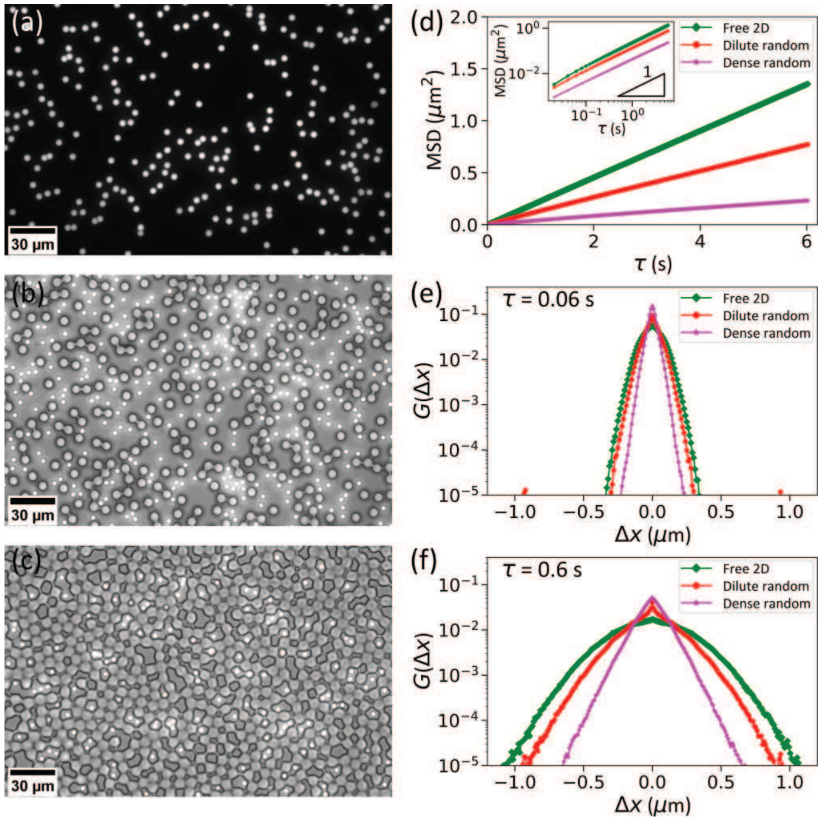


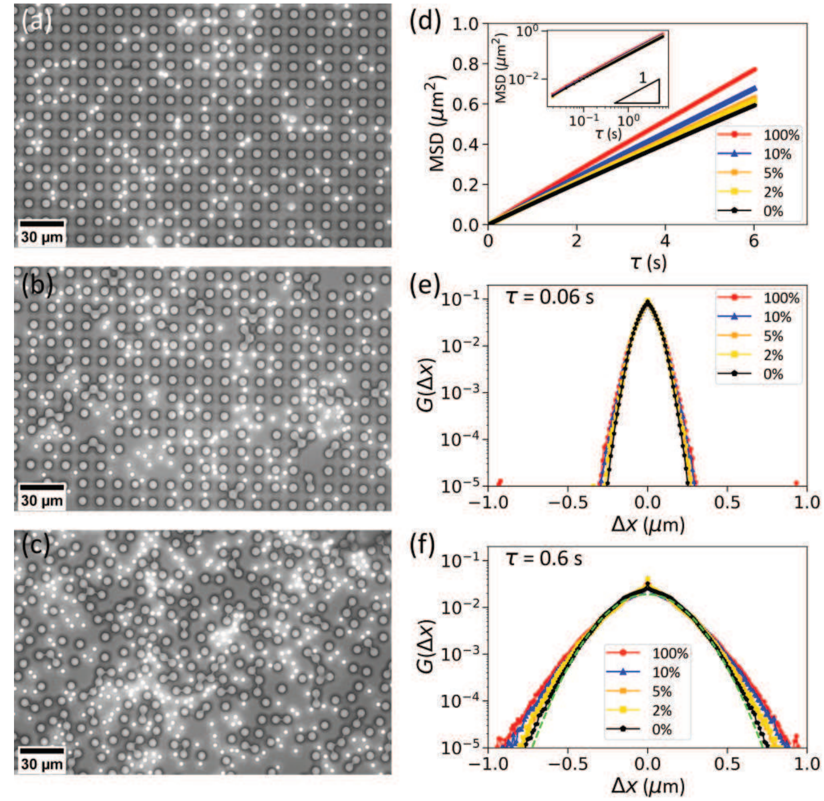
Wang et al, PNAS (2009); Nature Mat (2012)

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

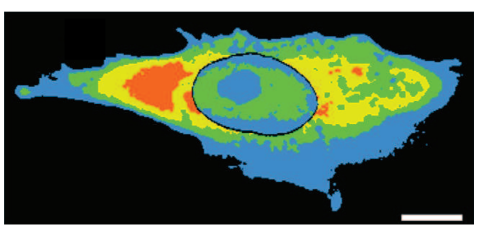
Fickian yet non-Gaussian diffusion in micropillar matrix

Increasing density ⟶



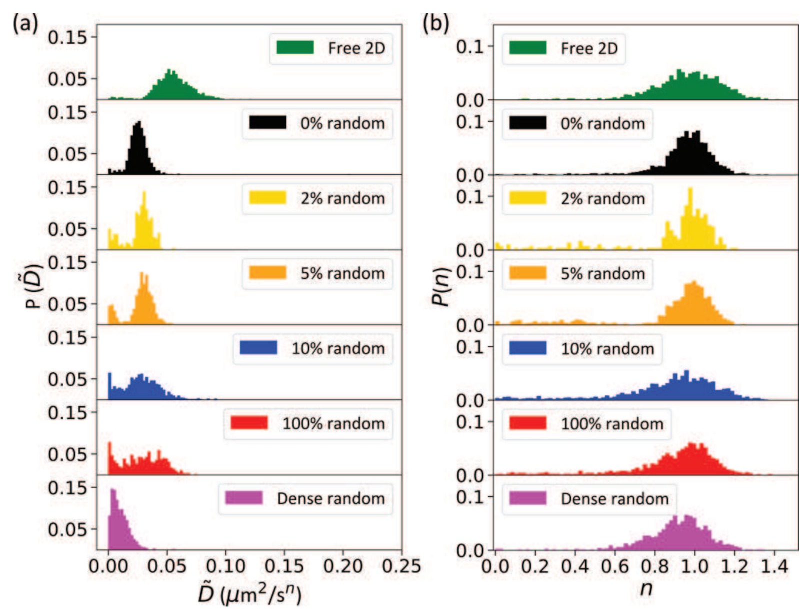


Increasing disorder ⟶



[Kühn et al, PLoS ONE (2011)]

I Chakraborty & Y Roichman, PRR (2020)



Superstatistics for non-Gaussian displacement PDFs

Superstatistical approach: patches of different diffusivities/mobilities or particles with different diffusivities (sizes/shapes) [$G(x,t|D)$ Gaussian Green's function for given D]:

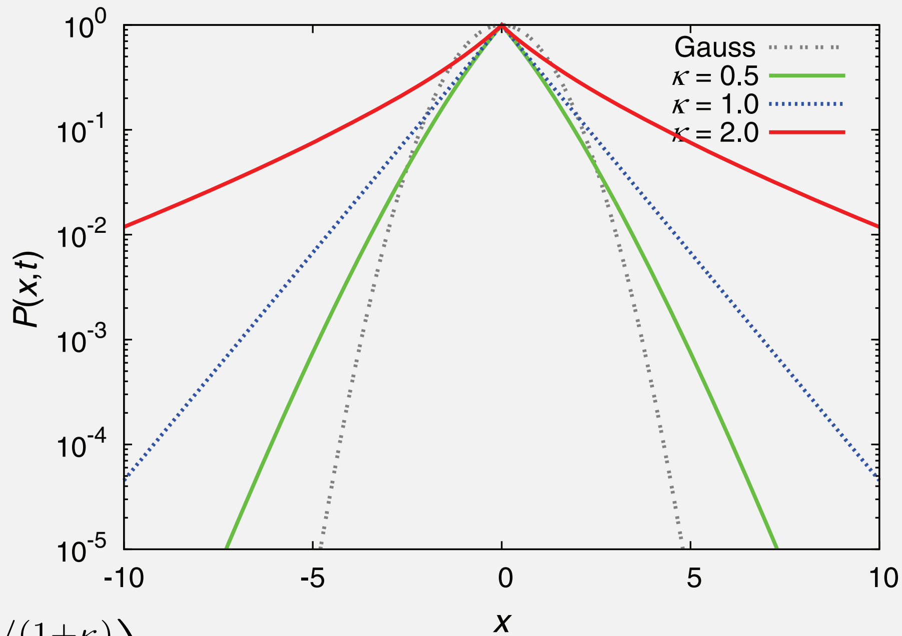
$$P(x,t)=\int_0^\infty G(x,t|D)p(D)dD$$

• $p(D)\propto\exp(-D/D^\star)\leadsto$

$$P(x,t)=(4D^\star t)^{-1/2}\exp\left(-\frac{|x|}{[D^\star t]^{1/2}}\right)$$

• $p(D)\propto\exp(-[D/D^\star]^\kappa)\leadsto$

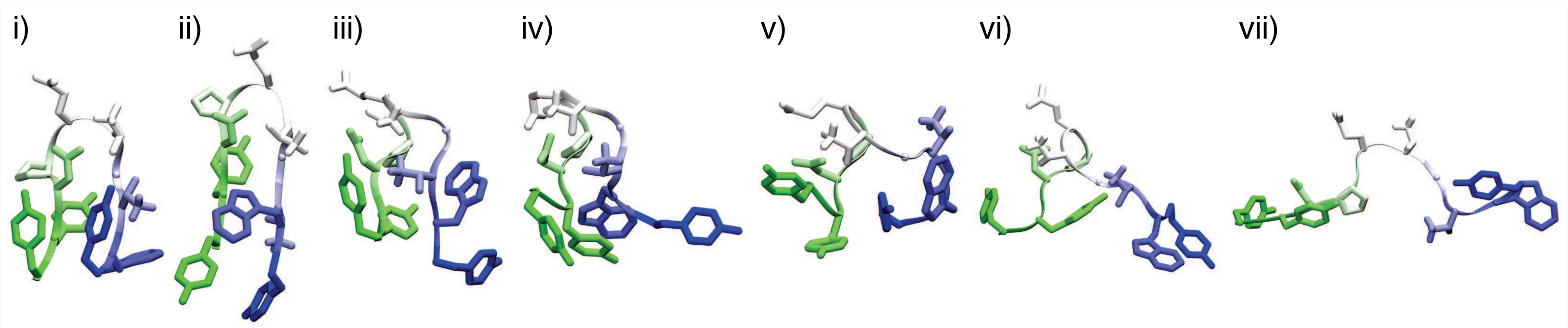
$$P(x,t)\simeq\frac{|x|^{(1-\kappa)/(1+\kappa)}}{(D^\star t)^{1/(1+\kappa)}}\times\exp\left(-a(\kappa)\left[\frac{x^2}{4D^\star t}\right]^{\kappa/(1+\kappa)}\right)$$



NB1: Superstatistics is closely related to (generalised) grey Brownian motion
[E.g., A Mura, MS Taqqu & F Mainardi, Physica (2008)]
NB2: $p(D)$ is static $\leadsto P(x,t)$ has fixed shape ↯ observed cross-over
NB3: ∃ also long history of superstatistics in turbulence

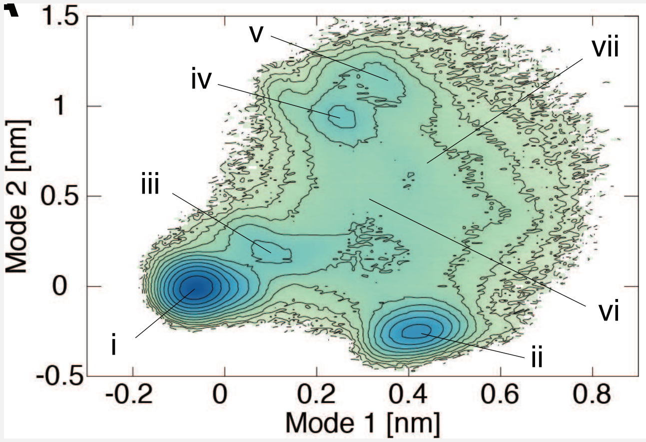
C Beck & EGD Cohen, Physica A (2003); AV Chechkin, F Seno, RM & IM Sokolov, PRX (2017)

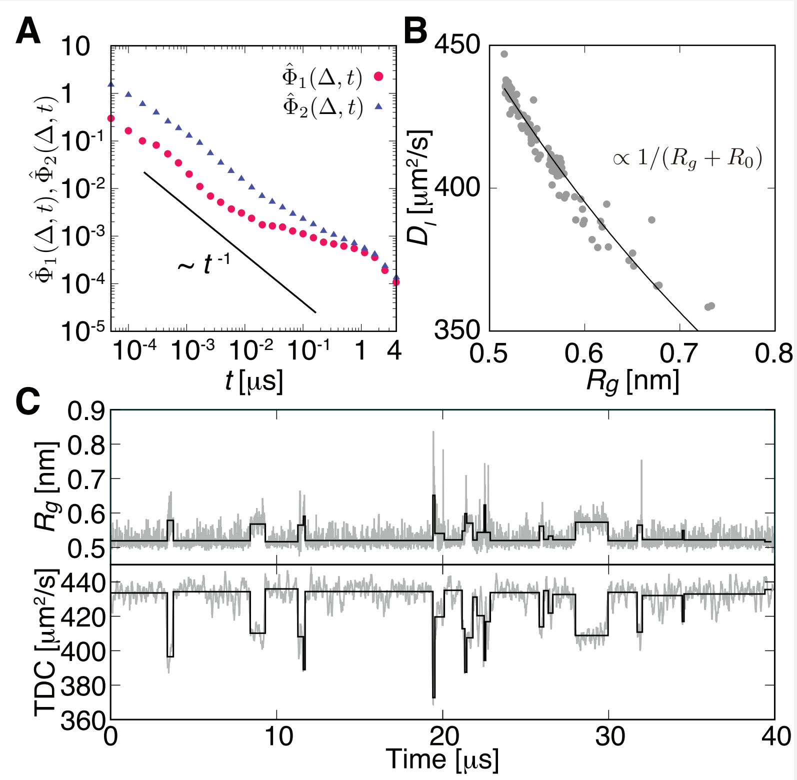
Instantaneous diffusivity of shape-fluctuating proteins



Instantaneous Einstein-Stokes-type relation (for different pressure & temperature):

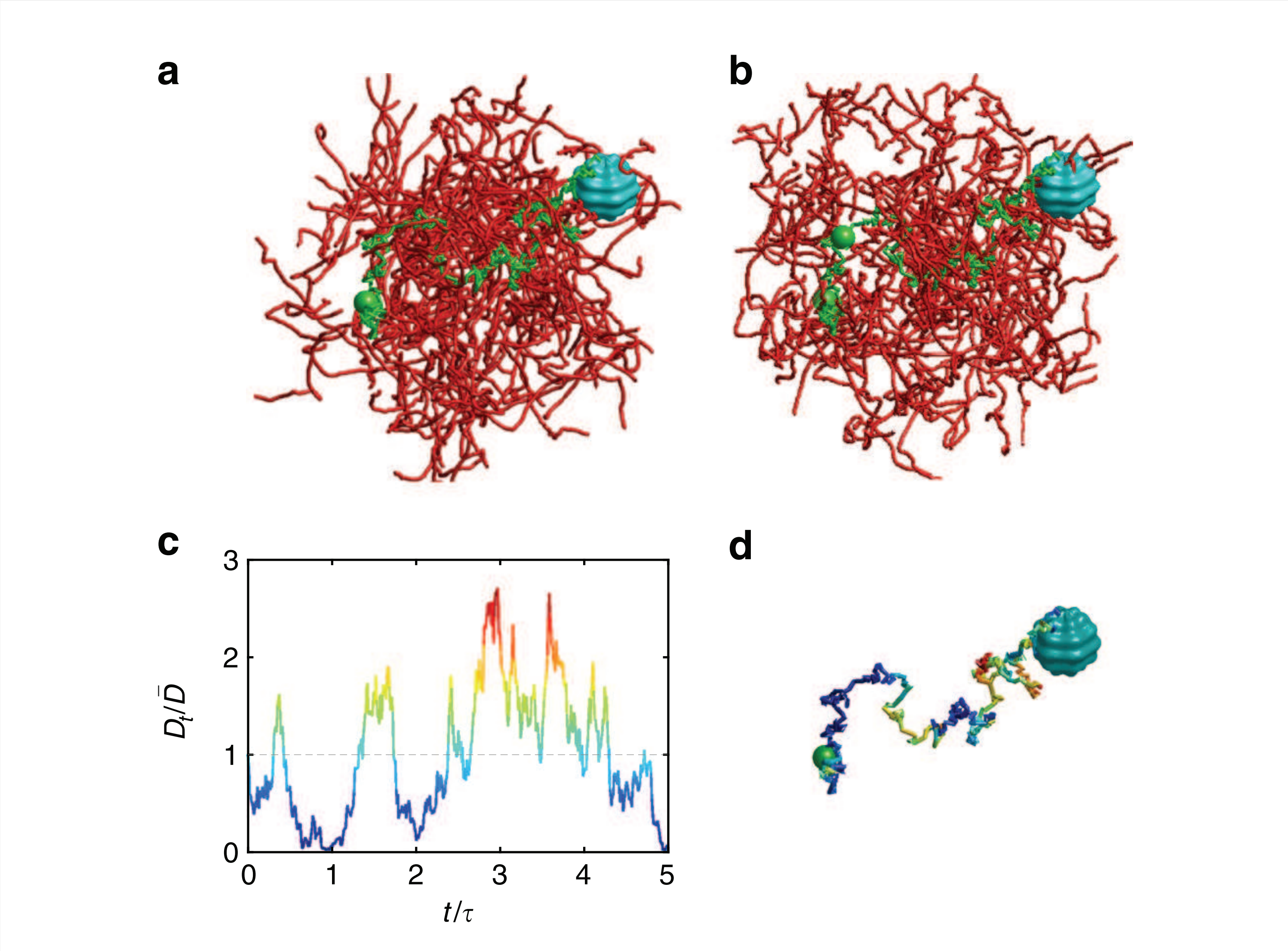
$$D \propto \frac{1}{R_g + R_0}, \quad R_0 \approx 0.3\text{nm}$$





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

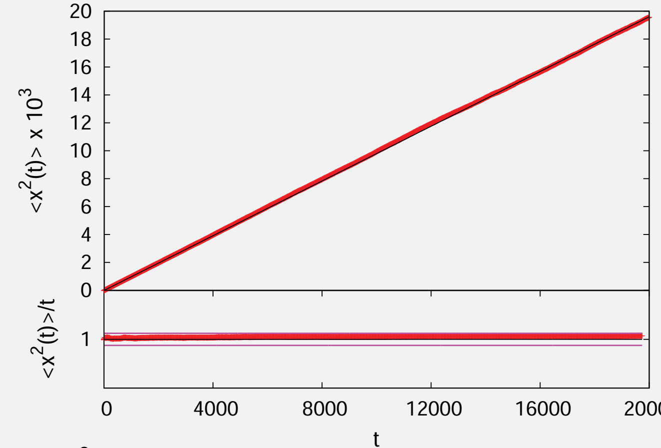
"Annealed" diffusing-diffusivity in rearranging heterogeneous enironment



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

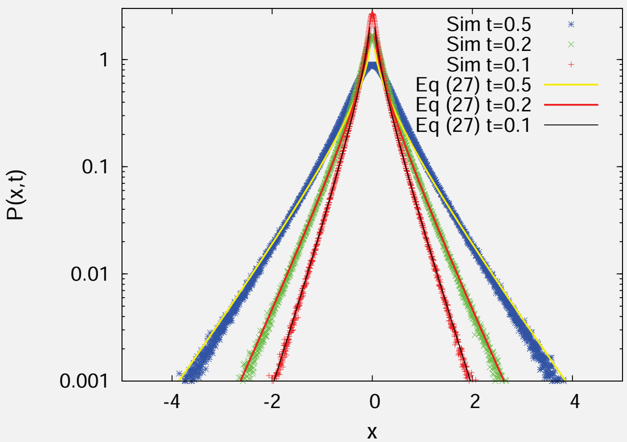
Fickian, non-Gaussian diffusion with diffusing diffusivity

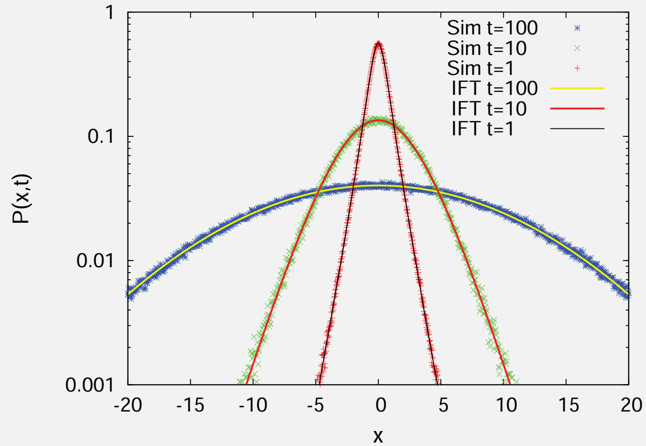
MV Chubinsky & G Slater, PRL (2014): diffusing diffusivity
[see also R Jain & KL Sebastian, JPC B (2016)]

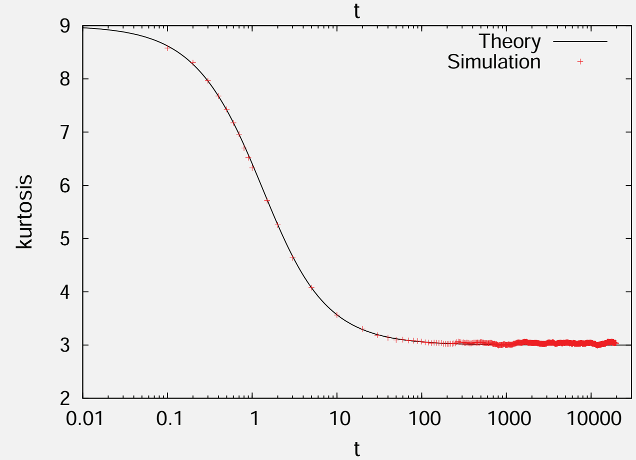


Our minimal model for diffusing diffusivity:

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





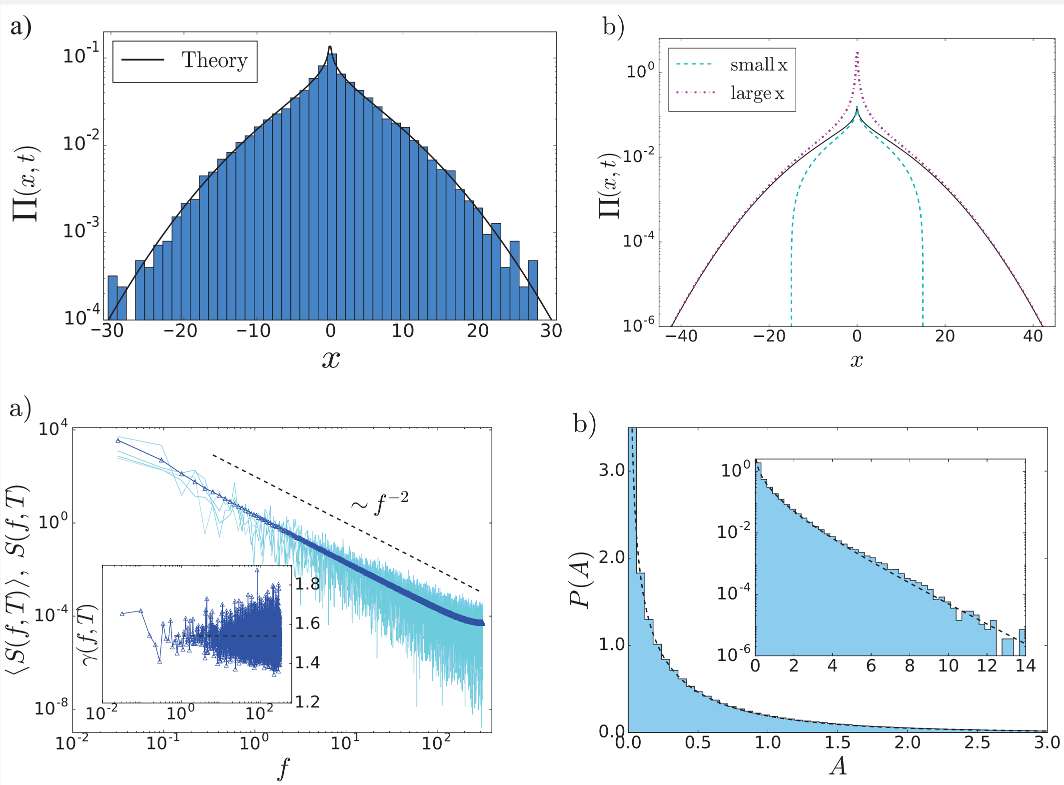


Generalised γ distribution & non-equilibrium diffusivity initial conditions: V Sposini, AV Chechkin, G Pagnini, F Seno & RM, NJP (2018)

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

Random-diffusivity models for non-Gaussian diffusion

1. Multimerisation of tracer [F Baldovin, F Seno & E Orlandini, Frontiers (2019); M Hidalgo-Soria & E Barkai, PRE (2020)]
2. Two-state model [A Sabri, X Xu, D Krapf & M Weiss, PRL (2020)]
3. Extreme value statistic of tails for small # jumps [E Barkai & S Burov, PRL (2020)]
4. Compartmenalisation model with partial reflectivity [J Ślęzak & S Burov, Sci Rep (2021)]
5. Jump processes & functionals of Brownian motion [V Sposini, D Grebenkov, RM, G Oshanin & F Seno, NJP (2020)]



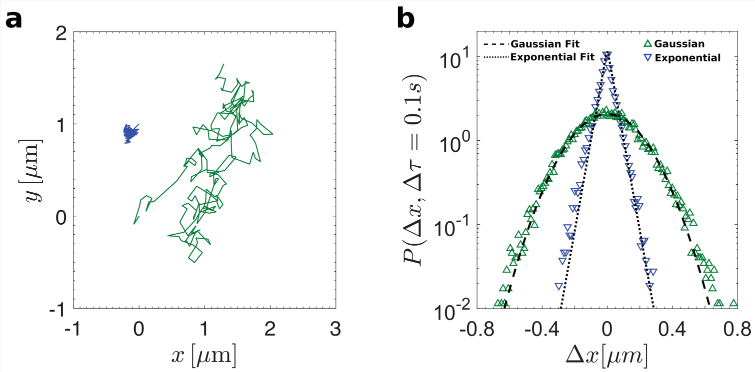
$$\dot{x}_t = \sqrt{2D_0\Psi_t}\xi_t \quad \therefore$$

Rectified BM: $\Psi_t\Theta(B_t)$:

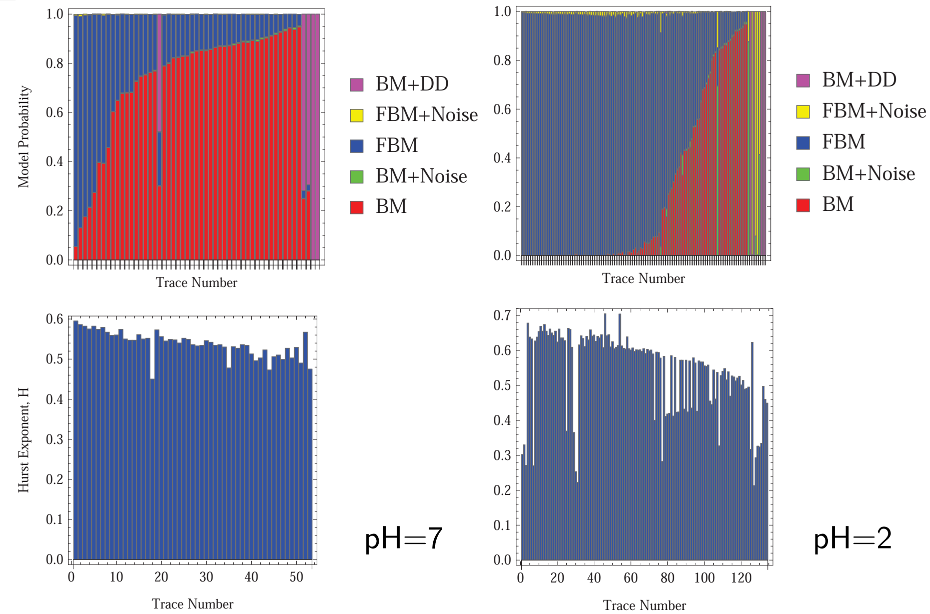
$$P(x,t) = \frac{\exp(-x^2/[8D_0t])}{2\sqrt{\pi^3 D_0 t}} \times K_0\left(\frac{x^2}{8D_0t}\right)$$

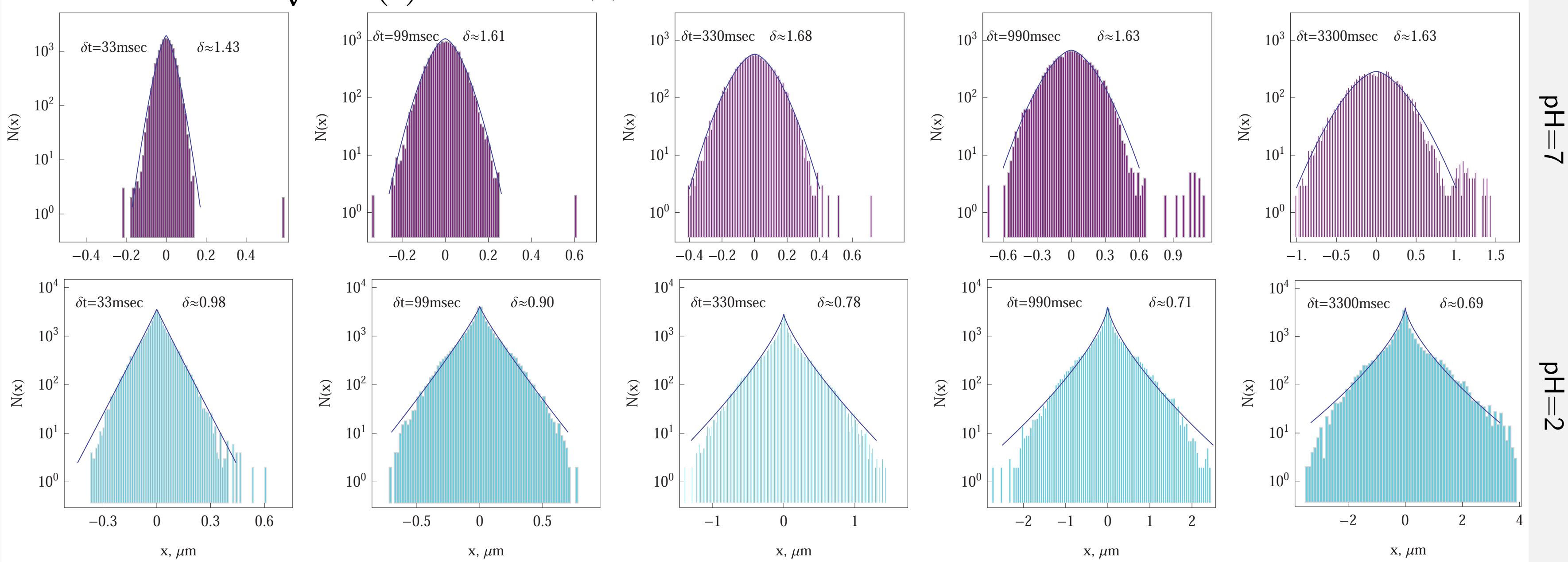
Non-Gaussian & non-Fickian diffusion in mucin hydrogels

CE Wagner et al, Biomacromol (2017)

