Some insights into the microscopic origin of anomalous diffusion in biomolecular systems

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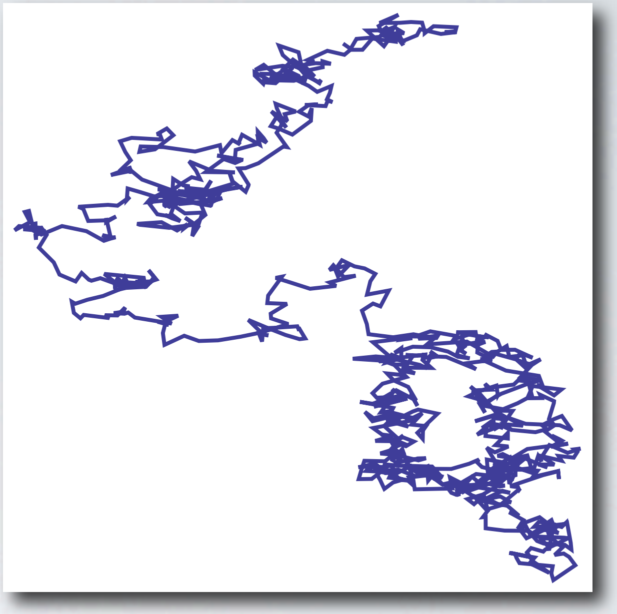
Sub- and superdiffusion in biomolecular systems



$$W(t) = \left\langle [x(t) - x(0)]^2 \right\rangle \overset{t\to\infty}{\to} 2D_\alpha t^\alpha$$

$0 < \alpha < 1$: **sub**diffusion (diffusion of molecules in membranes)

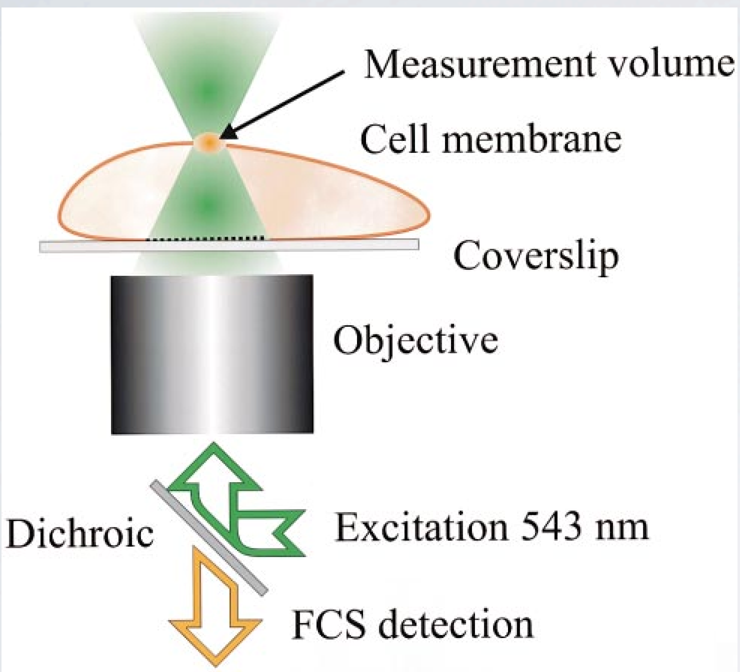
$\alpha = 1$: **normal** diffusion (diffusion of molecules in liquids)

