Random motion: from molecules to animals

—UP, 19th February 2022—

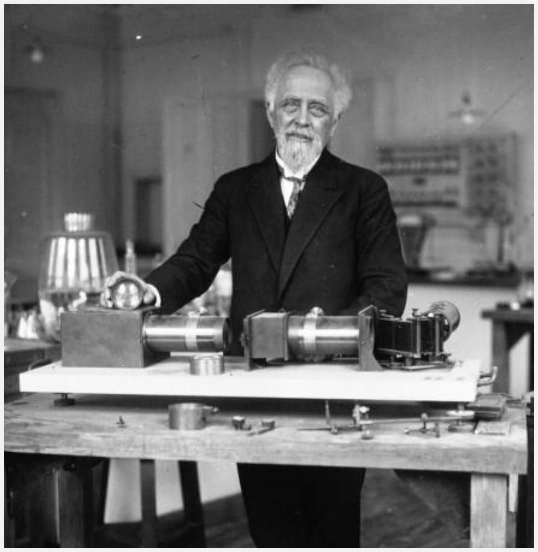
Fluxes, random walks, & fluctuating forces . . .

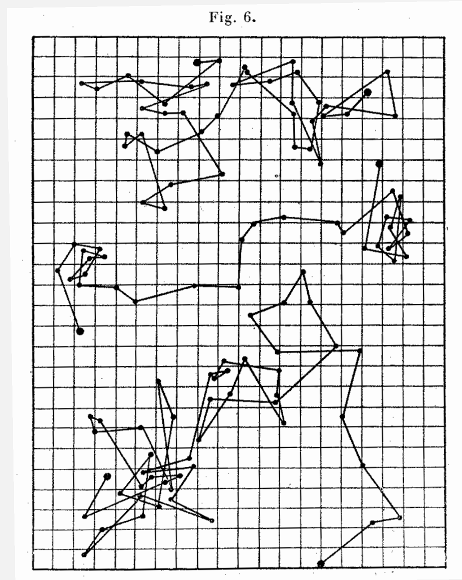
Paul Langevin (1872-1946)
Albert Einstein (1879-1955)

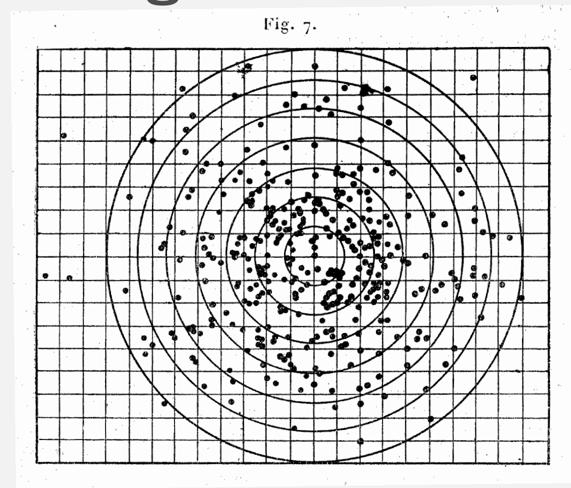
Marian Smoluchowski
(1872-1917)

William Sutherland
(1859-1911)

Les atomes: Brownian motion and Avogadro's number

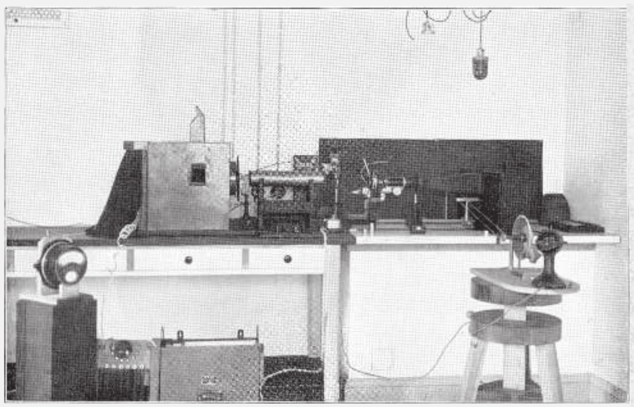


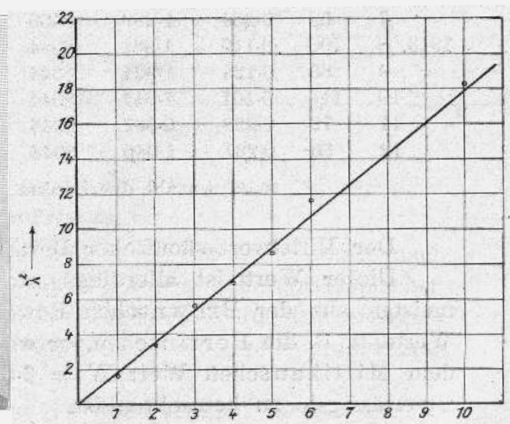


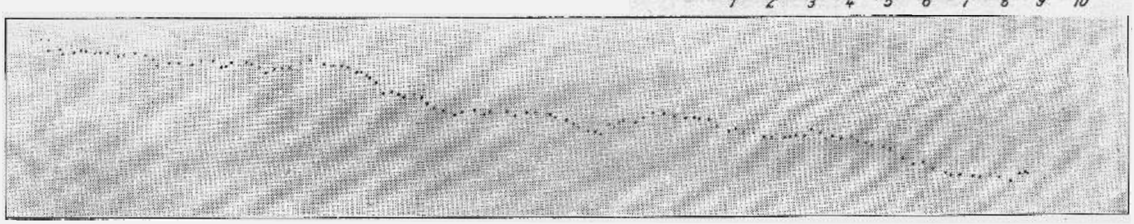


Δt=30 sec

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





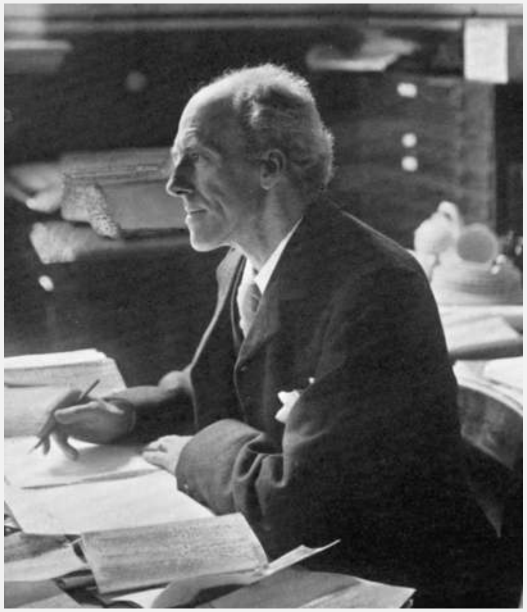


J Perrin, Comptes Rendus (Paris) 146 (1908) 967: $N_A = 70.5 \times 10^{22}$; I Nordlund, Z Physik (1914): $N_A = 5.91 \times 10^{23}$

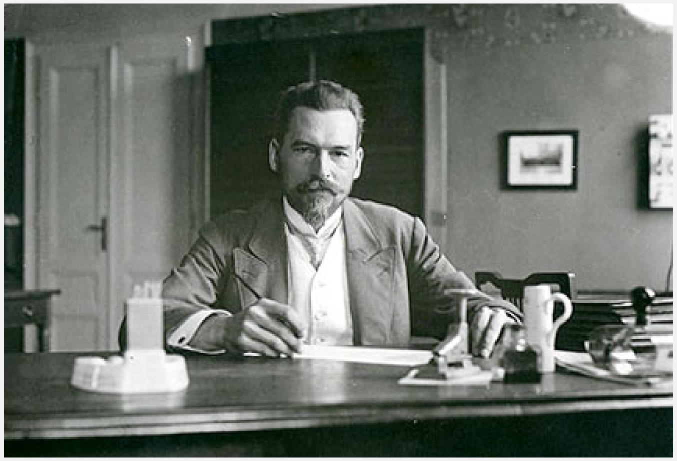
Brownian motion & random walks applied . . .

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

Ensemble versus single particle statistics

- Not all systems are ergodic: $\langle\cdot\rangle \neq \overline{\cdot}$ [RM et al, PCCP (2014)]
- Single particle statistics show useful fluctuations
- Some systems can only provide single time series:

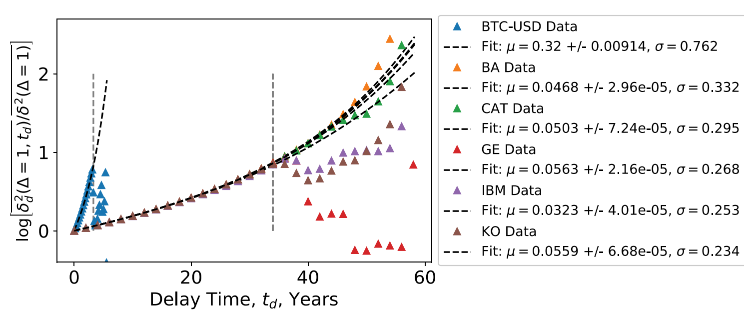
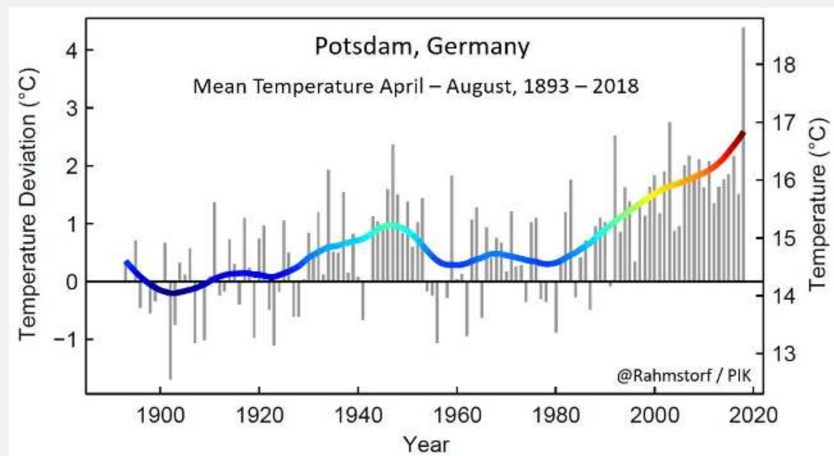


Figure 9. Delayed TAMSDs calculated for the stocks- and cryptocurrency-data plotted versus the delay time t_d. The time periods of the FTS used for the determination of optimal drift and volatilities are 1962–2020 and 2014–2019, for the classical stocks and cryptocurrencies (BitCoin), respectively. The optimal annualized volatility found from equation (C5) and the value of drift found from the single-parameter fit of $\overline{\delta^2_{d,i}}(\Delta)$ 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.

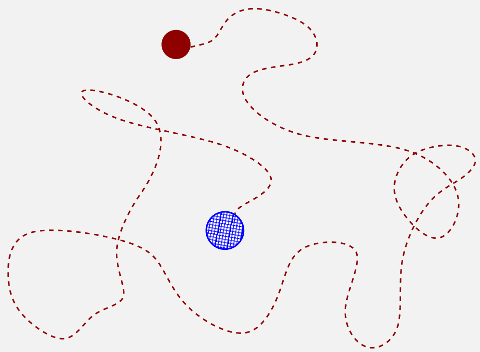


AG Cherstvy et al, NJP (2017); S Ritschel et al, J Phys Compl (2021); O Peters, Nature Phys (2019); V Stojkoski et al, Phil Trans A (2022)

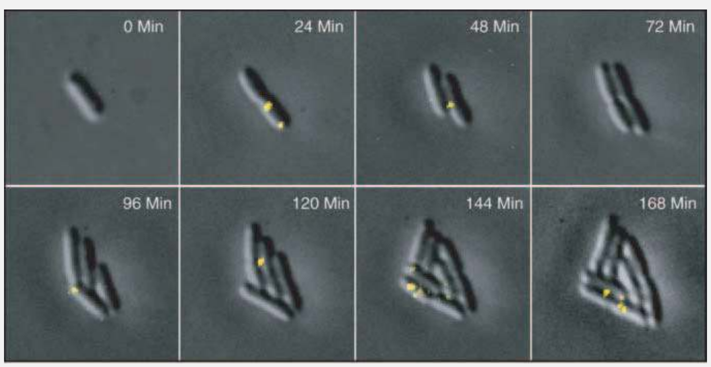
Molecular reaction times: macro vs micro

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

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



Yu et al, Science (2006)

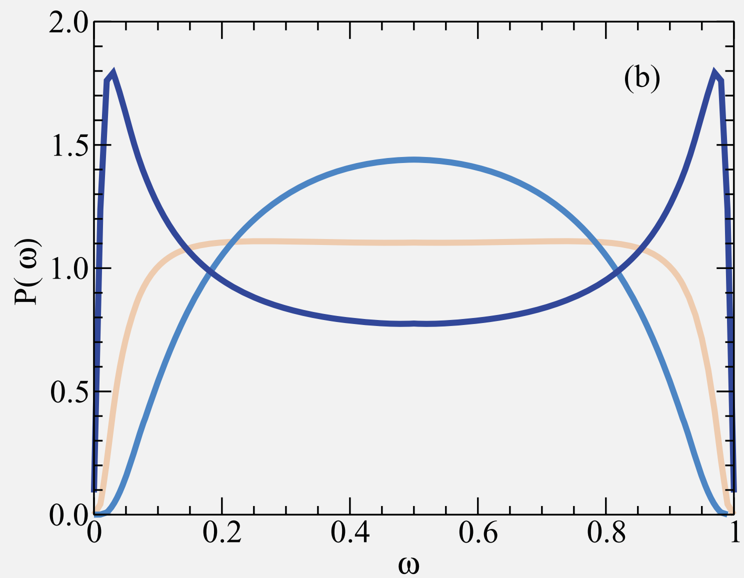


M v Smoluchowski, Physikal Zeitschr (1916)

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

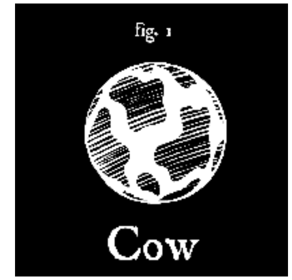
$$\omega = \frac{\tau_1}{\tau_1 + \tau_2}$$