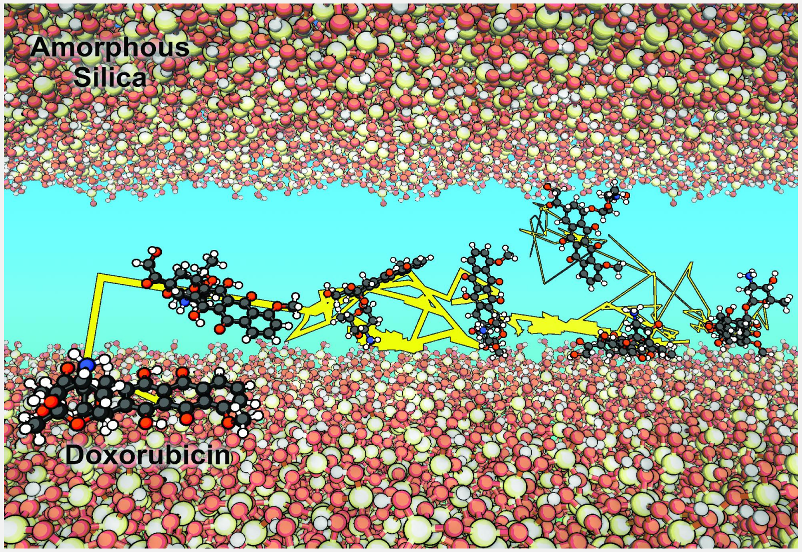


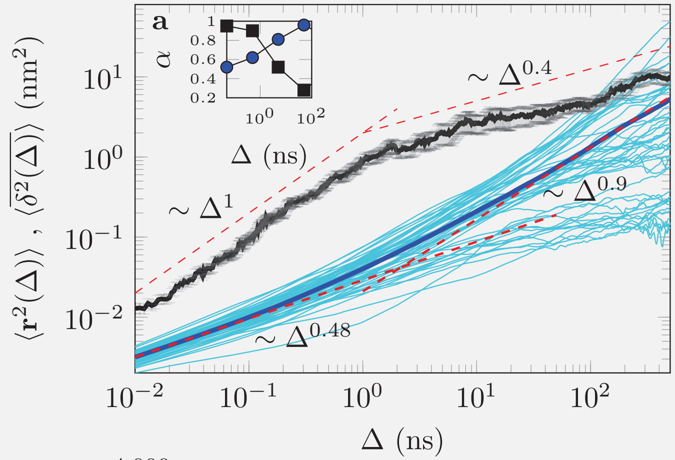
$$P(x,t) = \frac{A}{\sqrt{2\pi\sigma^2(t)}} \exp\left(-\frac{x^2}{2\sigma^2(t)}\right) + \frac{1-A}{\sqrt{4\lambda^2(t)}} \exp\left(-\frac{|x|}{\lambda(t)}\right)$$

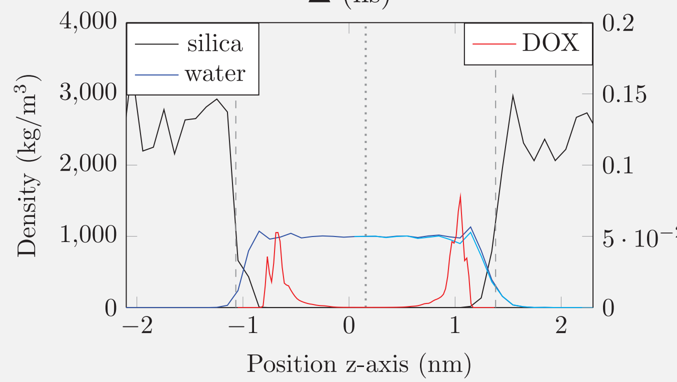


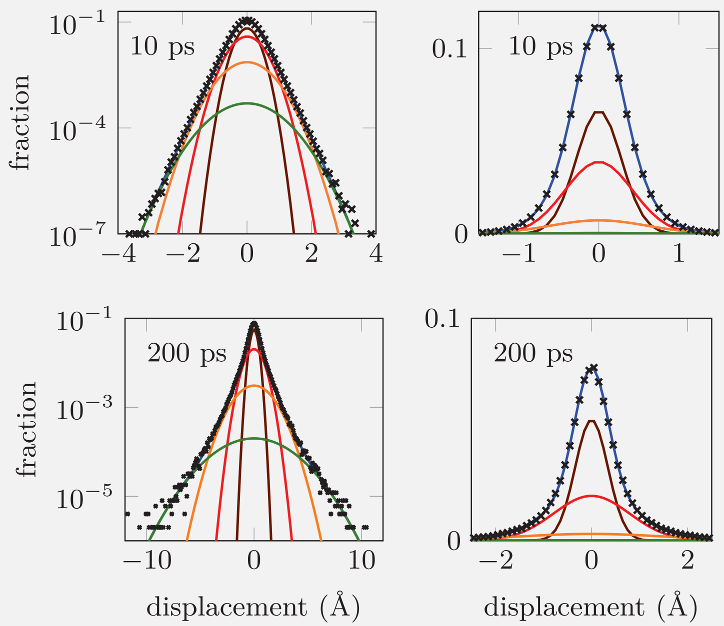


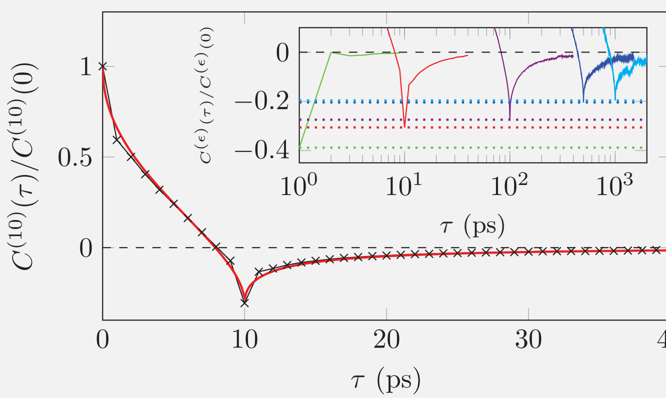
Doxorubicin drug molecule diffusion in silica nanochannels









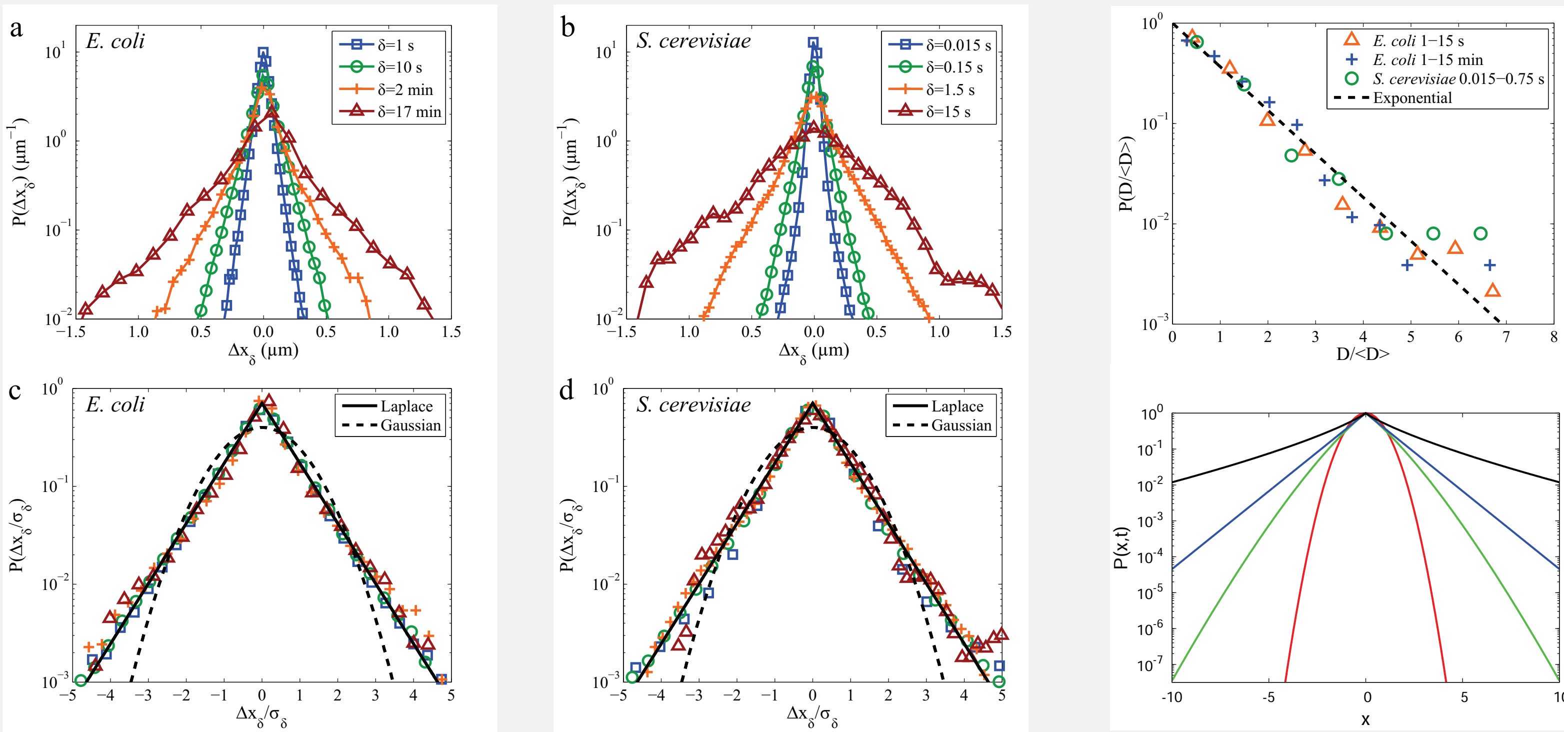


A Díez Fernández, P Charchar, AG Cherstvy, RM & MW Finnis, PCCP (2020)

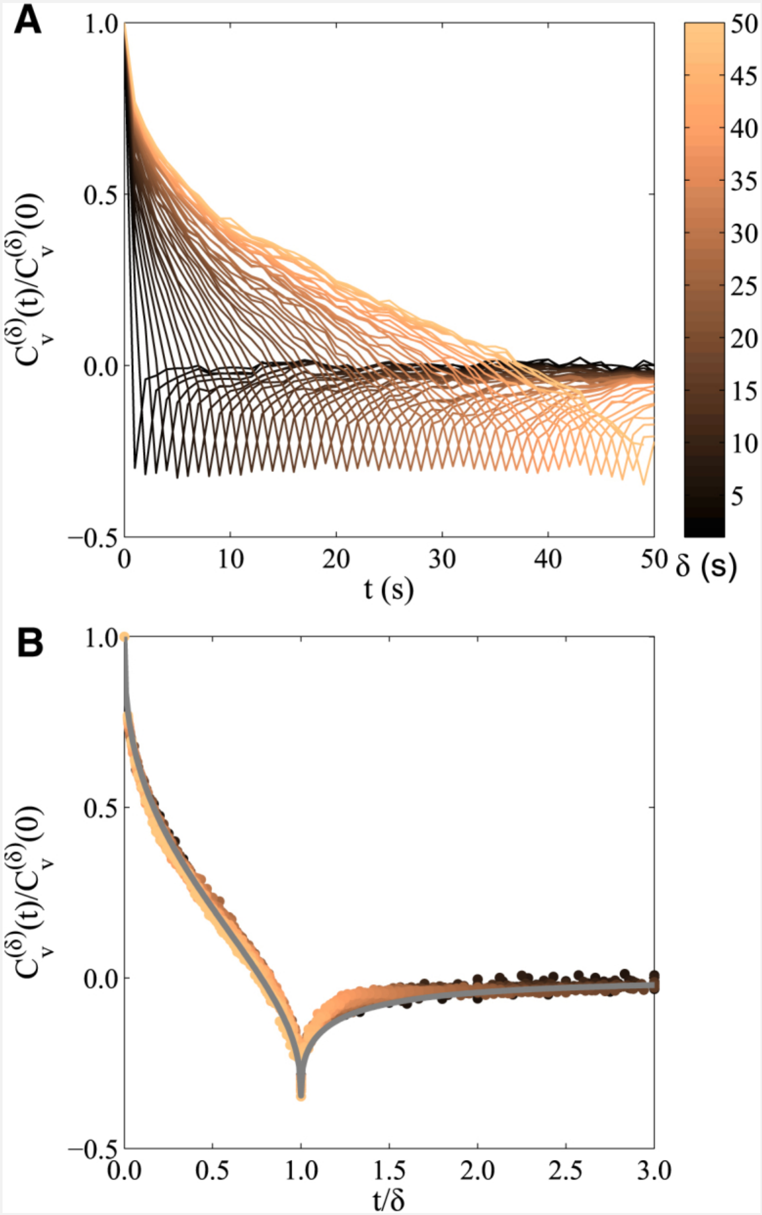
Non-Gaussian diffusion in viscoelastic systems

Passive motion of submicron tracers in the cytoplasm of living cells & crowded media is viscoelastic [L Oddershede & RM, PRL (2011); JH Jeon, N Leijnse, L Oddershede & RM, NJP (2013)]

RNA-protein particles in E.coli & S.cerevisiae perform exponential anomalous diffusion:



Non-Gaussian diffusion in viscoelastic systems



TJ Lampo, S Stylianidou, MP Backlund, PA Wiggins & AJ Spakowitz, BPJ (2017); N&V: RM, BPJ (2017)


Diverted
traffic
Diverted
traffic
Diverted
Traffic

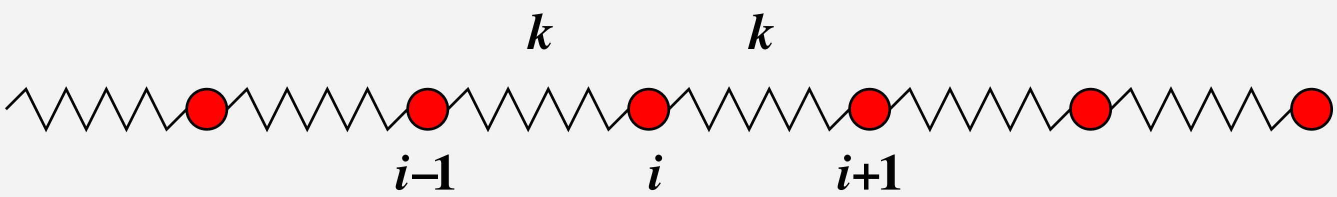
Fractional Langevin equations in viscoelastic systems

Coupled set of Markovian processes (e.g., Rouse model for polymers):

$$m_i\ddot{\mathbf{r}}_i(t) = k(\mathbf{r}_i - \mathbf{r}_{i+1}) + k(\mathbf{r}_{i-1} - \mathbf{r}_i) - \eta\dot{\mathbf{r}}_i + \sqrt{2\eta k_B T} \times \boldsymbol{\zeta}_i(t)$$

Integrating out all d.o.f. but one ↷ Generalised Langevin equation (GLE):

$$m\ddot{\mathbf{r}}(t) + \int_0^t \eta(t - t')\dot{\mathbf{r}}(t')dt' = \boldsymbol{\zeta}(t) \therefore \eta(t) = \sum_{i=1}^{N} a_i(k)e^{-\nu_i t} \to t^{-\alpha}$$



Kubo fluctuation dissipation theorem (in conti limit $\eta(t) \simeq t^{-\alpha}$ fractional Gaussian noise):

$$\langle \zeta_i(t)\zeta_j(t')\rangle = \delta_{ij} k_B T \eta(|t - t'|)$$

↷ fractional Langevin equation. Overdamped limit: Mandelbrot's FBM

Quantum mechanics: Nakajima-Zwanzig equation using projection operators

Hydrodynamics: Basset force with $\eta(t) \simeq t^{-1/2}$ due to hydrodynamic backflow

Viscoelastic diffusion $\langle \mathrm{r}^2(t)\rangle \simeq K_\alpha t^\alpha$ is asymptotically ergodic

Fractional Langevin equation:

$$\ddot{\mathbf{r}}(t) + \int_0^t \eta(t-t')\dot{\mathbf{r}}(t')dt' = \boldsymbol{\zeta}(t)$$

with $\eta(t) = \sum_{i=1}^N a_i(k)e^{-\nu_i t} \to t^{-\alpha}$ &
$\langle \zeta_i(t)\zeta_j(t')\rangle = \delta_{ij}k_BT\eta(|t-t'|)$, Gauss

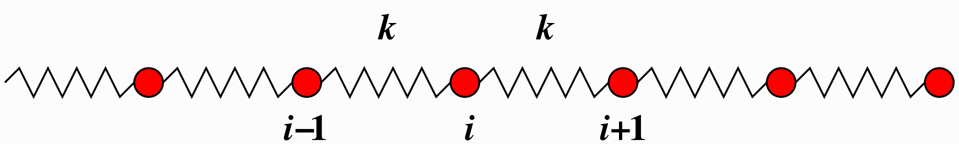
Fractional Brownian motion:

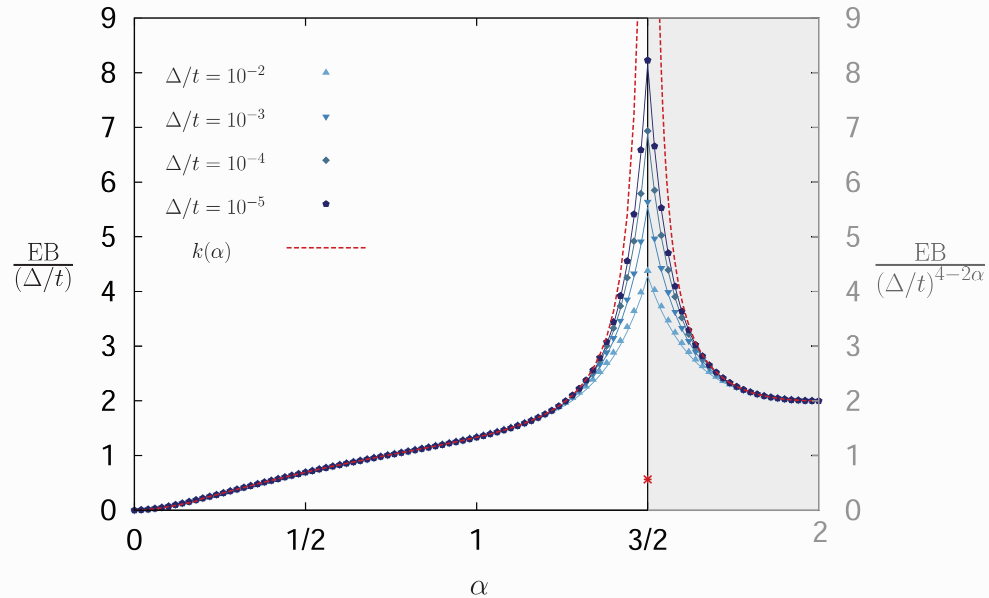
$$\dot{\mathbf{r}}(t) = \boldsymbol{\zeta}(t)$$

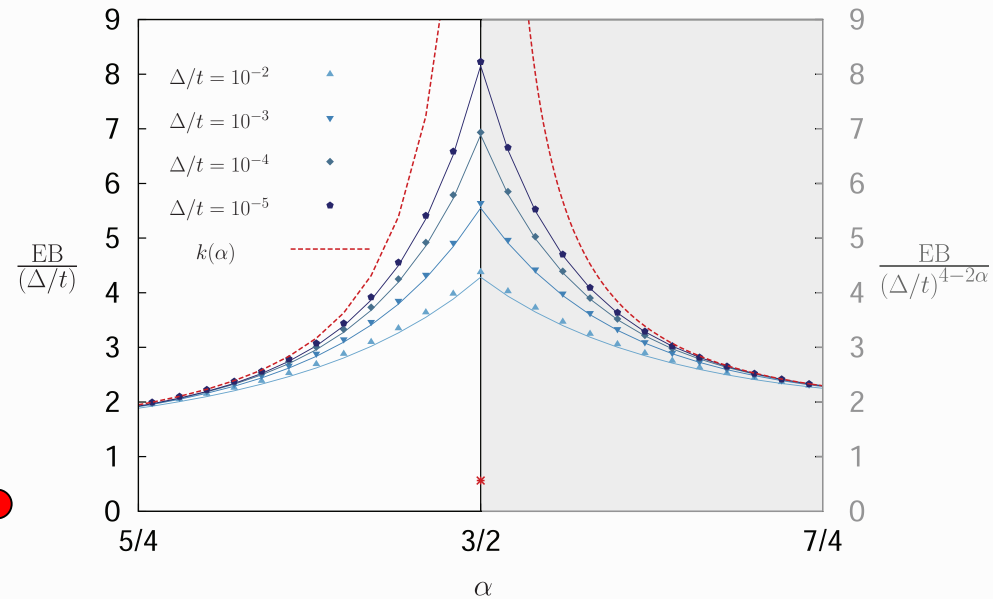
In both cases: $\lim_{T\to\infty}\overline{\delta^2(\Delta)} = \langle \mathrm{r}^2(\Delta)\rangle$

Ergodicity breaking parameter:

$$\mathrm{EB} = \langle \xi^2\rangle - 1, \xi = \overline{\delta^2(\Delta)} \Big/ \left\langle \overline{\delta^2(\Delta)} \right\rangle$$







W Deng & E Barkai, PRE (2009); JH Jeon & RM, PRE (2010); M Schwarzl, A Godec & RM, Sci Rep (2017)

Fractional Brownian motion

FLE: fluctuation-dissipation $\rightsquigarrow$ asymptotic thermal equilibrium [books by Zwanzig, Kubo]

FBM: "external noise" for non-equilibrium systems or "open systems" [Klimontovich, Statistical physics of open systems]

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

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

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

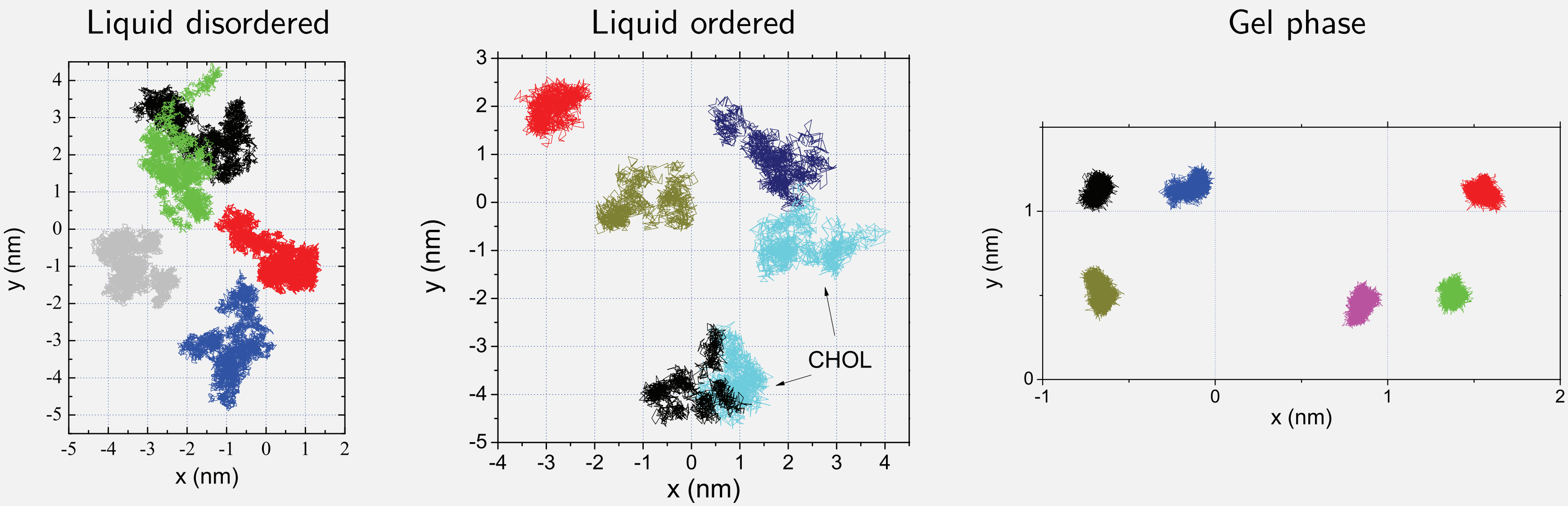
$$\langle \xi_H(t)\xi_H(t+\tau)\rangle = \frac{1}{2\delta}\Big(|t+\delta|^{2H} - 2|\tau|^{2H} + |t-\delta|^{2H}\Big) \sim H(2H-1)\tau^{2H-2}$$

Displacement correlator:

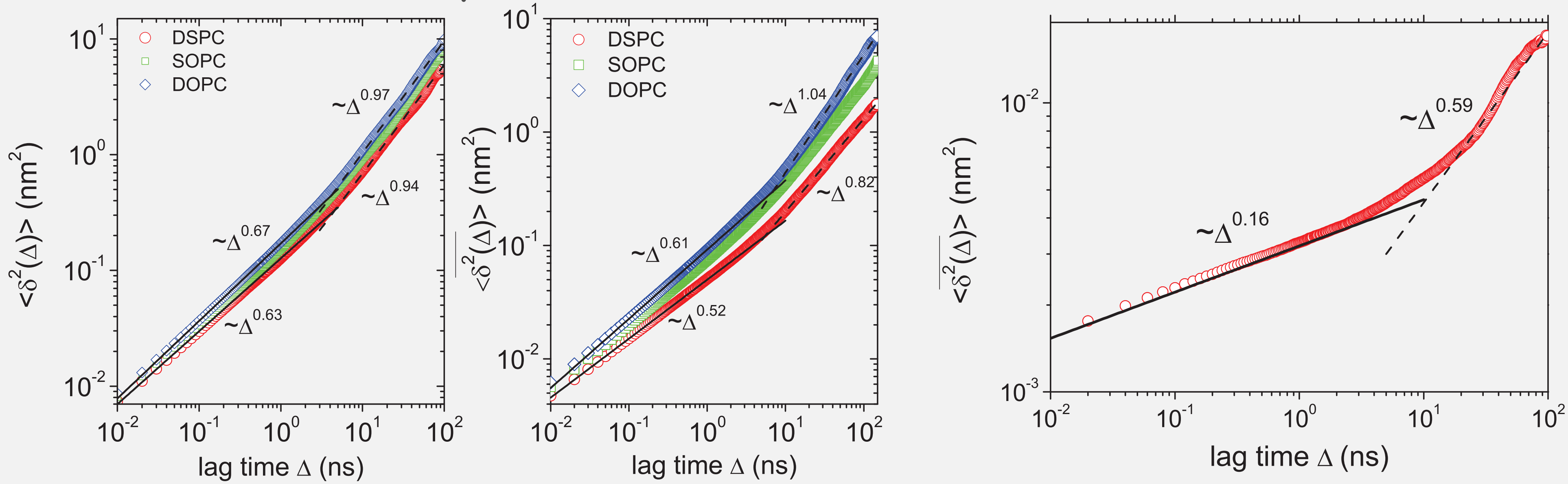
$$C_{\delta t}(t) = \frac{\langle[\mathbf{r}(t+\delta t) - \mathbf{r}(t)]\cdot \mathbf{r}(\delta t) - \mathbf{r}(0)]\rangle}{\delta t^2}$$

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

Sample trajectories for the lipid & cholesterol motion

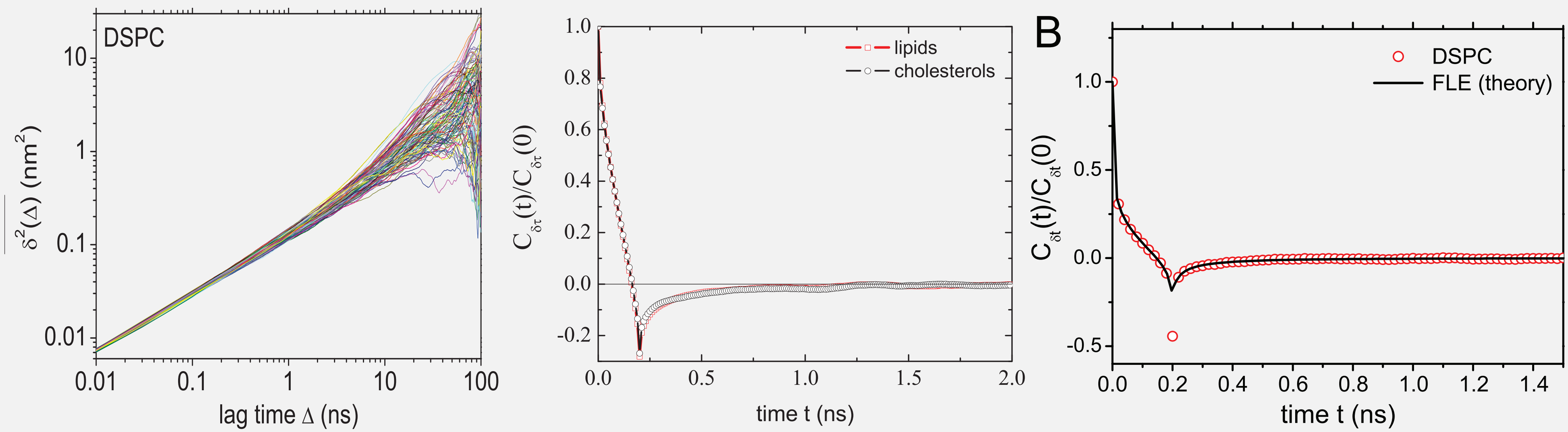


Liquid ordered/gel phases: extended anomalous diffusion

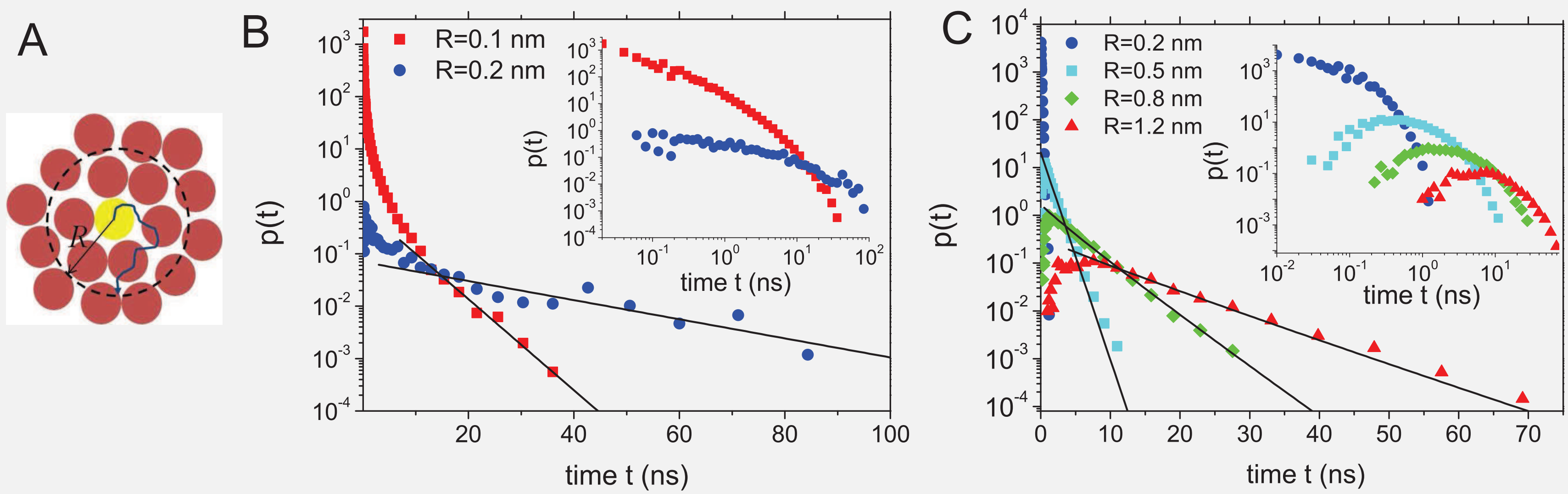


JH Jeon, H Martinez-Seara Monne, M Javanainen & RM, PRL (2012)

Reproducible TA MSD & antipersistent correlations

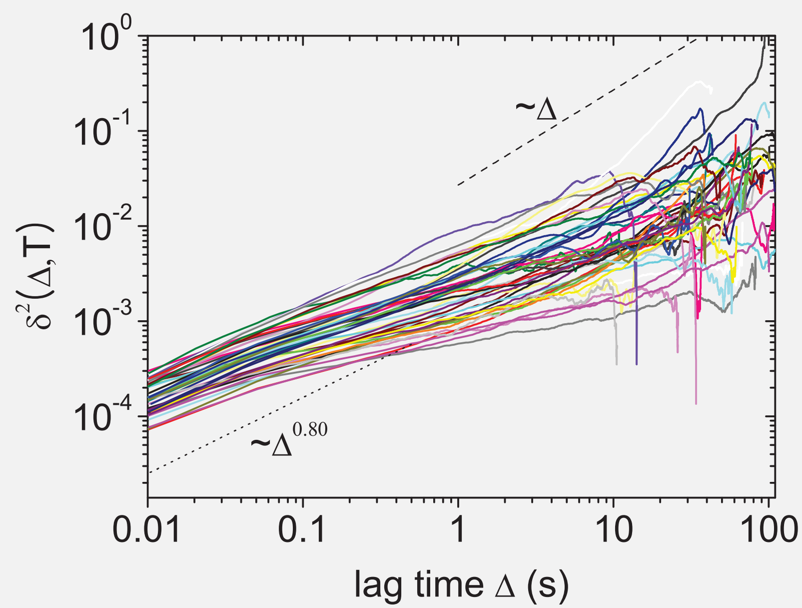


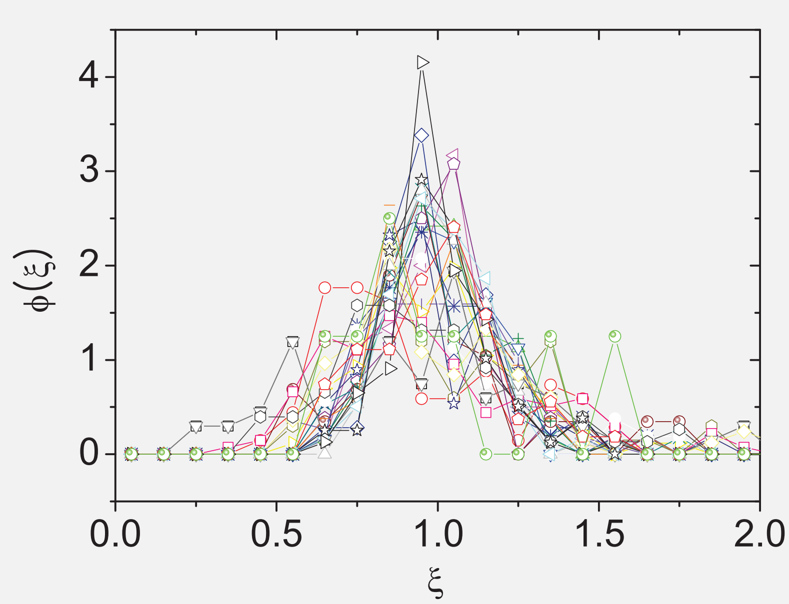
Rattling dynamics: exptl first passage PDF ↷ FLE motion