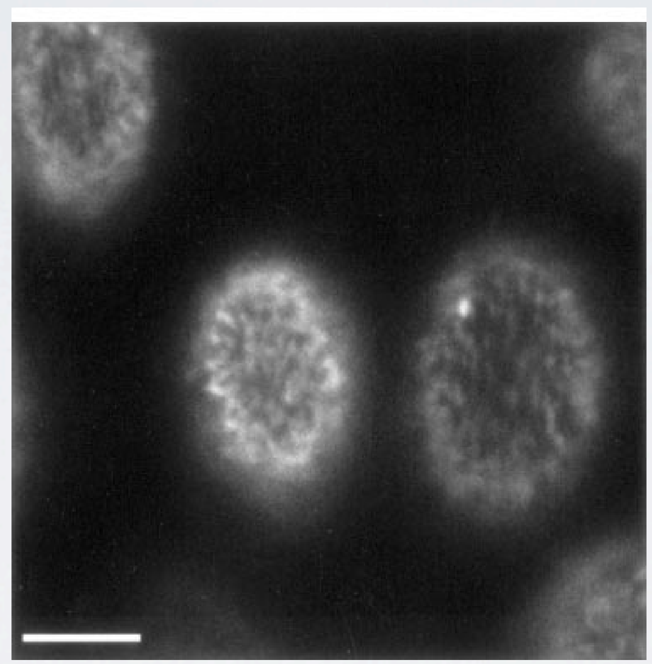
$1 < \alpha < 2$: **super**diffusion (target-site search by DNA-binding proteins)

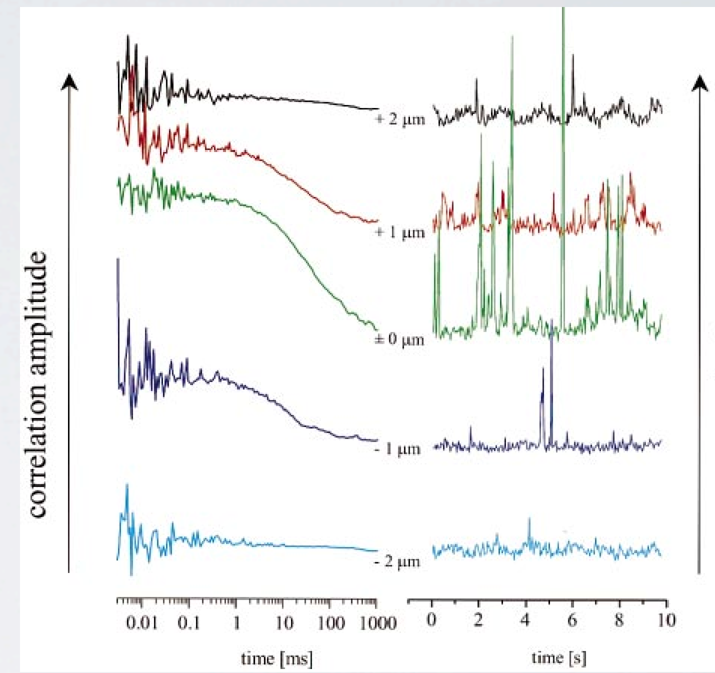
Cytometry 36:176–182 (1999)

Fluorescence Correlation Spectroscopy With Single-Molecule Sensitivity on Cell and Model Membranes

Petra Schwille,* Jonas Korlach, and Watt W. Webb
Cornell University, School of Applied and Engineering Physics, Ithaca, New York