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



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

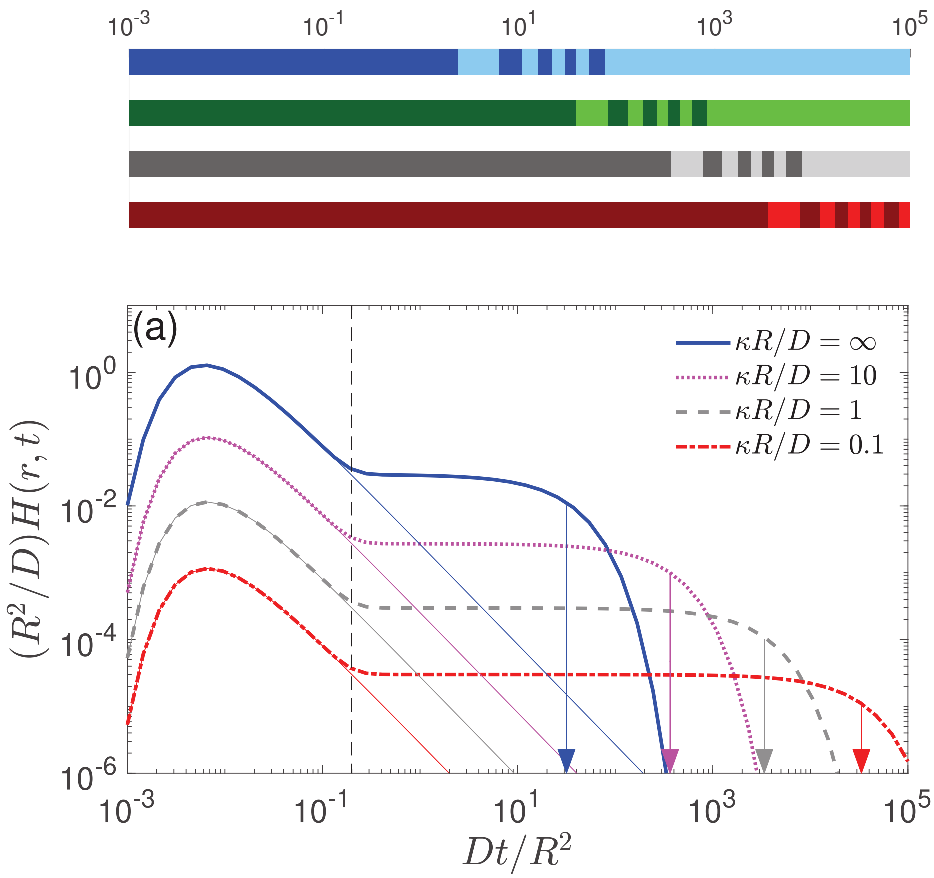
Strongly defocused (fluctuating) reaction times



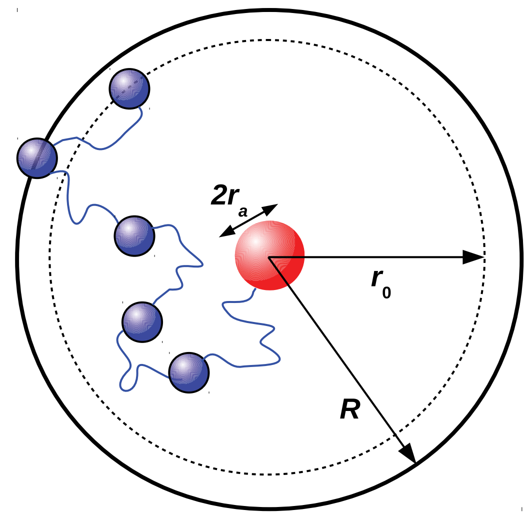
Geometry control: direct trajectories independent of outer boundary

Reaction control: finite reactivity requires multiple collisions

Full first passage time density:



Direct vs indirect trajectories:



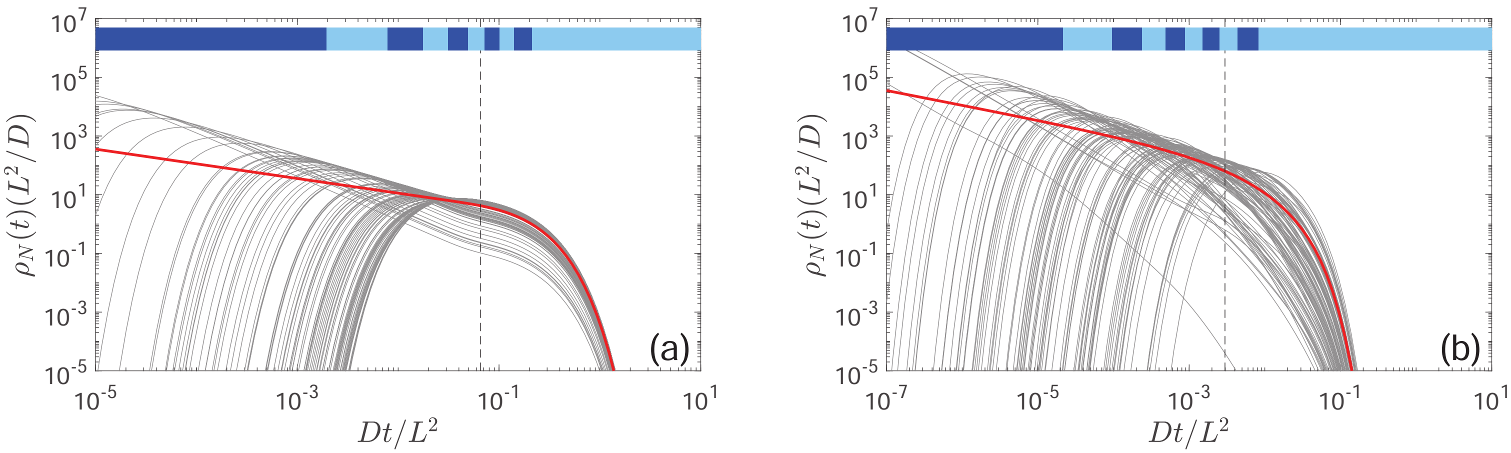
$$\langle t\rangle=\frac{(r_0-r_a)(2R^3-r_0r_a[r_0+r_a])}{6Dr_0r_a}+\frac{R^3-r_a^3}{3\kappa r_a}$$

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



$N = 1$ $\qquad$ $N = 10$

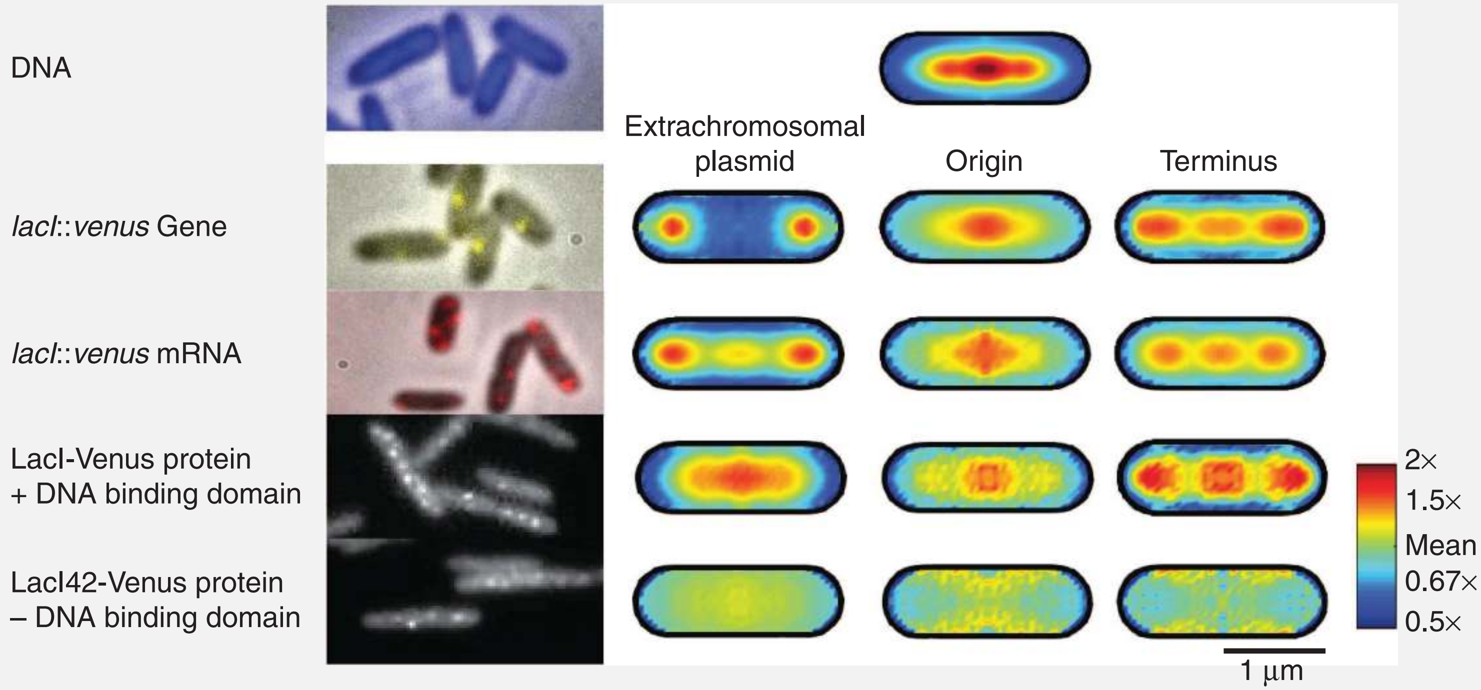
Grey lines: 100 random initial configurations

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

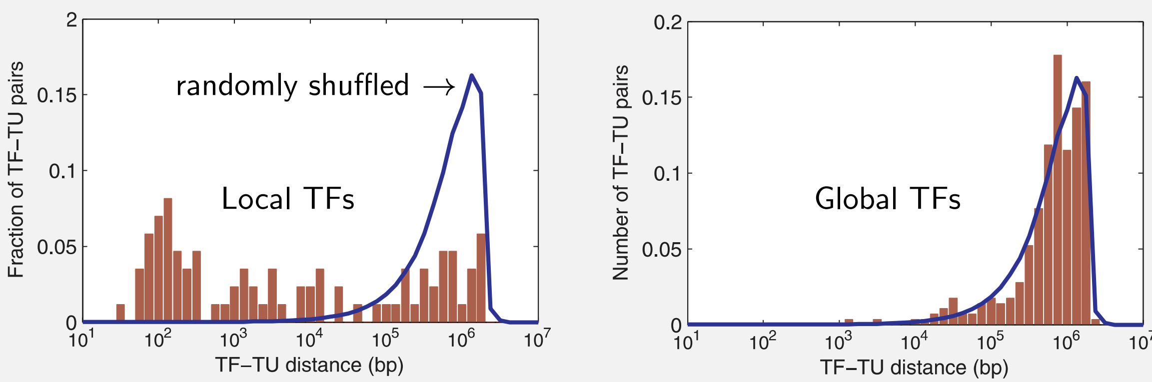
$\rightsquigarrow$ Initial conditions matter significantly & chemical rate approach requires sufficiently high concentrations

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

Inhomogeneous TF location, rapid search hypothesis

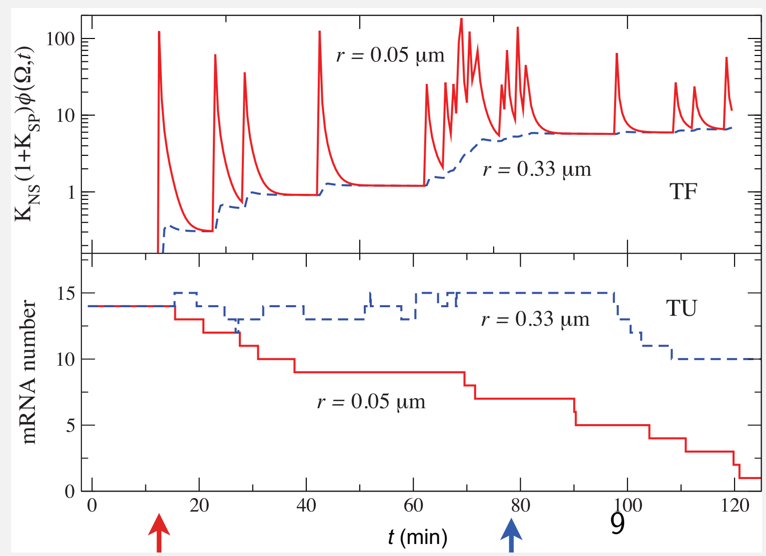


Kuhlman & Cox, Mol Sys Biol (2012)

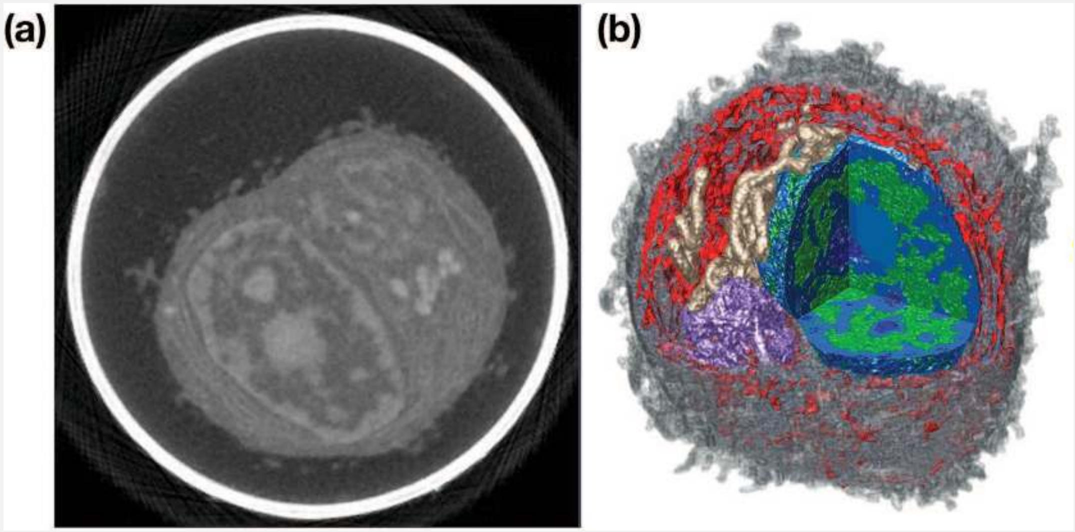


TF-TU gene-gene distance [G Kolesov . . . LA Mirny, PNAS (2007)]