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

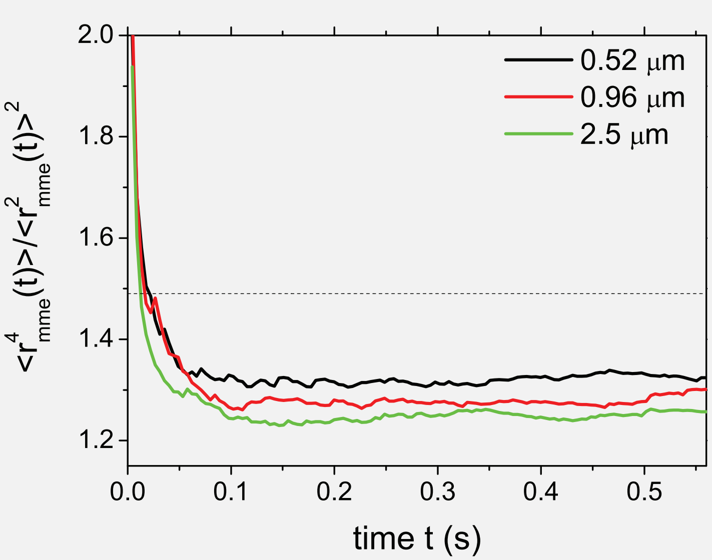
Passive motion of submicron tracers in cells is viscoelastic

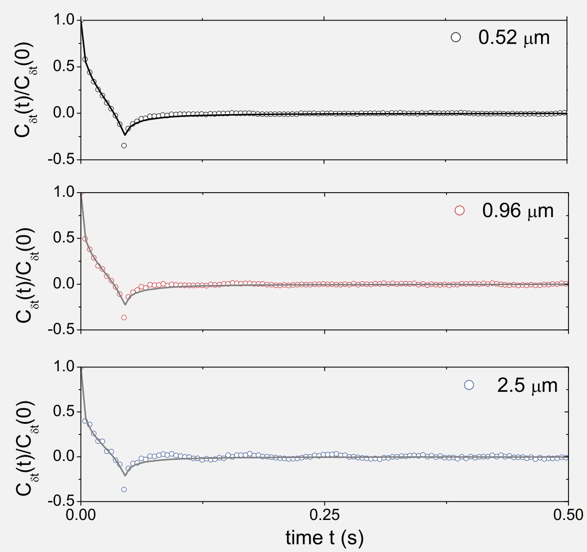


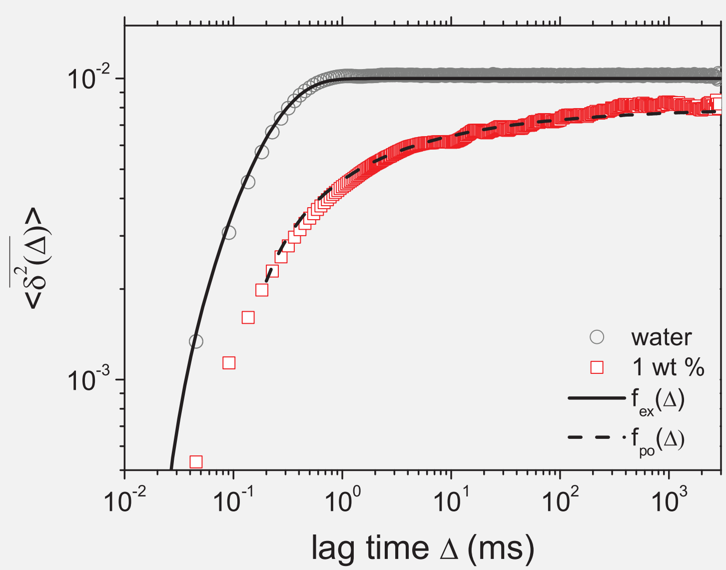


Lipid granules in living yeast cells ←

Tracer beads in wormlike micellar solution →

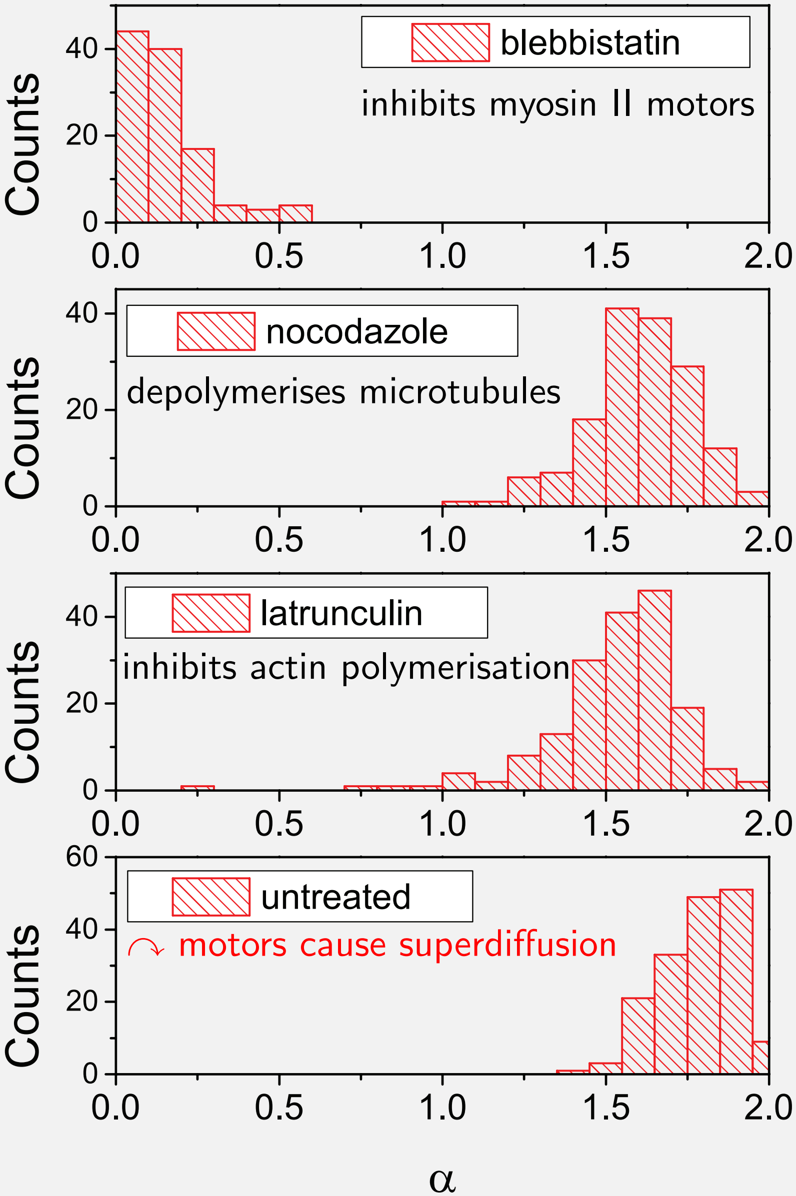


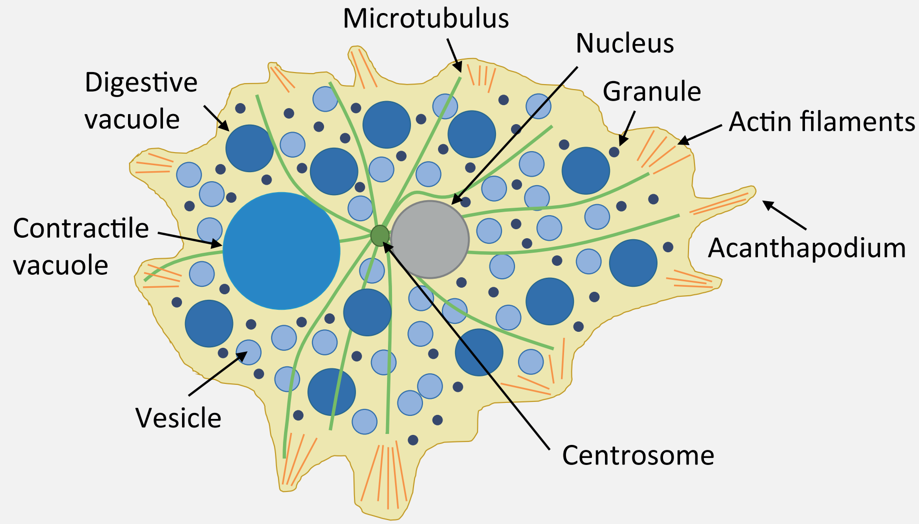


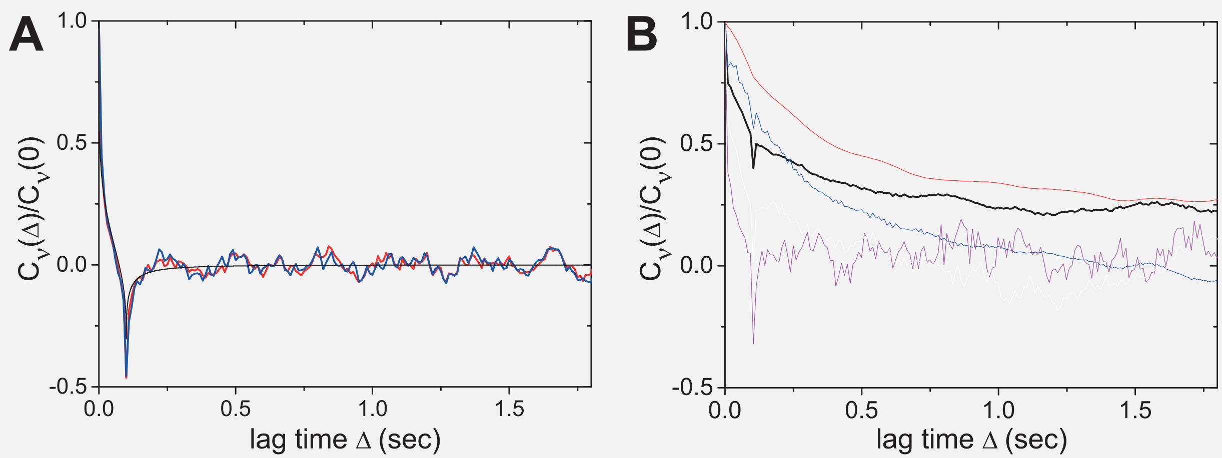


JH Jeon, . . . L Oddershede & RM, PRL (2011); JH Jeon, N Leijnse, L Oddershede & RM, NJP (2013)

Superdiffusion in supercrowded Acanthamoeba castellani





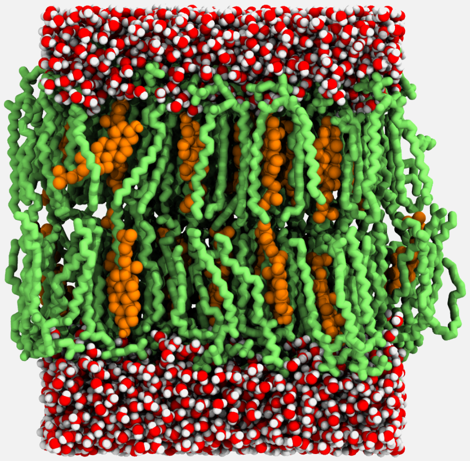


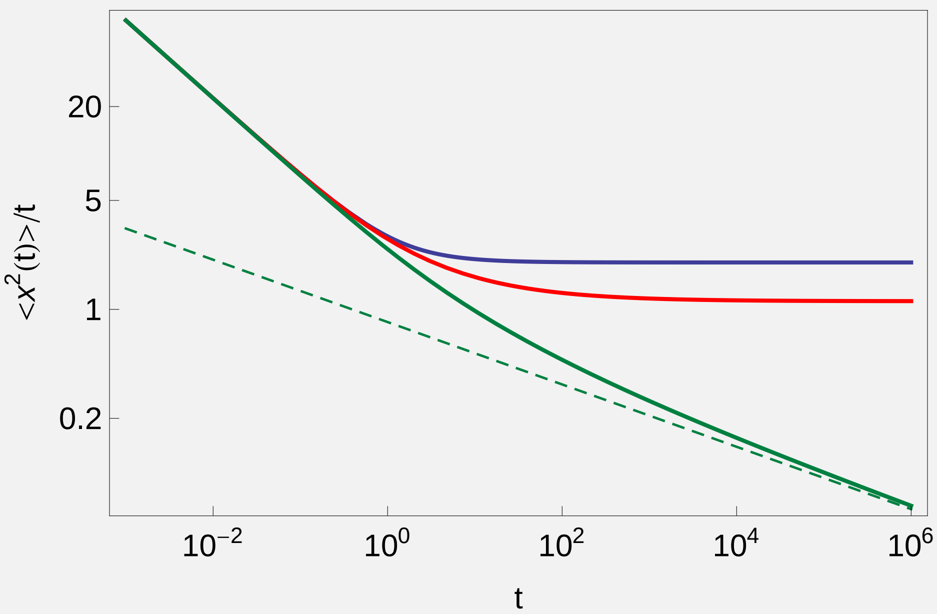
JF Reverey, J-H Jeon, H Bao, M Leippe, RM & C Selhuber-Unkel, Sci Rep (2015)

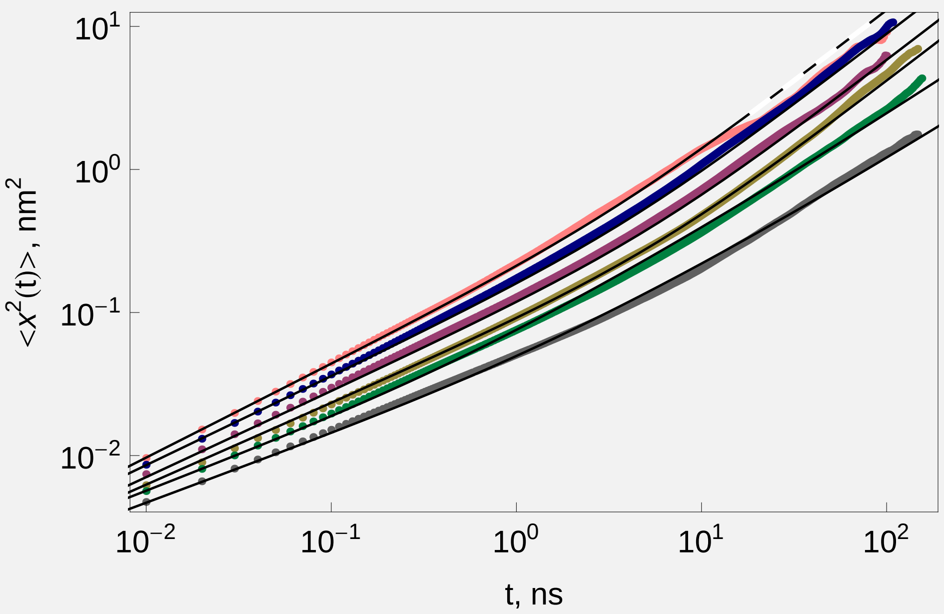
Tempered FLE motion: crossover to faster diffusion

Tempered fractional Gaussian noise:

$$\langle \xi(t)\xi(t+\tau)\rangle = \begin{cases} \dfrac{C}{\Gamma(2H-1)}\tau^{2H-2}e^{-\tau/\tau_\star} \\ \dfrac{C}{\Gamma(2H-1)}\tau^{2H-2}\left(1+\dfrac{\tau}{\tau_\star}\right)^{-\mu} \end{cases}$$



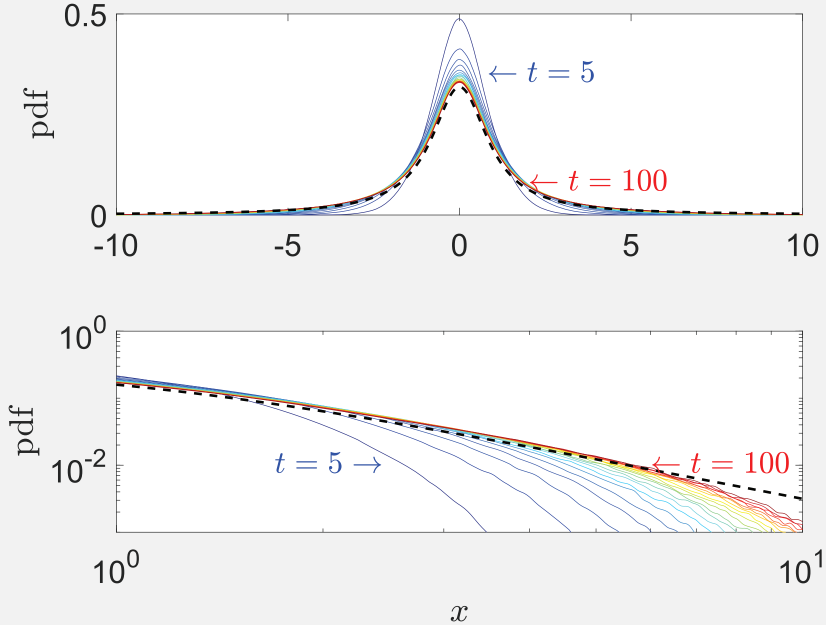


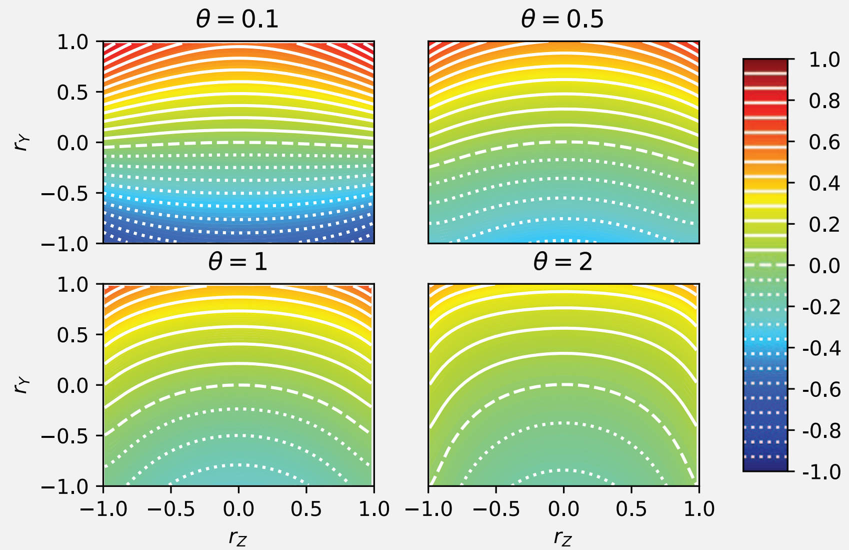


D Molina-Garcia, T Sandev, H Safdari, G Pagnini, AV Chechkin & RM, NJP (2018)


Umleitung
ca. Mai 2012 bis Nov. 2012
Stadeln
Fischer
berg
Erlangen
Stadelner Hauptstrasse
Umleitung
Fürth
Nürnberg
Regnitz
Vach
Atzenhof
U

Non-Gaussian dynamics in the presence of correlated noise

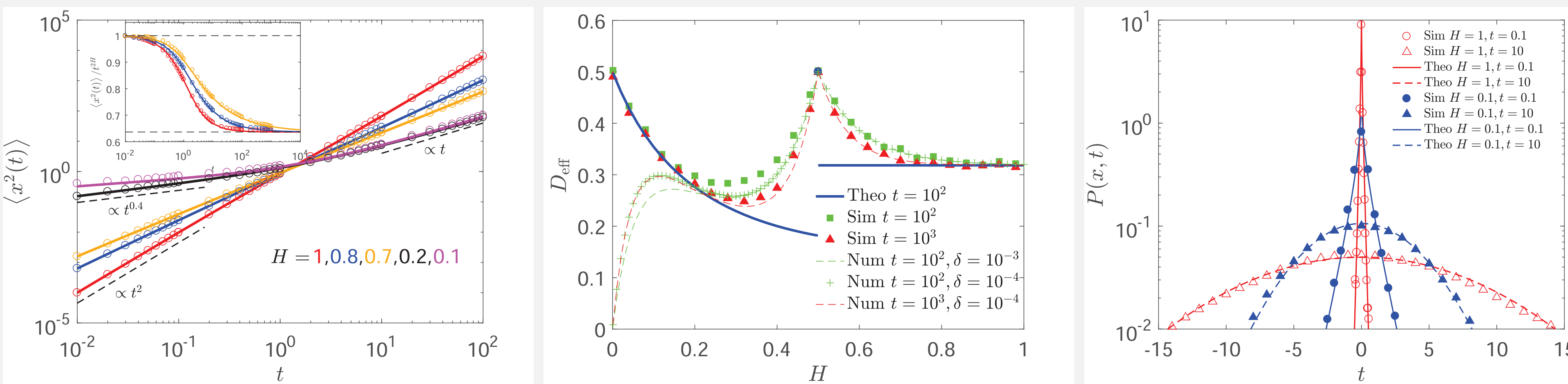




Codiffererence detects non-Gaussianity & non-ergodicity

Viscoelastic diffusing-diffusivity model

Prosecco-DD



J Ślęzak, M Magdziarz & RM, NJP (2018), NJP (2019); W Wang, AV Chechkin, F Seno, IM Sokolov & RM, NJP (2020)

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 $Y(t)$:

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

Here, $\eta(t)$ is white Gaussian noise with zero mean & unit variance

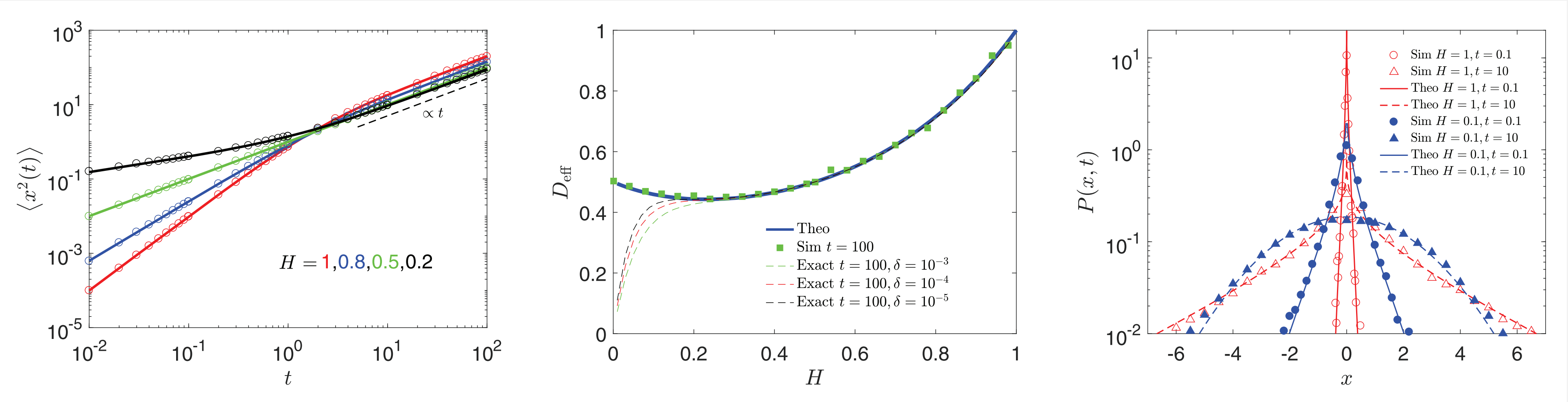
$\xi_H(t)$ is fractional Gaussian noise, understood as the derivative of the Mandelbrot-van Ness smoothed FBM [SIAM Rev (1968)]:

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

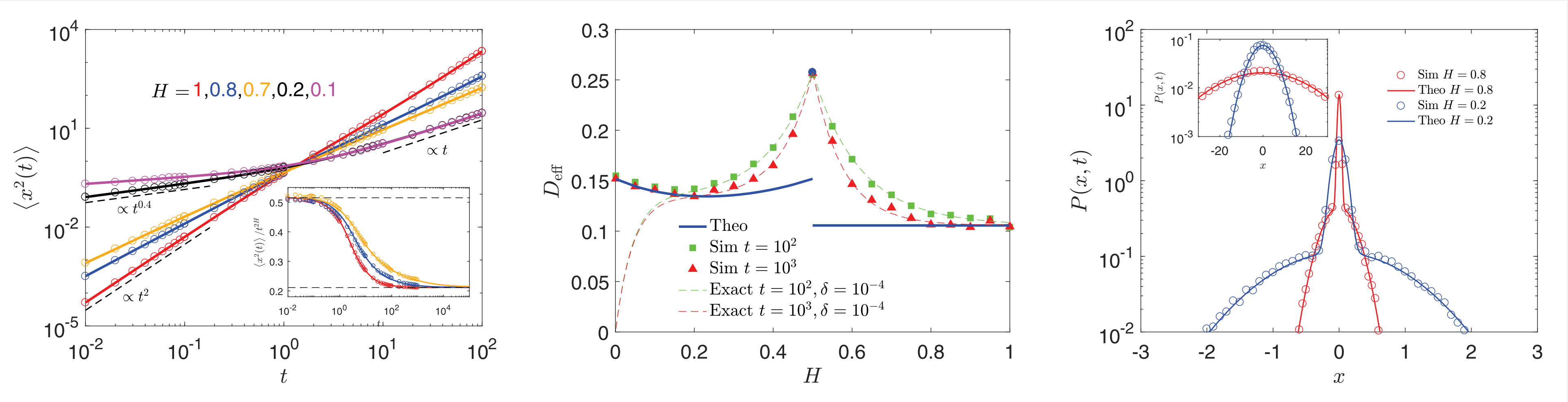
J Ślęzak, M Magdziarz & RM, NJP (2018), NJP (2019); W Wang, AV Chechkin, F Seno, IM Sokolov & RM, NJP (2020)

Viscoelastic diffusing-diffusivity model

Tyagi model

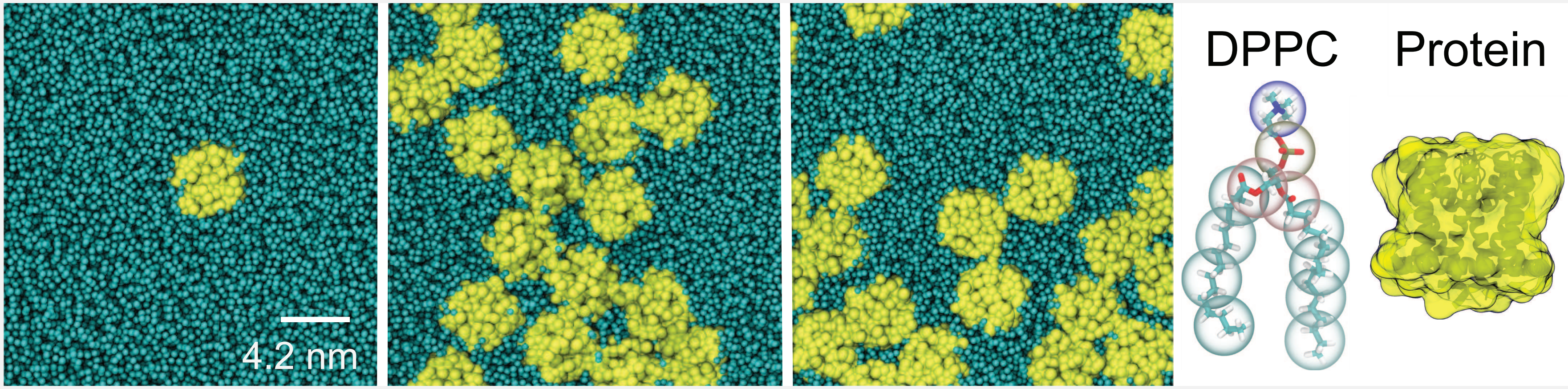


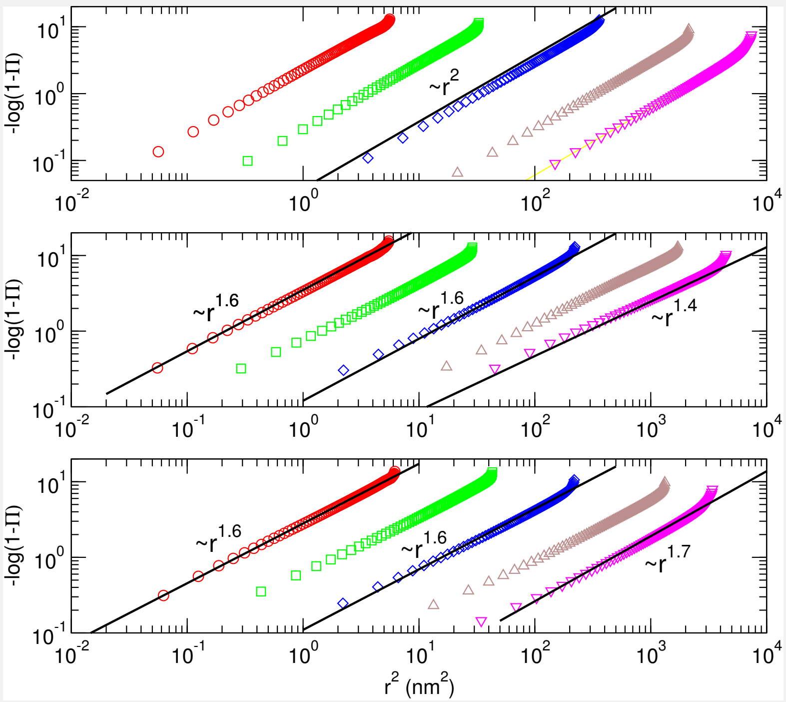
Switching model



J Ślęzak, M Magdziarz & RM, NJP (2018), NJP (2019); W Wang, AV Chechkin, F Seno, IM Sokolov & RM, NJP (2020)

Crowding in membranes: non-Gaussian lipid/protein diffusion

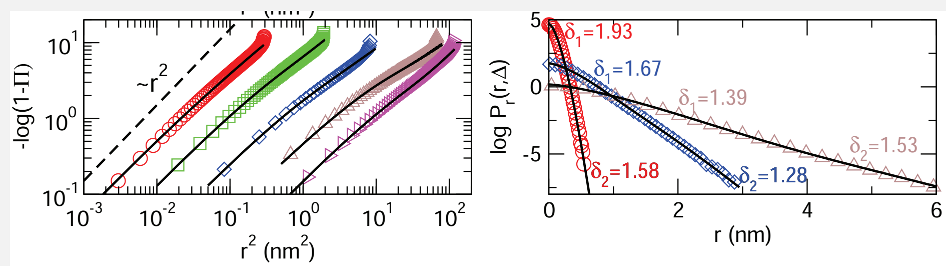




Dilute membrane: $P(r,t)$ Gauss

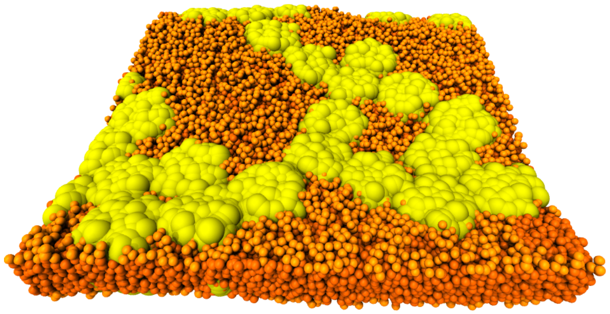
Crowded membrane ($\delta \approx 1.3 \ldots 1.7$):

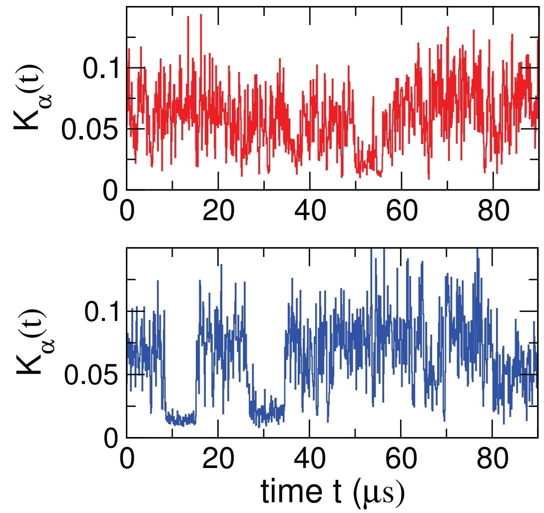
$$P(r,t) \propto \exp\left(-\left[\frac{r}{ct^{\alpha/2}}\right]^{\delta}\right)$$

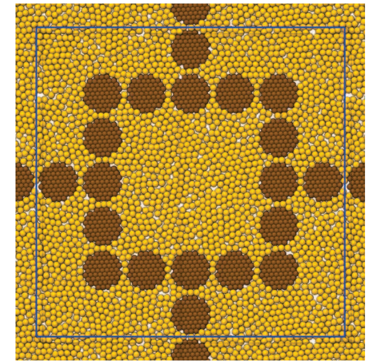


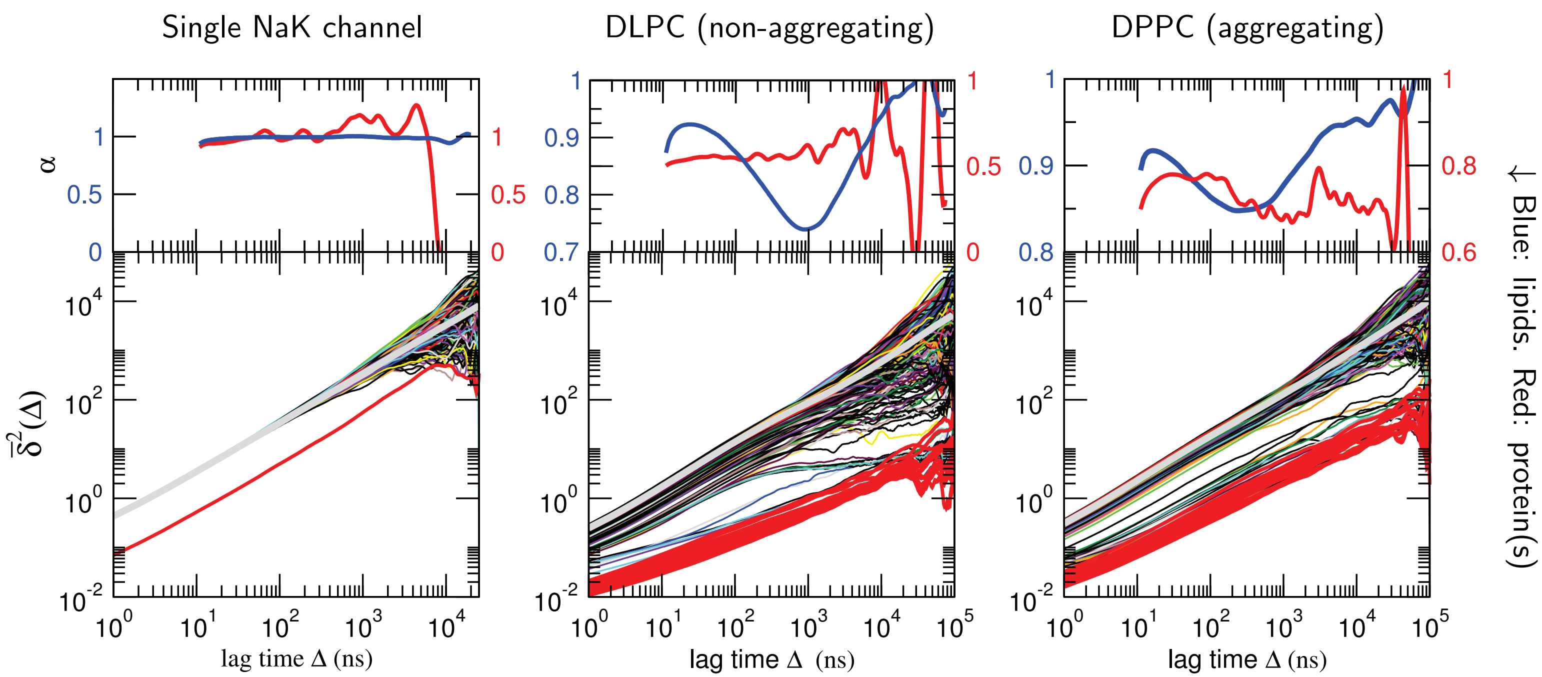
J-H Jeon, M Javanainen, H Martinez-Seara, RM & I Vattulainen, PRX (2016); compare Faraday Disc (2013)

Intermittent lipid diffusion in protein-crowded membranes



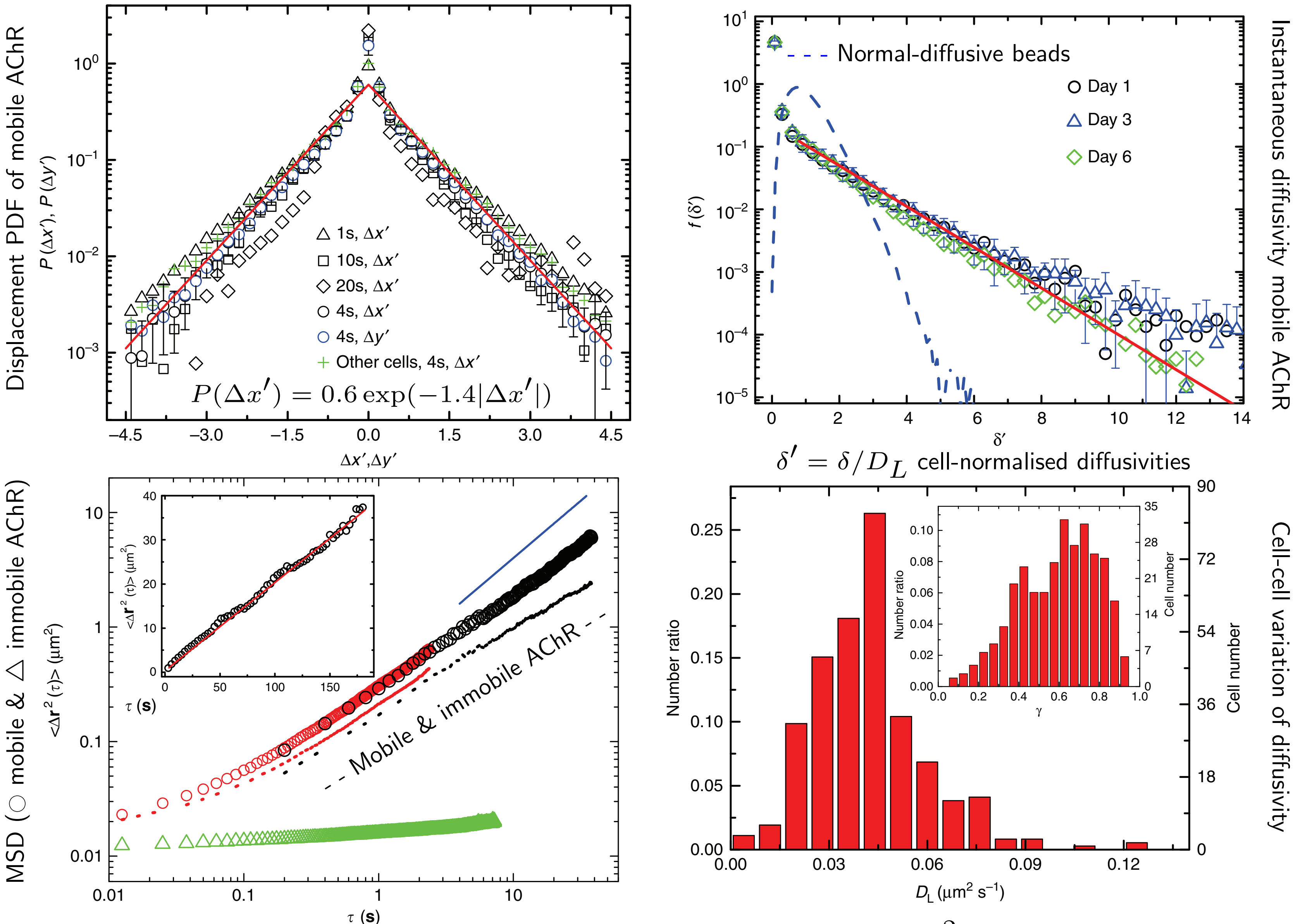






J-H Jeon, M Javanainen, H Martinez-Seara, RM & I Vattulainen, PRX (2016); compare Faraday Disc (2013)

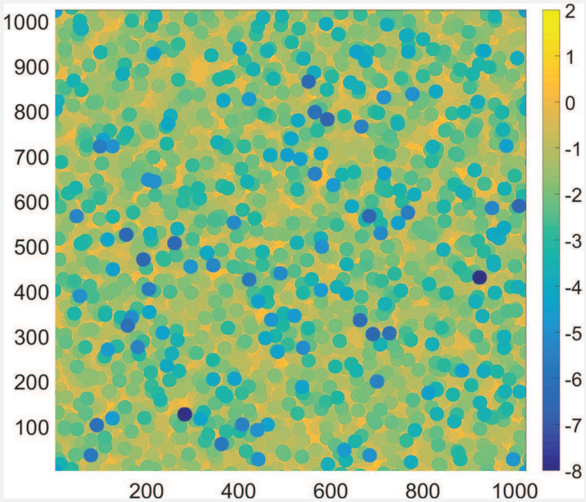
Non-Gaussianity of acetylcholine receptors in Xenopus cells

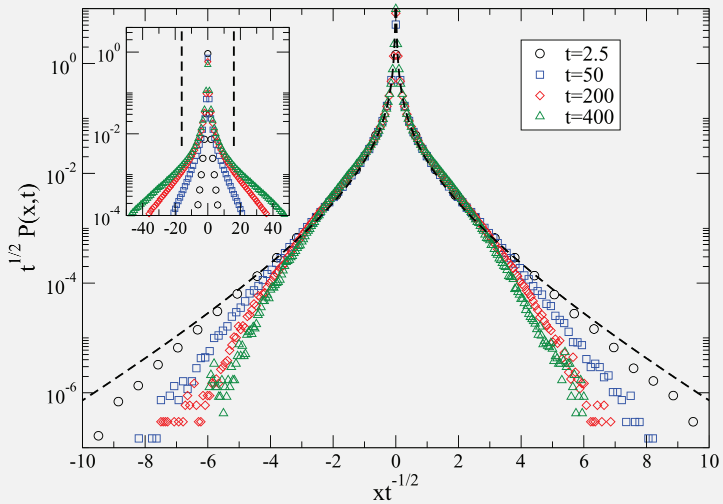


D_L from $\langle \mathbf{r}^2(\tau)\rangle = 2D_L\tau$

W He, H Song, Y Su, L Geng, BJ Ackerson, HB Peng & P Tong, Nat Comm (2016)

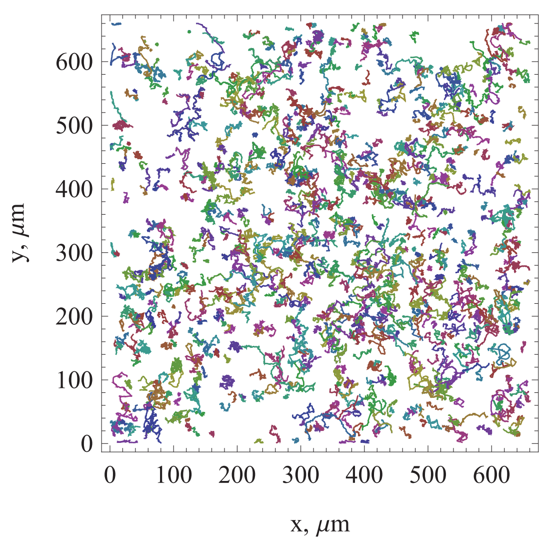
Non-Gaussian diffusion in quenched landscape models

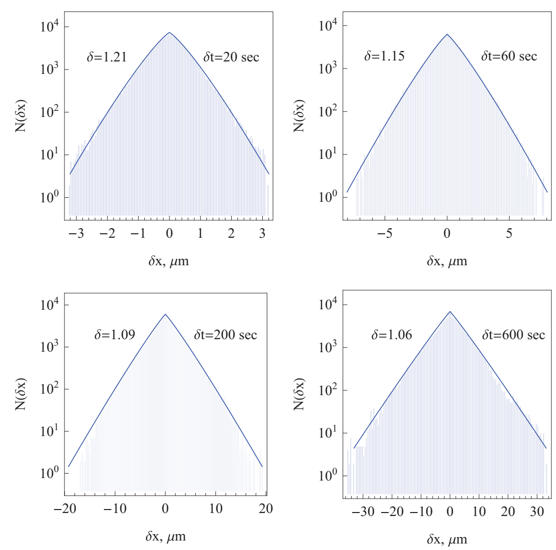


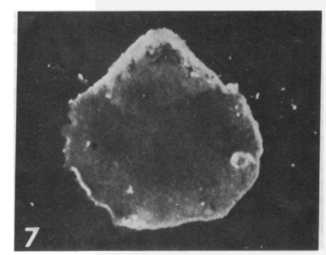


L Luo & M Yi, PRE (2018,2019); see also EB Postnikov, A Chechkin & IM Sokolov, NJP (2020)

Increasing non-Gaussianity in moving amoeba cells







AG Cherstvy, O Nagel, C Beta & RM, PCCP (2018)

Inertial and active Brownian particles /w distributed speeds

Inertial model [Mikhailov & Meinköhn (1997)]:

$$\dot{\mathbf{r}}(t) = v_0 \mathbf{e}_v, \quad \dot{\phi}(t) = \frac{\sqrt{2\sigma}}{m v_0}\Big(\xi_y \cos\phi - \xi_x \sin\phi\Big)$$

$$\langle \Delta \mathbf{r}^2(t) \rangle = \frac{2 v_0^4 m^2 t}{\sigma} + \frac{v^6 m^4}{\sigma^2}\left[\exp\left(-\frac{2\sigma t}{m^2 v_0^2}\right) - 1\right] \sim v_0^2 t^2 \ldots \frac{2 v_0^4 m^2}{\sigma} t$$

Active Brownian particle [Sevilla & Sandoval (2015)]:

$$\dot{\mathbf{r}}(t) = v_0 \mathbf{e}_v + \sqrt{2 D_T} \boldsymbol{\xi}_T(t), \quad \dot{\phi}(t) = \sqrt{2 D_R} \xi_R(t)$$

$$\langle \Delta \mathbf{r}^2(t) \rangle \sim 4 D_T t + (2 D_T D_R + v_0^2) t^2 \ldots 4\left(D_T + \frac{v_0^2}{2 D_R}\right) t$$

Consider (i) distribution of diffusivities $p(D)$ or (ii) of speeds $p(v_0)$

Inertial and active Brownian particles /w distributed speeds

Inertial case:

$$p(D) = \frac{1}{D_\star}\exp\left(-\frac{D}{D_\star}\right) \quad \rightsquigarrow \quad P(\mathbf{r},t) = \frac{2v_0^4 t}{\pi D_\star(\mathbf{r}^2 + 2v_0^4 t/D_\star}$$

To get asymptotic exponential PDF: Inertial case uses Weibulll-$p(v)$

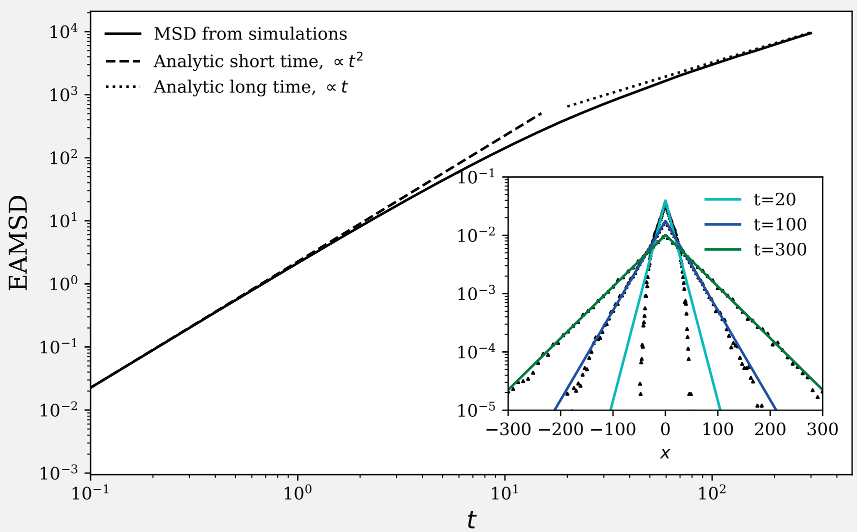
$$p(v) = \frac{4v^3}{2DD_\star^{\text{eff}}}\exp\left(-\frac{v^4}{2DD_\star^{\text{eff}}}\right)$$

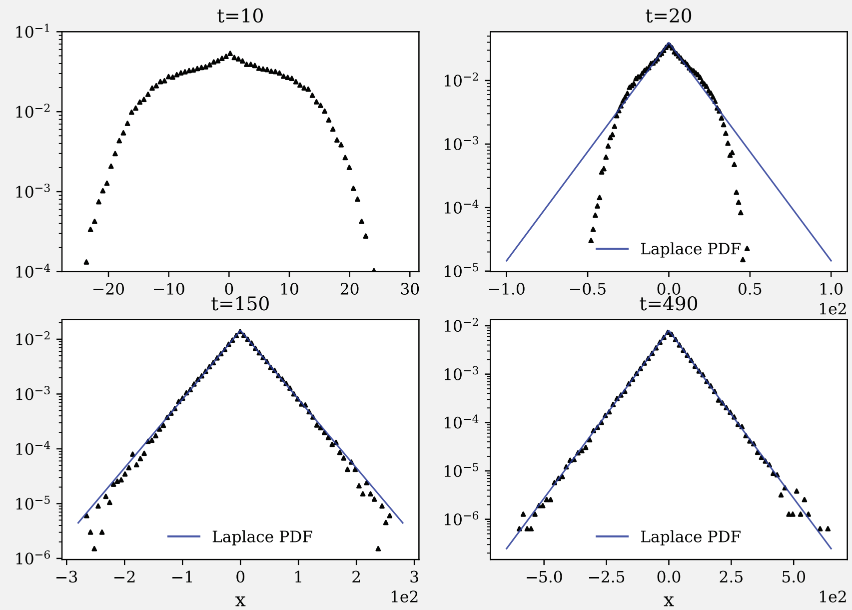
ABP Rayleigh-$p(v)$:

$$p(v) = \frac{\exp(-D_T/D_\star^{\mathbf{eff},o})}{D_R D_\star^{\mathbf{eff},o}} v \exp\left(-\frac{v^2}{2D_R D_\star^{\mathbf{eff},o}}\right)$$

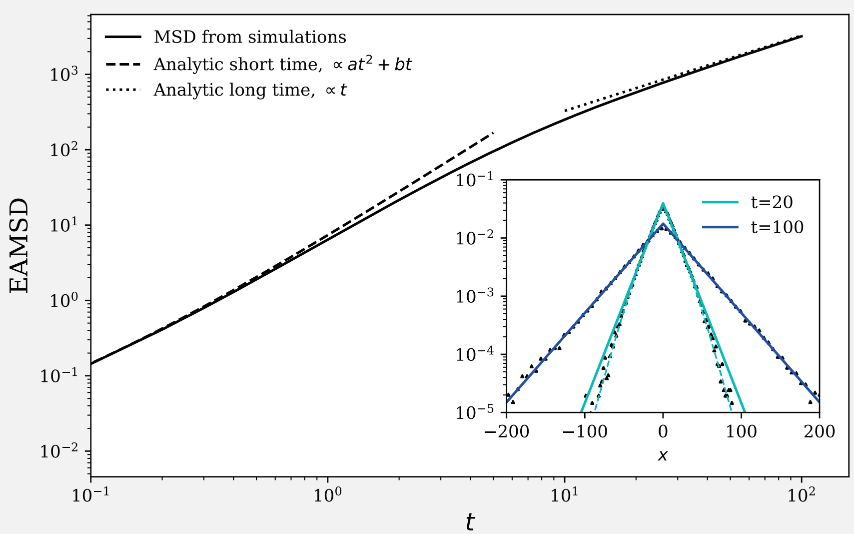
Inertial and active Brownian particles /w distributed speeds

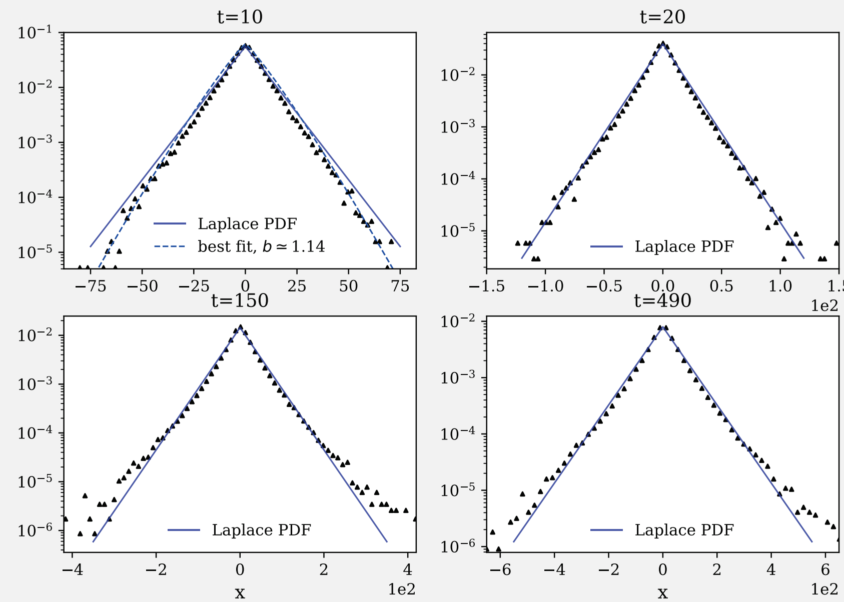
Inertial





ABP

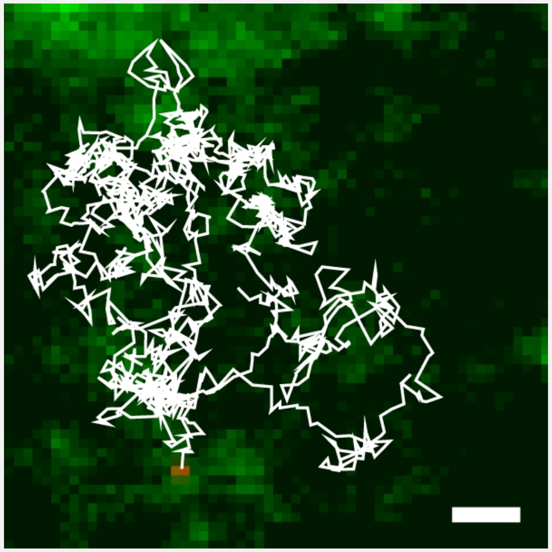


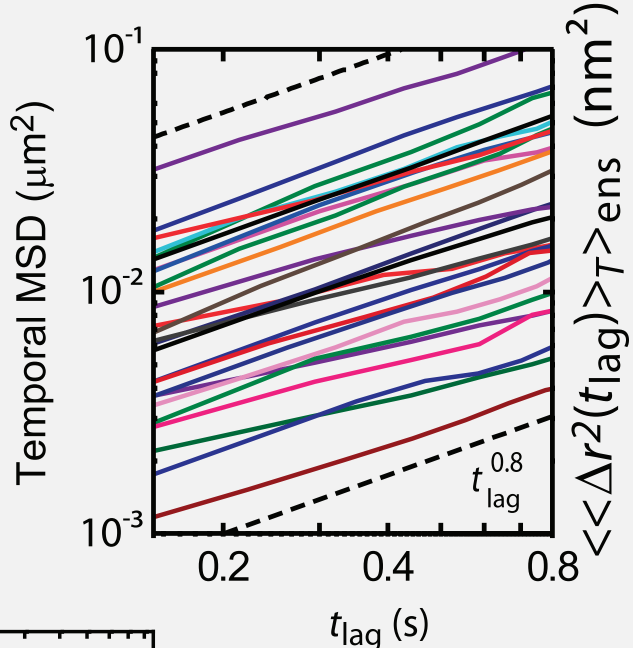


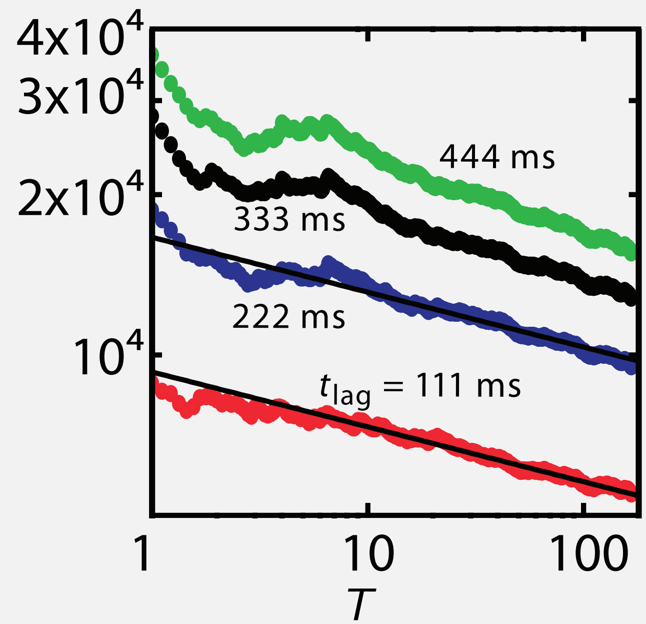
E Lemaitre, AV Chechkin, IM Sokolov & RM, (2022)

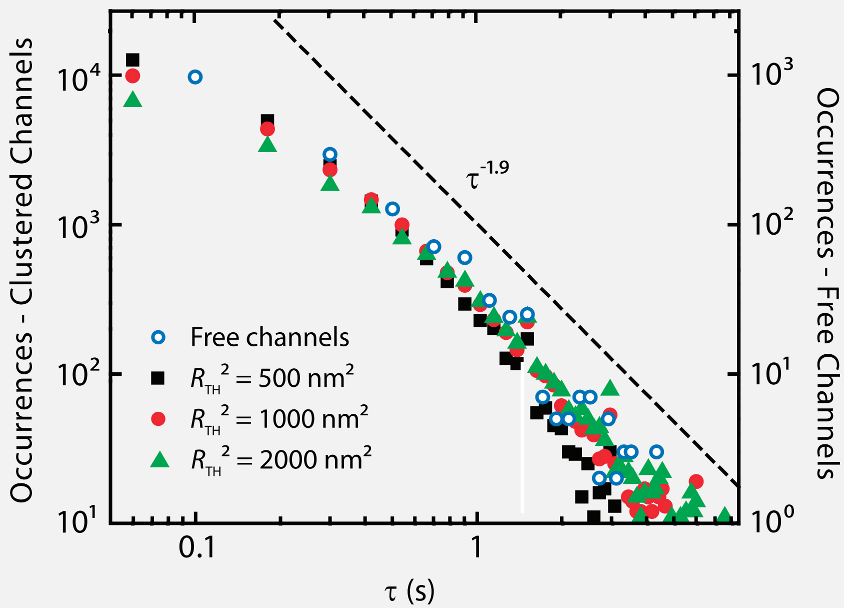

#BURNISTOUN
"Hauns up if yer da's in the jail"
POLICE
BBC Scotland

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)

Time averaged MSD & weak ergodicity breaking (WEB)

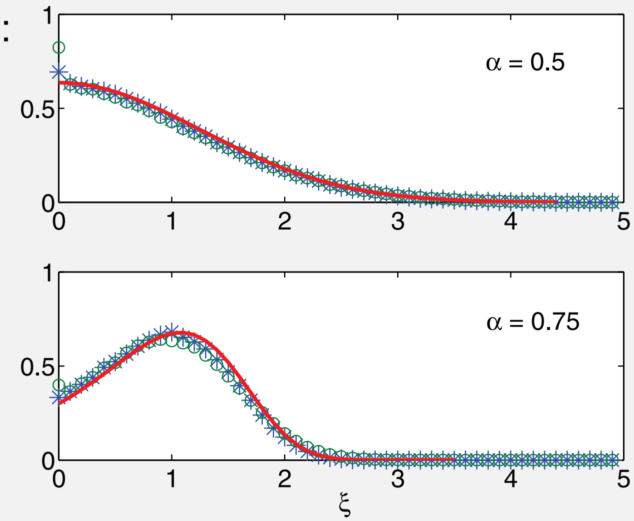
Time averaged MSD $\simeq \Delta$ is pseudo-Brownian and ageing ($\langle x^2(t)\rangle \simeq K_\alpha t^\alpha$):

$$\left\langle \overline{\delta^2(\Delta)} \right\rangle \sim \frac{1}{N}\sum_i^N \overline{\delta_i^2(\Delta)} \sim \frac{2dK_\alpha}{\Gamma(1+\alpha)}\frac{\Delta}{T^{1-\alpha}} \quad \therefore \quad K_\alpha \equiv \frac{\langle \delta \mathbf{r}^2\rangle}{2\tau^\alpha}$$

Amplitude distribution $\overline{\delta^2}$ of trajectories ($\xi \equiv \overline{\delta^2}/\langle\overline{\delta^2}\rangle$):

$$\phi_\alpha(\xi) \sim \frac{\Gamma^{1/\alpha}(1+\alpha)}{\alpha \xi^{1+1/\alpha}} L_\alpha^+\left(\frac{\Gamma^{1/\alpha}(1+\alpha)}{\xi^{1/\alpha}}\right)$$

$$\phi_{1/2}(\xi) = \frac{2}{\pi}\exp\left(-\frac{\xi^2}{\pi}\right); \quad \phi_1(\xi) = \delta(\xi - 1)$$

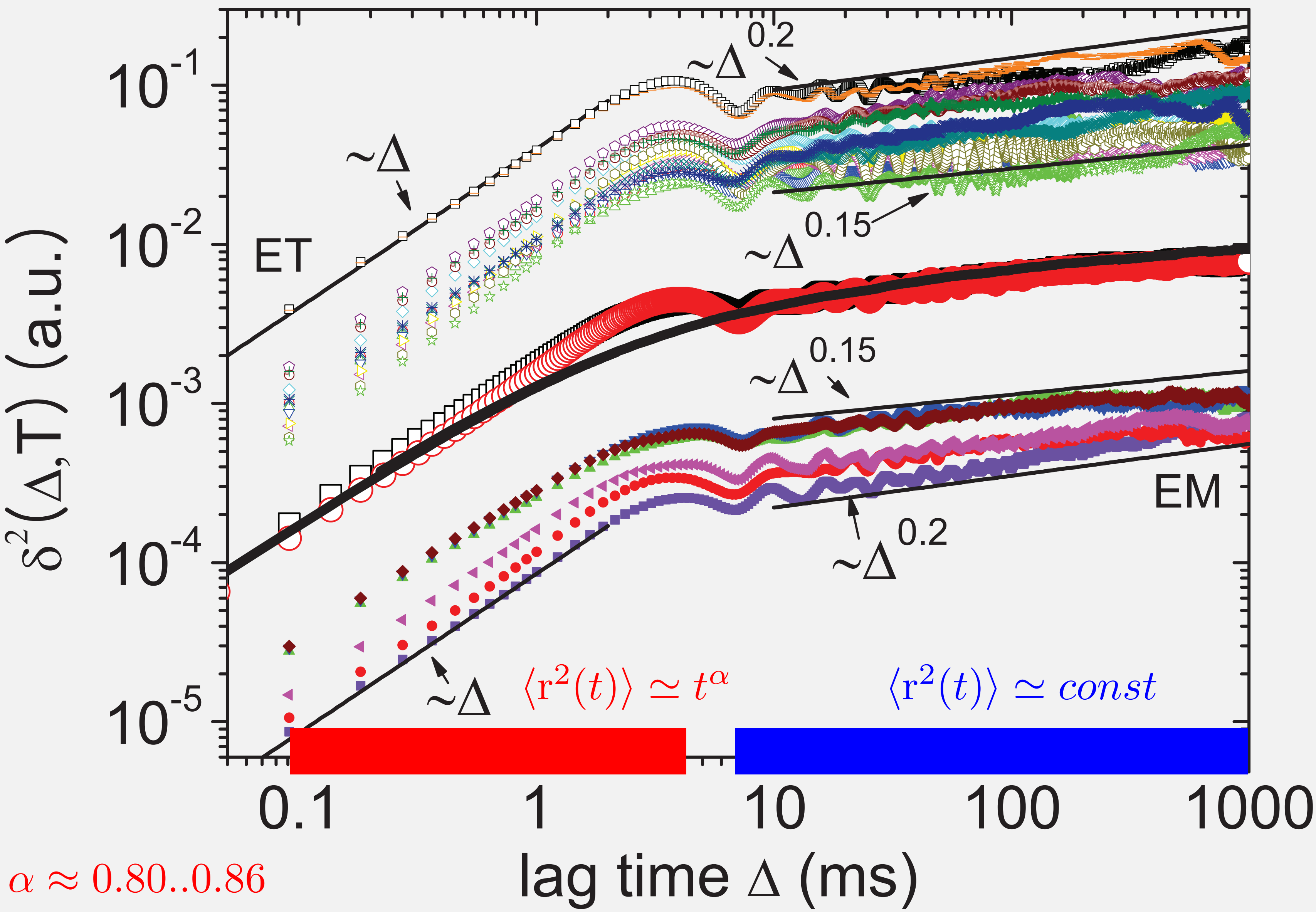


Confinement does not effect a plateau ($\langle x^2(t)\rangle \simeq \mathrm{const}(T)$):

$$\left\langle \overline{\delta^2(\Delta)} \right\rangle \sim \left(\left\langle x^2 \right\rangle_B - \langle x \rangle_B^2 \right) \frac{2\sin(\pi\alpha)}{(1-\alpha)\alpha\pi}\left(\frac{\Delta}{T}\right)^{1-\alpha}; \quad \frac{1}{(K_\alpha \lambda_1)^{1/\alpha}} \ll \Delta \ll T$$