O Pulkkinen & RM, PRL (2013): Distance TF-TU matters →

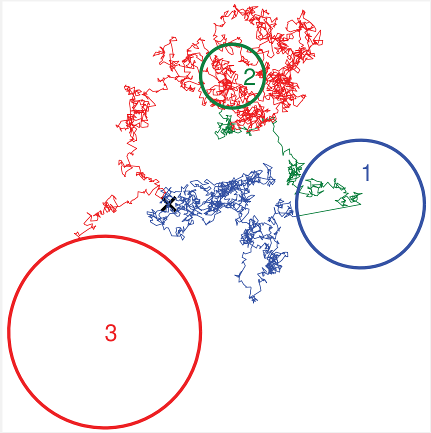


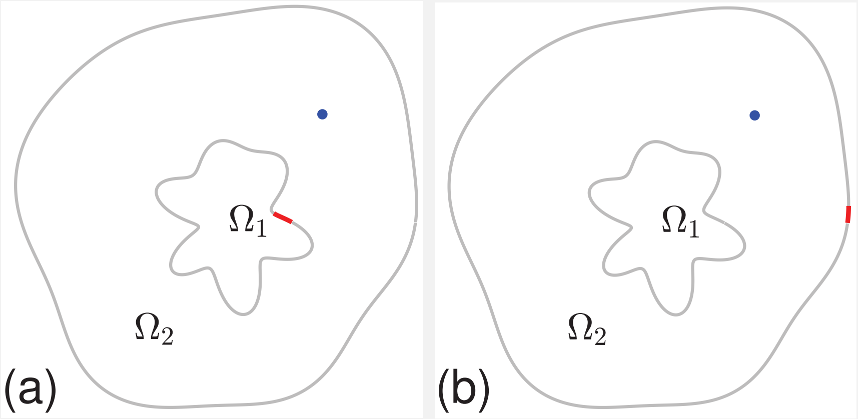
Computational models for intracellular signalling



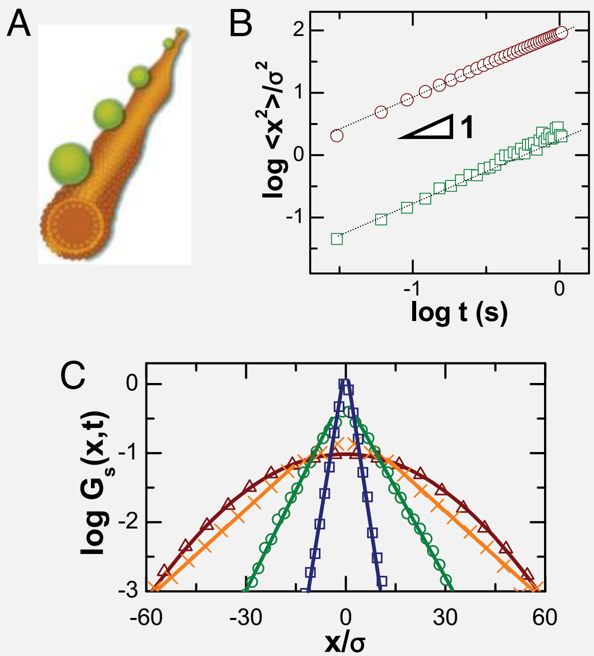
[J Ma . . . SA Isaacson, PLoS Comp Biol (2021)]

Reaction cascades & reaction in onion-like shell regions

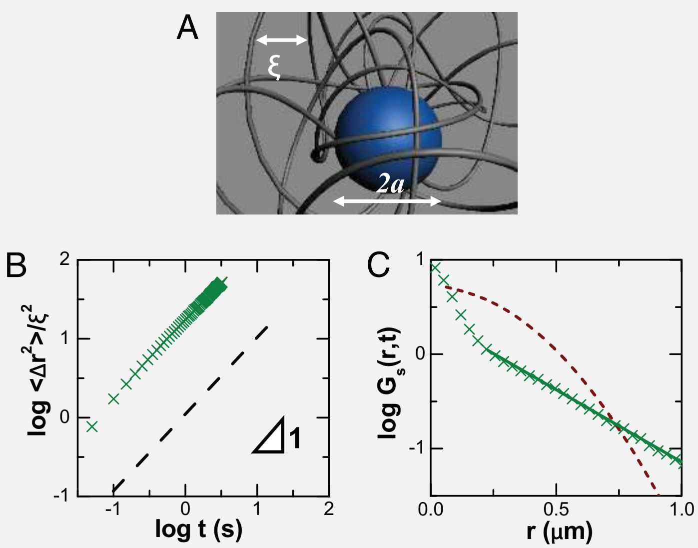




Brownian yet non-Gaussian diffusion in soft & bio-matter

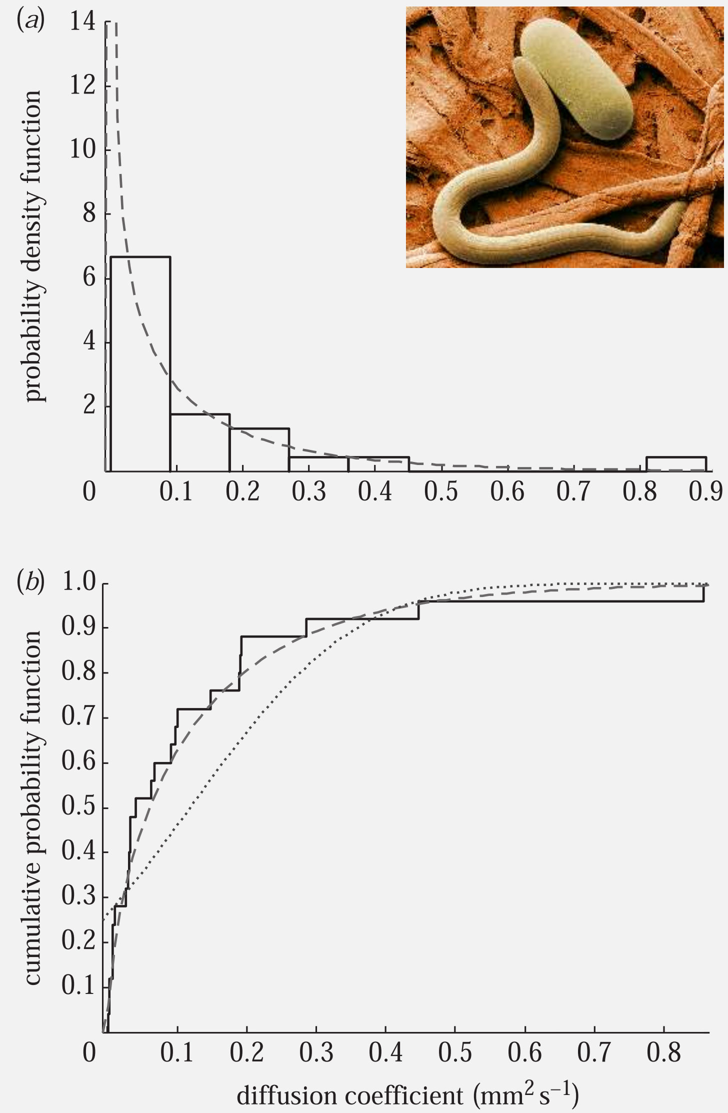


Colloidal beads on nanotubes



Nanospheres in entangled actin

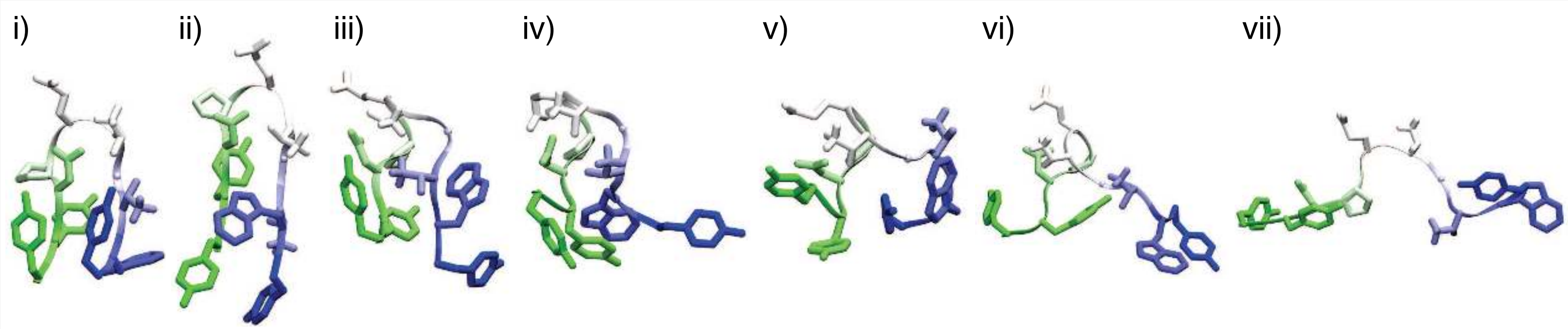
Motion of *Phasmarhabditis* nematodes



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

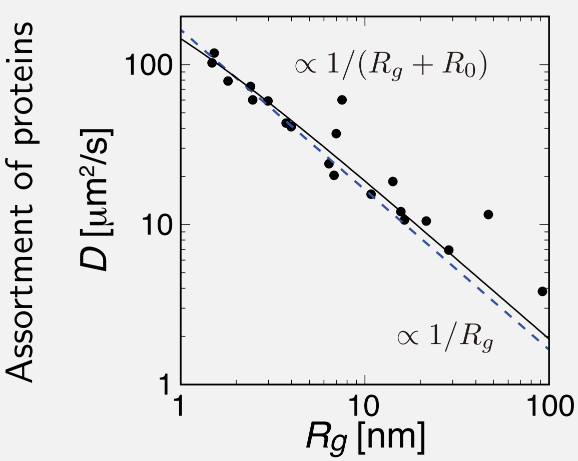
S Hapca, JW Crawford & IM Young, Interface (2009)

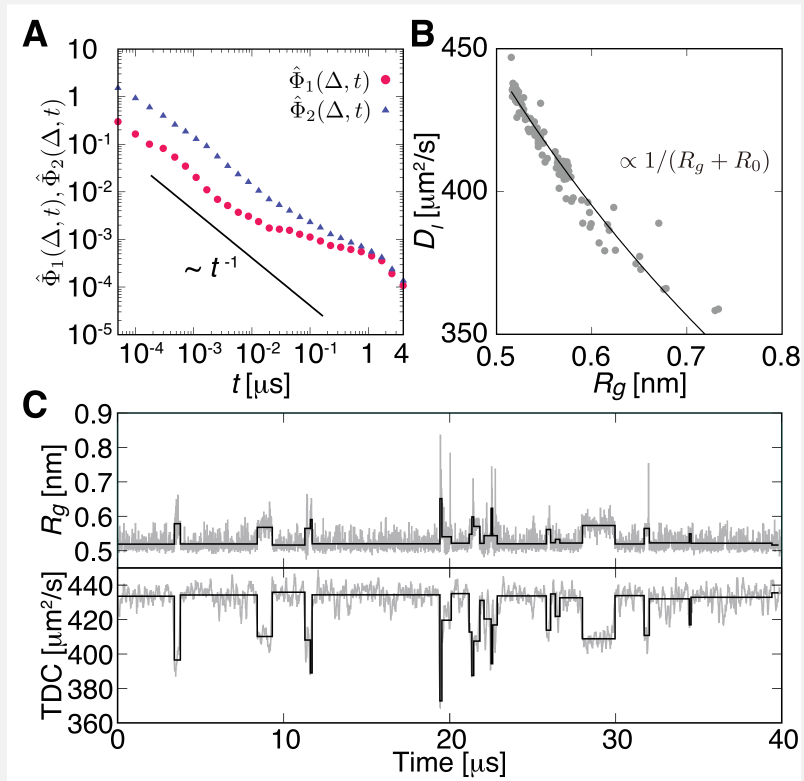
Instantaneous diffusivity of shape-fluctuating proteins



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

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

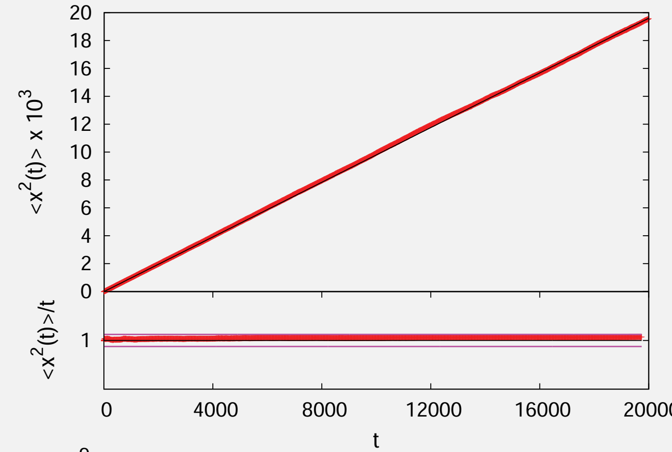




E Yamamoto, T Akimoto, A Mitsutake & RM, PRL (2021)

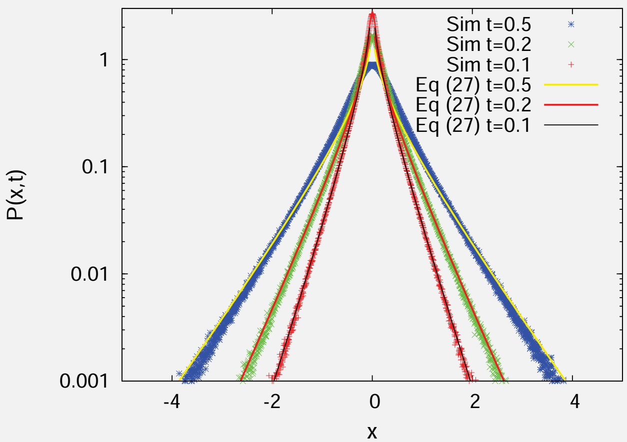
Fickian, non-Gaussian diffusion with diffusing diffusivity

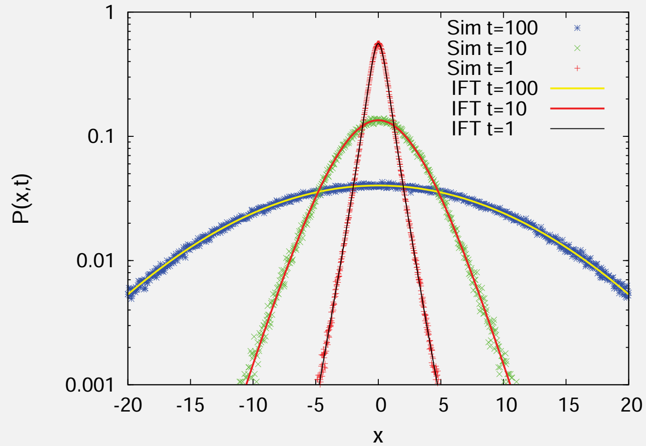
MV Chubinsky & G Slater, PRL (2014): diffusing diffusivity
[see also R Jain & KL Sebastian, JPC B (2016)]

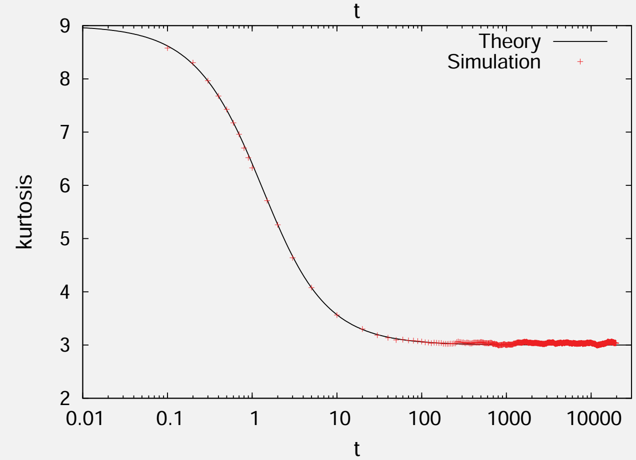


Our minimal model for diffusing diffusivity:

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



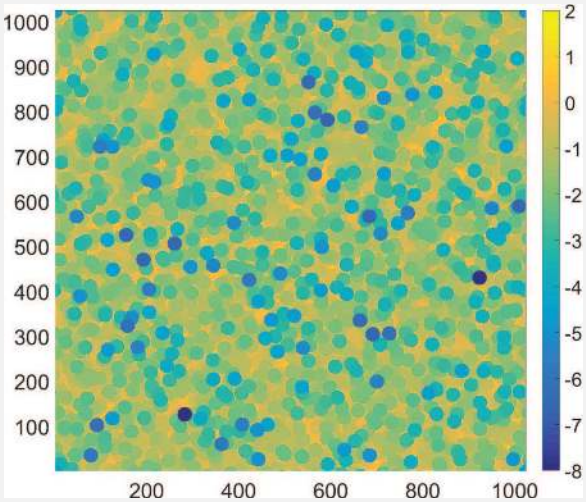


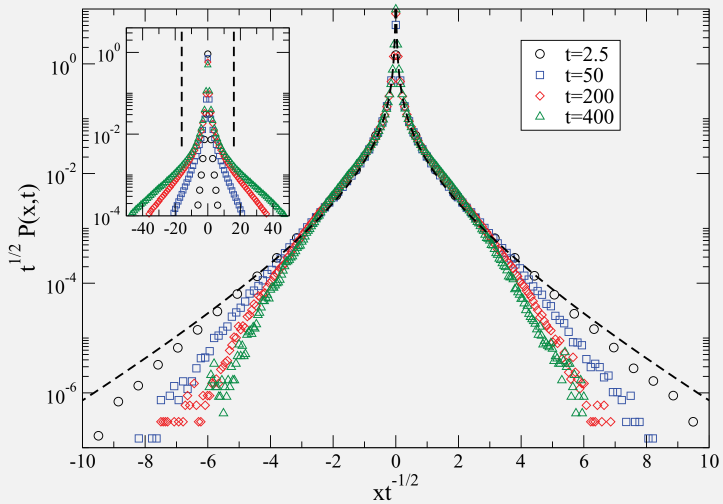


Generalised γ distribution & non-equilibrium diffusivity initial conditions: V Sposini, AV Chechkin, G Pagnini, F Seno & RM, NJP (2018)

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

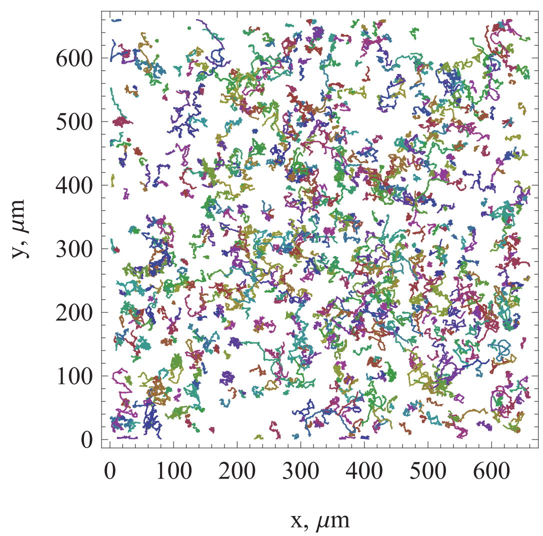
Non-Gaussian diffusion in quenched landscape models

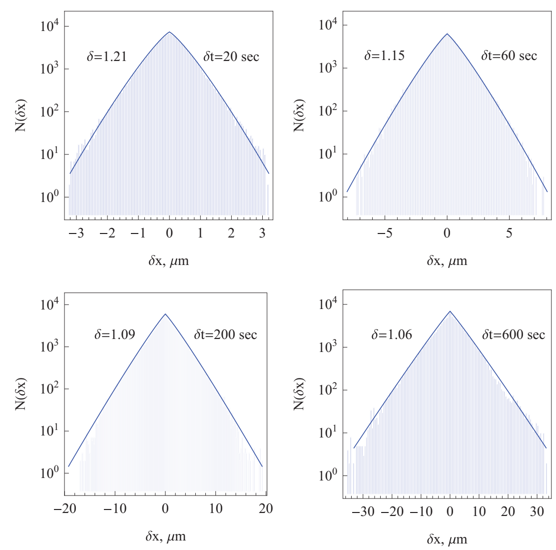


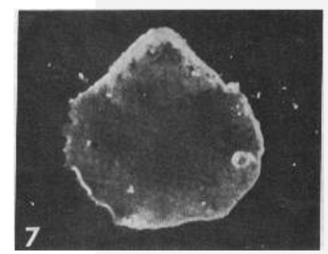


L Luo & M Yi, PRE (2018,2019); see also EB Postnikov, A Chechkin & IM Sokolov, NJP (2020)

Increasing non-Gaussianity in moving amoeba cells

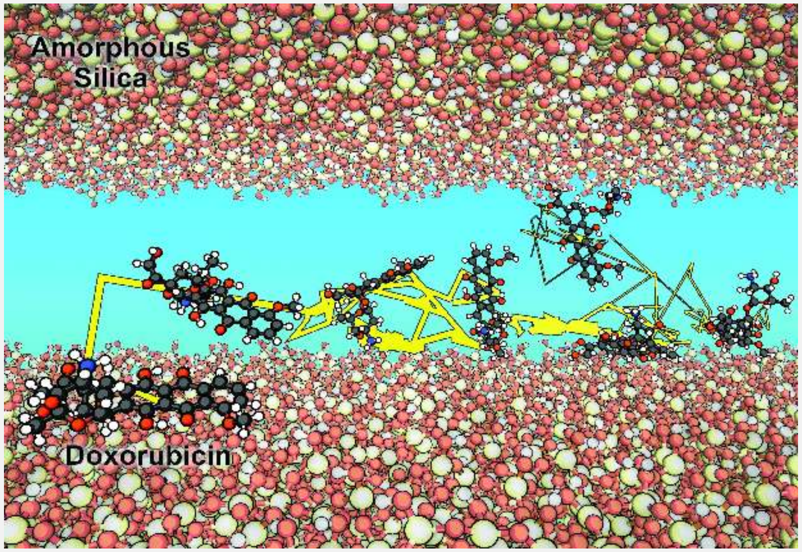


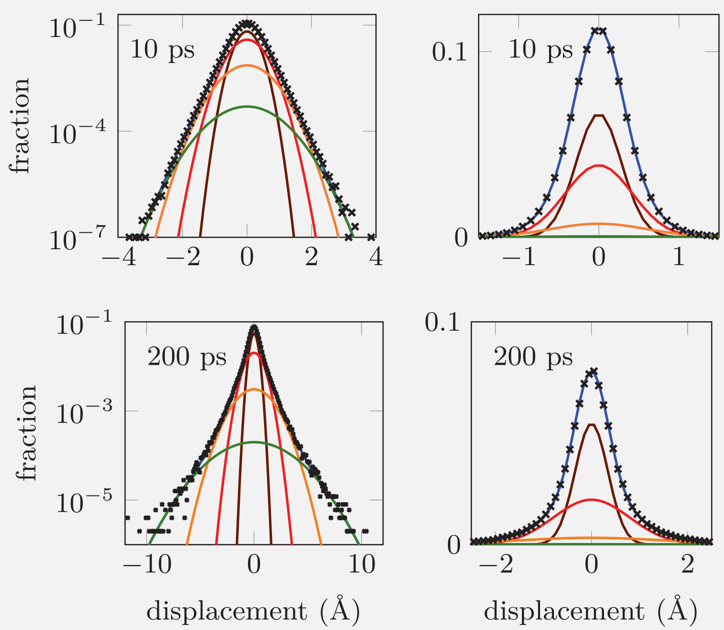


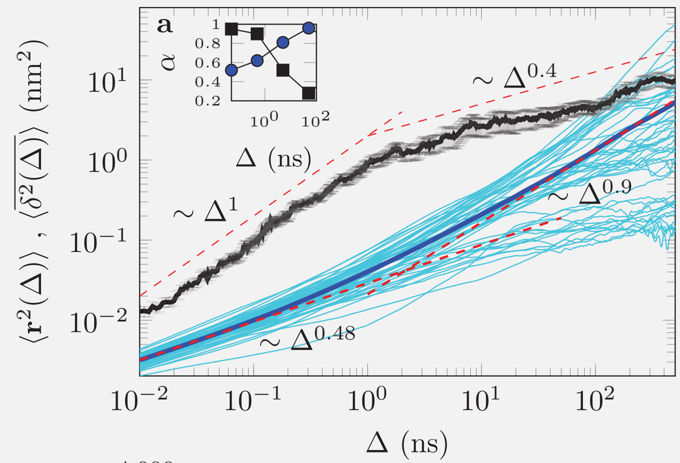


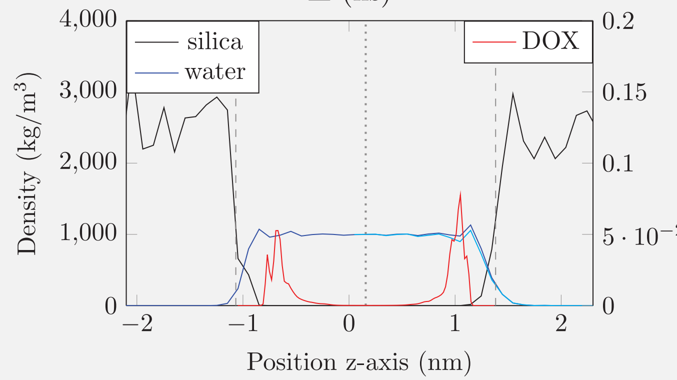
AG Cherstvy, O Nagel, C Beta & RM, PCCP (2018)

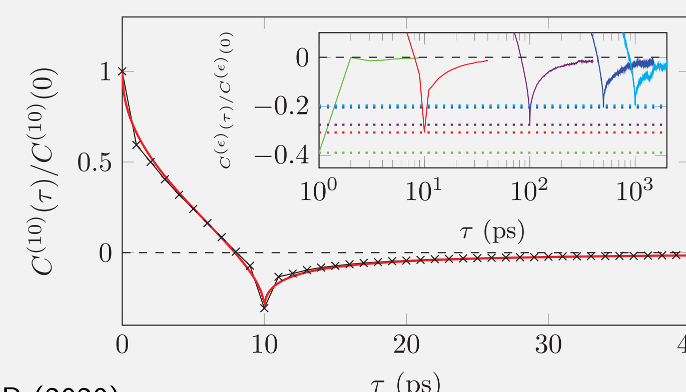
Doxorubicin drug molecule diffusion in silica nanochannels











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

Lévy foraging hypothesis: to avoid oversampling

Shlesinger & Klafter (1986): Lévy flights as efficient search mechanism

Lévy foraging hypothesis: *Superdiffusive motion governed by fat-tailed propagators optimise encounter rates under specific (but common) circumstances: hence some species must have evolved mechanisms that exploit these properties* [. . .].