Y He, S Burov, RM & E Barkai, PRL (2008); Generalised Khinchin theorem: S Burov, RM, & E Barkai, PNAS (2010)

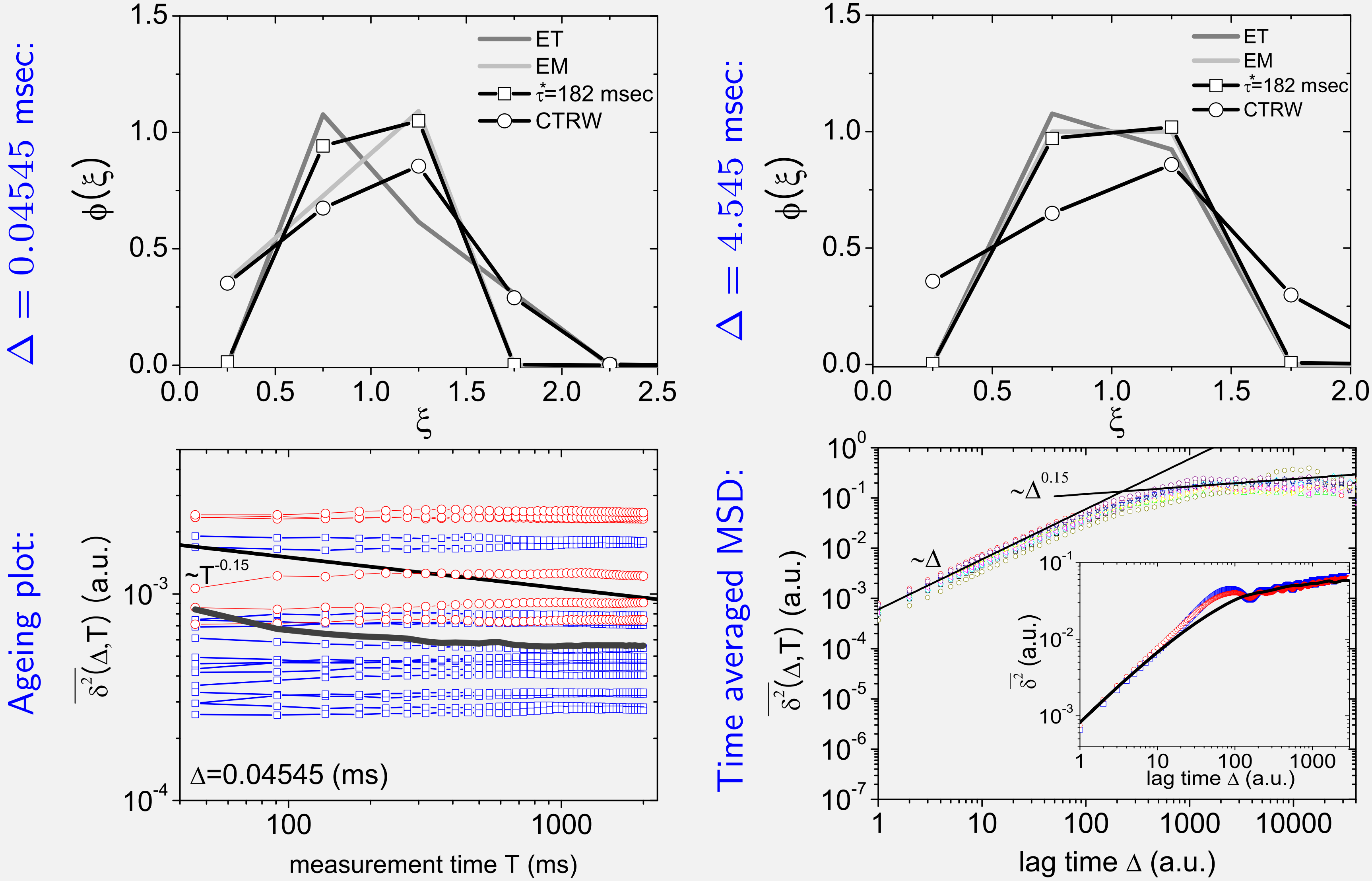
Granule subdiffusion in harmonic optical tweezer potential



$\alpha \approx 0.80..0.86$

J-H Jeon, . . . , K Berg-Sørensen, L Oddershede & RM, PRL (2011); S Burov, RM, & E Barkai, PNAS (2010)

Further analysis of the lipid granule data

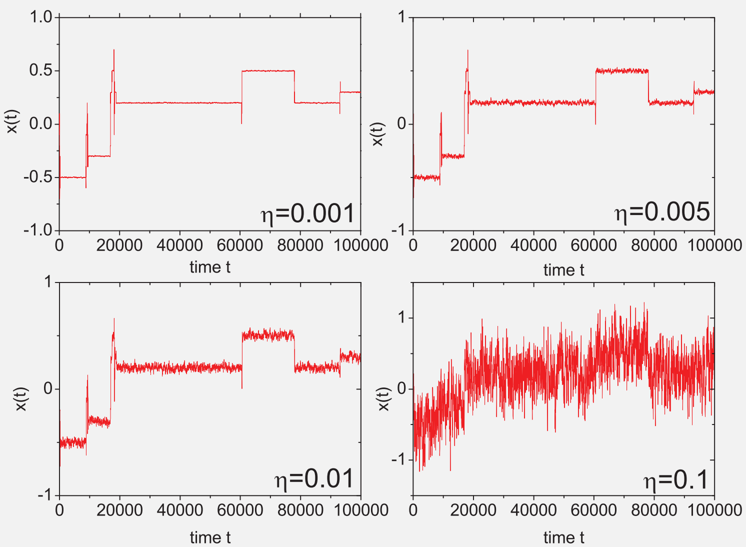


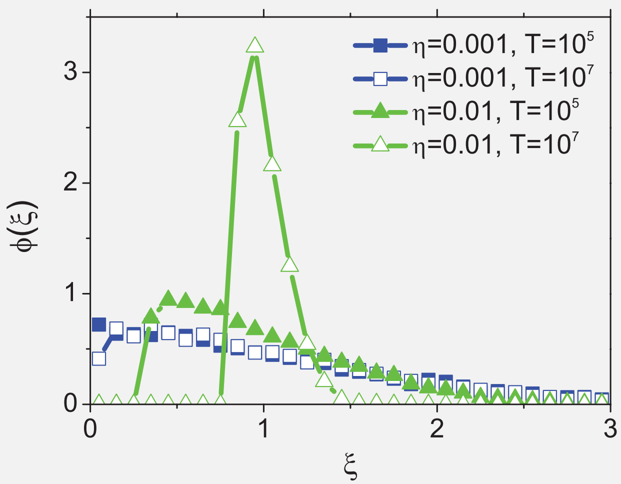
$$\psi(t) = \frac{d}{dt}\left[1 - \tau^{\alpha}(\tau + t)^{-\alpha}\exp\left(-\frac{t}{\tau^*}\right)\right] \quad \therefore \quad \tau^* \approx 182\text{msec}$$

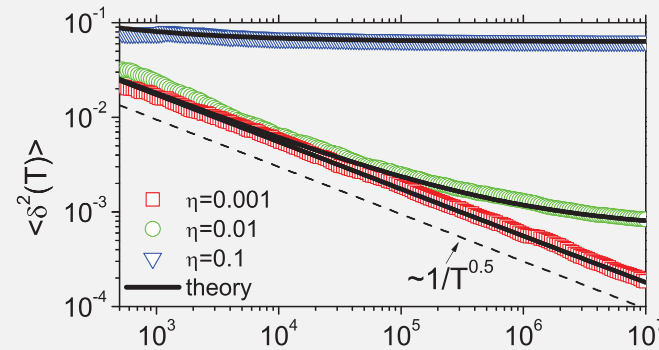
J-H Jeon, V Tejedor, S Burov, E Barkai, C Selhuber-Unkel, K Berg-Sørensen, L Oddershede & RM, PRL (2011)

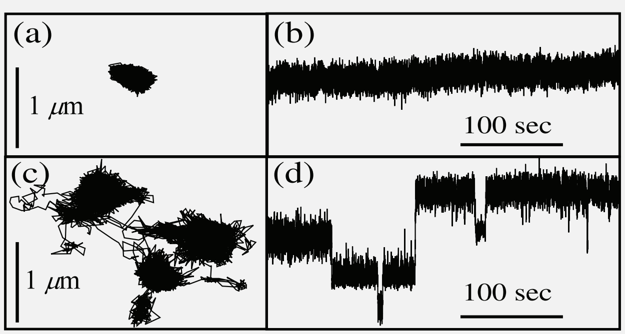
Noisy CTRW processes /w Ornstein-Uhlenbeck-noise

$$\langle x^2(t)\rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)}t^\alpha + \frac{\eta^2 D}{k}\left(1-e^{-2kt}\right)$$

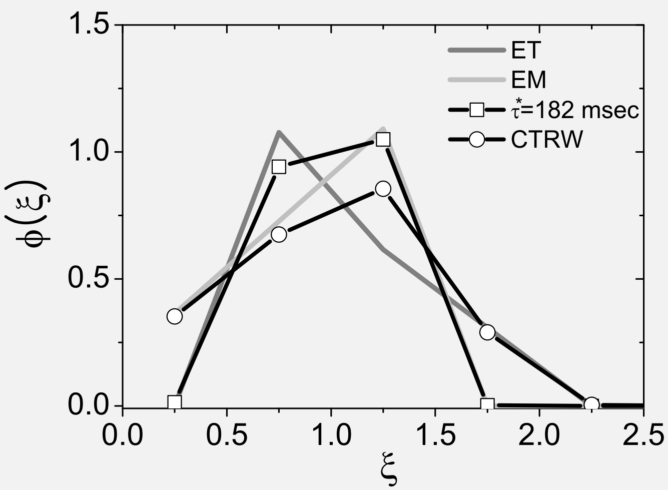


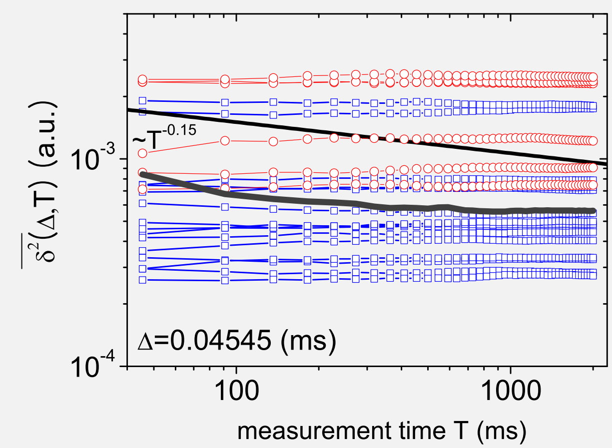






IY Wong . . . DA Weitz, PRL (2004)

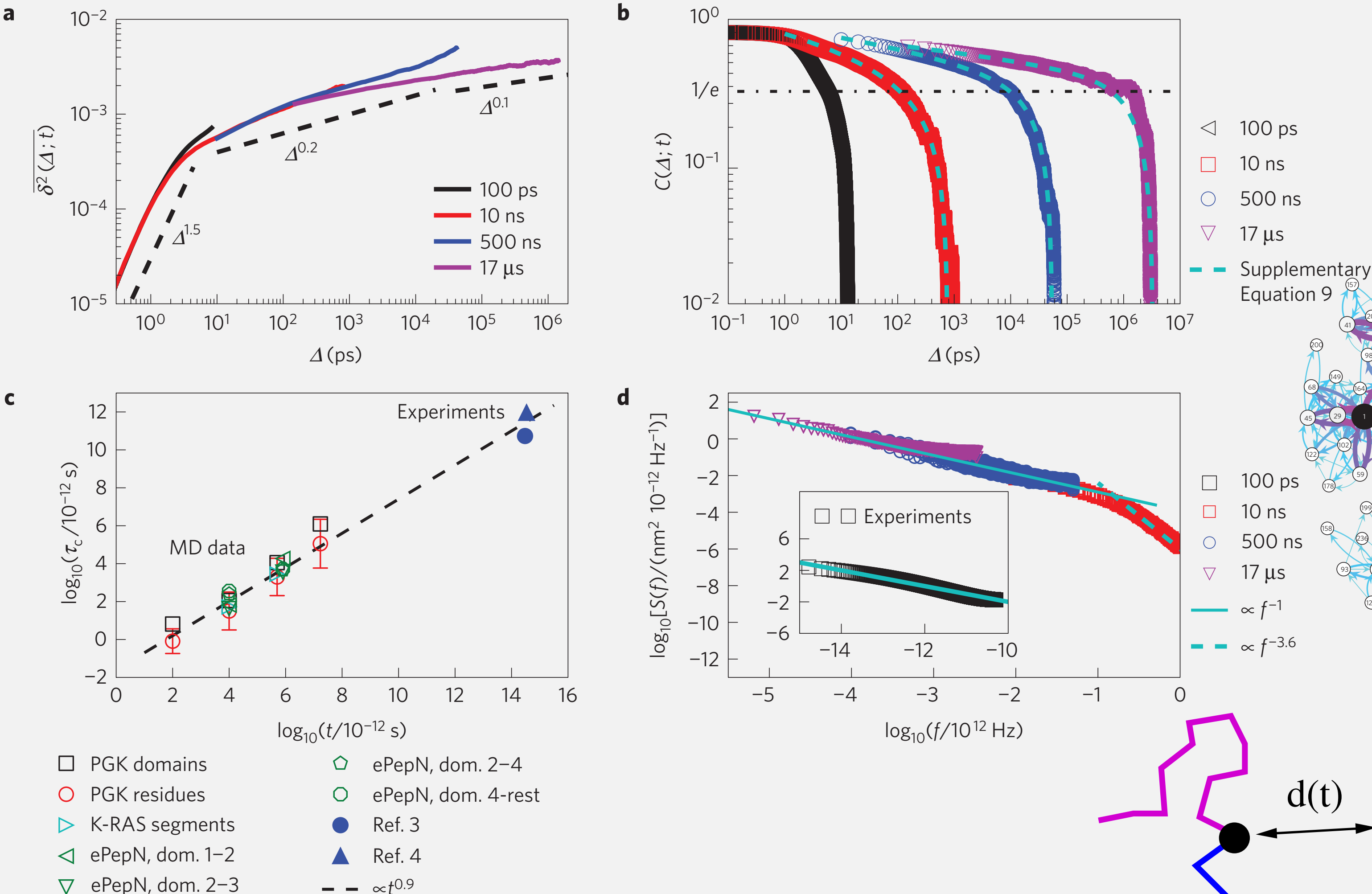


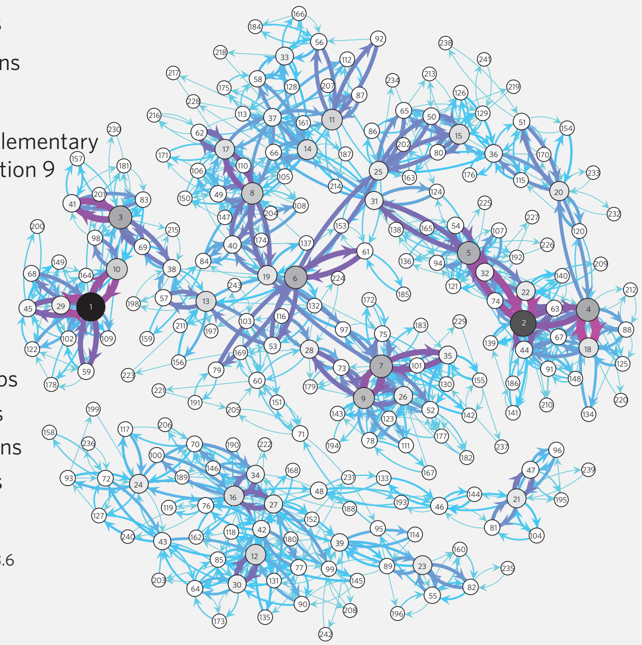


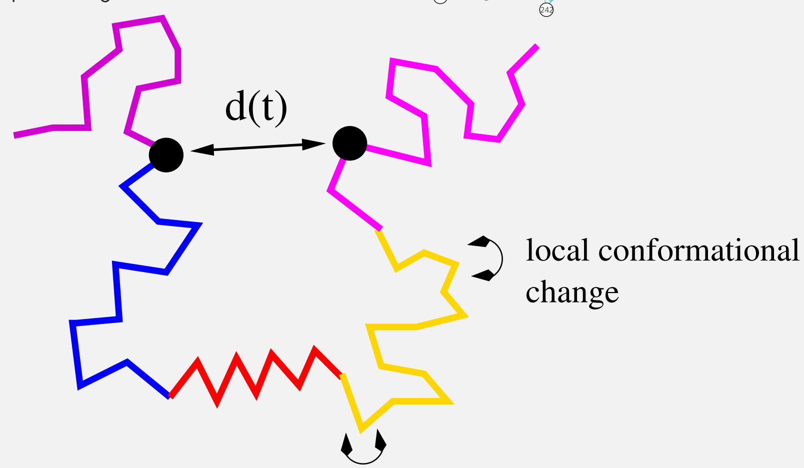
JH Jeon . . . K Berg-Sørensen, L Oddershede & RM, PRL (2011)

JH Jeon, E Barkai & RM, JCP (2013)

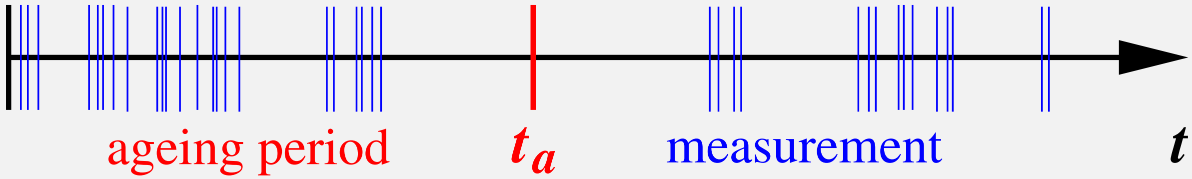
Self-similar internal protein dynamics: 13 decades of ageing







Ageing effects in single trajectory time averages

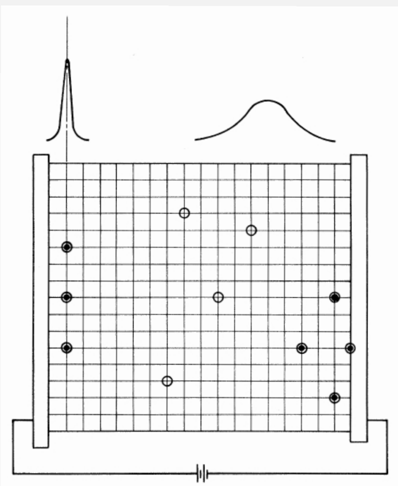


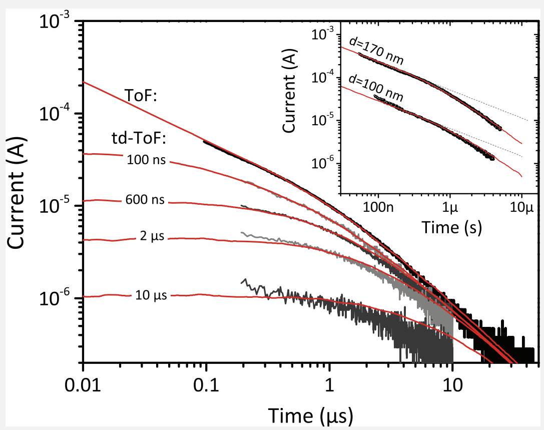
Ageing mean squared displacement ($\Lambda(z) = (1+z)^\alpha - z^\alpha$)

$$\left\langle \overline{\delta^2(\Delta)} \right\rangle_a = \frac{\Lambda_\alpha(t_a/T)}{\Gamma(1+\alpha)} \frac{g(\Delta)}{T^{1-\alpha}} \quad \not\Leftrightarrow \quad \langle x^2(t) \rangle_a \simeq \begin{cases} t^\alpha, & t_a \ll t \\ t_a^{\alpha-1} t, & t_a \gg t \end{cases}$$

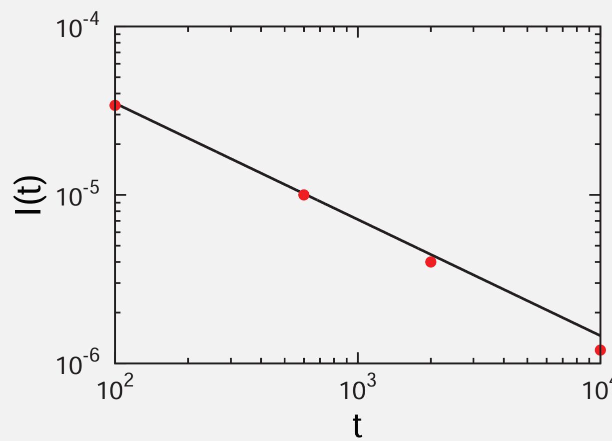
Probability to make at least one step during $[t_a, t_a + T]$: *population splitting*

$$m_\alpha(T/t_a) \simeq (T/t_a)^{1-\alpha}, \quad T \ll t_a$$





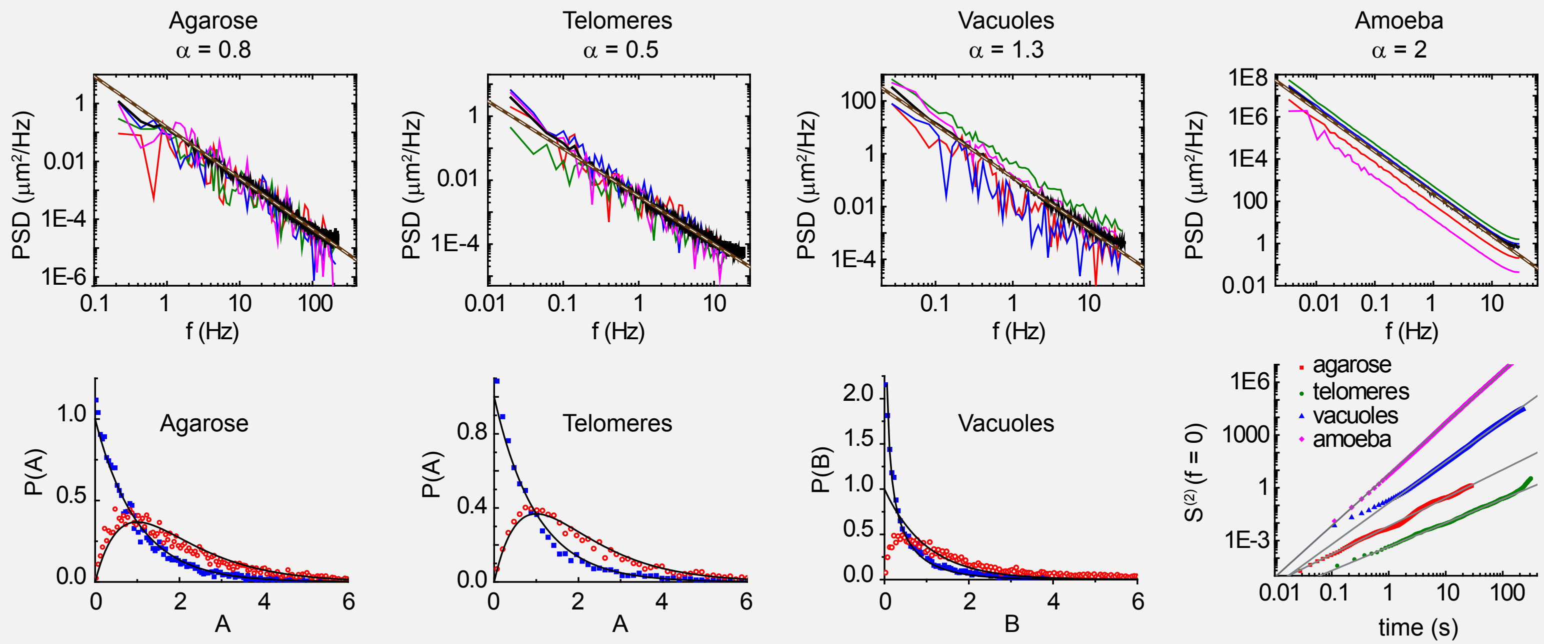
M Schubert, . . . & D Neher, Phys Rev B (2013)

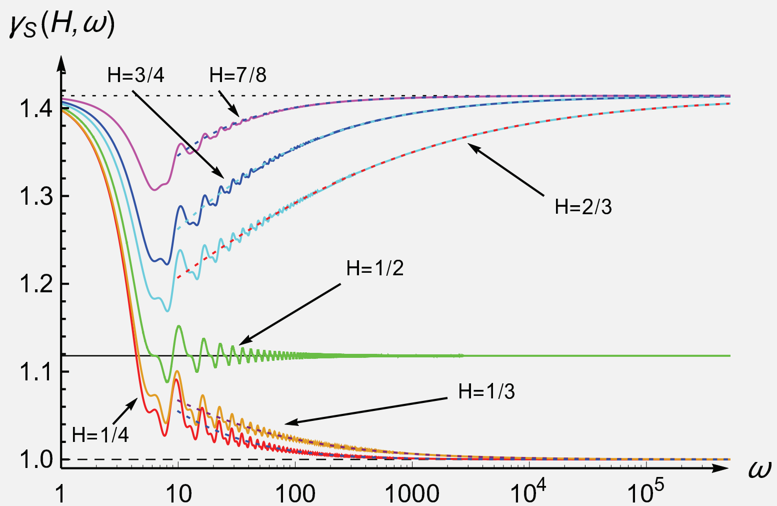


H Krüsemann, R Schwarzl & RM, Transp Porous Media (2016), PRE (2015)

J Schulz, E Barkai & RM, PRL (2013), PRX (2014)

Power spectral density of a single FBM trajectory



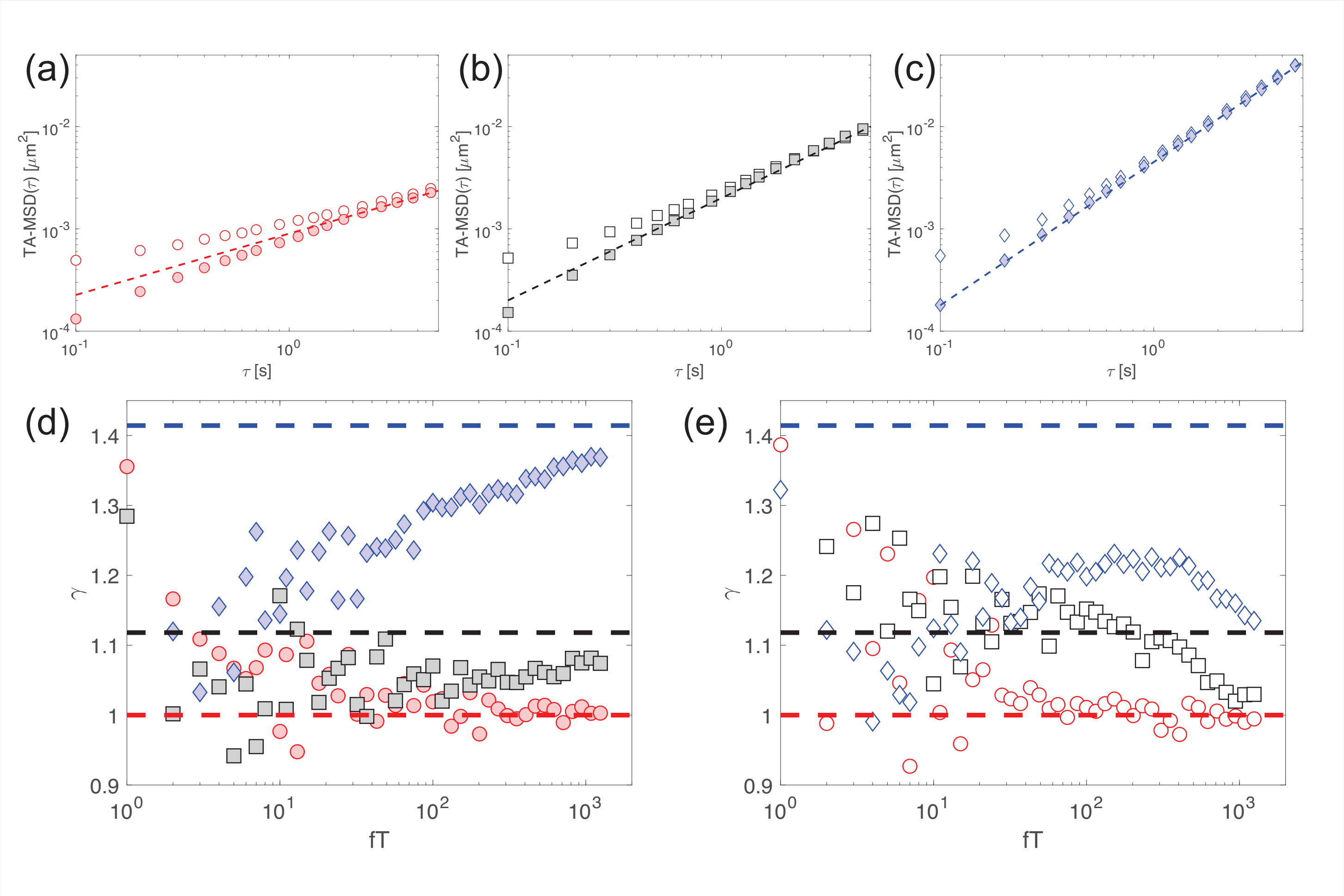


$$S(f,T) = \frac{1}{T}\left|\int_0^T \exp(ift)X_t dt\right|^2$$

$$\gamma = \frac{\left(\langle S_T^2(f)\rangle - \langle S_T(f)\rangle^2\right)^{1/2}}{\langle S_T(f)\rangle}$$

D Krapf, N Lukat, E Marinari, RM, G Oshanin, C Selhuber-Unkel, A Squarcini, L Stadler, M Weiss & X Xu, PRX (2019)

PSD analysis of *noisy* FBM trajectories



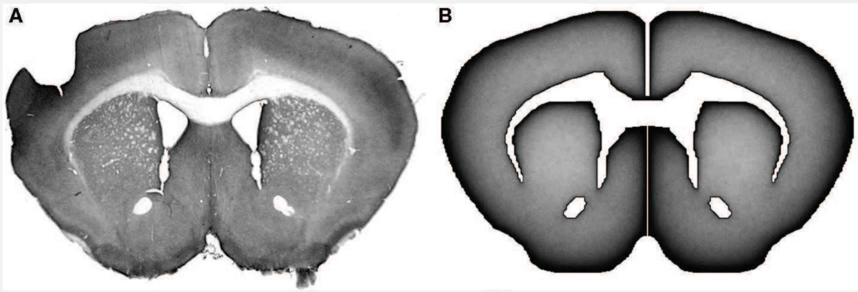
Open symbols: dominant static error
Filled symbols: dominant dynamic error

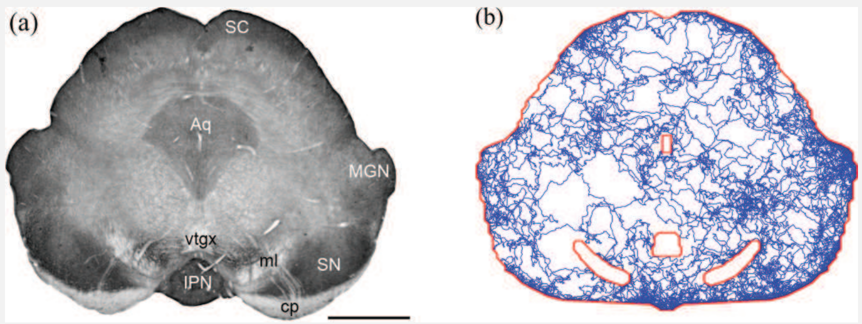
V Sposini, D Krapf, E Marinari, R Sunyer, F Ritort, F Taheri, C C Selhuber-Unkel, M Weiss, RM & G Oshanin, (2022)