Lévy flight (Mandelbrot): $\psi(t) = \tau^{-1}\exp(-t/\tau) \wedge$

$$\lambda(x) \simeq |x|^{-1-\mu}, \;\; 0 < \mu < 2 \;\; \curvearrowright \;\; \langle x^2(t)\rangle \to \infty$$

Lévy walk (Shlesinger, Klafter & Wong, JSP, 1982): spatiotemporal coupling

$$\psi(x,t) = \lambda(x)\delta(|x| - vt) \;\; \curvearrowright \;\; \langle x^2(t)\rangle \simeq t^{3-\alpha}; \;\; 1 < \alpha < 2$$

Viswanathan GE, da Luz MGE, Raposo EP, Stanley HE, The physics of foraging (CUP, 2011)

Lévy flight/walk as random search model

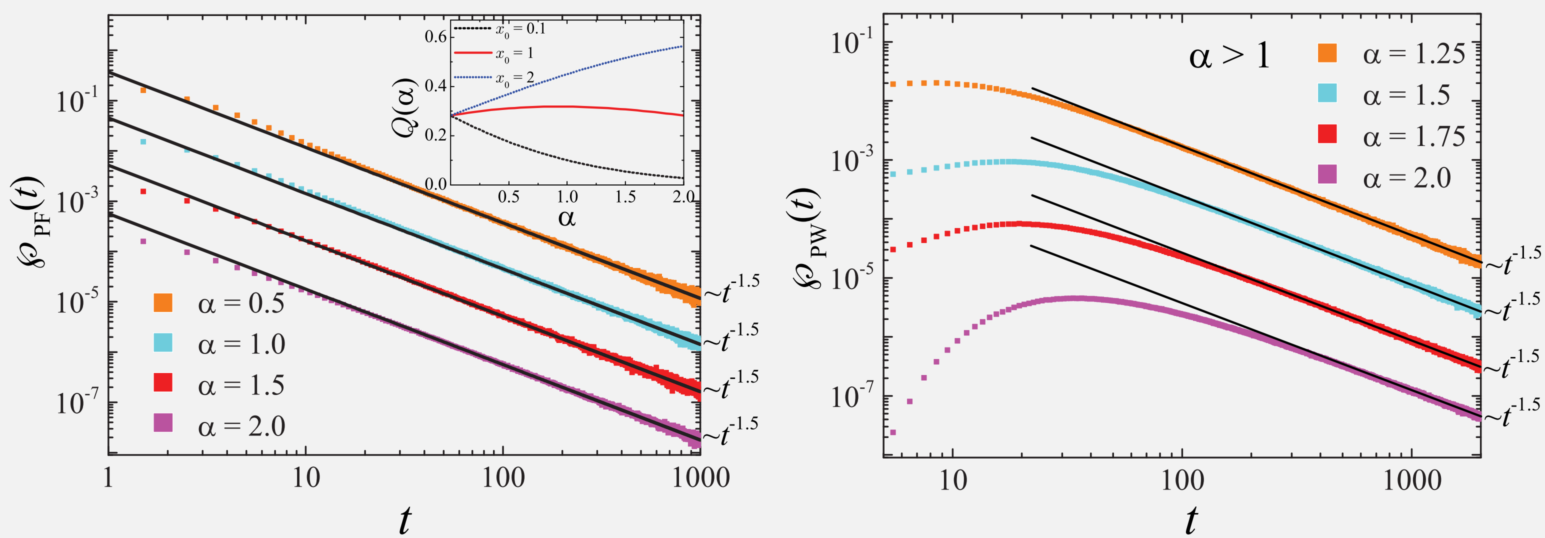
I First-passage & first-arrival (-hitting) are different; leapovers [AV Chechkin et al, JPA (2003); T Koren et al, Phys Rev Lett (2007)]

II Statistical model transcription factor search leads to Lévy flights [MA Lomholt et al, Phys Rev Lett (2005)]

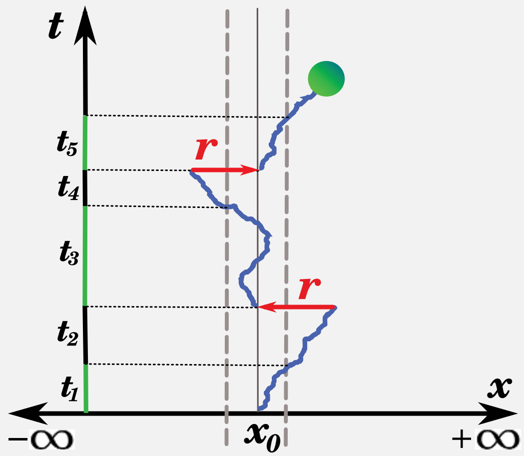
III Lévy flights do not always optimise random search for sparse targets [VV Palyulin et al, PNAS (2014)]

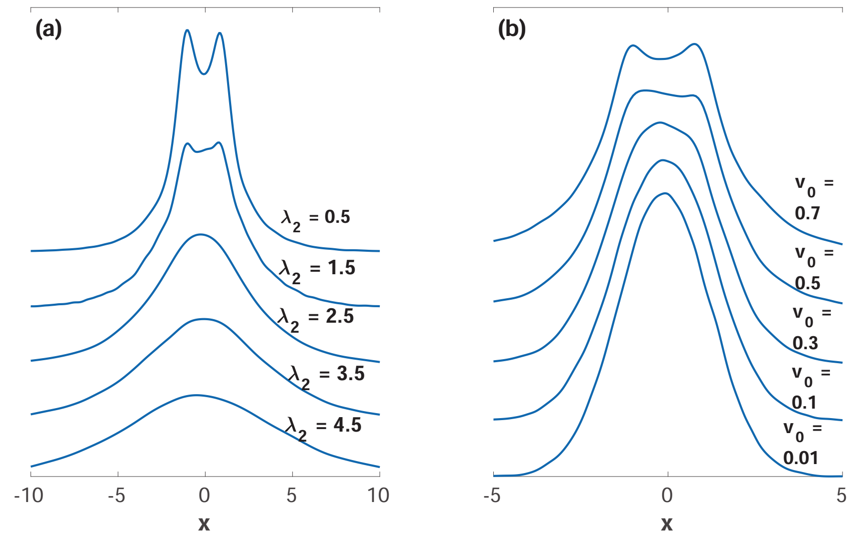
IIII First-passage statistics of asymmetric Lévy flights [A Padash et al, J Phys A (2019), (2020)]

IIIII First-passage & first-hitting time densities for Lévy flights & Lévy walks [VV Palyulin et al, New J Phys (2019)]



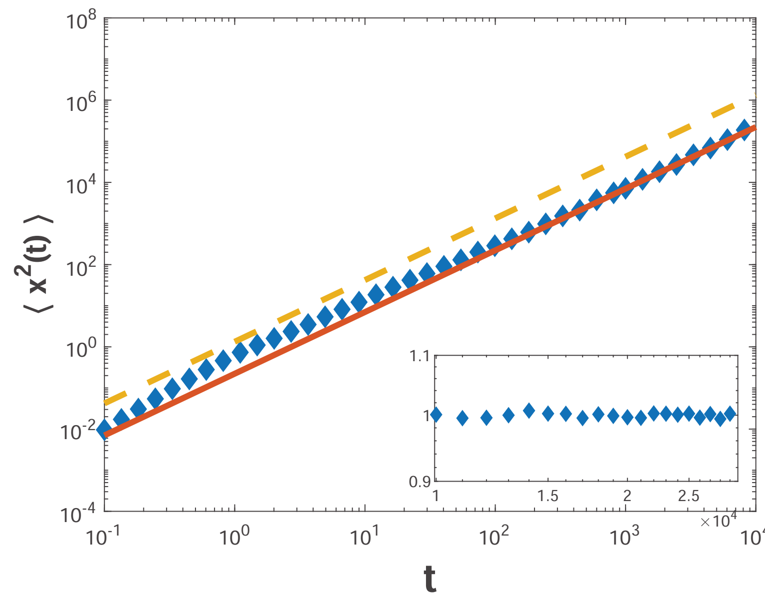
Soft resets of Lévy walk





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

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

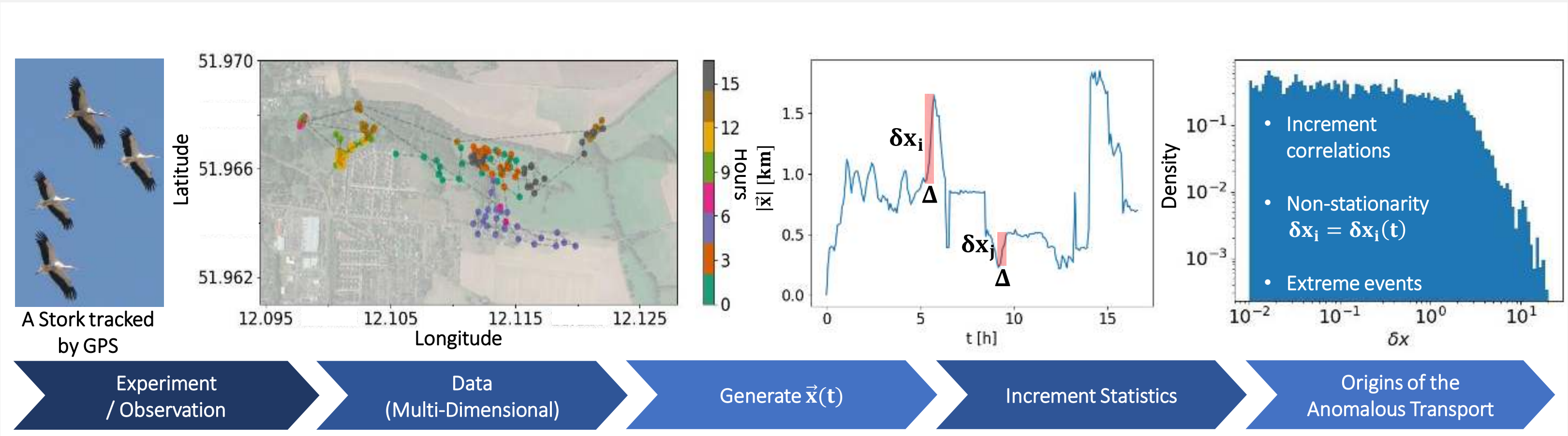


Free Lévy walk phase:

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

P Xu, T Zhou, RM & W Deng, NJP (2022)

Scaling analysis of anomalous diffusion



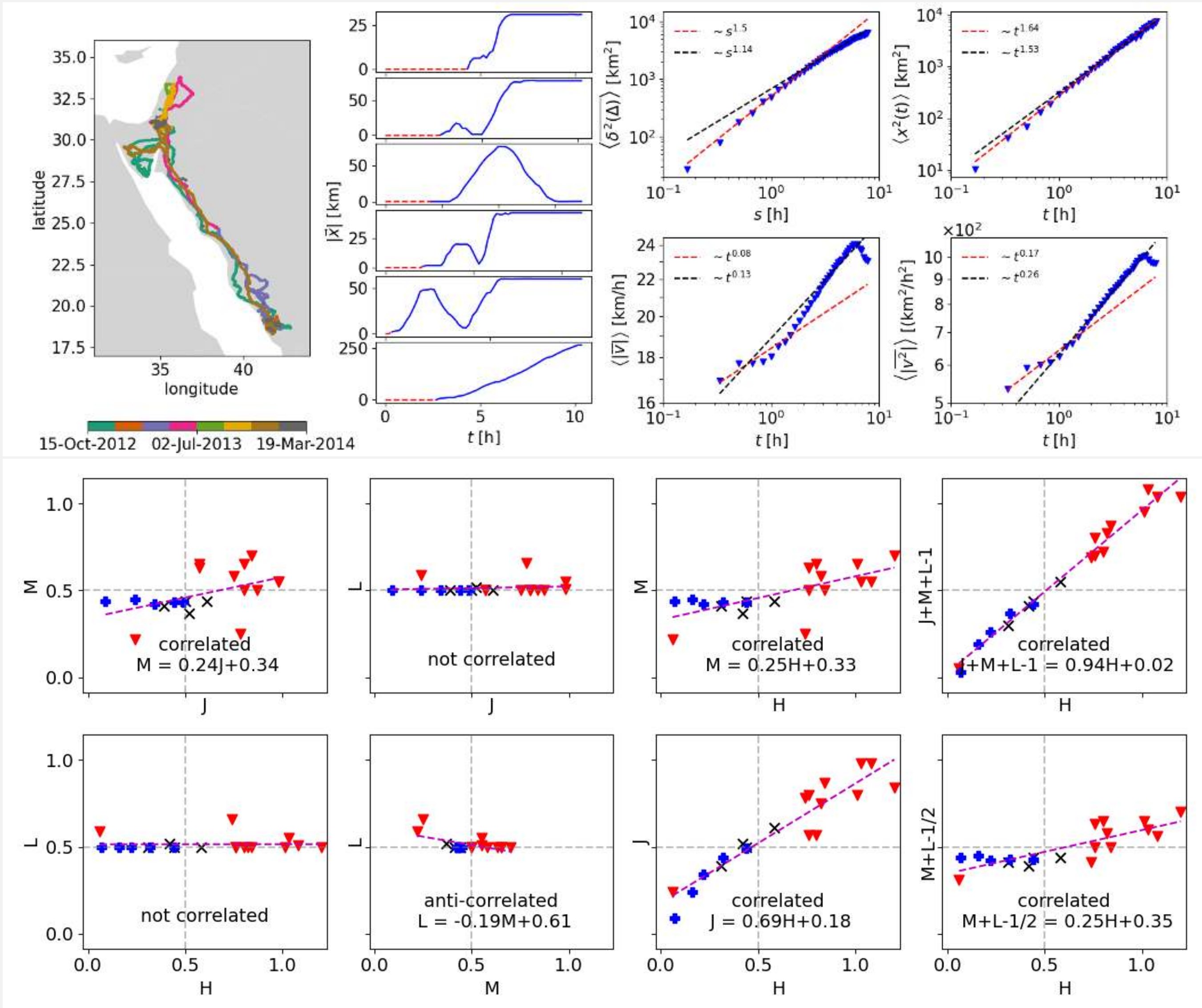
Moses
- M<1/2: Process slowing down/ Statistical aging
- M=1/2: No effect of non-stationarity
- M>1/2: Process is accelerating with time

Noah
- L=1/2: No effect from extreme events
- L>1/2: Rare extreme events

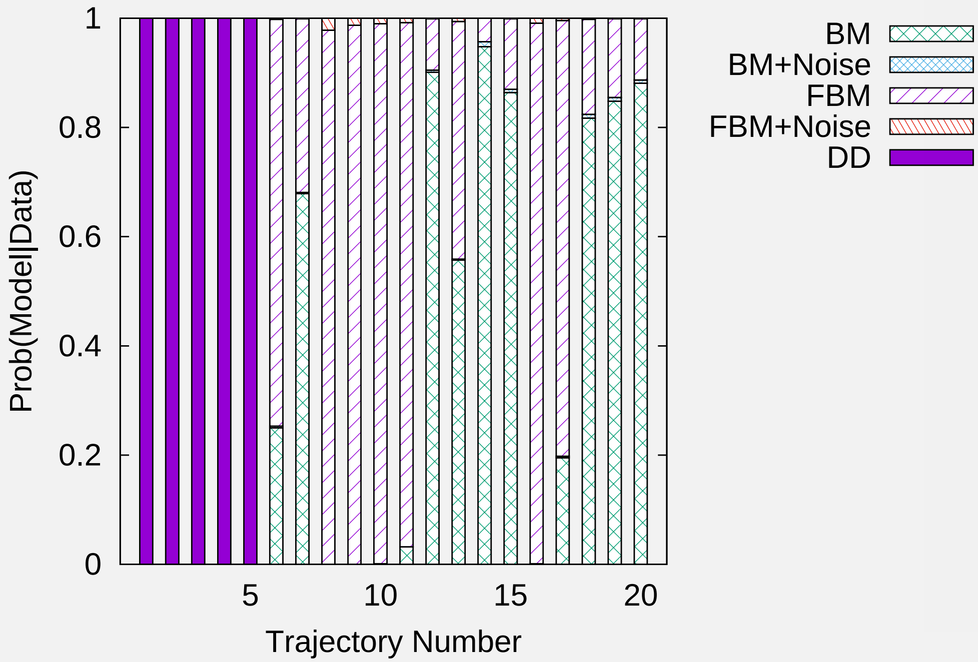
Joseph
- J<1/2: Anti-correlations
- J=1/2: No effect of temporal correlations
- J>1/2: Positive, long-ranged correlations

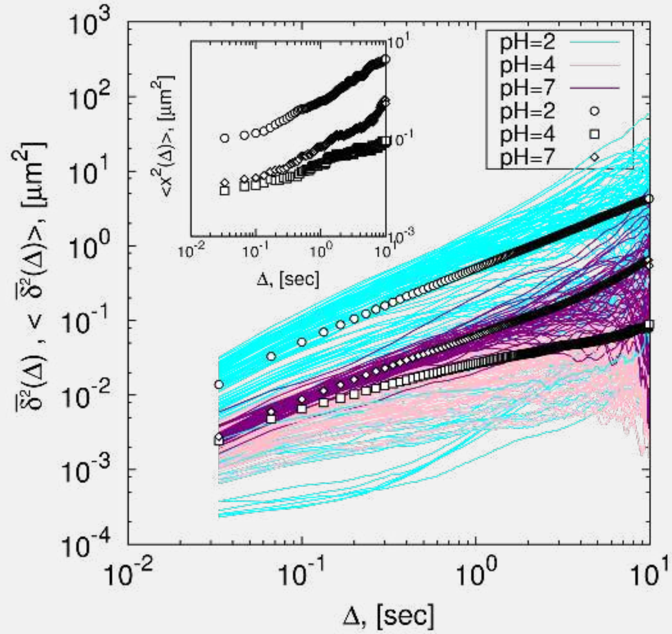
data set	ensemble size	regime	J	L	M	H measured	H prediction	$\frac{\|H_p - H\|}{H}$
Rhodamine 100%	174	$50 < t < 1500$ ms	0.50	0.50	0.41	0.38 $\pm$ 0.02	0.42 $\pm$ 0.04	10%
Rhodamine 90%	298	$50 < t < 1500$ ms	0.38	0.50	0.42	0.28 $\pm$ 0.02	0.30 $\pm$ 0.03	7%
Rhodamine 85%	239	$50 < t < 1500$ ms	0.34	0.50	0.40	0.22 $\pm$ 0.02	0.24 $\pm$ 0.05	9%
Rhodamine 75%	258	$50 < t < 1500$ ms	0.22	0.51	0.44	0.18 $\pm$ 0.02	0.18 $\pm$ 0.01	$>$1%
Rhodamine 30%	436	$50 < t < 1500$ ms	0.09	0.50	0.44	0.07 $\pm$ 0.02	0.04 $\pm$ 0.03	**
Tracers in	200	0.1 $< t <$ 5 s	0.39	0.50	0.41	0.31 $\pm$ 0.01	0.30 $\pm$ 0.02	3%
treated cells		5 $< t <$ 50 s	0.50	0.50	0.44	0.44 $\pm$ 0. 01	0.44 $\pm$ 0.01	$<$1%
Tracers in	1000	0.1 $< t <$ 2 s	0.39	0.50	0.44	0.31 $\pm$ 0.01	0.33 $\pm$ 0.02	6%
untreated cells		2 $< t <$ 8 s	0.60	0.50	0.47	0.55 $\pm$ 0.01	0.57 $\pm$ 0.01	4%
Amoeba	1142	1 $< t <$ 6 min	0.61	0.50	0.44	0.58 $\pm$ 0.01	0.55 $\pm$ 0.03	5%
		10 $< t <$ 100 min	0.52	0.52	0.37	0.42 $\pm$ 0.02	0.40 $\pm$ 0.02	5%
Harvester ants	67	10 $< t <$ 100 s	0.88	0.50	0.57	0.92 $\pm$ 0.12	0.95 $\pm$ 0.08	3%
		100 $< t <$ 400 s	0.59	0.51	0.35	0.47 $\pm$ 0.03	0.45 $\pm$ 0.03	4%
Commuting kite	107	$0.1 < t < 3$ min	0.87	0.50	0.49	0.84 $\pm$ 0.02	0.86 $\pm$ 0.02	2%
		$3 < t < 12$ min	0.80	0.50	0.50	0.76 $\pm$ 0.01	0.80 $\pm$ 0.02	5%
Searching kite	587	$0.5 < t < 20$ min	0.24	0.59	0.22	0.06 $\pm$ 0.02	0.06 $\pm$ 0.01	$<$1%
Stork (Jun-Jul)	455	$0.2 < t < 2$ h	0.46	0.88	-0.24	*	0.10 $\pm$ 0.03	–
		$2 < t < 10$ h	0.18	0.50	0.48	*	0.16 $\pm$ 0.08	–
Stork (Aug-Sep)	394	$0.2 < t < 2$ h	0.98	0.55	0.55	1.20 $\pm$ 0.03	1.08 $\pm$ 0.02	10%
		$2 < t < 10$ h	0.84	0.50	0.70	1.03 $\pm$ 0.01	1.04 $\pm$ 0.06	1%
Stork (Oct-Jan)	854	$0.2 < t < 2$ h	0.78	0.66	0.25	0.74 $\pm$ 0.02	0.68 $\pm$ 0.03	8%
		$2 < t < 10$ h	0.57	0.50	0.65	0.80 $\pm$ 0.02	0.73 $\pm$ 0.10	9%
Stork (Mar-Apr)	391	$0.2 < t < 2$ h	0.98	0.51	0.55	1.08 $\pm$ 0.02	1.04 $\pm$ 0.02	4%
		$2 < t < 10$ h	0.80	0.50	0.65	1.01 $\pm$ 0.01	0.95 $\pm$ 0.07	6%
Vulture	444	$0.1 < t < 2$ h	0.75	0.50	0.58	0.82 $\pm$ 0.02	0. 84 $\pm$ 0.02	1%
		$2 < t < 5.5$ h	0.57	0.50	0.63	0.76 $\pm$ 0.02	0.70 $\pm$ 0. 04	9%