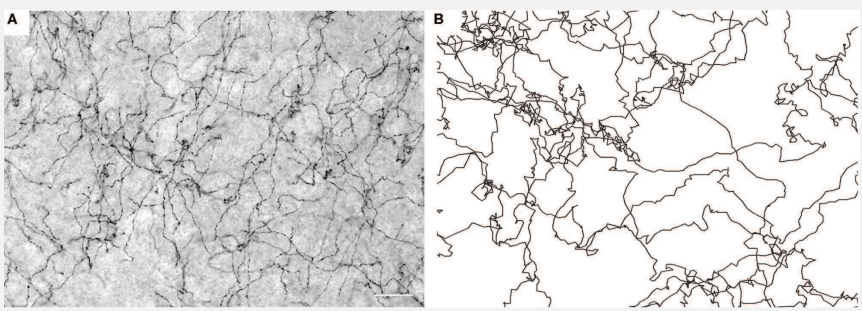
Brain serotonergic axons as FBM paths

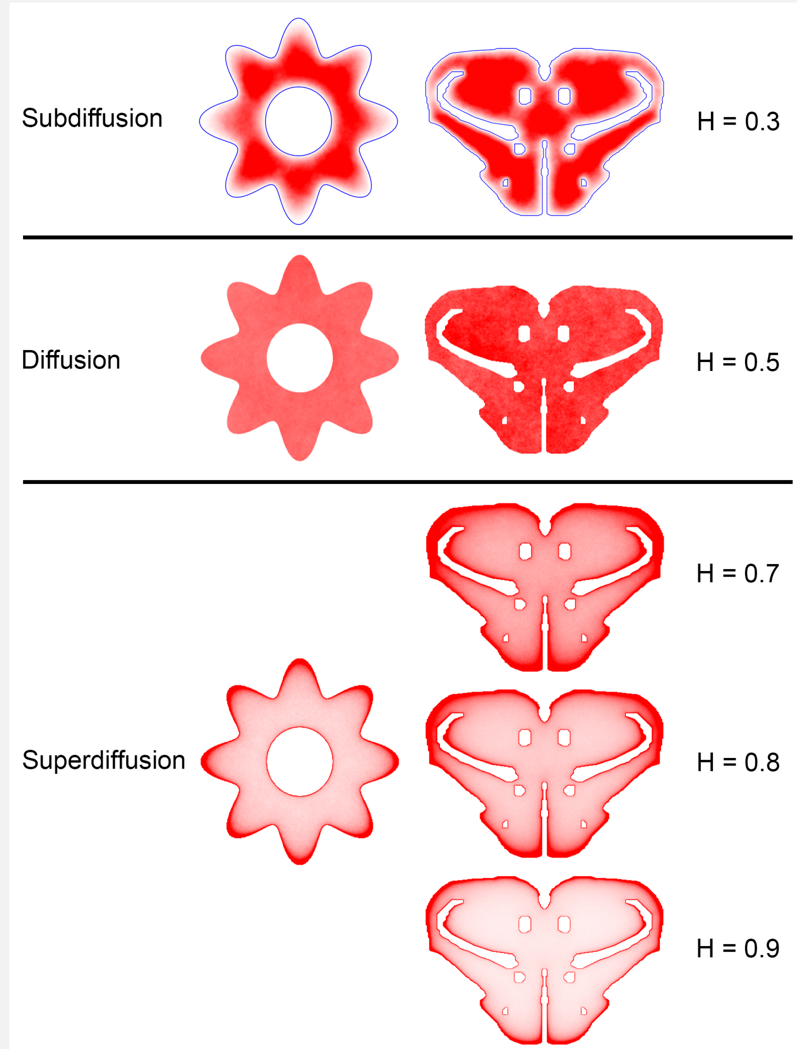
DIVERSION AHEAD

Correlated fluctuations effect non-flat profile









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

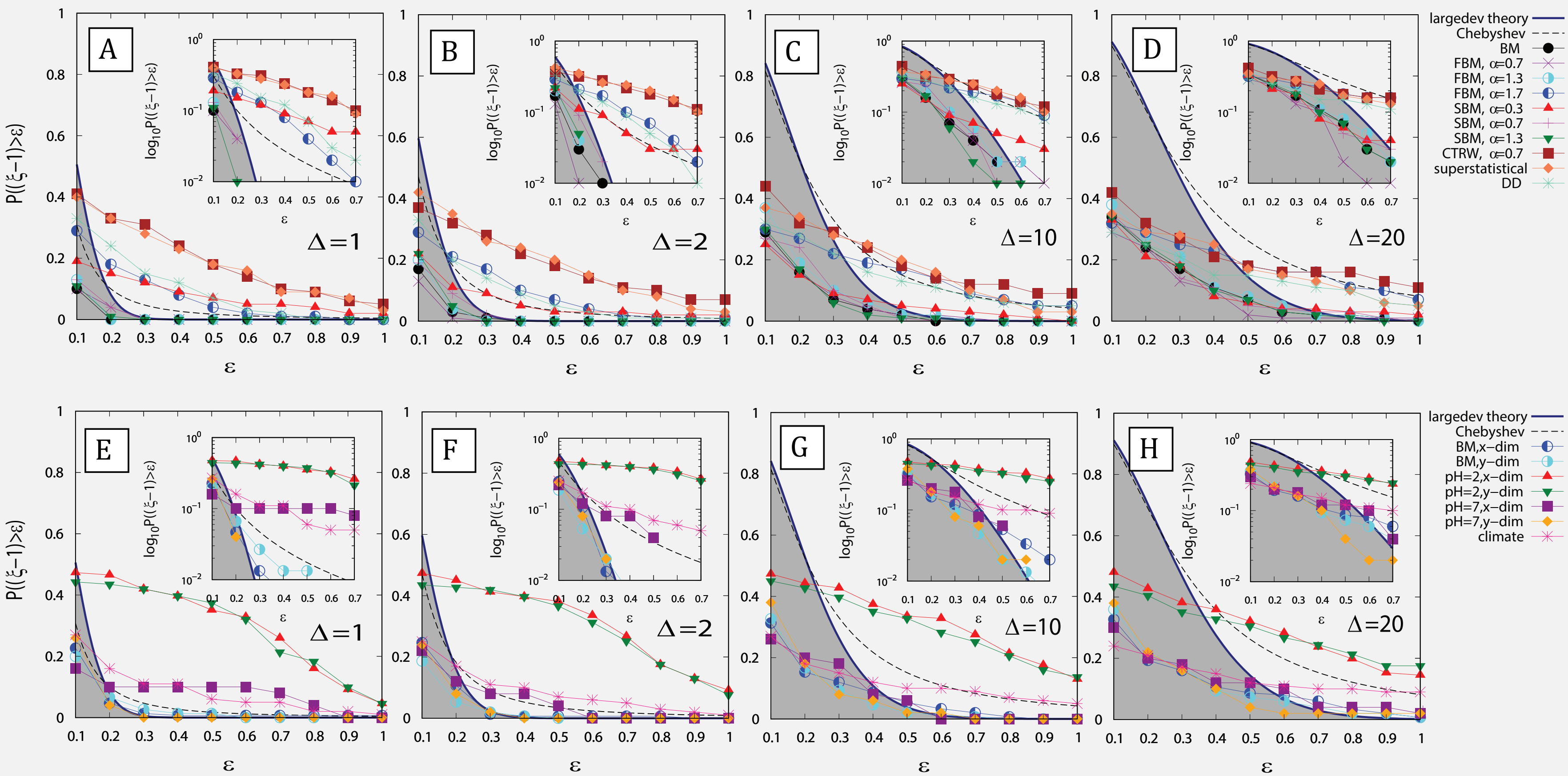
Large-deviation statistics for TAMSD

Chebyshev's inequality for Brownian motion $X(1), X(2), \dots, X(N)$, given deviation ε:

$$P\Big((\xi-1)\geq\varepsilon\Big)\leq\frac{4\Delta}{4\Delta+3N\varepsilon^2},\quad \xi=\frac{\overline{\delta^2(\Delta)}}{\langle\overline{\delta^2(\Delta)}\rangle},\quad \langle\xi\rangle=1$$

Large-deviation result:

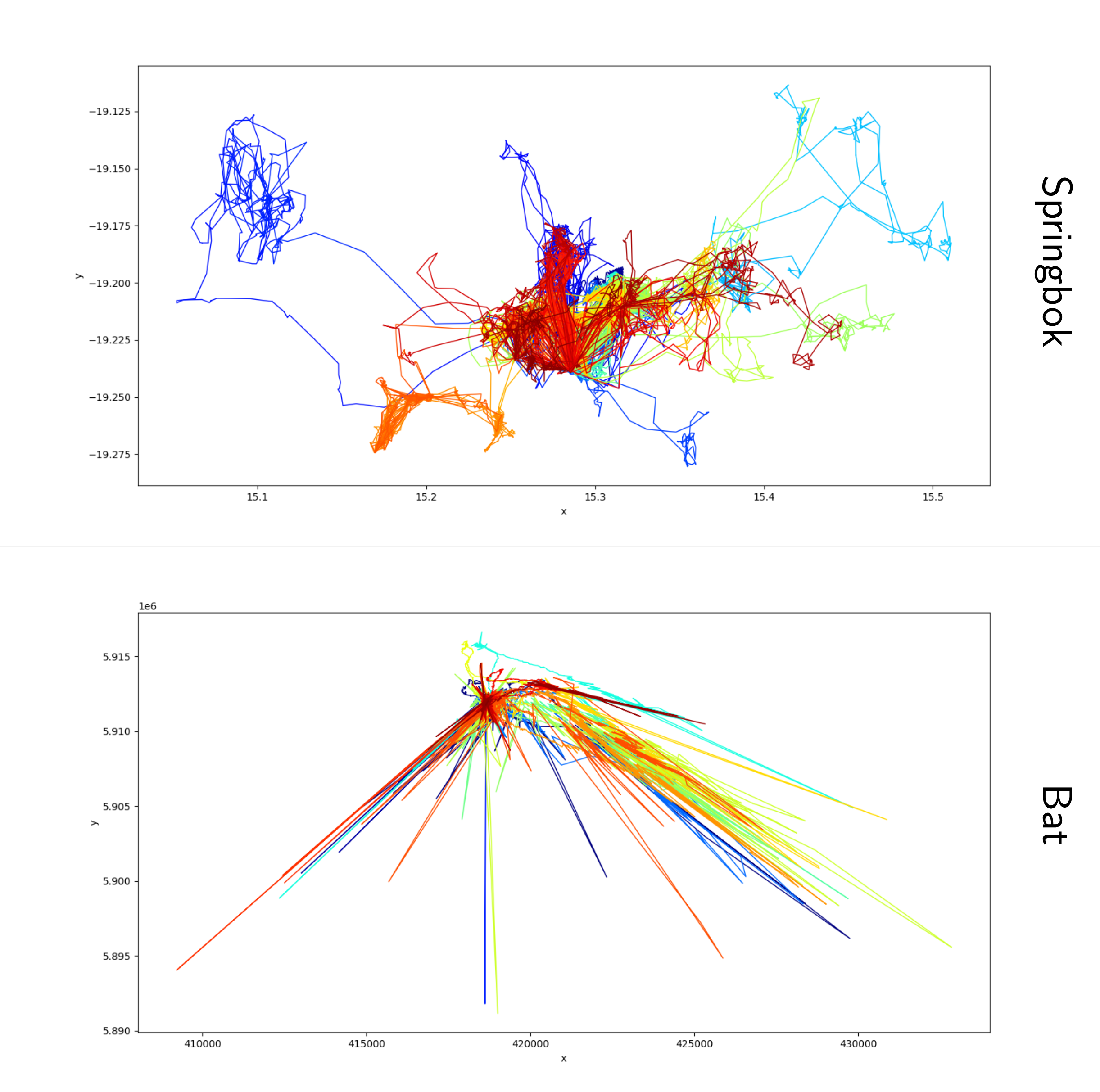
$$P\Big((\xi-1)\geq\varepsilon\Big)\leq\exp\Big(-a\mathcal{H}(b)\Big),\quad \mathcal{H}(b)=1+b-\sqrt{1+2b};\quad a,b=f(\Delta,\dots)$$



S Thapa, A Wyłomańska, G Sikora, CE Wagner, D Krapf, H Kantz, AV Chechkin & RM, NJP (2021)

Most scientists regarded the new streamlined peer-review process as ‘quite an improvement’. . .

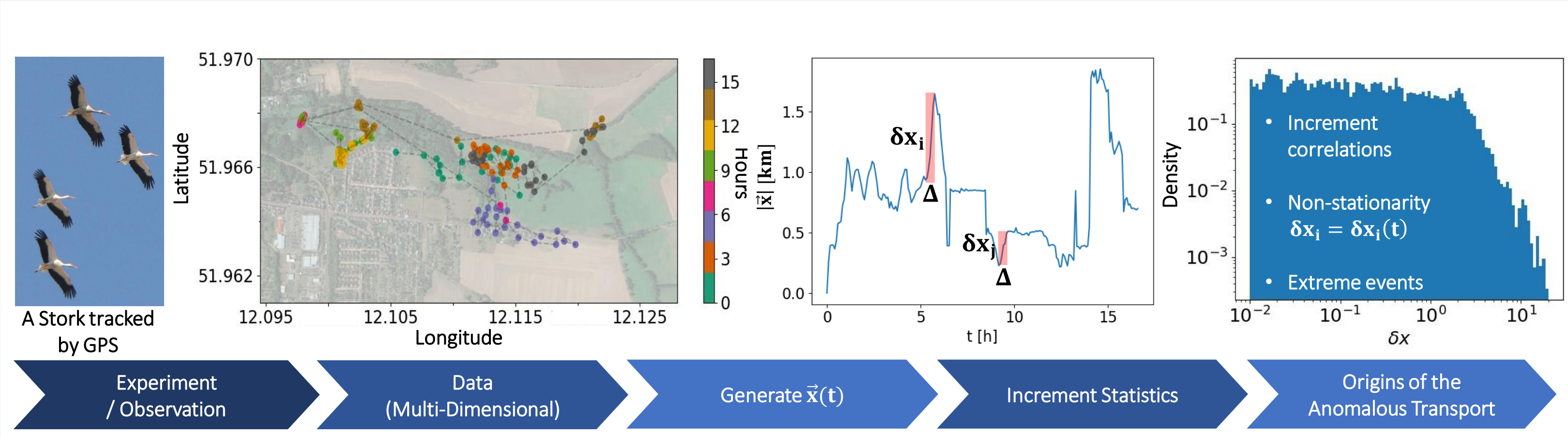
A word on input data for analyses

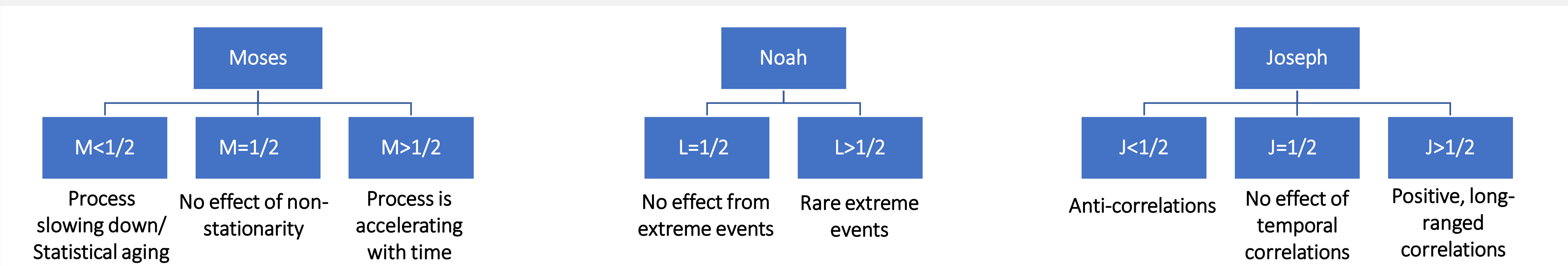


- I Gaps in trajectories
- II Smoothing artifacts
- III Different resolution along trajectory
- IIII Trajectories of different length
- ~~IIII~~ Different regimes in single trajectory (e.g., nesting, cruising, eating . . .)
- ~~IIII~~ I Ageing effects (trajectory record starts after system initiation

Data from Florian Jeltsch & Damaris Zurell's groups

Scaling analysis of anomalous diffusion

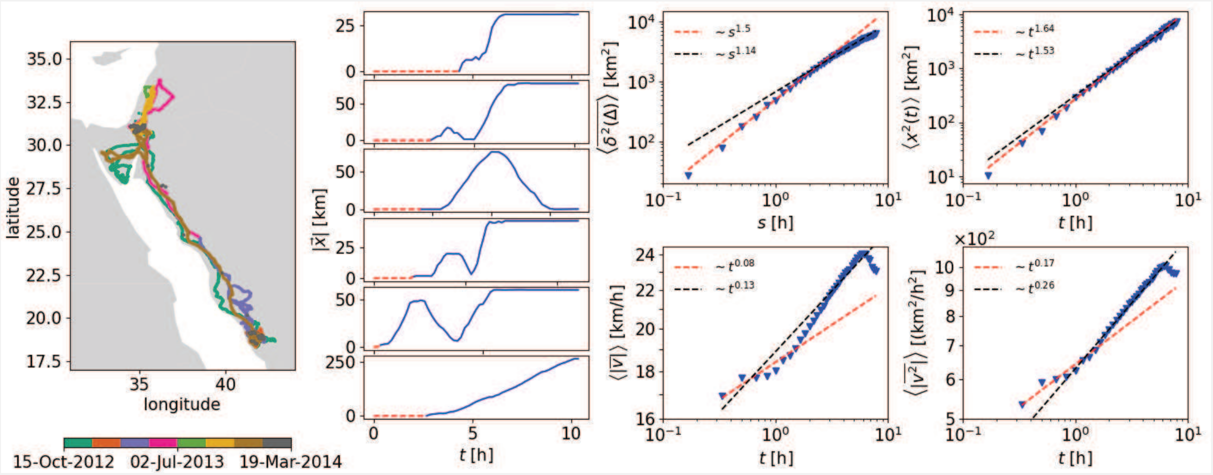


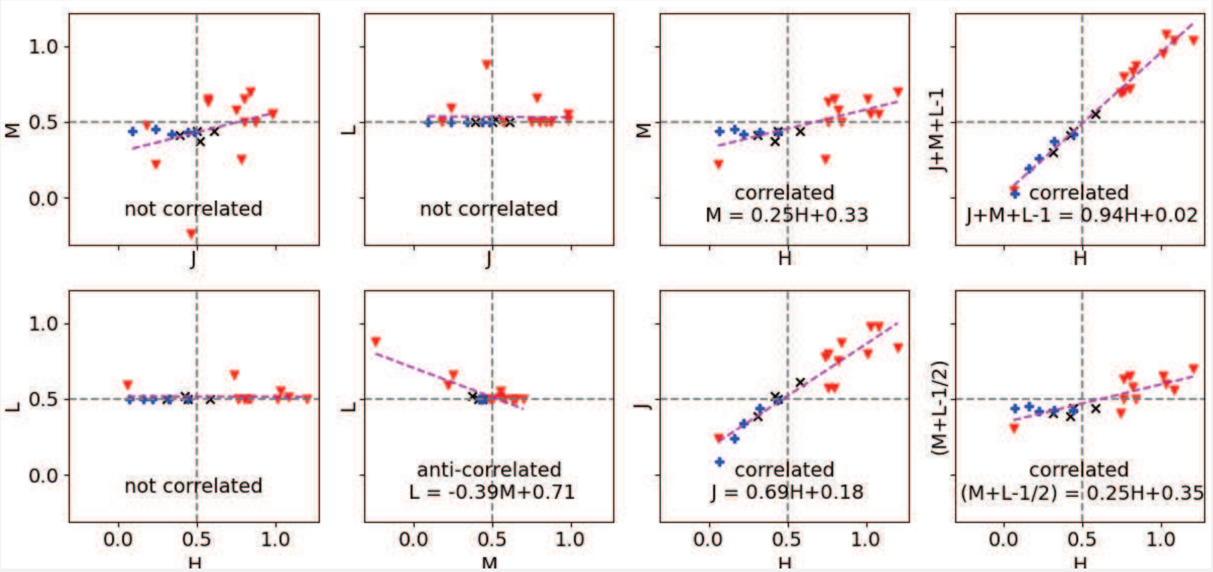


O Vilk, E Aghion, T Avgar, C Beta, O Nagel, M Weiss, A Sabri, D Krapf, R Sarfati, DK Schwartz, RM, R Nathan, M Assaf, E-print (2021)

Scaling analysis of anomalous diffusion

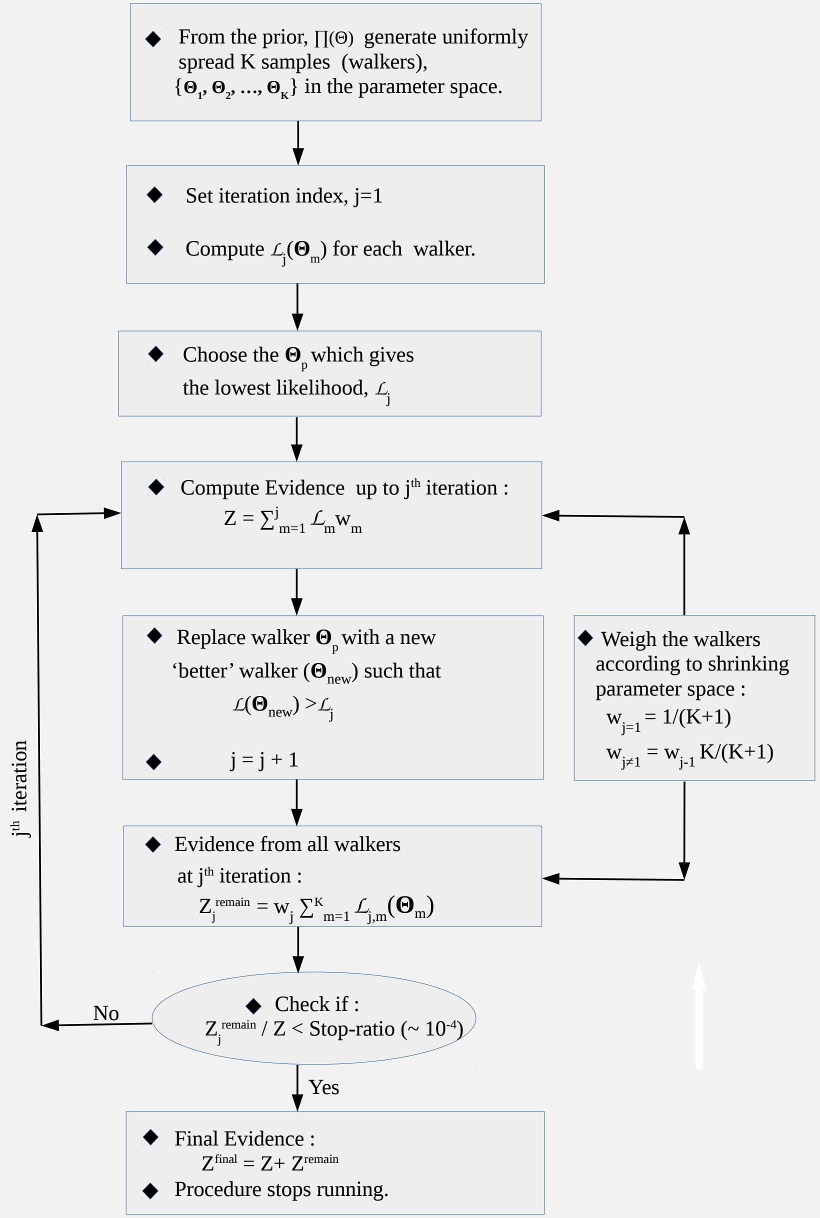
Joseph: long-range correlations; Noah: fat tails of increment PDF; Moses: non-stationarity





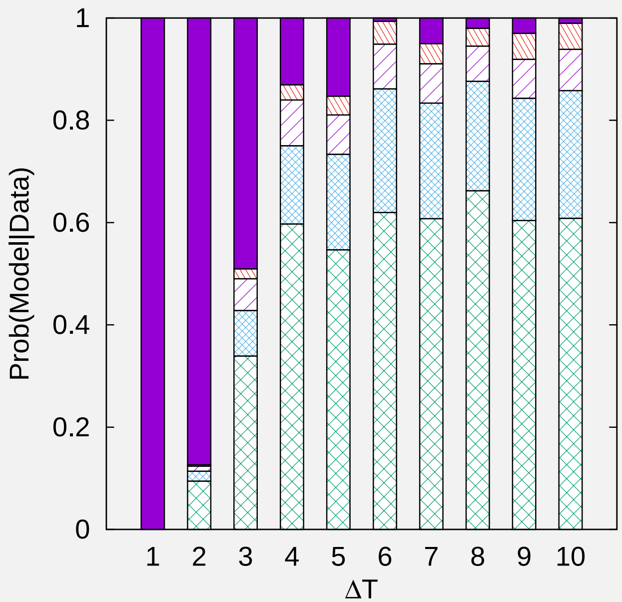
O Vilk, E Aghion, T Avgar, C Beta, O Nagel, M Weiss, A Sabri, D Krapf, R Sarfati, DK Schwartz, RM, R Nathan, M Assaf, E-print (2021)

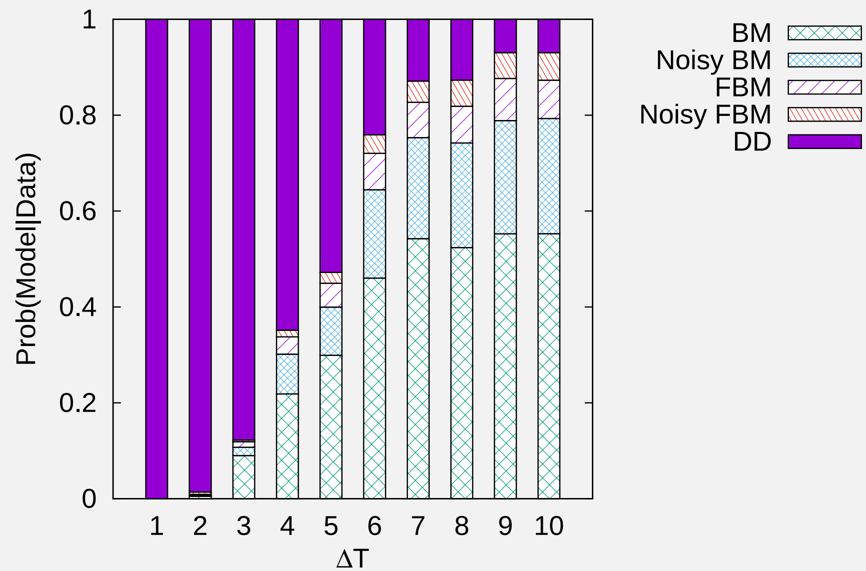
Maximum likelihood Bayesian data analyses

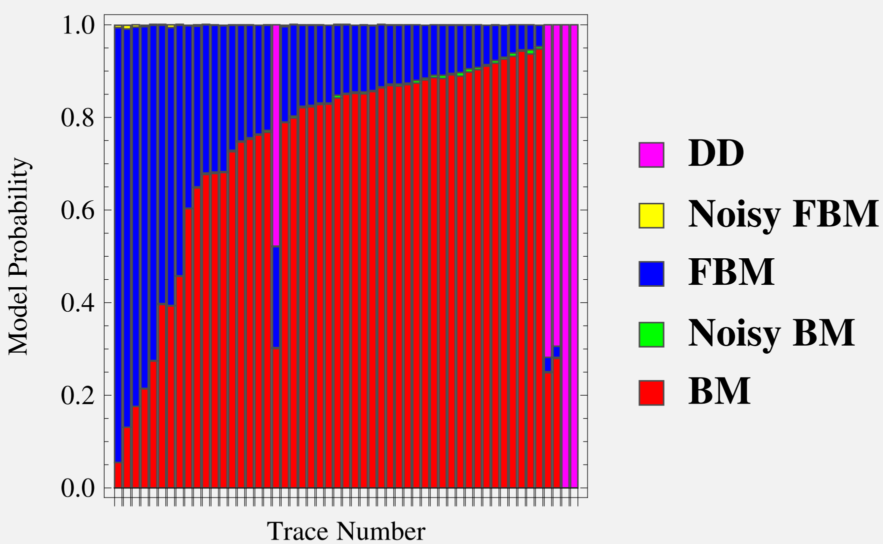


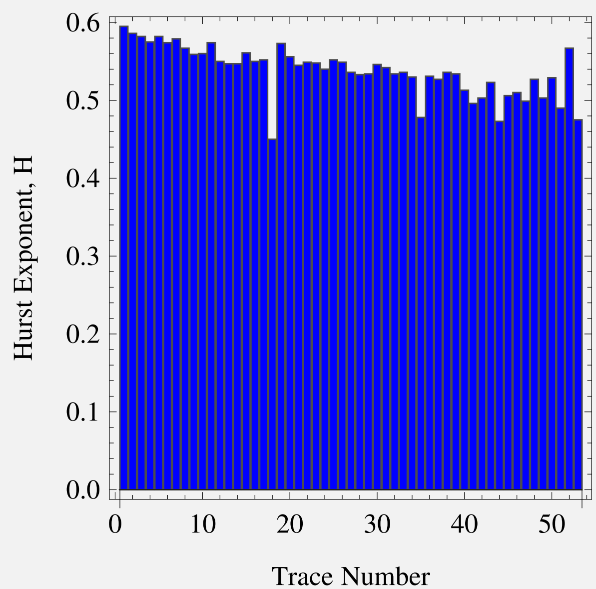
S Thapa, AG Cherstvy & RM (2018); AG Cherstvy, S Thapa, CE Wagner & RM, Soft Matter (2019)

Maximum likelihood Bayesian data analyses









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

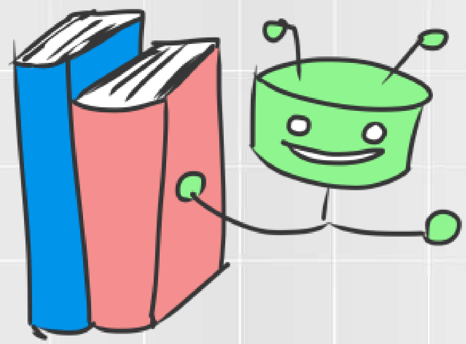
Wroclaw University of Science and Technology

Machine learning approach to classification

Training data

Input (trajectories) →

Output (diff. modes) →

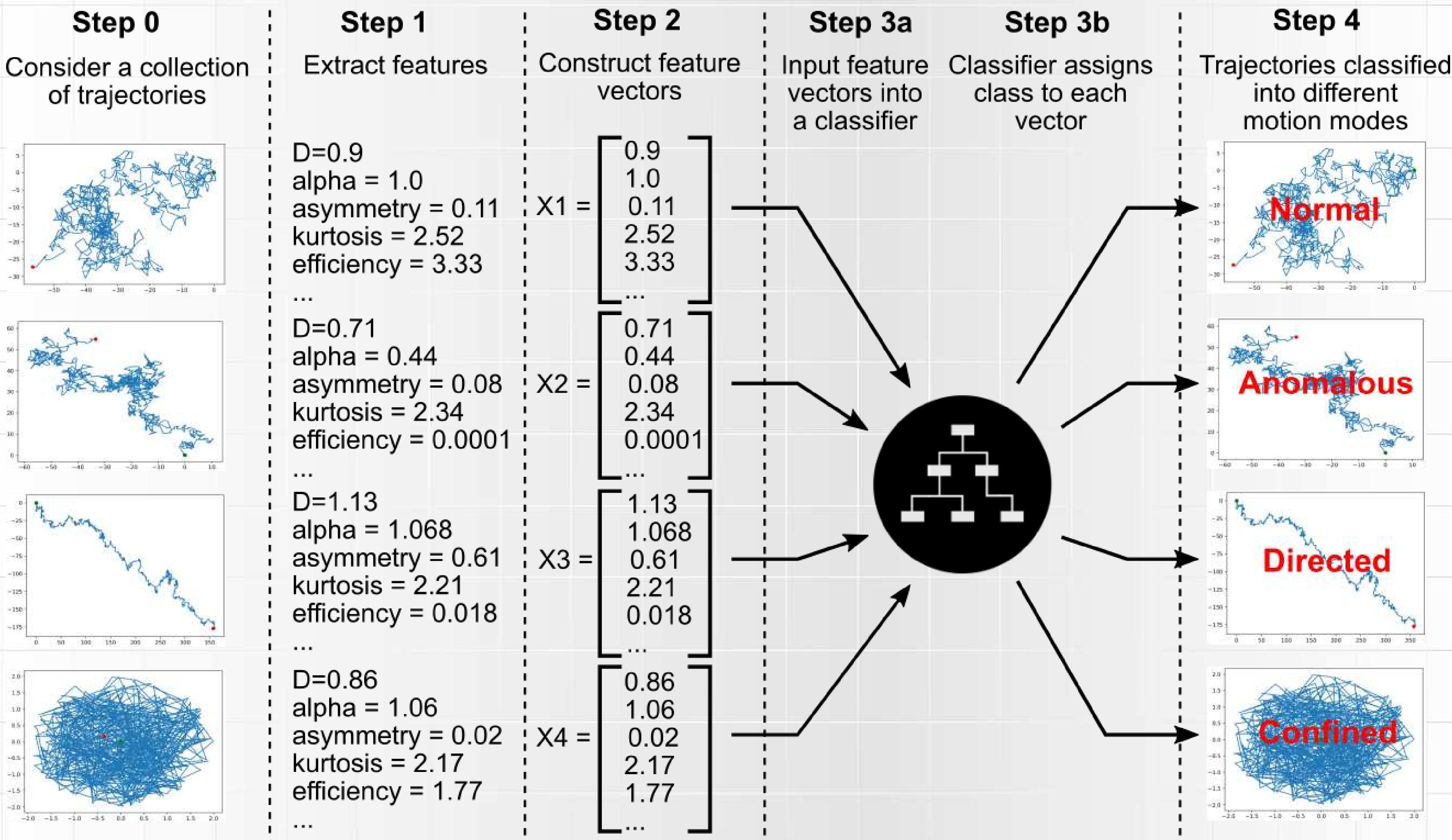


ML algorithm learns the parameters and produces a **trained model** that could **generalize** data