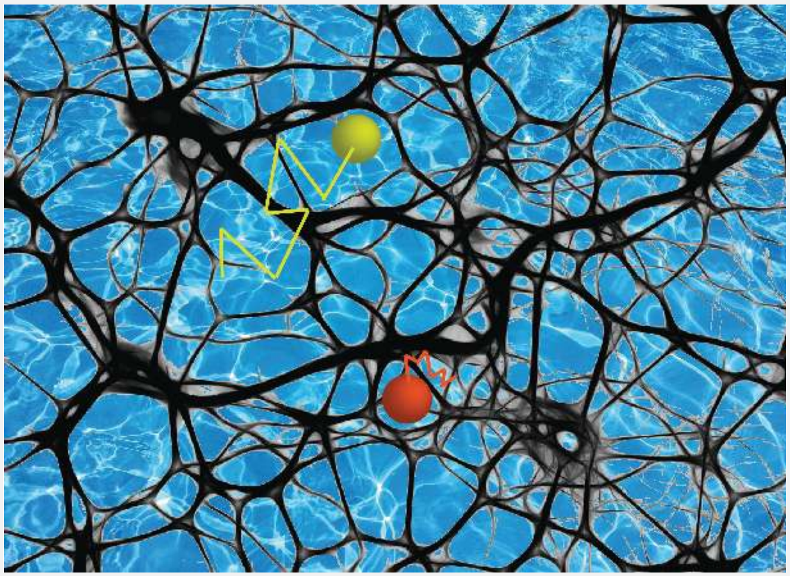
Scaling analysis of anomalous diffusion



Maximum likelihood Bayesian data analyses







Nested sampling à la Skilling

Objective model selection

Parameter estimation

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

The ANomalous DIffusion challenge

nature COMMUNICATIONS

ARTICLE

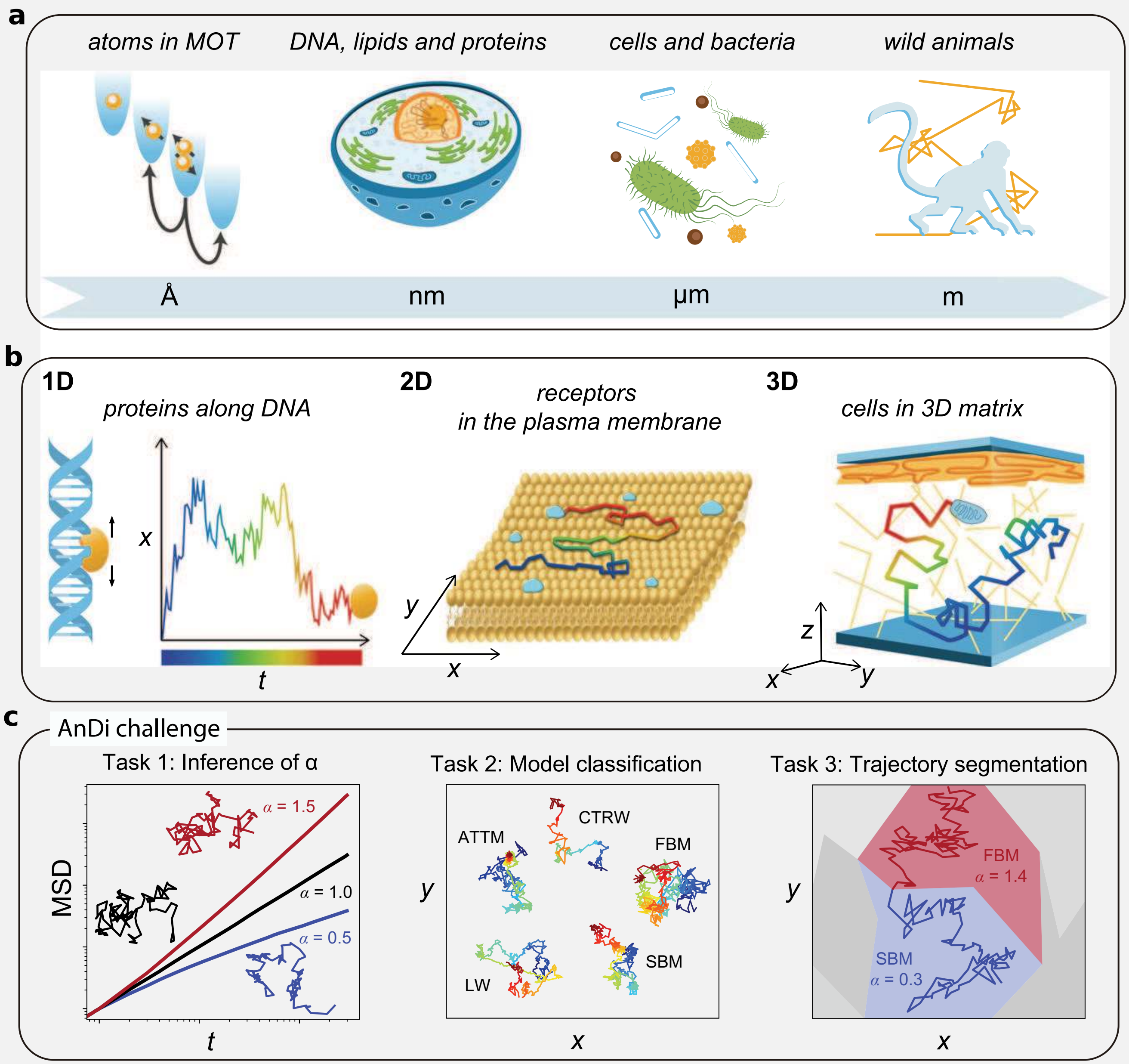
Check for updates

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

Objective comparison of methods to decode anomalous diffusion

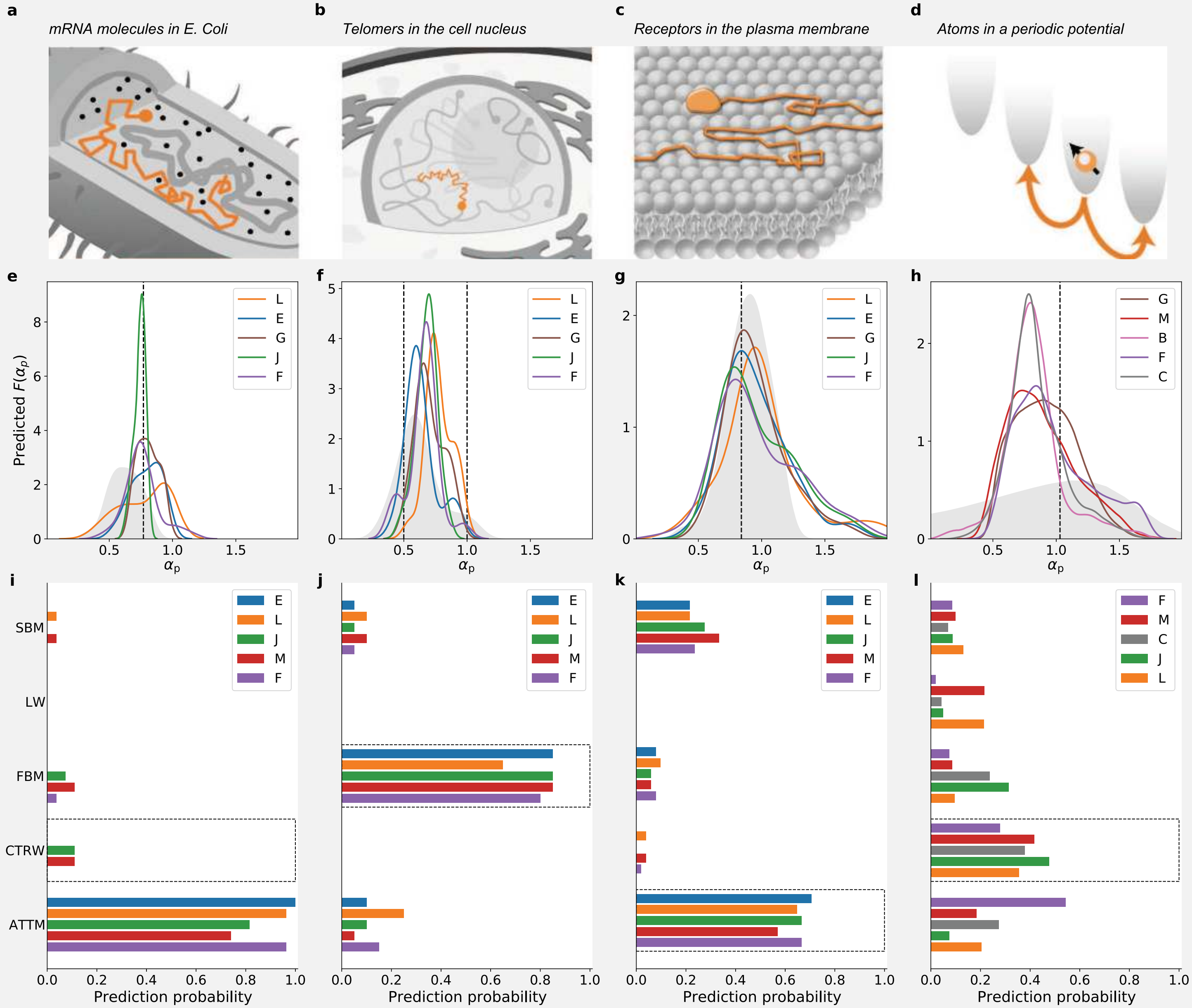
Gorka Muñoz-Gil[1], Giovanni Volpe[2✉], Miguel Angel Garcia-March[3], Erez Aghion[4], Aykut Argun[2], Chang Beom Hong[5], Tom Bland[6], Stefano Bo[4], J. Alberto Conejero[3], Nicolás Firbas[3], Òscar Garibo i Orts[3], Alessia Gentili[7], Zihan Huang[8], Jae-Hyung Jeon[5], Hélène Kabbech[9], Yeongjin 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 Commun (2021)

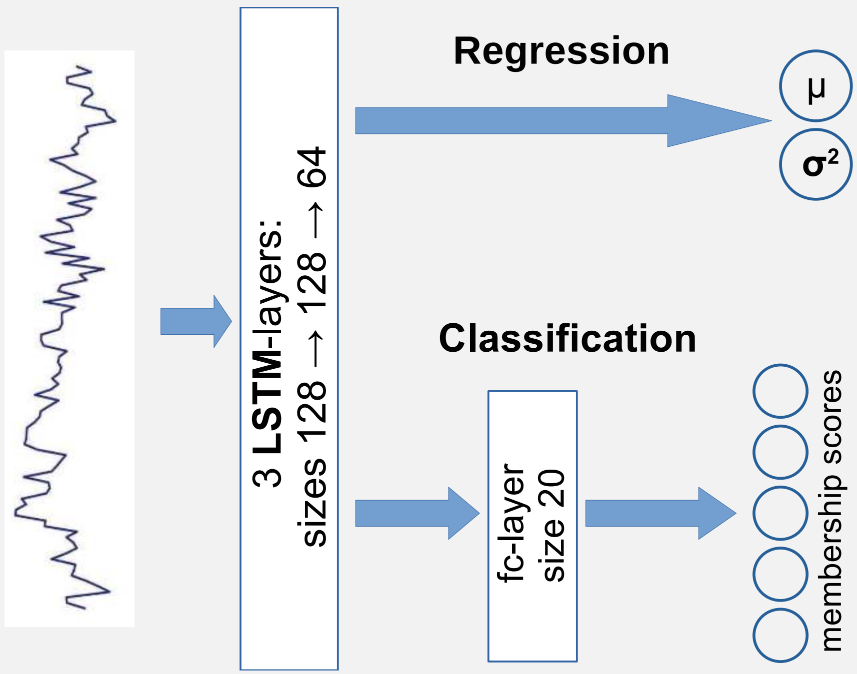
The ANomalous DIffusion challenge



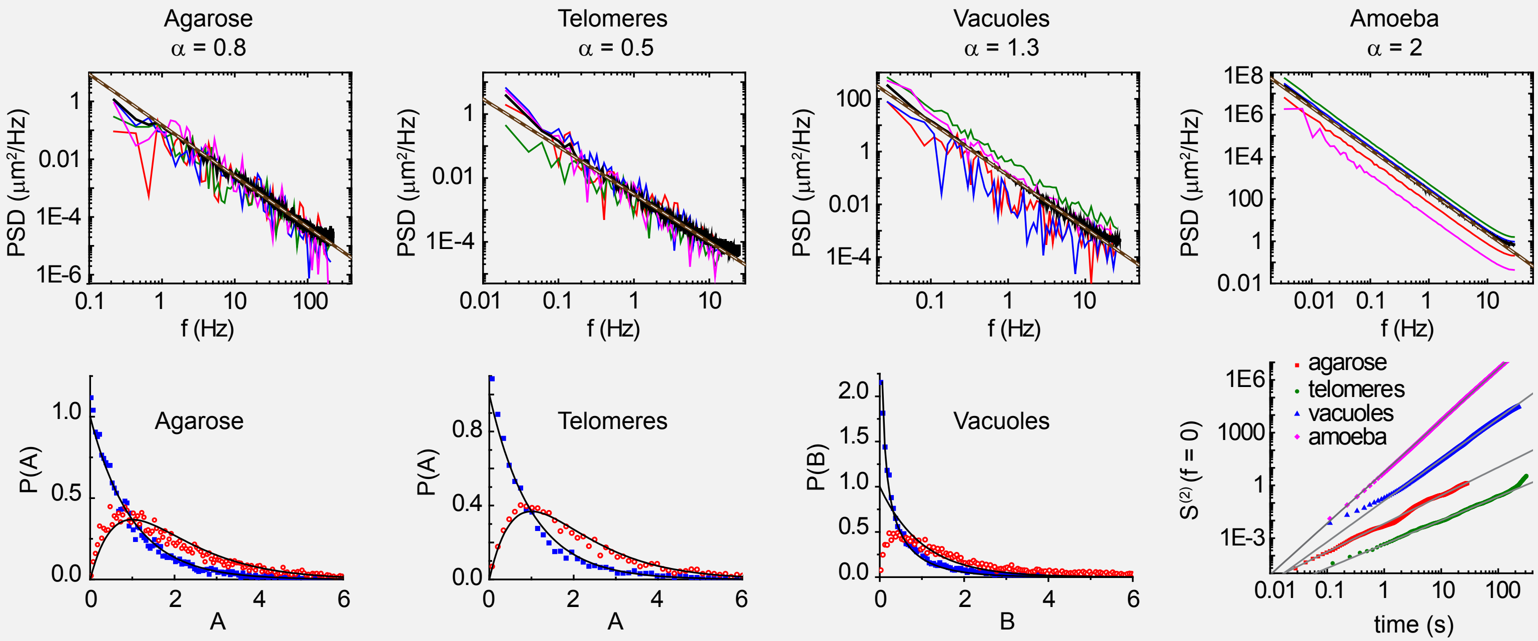
G Muñoz-Gil et al., Nat Commun (2021)

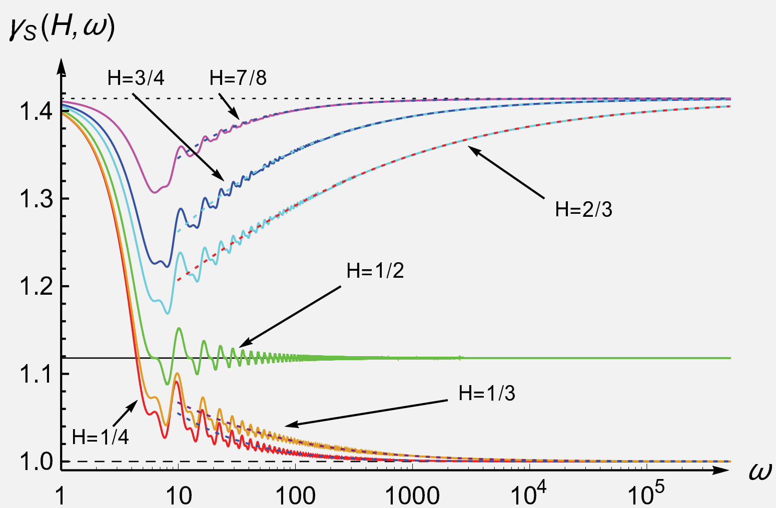
Bayesian-weighted deep learning model selection

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



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)

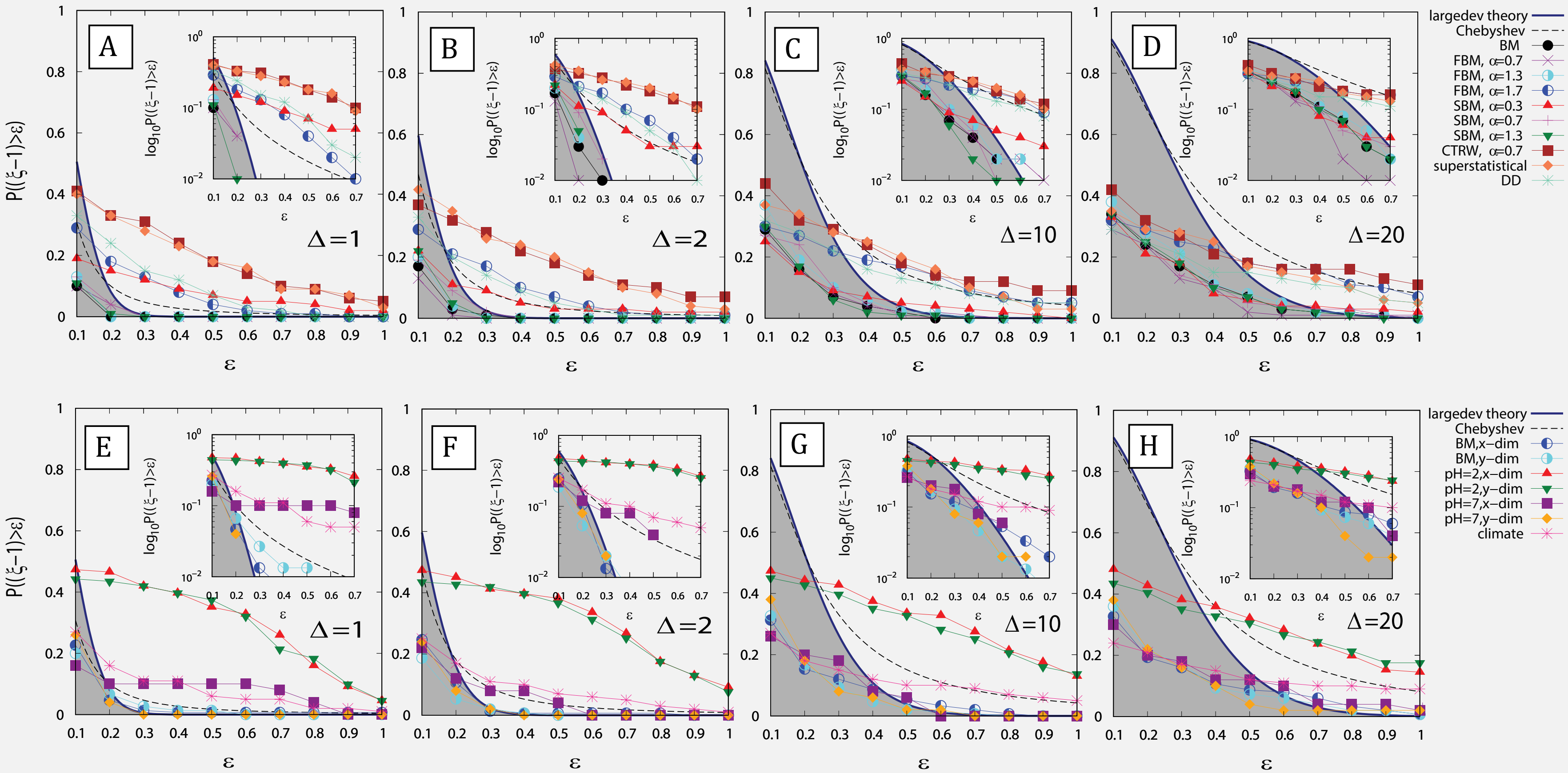
Large-deviation statistics for TAMSD

Chebyshev's inequality for Brownian motion $X(1), X(2), \ldots, X(N)$, 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:

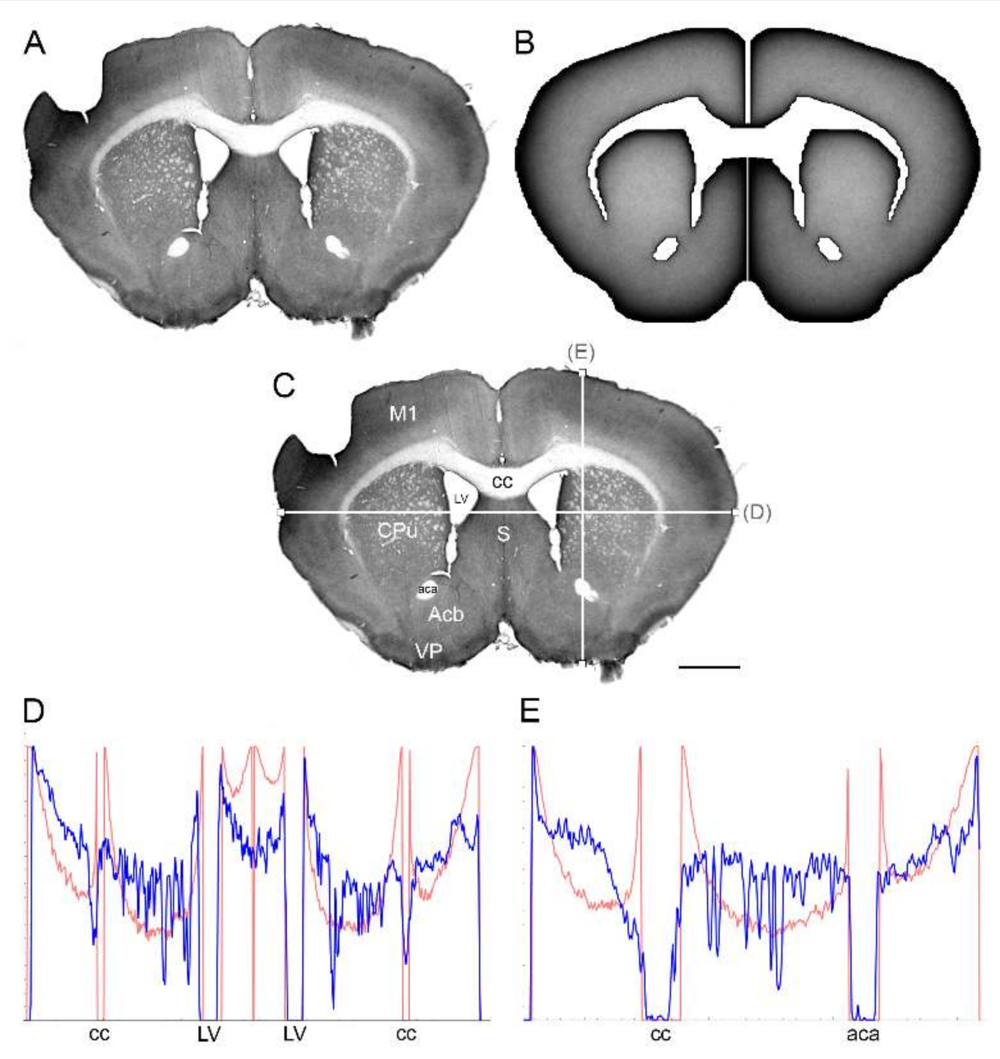
$$P\Big((\xi-1)\geq\varepsilon\Big)\leq\exp\Big(-a\mathcal{H}(b)\Big),\quad \mathcal{H}(b)=1+b-\sqrt{1+2b};\quad a,b=f(\Delta,\ldots)$$

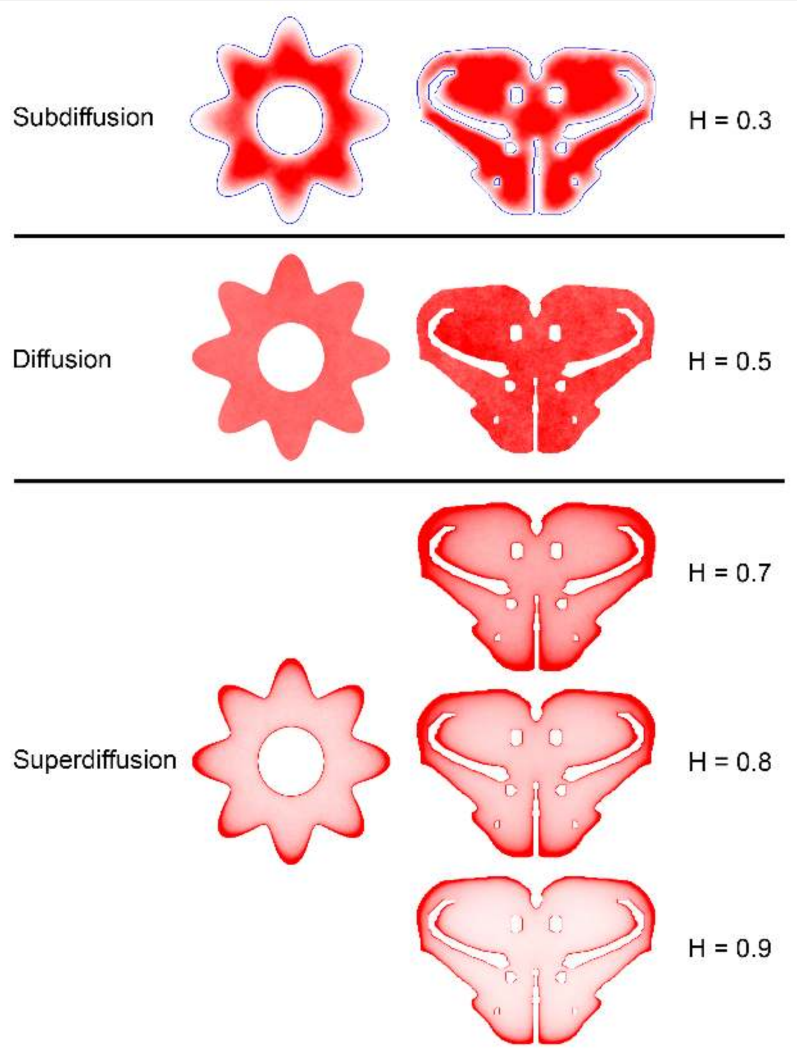


S Thapa, A Wyłomańska, G Sikora, CE Wagner, D Krapf, H Kantz, AV Chechkin & RM, NJP (2021)

Brain serotonergic axons as FBM paths

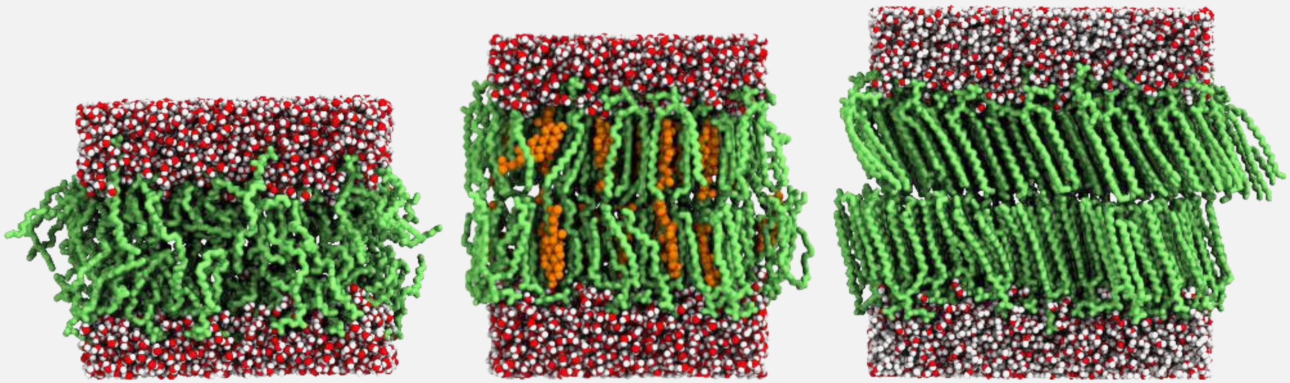
Correlated fluctuations effect non-flat profile

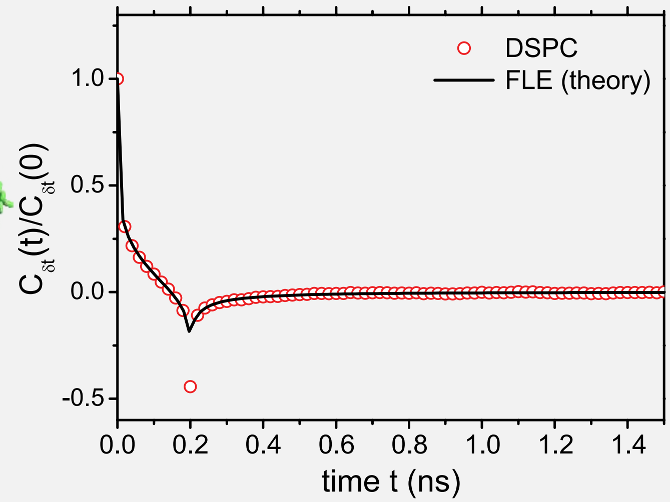


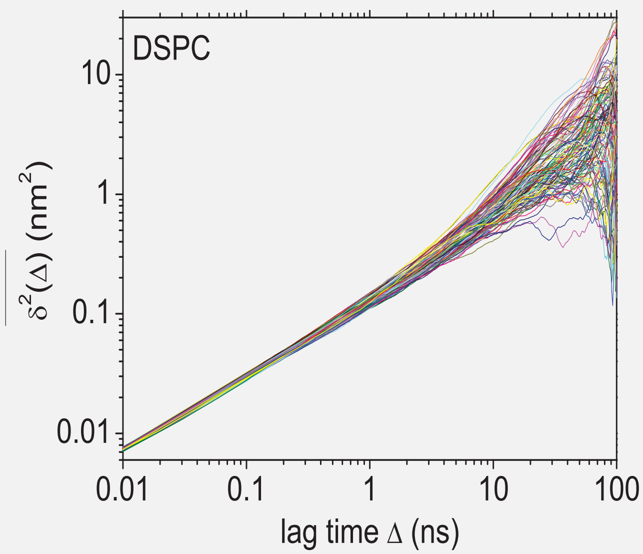


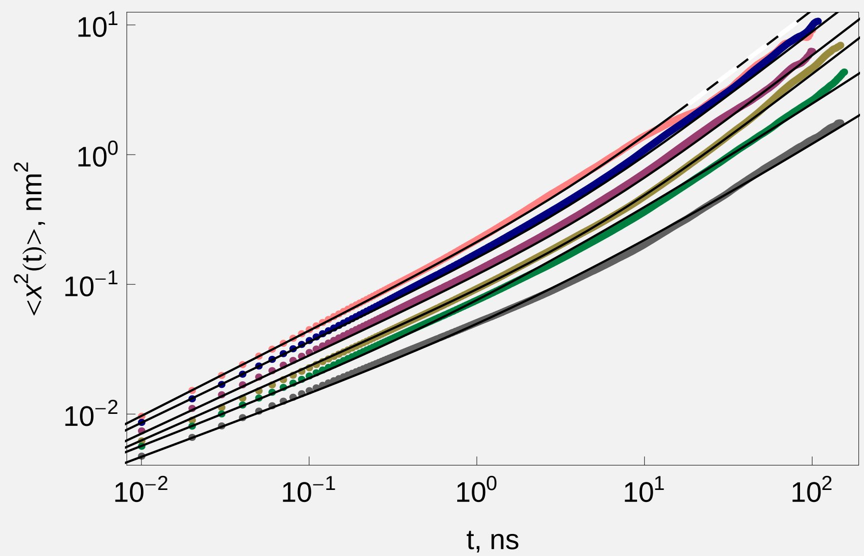
S Janušonis, N Detering, RM & T Vojta, Frontiers Comp Neurosc (2020); T Guggenberger, T Vojta & RM, NJP (2019)

Single lipid motion in bilayer membrane MD simulations









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)

$\sum$ummary

- I Random search processes have characteristic search/reaction times that may differ by orders of magnitude $\rightsquigarrow$ chemical rates or (global) mean search times inappropriate for quantitative description
- II Lévy walk search processes can be adequately quantified by stochastic observables, including the first-passage & first-hitting time statistics
- III Instead of Lévy walks persistent fractional Brownian motion may be relevant for the search dynamics of larger animals
- IIII Random-parameter models may adequately describe ensembles of animals, or different trajectories of the same animal
- ~~IIII~~ Objective data analysis methods aid in identification of models & parameters: Bayesian-maximum likelihood, deep learning, & their combinations

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

Group

Prof Aleksei Chechkin (Ukraine)
Dr Andrey Cherstvy (Belarus)
Marcus Dahlenburg (Germany)
Costantino Di Bello (Italy)
Timo Doerries (Germany)
Koushik Goswami (India)
Tobias Guggenberger (Germany)
Dr Yingjie Liang (China)
Dr Philipp Meyer (Germany)
Dr Yousof Mardoukhi (Iran)
Henrik Seckler (Germany)
Prof Trifce Sandev (Macedonia)
Dr Helena Stage (Denmark)
Dr Wei Wang (China)

Humboldt fellows/guests:
Prof Michael Assaf (Israel)
Prof Guillermo Chacon (Mexico)
Prof Denis Grebenkov (France)
Elisabeth Lemaitre (France)
Dr Gleb Oshanin (France)

Projects

1. Stochastic models for normal & anomalous diffusion, with deterministically & randomly varying $D(\mathbf{r}, t)$

2. Analysis of physical observables, first-passage & reaction dynamics, ergodicity, ageing, . . .

3. Stochastic resetting strategies (hard/soft/distributed)

4. Data-science approaches such as Bayesian & machine (deep) learning strategies $\rightsquigarrow$ physical models

5. Simulations of stochastic processes for brain fibre distribution

6. MD/LD/BD simulations: crowded environments,

7. Applications to: biological cells & tissues, gene regulation; quorum sensing; membrane dynamics; geophysics; finance; movement ecology

Acknowledgements

Eli Barkai (Bar-Ilan U Ramat Gan)
Carsten Beta (U Potsdam)
Krzysztof Burnecki (Politechnika Wrocławska)
Aleksei Chechkin, Andrey Cherstvy (U Potsdam)
Aljaz Godec (MPIBC Göttingen)
Denis Grebenkov (École Polytechnique)
Jae-Hyung Jeon (POSTECH Pohang)
Michael Lomholt (Syddansk U Odense)
Marcin Magdziarz (Politechnika Wrocławska)
Lene Oddershede (NBI København U)
Gleb Oshanin (Sorbonne)
Gianni Pagnini (BCAM Bilbao)
Christine Selhuber-Unkel (U Heidelberg)
Flavio Seno (Universitá di Padova)
Igor Sokolov (Humboldt U Berlin)
Ilpo Vattulainen (Helsingin Yliopisto)
Caroline Wagner (McGill)
Matthias Weiss (U Bayreuth)
Agnieszka Wyłomańska (Politechnika Wrocławska)
Yong Xu (NWPU Xi'an)

DFG Deutsche Forschungsgemeinschaft

Universität Potsdam

Tampere University of Technology

FNP Fundacja na rzecz Nauki Polskiej

Suomen Akatemia

FIDIPRO Finland Distinguished Professor Programme