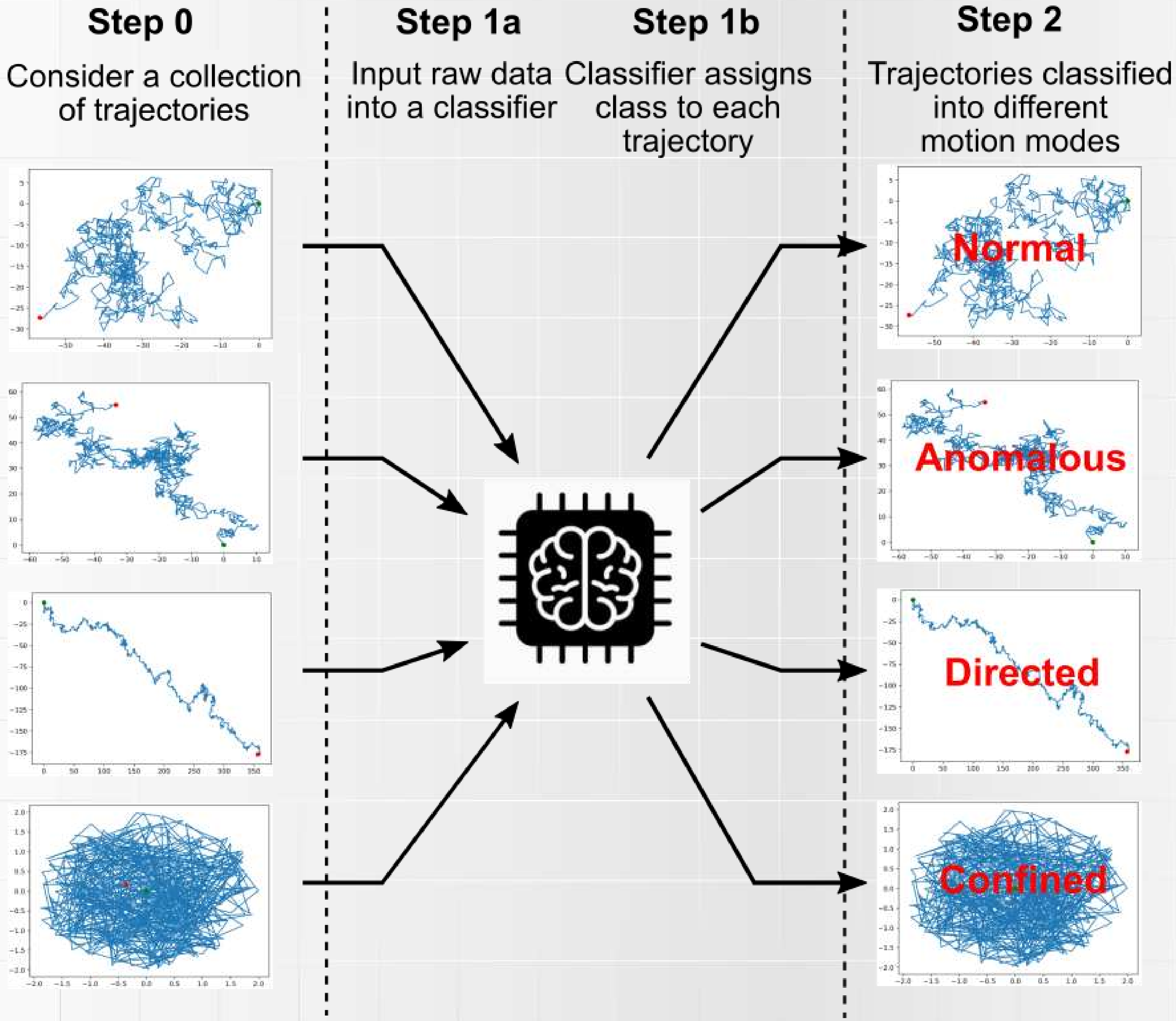
Unseen data

New input (trajectory) → Trained model → Predicted output (diffusion type)

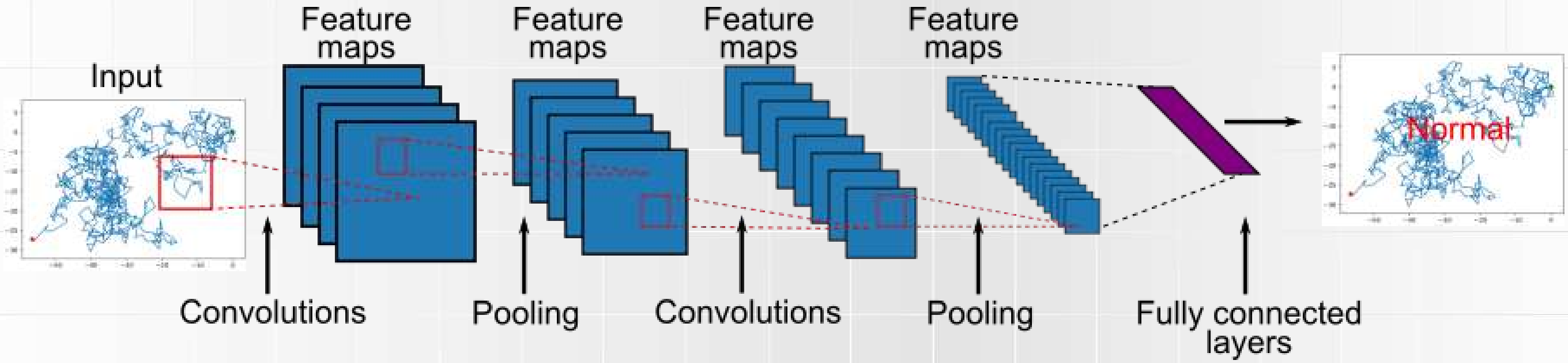
Feature-based methods



Deep learning methods



Convolutional neural networks



- each convolution uses a different filter sliding over the input and producing its own feature map
- pooling reduces the dimensionality of feature maps
- state-of-the-art in image processing

nature COMMUNICATIONS

ARTICLE

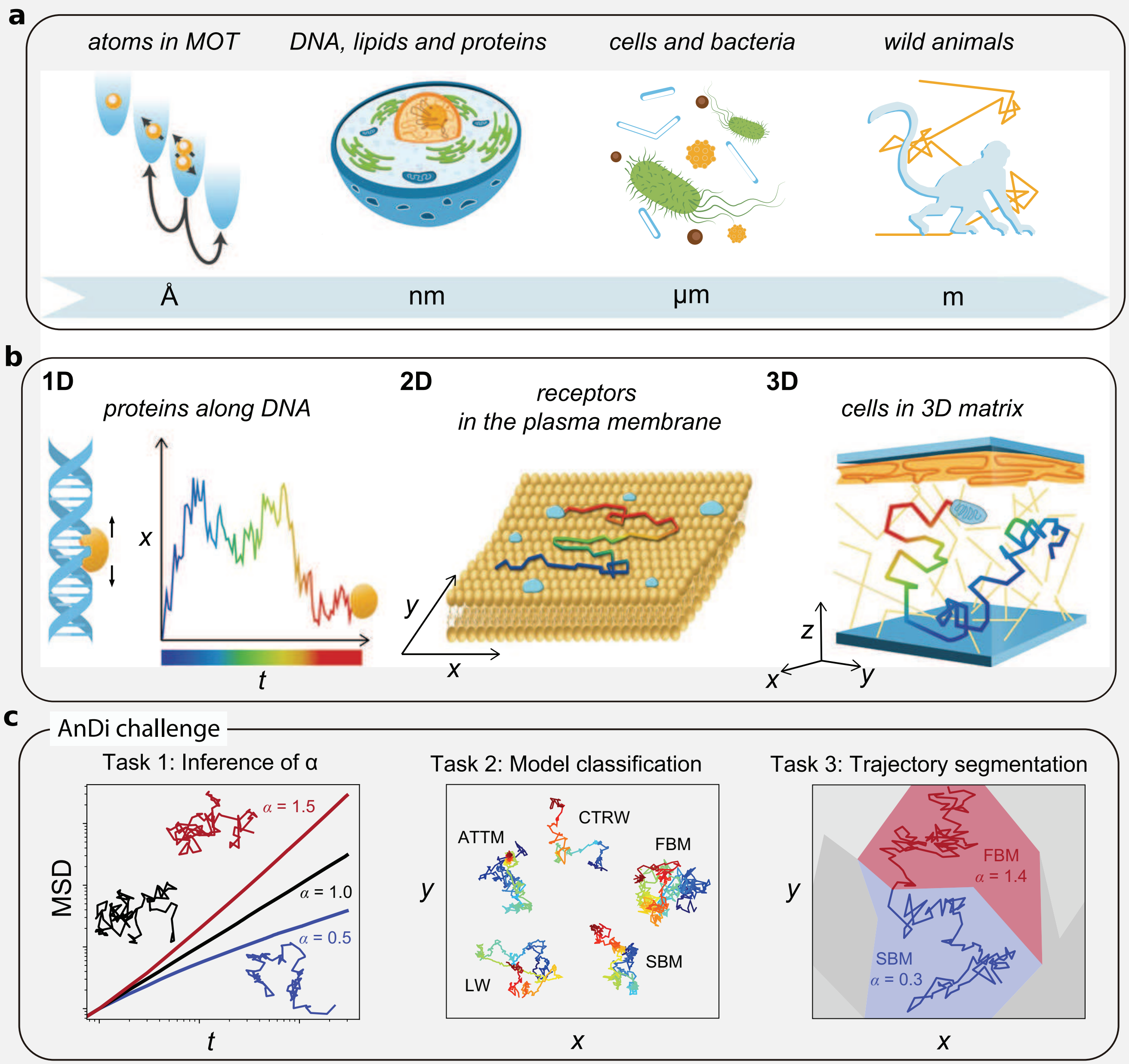
https://doi.org/10.1038/s41467-021-26320-w OPEN

Check for updates

Objective comparison of methods to decode anomalous diffusion

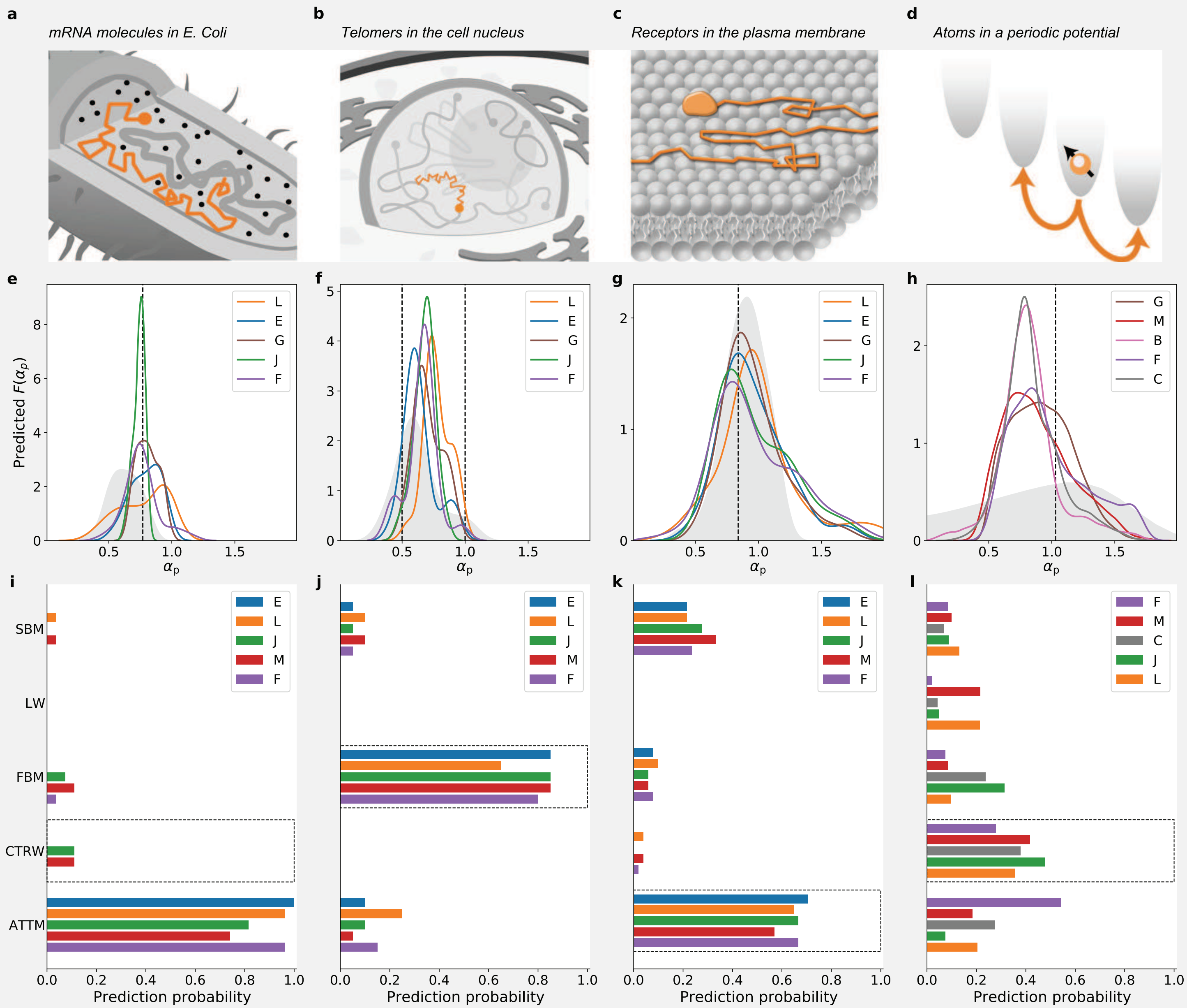
Gorka Muñoz-Gil[1], Giovanni Volpe[2✉], Miguel Angel Garcia-March[3], Erez Aghion[4], Aykut Argun[2], Chang Beom Hong[5], Tom Bland[6], Stefano Bo[4], J. Alberto Conejero[3], Nicolás Firbas[3], Òscar Garibo i Orts[3], Alessia Gentili[7], Zihan Huang[8], Jae-Hyung Jeon[5], Hélène Kabbech[9], Yeongjin 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✉]

The ANomalous DIffusion challenge



G Muñoz-Gil et al., Nat Comm (2021)

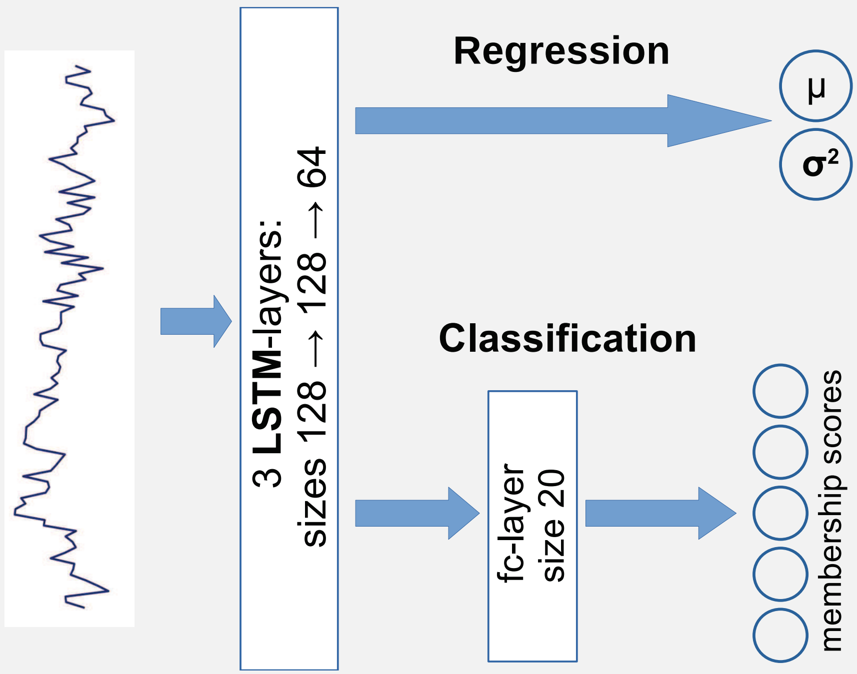
The ANomalous DIffusion challenge

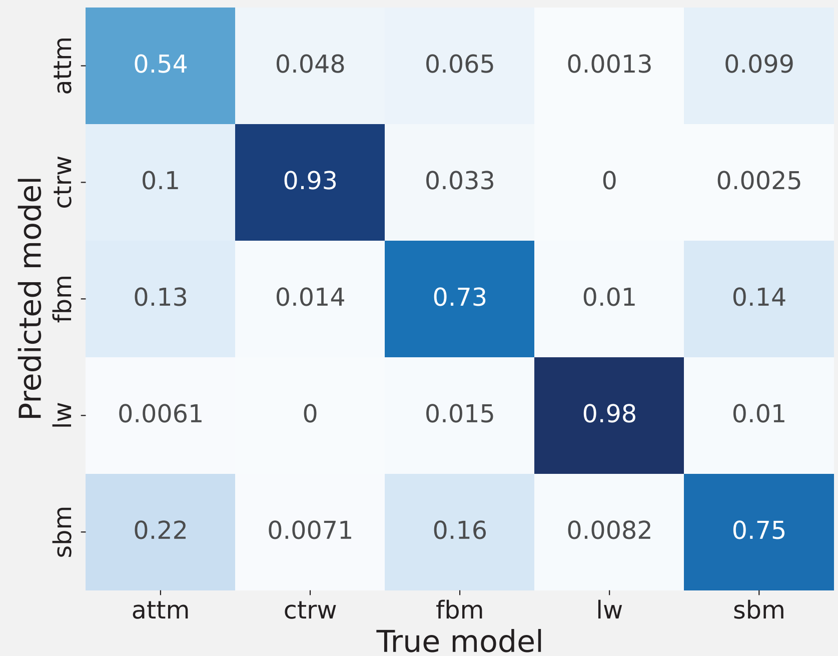


G Muñoz-Gil et al., Nat Comm (2021)

Bayesian-weighted deep learning model selection

Long **S**hort-**T**erm **M**emory approach (recurrent neural network architecture)





Feature-based classification schemes

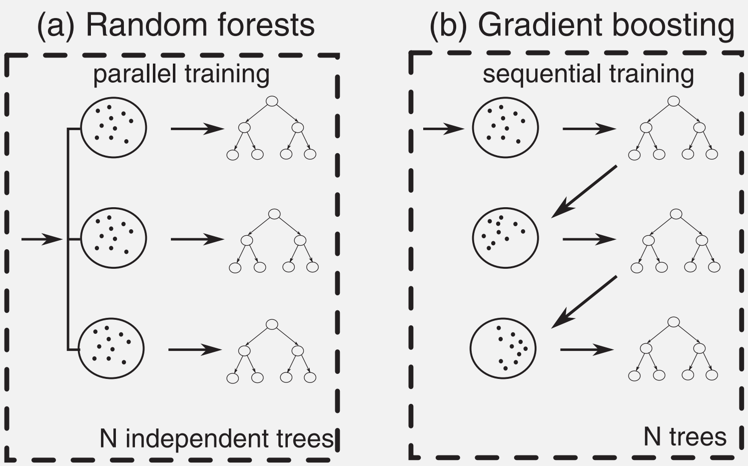


FIG. 1. Comparison between (a) random forest and (b) gradient boosting methods. In the random forest, N independent learners (trees) are built in parallel from random subsets of the input data set. In gradient boosting, the next tree is constructed from the pseudoresiduals of the ensemble and added to it.

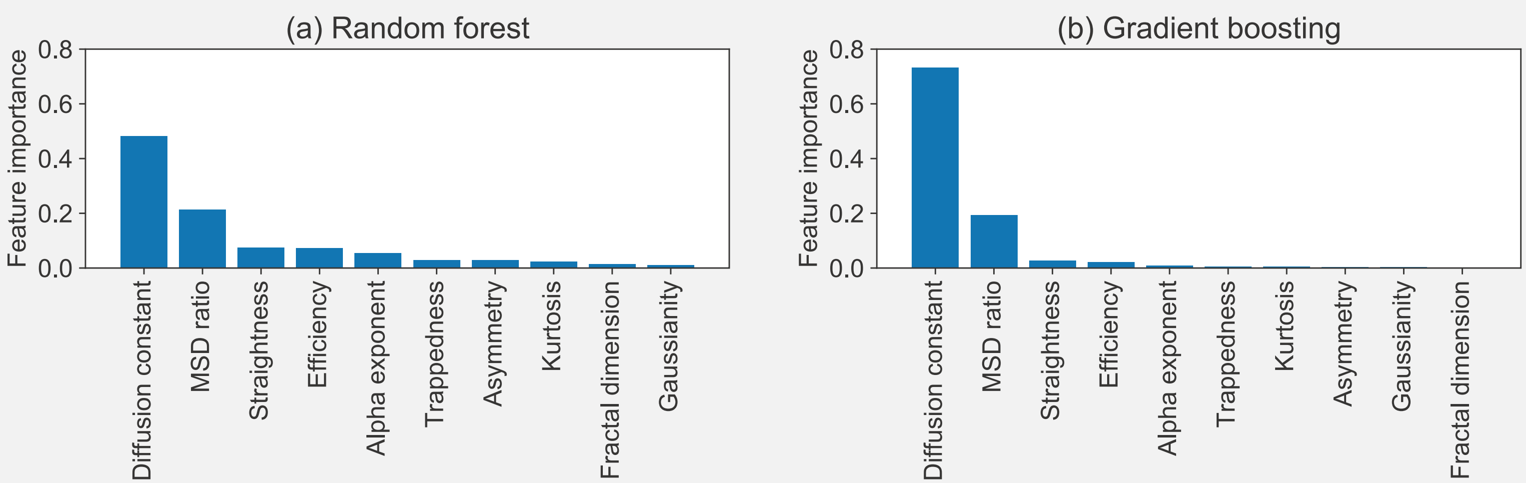
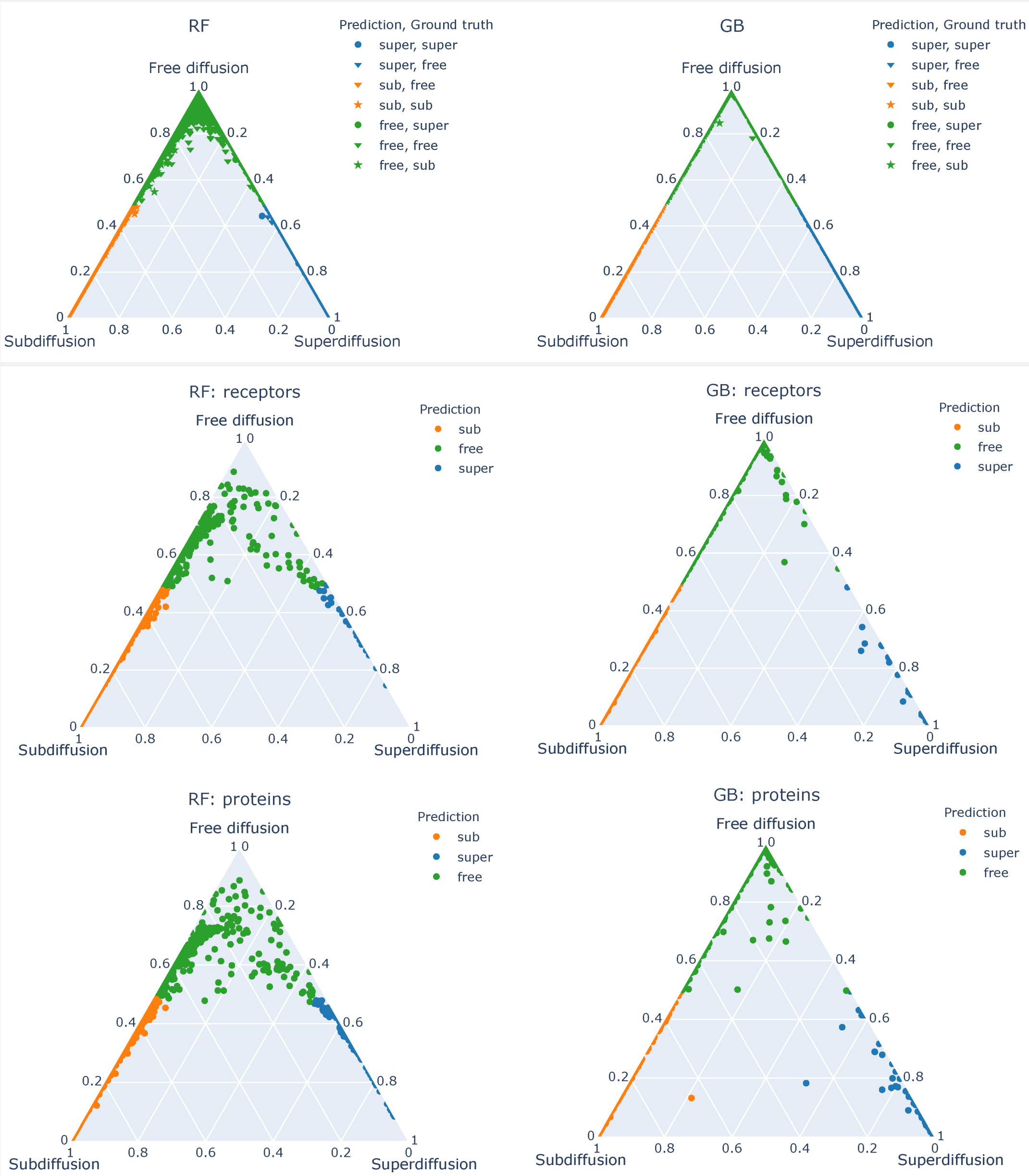


FIG. 4. Feature importance in (a) the random forest model and (b) the gradient boosting models.

P Kowalek, H Loch-Olszewska & J Szwabiński, PRE (2019)

Feature-based classification schemes



H Loch-Olszewska & J Szwabiński, Entropy (2020)

List of the features - Table

The features used to characterize the SPT trajectories. The original set of features for the AnDi challenge (left column) have been extended afterwards (right columns) to improve the performance of the classifier. See [1] for definitions and further details

Original features	Additional features
Anomalous exponent	D'Agostino-Pearson test statistic
Diffusion coefficient	Kolmogorov-Smirnov statistic against χ^2 distribution
Asymmetry	Noah exponent
Efficiency	Moses exponent
Empirical velocity autocorrelation function	Joseph exponent
Fractal dimension	Detrending moving average
Maximal excursion	Average moving window characteristics
Mean maximal excursion	Maximum standard deviation
Mean gaussianity	
Mean squared displacement ratio	
Kurtosis	
Statistics based on p-variation	
Straightness	
Trappedness	

Confusion matrices

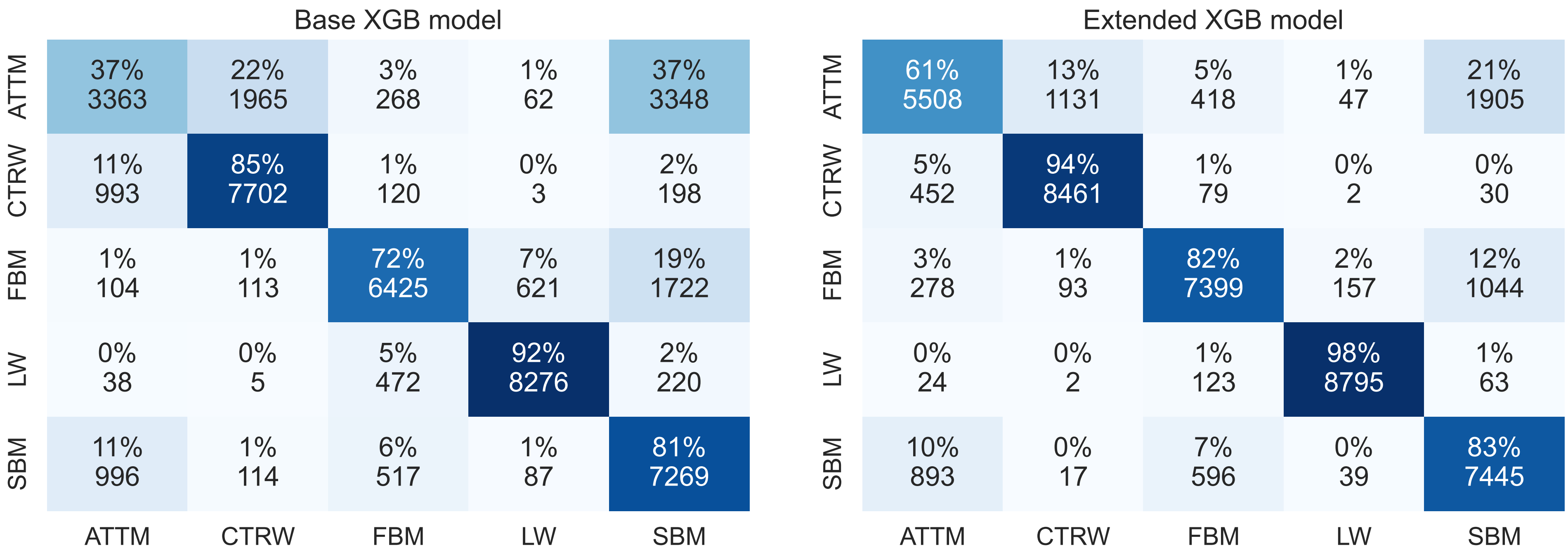


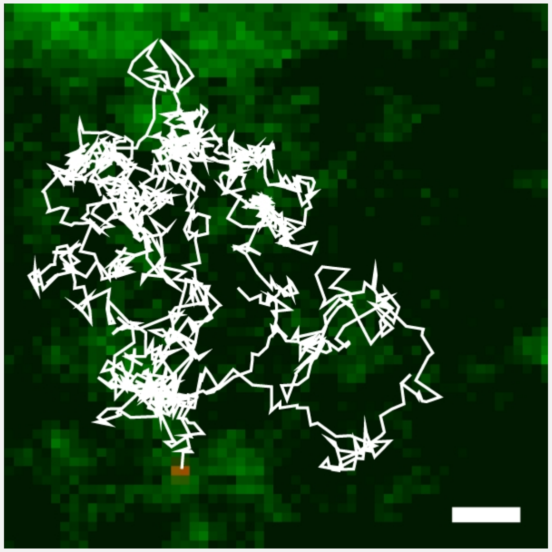
Figure: Normalized confusion matrices for the AnDi contribution (left) and the extended model (right). Rows correspond to the true labels and columns to the predicted ones.

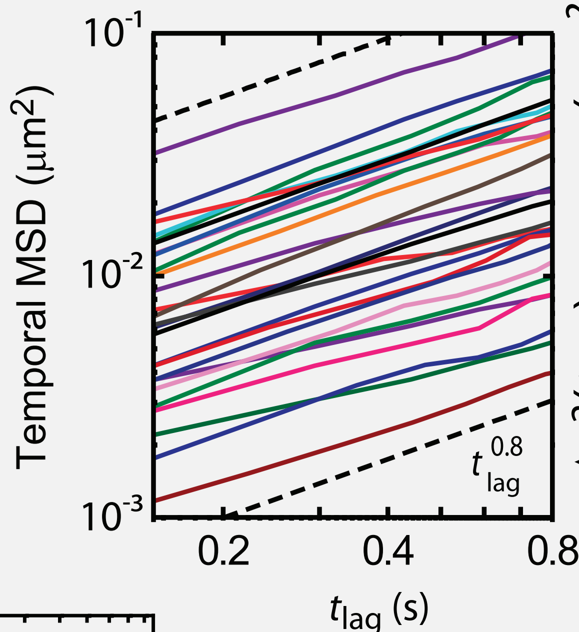
Feature importances

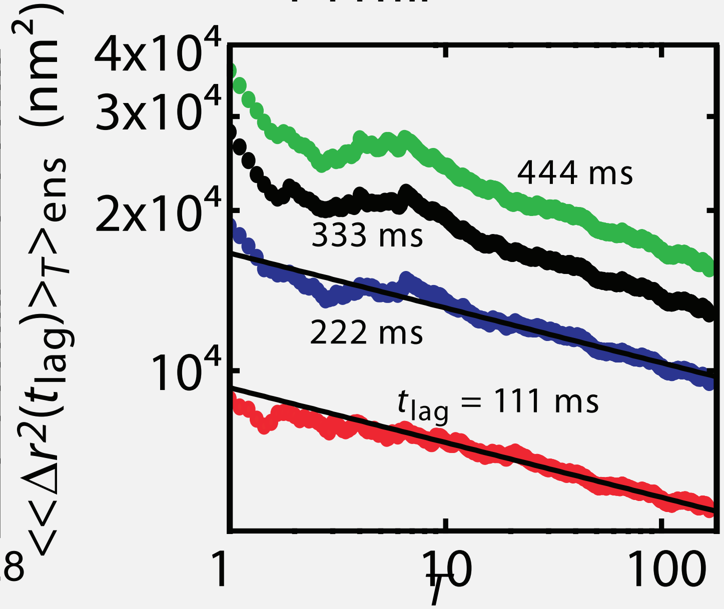
ATTM		**FBM**		**SBM**	
feature	importance	feature	importance	feature	importance
M	0.13	M	0.07	M	0.20
max_std_x	0.08	alpha	0.06	dagostino_y	0.05
max_std_y	0.08	dagostino_y	0.06	dagostino_x	0.04
dagostino_y	0.07	dagostino_x	0.06	alpha	0.03
mw_x_mean10	0.06	max_std_x	0.05	max_std_y	0.03
mw_y_mean10	0.06	max_std_y	0.05	max_std_x	0.03
mean_gaussianity	0.06	max_std_change_y	0.03	mw_y_mean10	0.02
dagostino_x	0.06	mean_gaussianity	0.03	ksstat_chi2	0.02
p_var_1	0.05	p_var_1	0.03	vac_lag_1	0.02
alpha	0.05	vac_lag_1	0.03	mean_gaussianity	0.02
CTRW		**LW**			
feature	importance	feature	importance		
mw_x_mean10	0.07	max_std_x	0.05		
mw_y_mean10	0.07	max_std_y	0.05		
fractal_dimension	0.04	dagostino_y	0.02		
dagostino_x	0.03	p_var_1	0.02		
ksstat_chi2	0.02	dagostino_x	0.02		
mw_x_mean20	0.02	alpha	0.02		
mw_y_mean20	0.02	vac_lag_2	0.01		
dagostino_y	0.02	max_std_change_y	0.01		
mean_gaussianity	0.02	max_std_change_x	0.01		
p_var_1	0.01	mw_y_mean10	0.01		

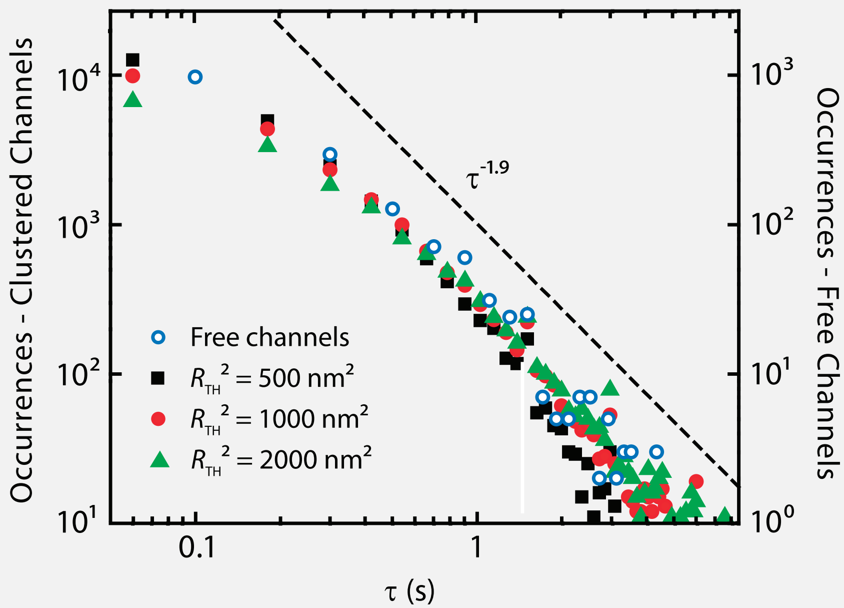
Table: Ranking of most important features (based on SHAP values) in case of the extended classifier.

But: clear feature-extraction possible despite $\alpha = 0.9$









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

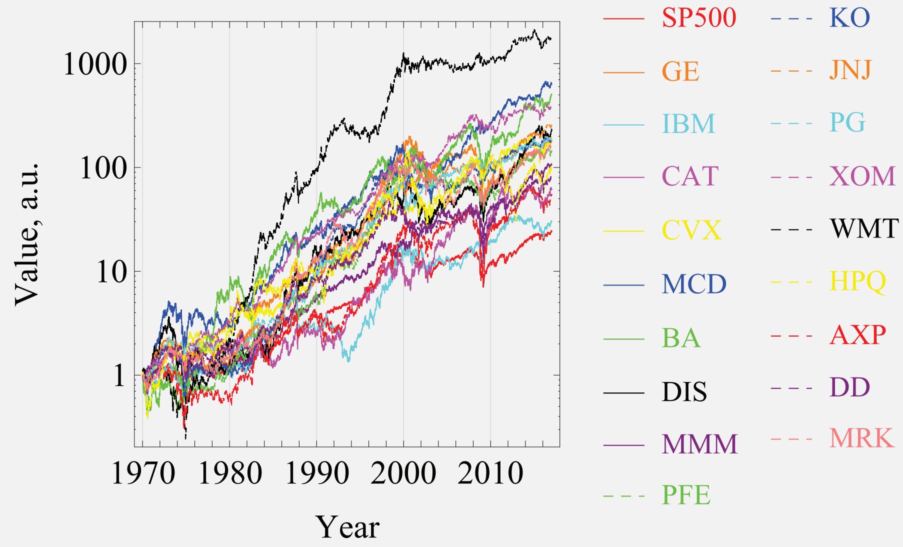
$\overline{\delta^2(\Delta)}$ apparently random

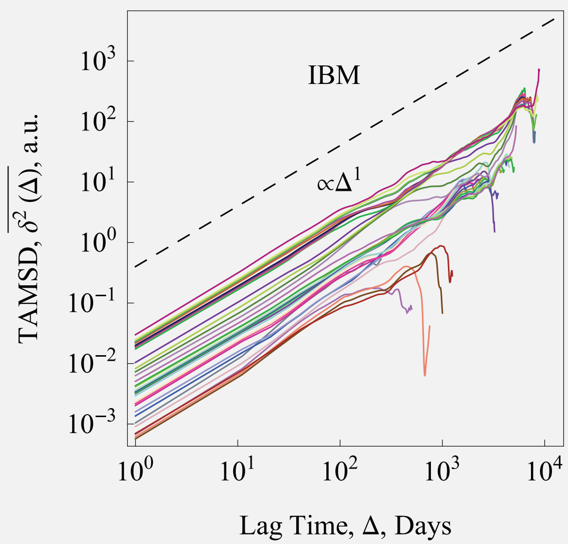
$\Delta / T^{1-\alpha} \simeq \overline{\delta^2(\Delta)} \neq \langle \mathbf{r}^2(\Delta) \rangle \simeq \Delta^\alpha$

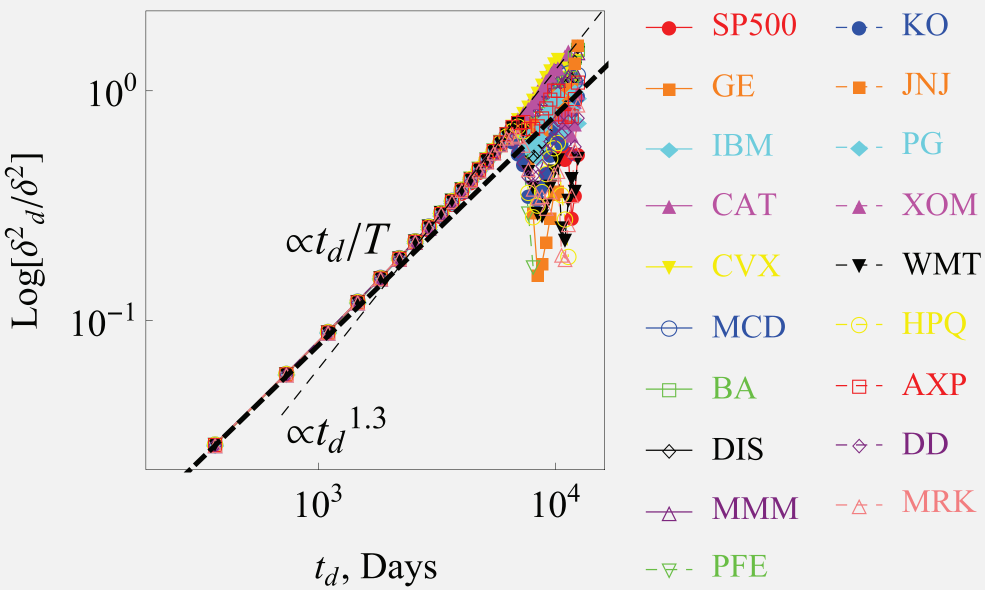
$P(\mathbf{r}, t) \simeq \exp\left(-\beta r^{1/[1-\alpha/2]}\right)$

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

Time averages & ageing in financial market time series







$$dX(t) = \mu X(t)dt + \sigma X(t)dW(t)$$

$$\overline{\delta_d^2(\Delta)} = \frac{\int_{t_d}^{T-\Delta} [X(t+\Delta) - X(t)]^2\, dt}{T - t_d - \Delta} \sim \frac{\Delta}{T - t_d} X_0^2 \left(e^{\sigma^2 T} - e^{\sigma^2 t_d}\right)$$

$$\log\left[\left\langle \overline{\delta_d^2(\Delta, t_d)} \right\rangle \Big/ \left\langle \overline{\delta^2(\Delta)} \right\rangle\right] \sim t_d/T$$

AG Cherstvy, D Vinod, E Aghion, AV Chechkin & RM, NJP (2017)

Universality of delay-time averages for financial time series

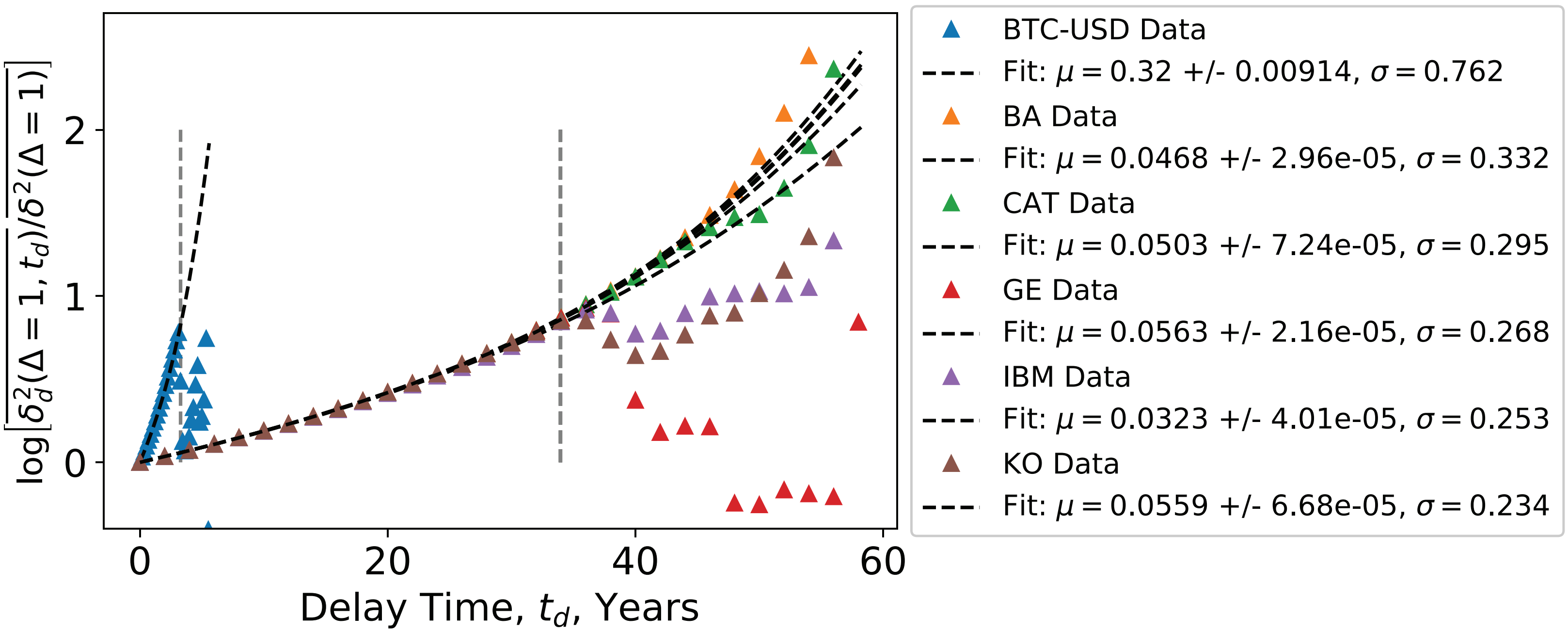
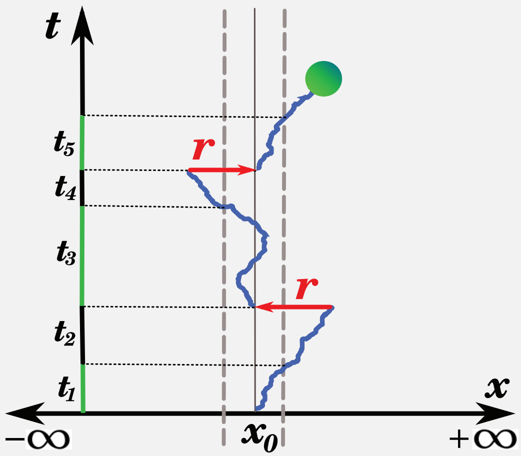


Figure 9. Delayed TAMSDs calculated for the stocks- and cryptocurrency-data plotted versus the delay time t_d. The time periods of the FTS used for the determination of optimal drift and volatilities are 1962–2020 and 2014–2019, for the classical stocks and cryptocurrencies (BitCoin), respectively. The optimal annualized volatility found from equation (C5) and the value of drift found from the single-parameter fit of $\overline{\delta_{d,i}^2}(\Delta)$ are listed in the legend. The two vertical dashed lines shown on the t_d-axis at the end of 1995 and 2017 help to assess the positions, respectively, of the 1997–1999 financial crisis for the stocks and of the crash late December 2017 for BitCoin. These lines define the range of the delayed-TAMSD data used to obtain the parameter μ from the respective fits to the data, see appendix C for details.

Soft resets of Lévy walk

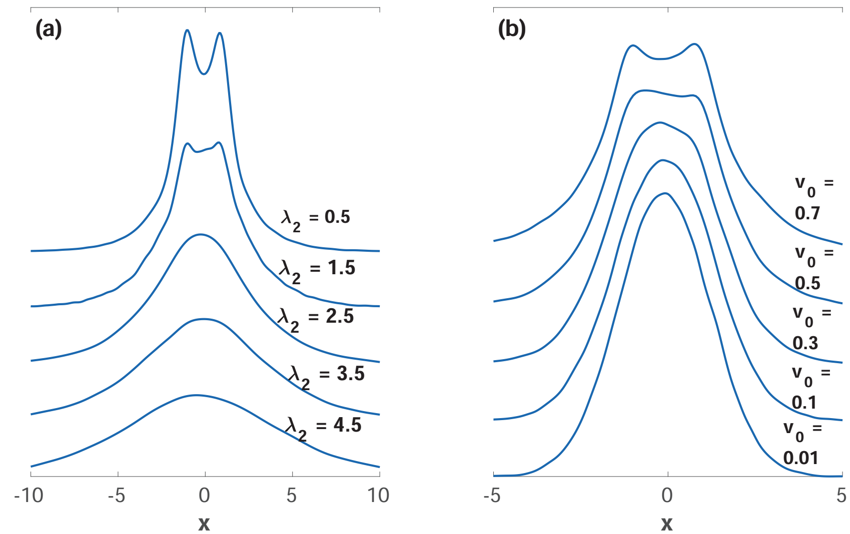


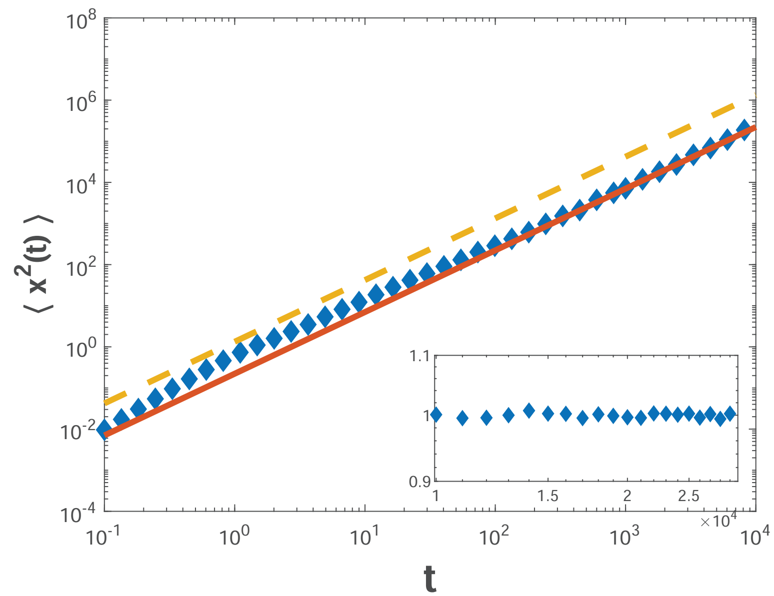
Soft reset phase: motion in harmonic potential with Hooke constant γ:

$$m\frac{d^2x}{dt^2} = -\gamma x$$

Free Lévy walk phase:

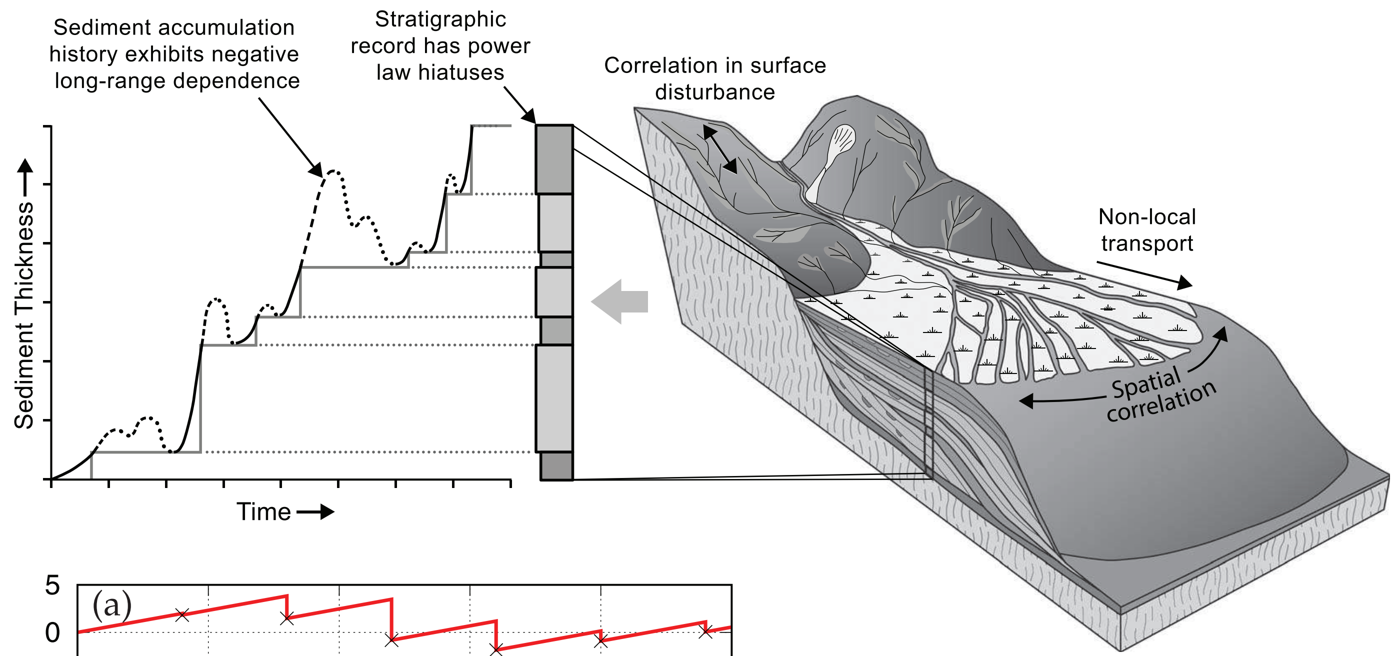
$$\frac{dx}{dt} = \pm v_0$$

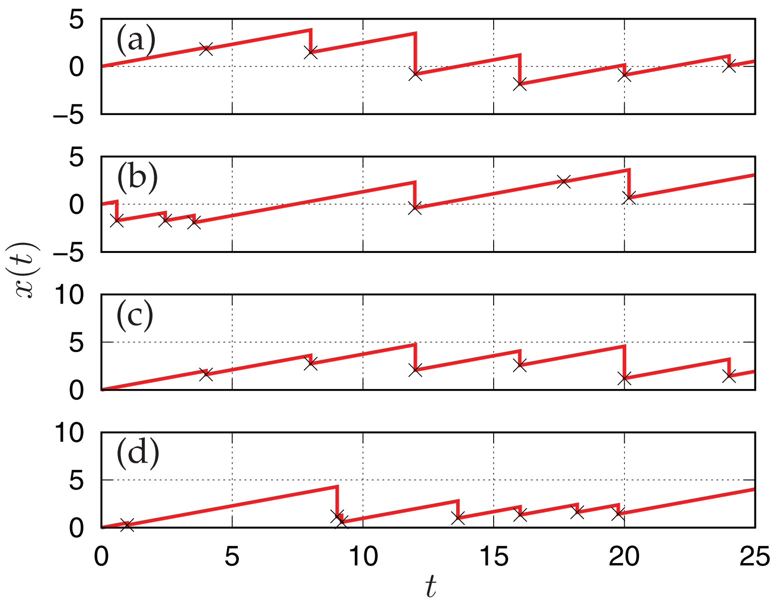




P Xu, T Zhou, RM & W Deng (2021)

Stochastic resets with random amplitude & stratigraphy

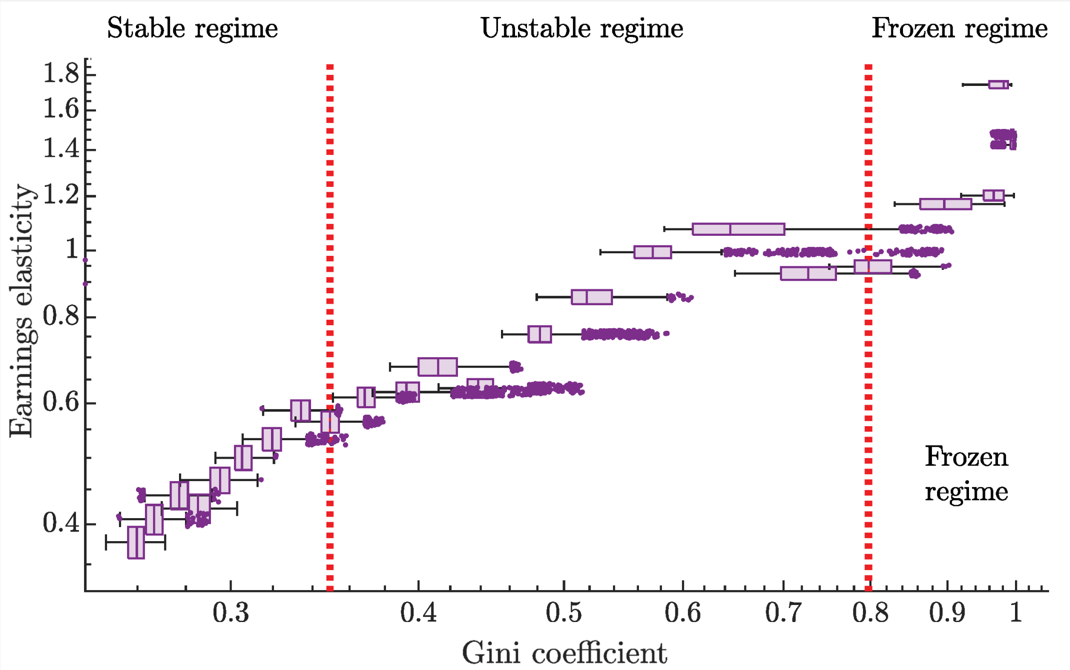


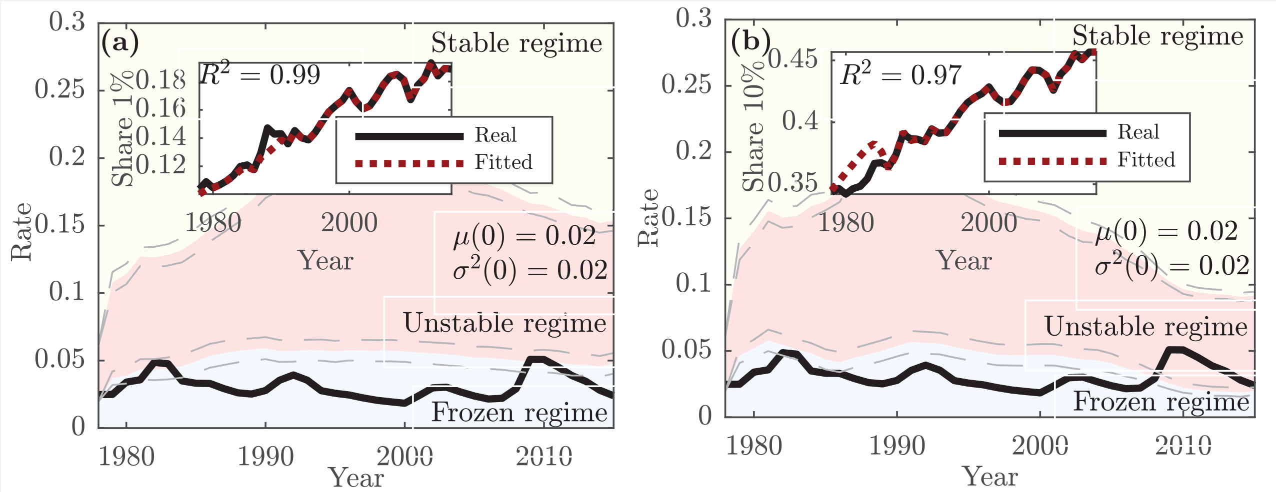


NB: ∃ ample applications in finance

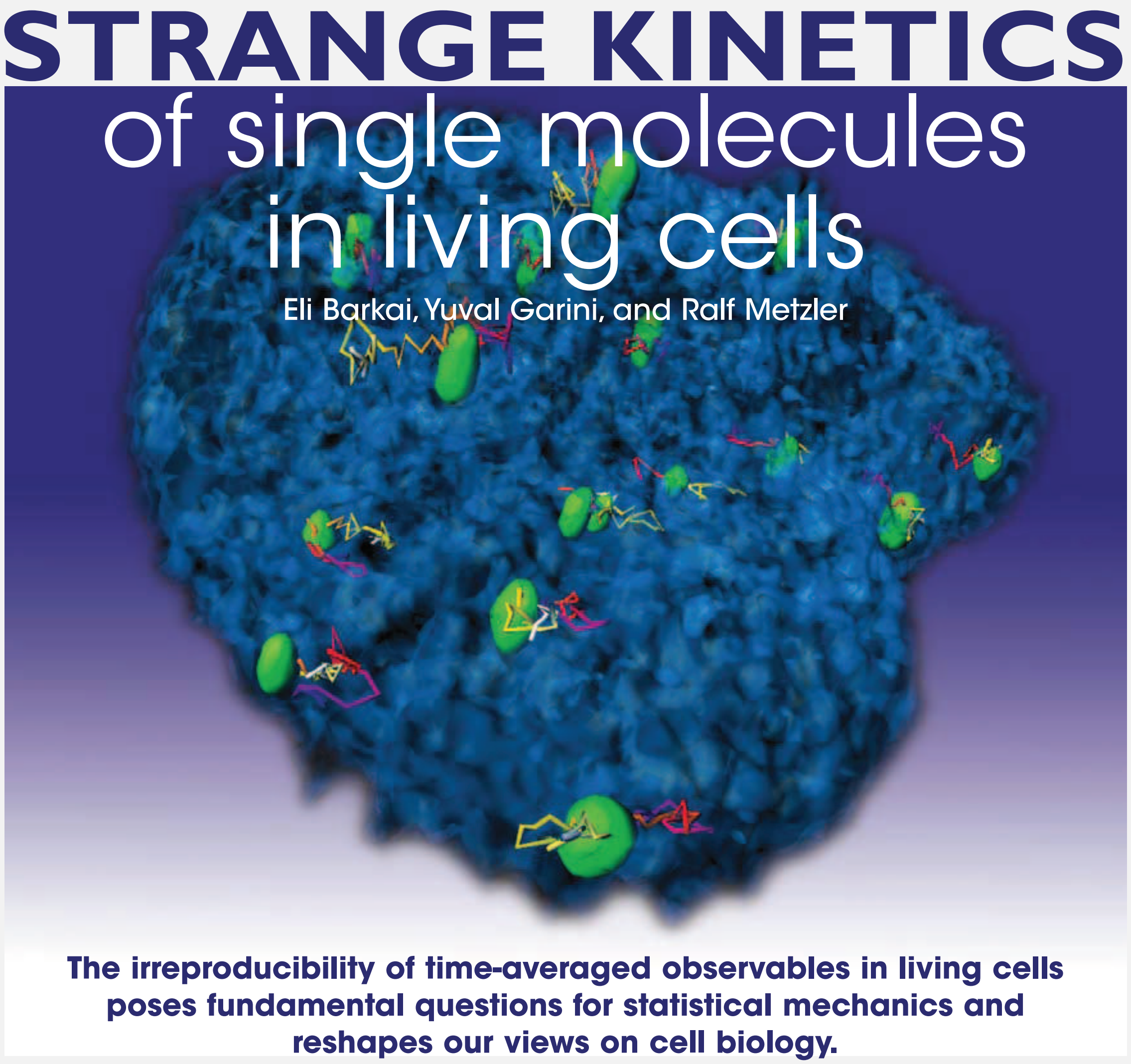
M Dahlenburg, R Schumer, A Chechkin & RM, PRE (2021)

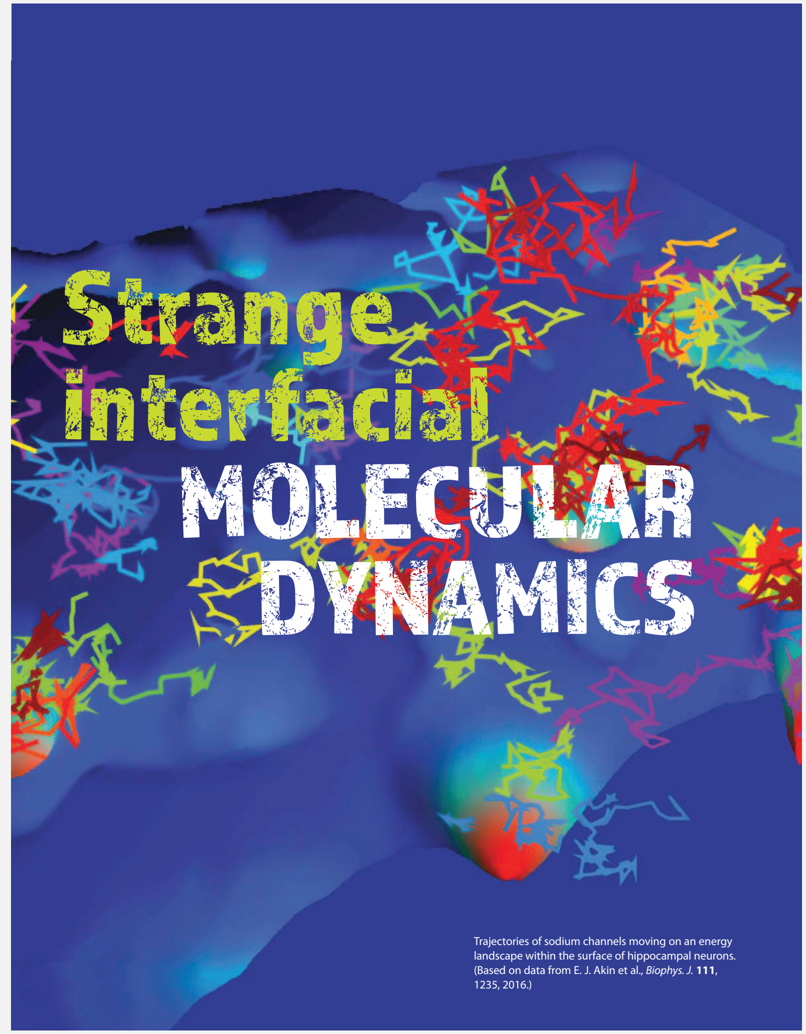
Income inequality & mobility in GBM /w stochastic resetting





V Stojkoskim P Jolakoski, A Pal, T Sandev, L Kocarev & RM (2021)





E Barkai, Y Garini & RM, Phys Today (2012); D Krapf & RM, Phys Today (2019)

∑ummary

I General theme: modelling, i.e., from data to models

II Ever better data from experiments & simulations, especially single time series $\mathbf{r}(t)$. Finite measurement time & often few

III Anomalous diffusion is non-universal: big question what is the underlying physical process

IIII Classical observables ("features") $\rightsquigarrow$ decision trees

卌 Deep learning strategies combined with random forest or gradient boosting: many imponderables. Feature-based approaches allow for physical interpretation

卌I Bayesian evaluation of deep learning. More approaches?

For slides or questions: write to rmetzler@uni-potsdam.de

Thank you!

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Gleb Oshanin (Sorbonne)
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Christine Selhuber-Unkel (U Heidelberg)
Flavio Seno (Universitá di Padova)
Igor Sokolov (Humboldt U Berlin)
Ilpo Vattulainen (Helsingin Yliopisto)
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