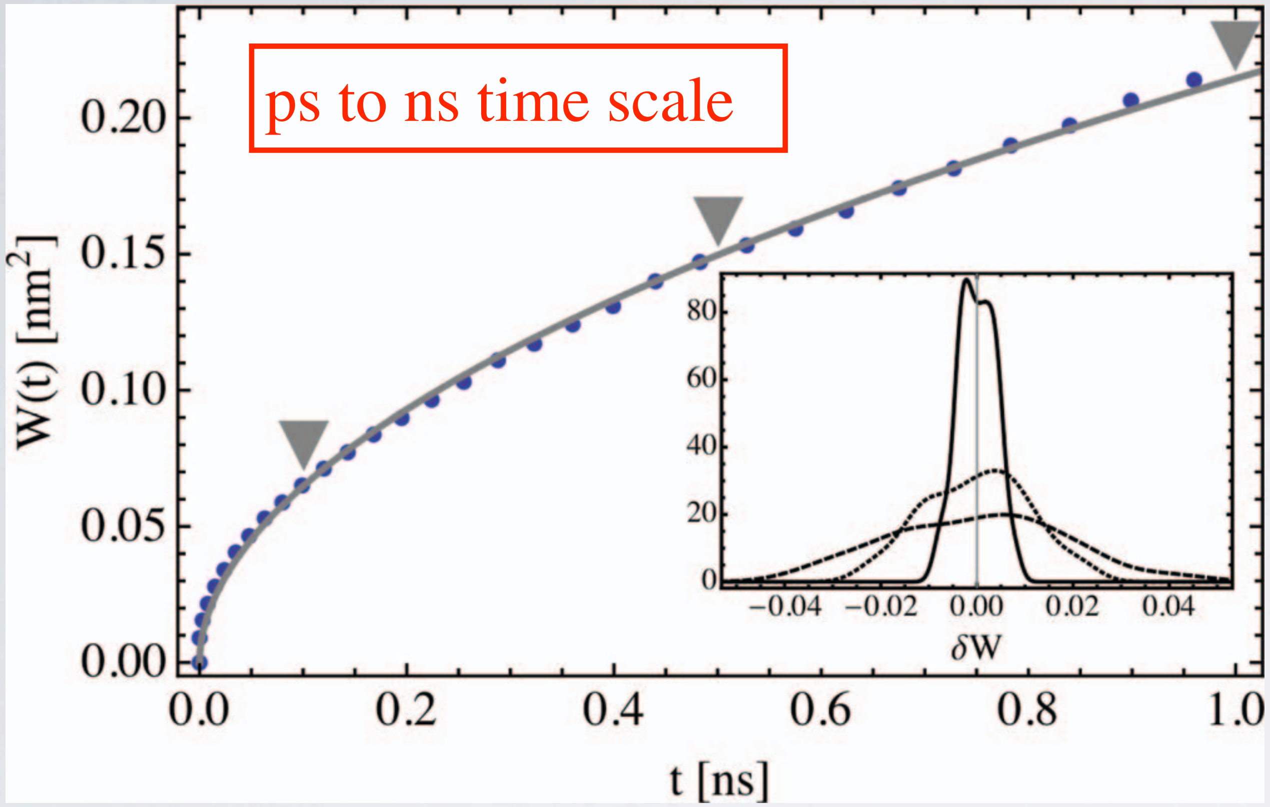
ms to s time scale

$$P_{anom}[\underline{r}', (t+\tau) \,|\, \underline{r}, t] = \frac{1}{(\pi \Gamma \tau^{\alpha})^{n/2}} e^{\frac{-(\underline{r}-\underline{r}')^2}{\Gamma \tau^{\alpha}}}$$

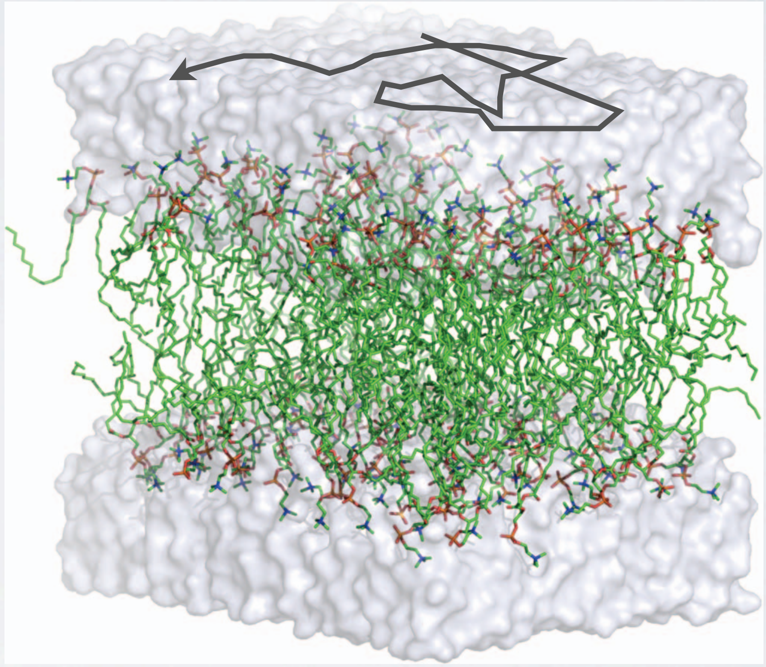
$\alpha = 0.74 \pm 0.08.$

Anomalous Brownian motion

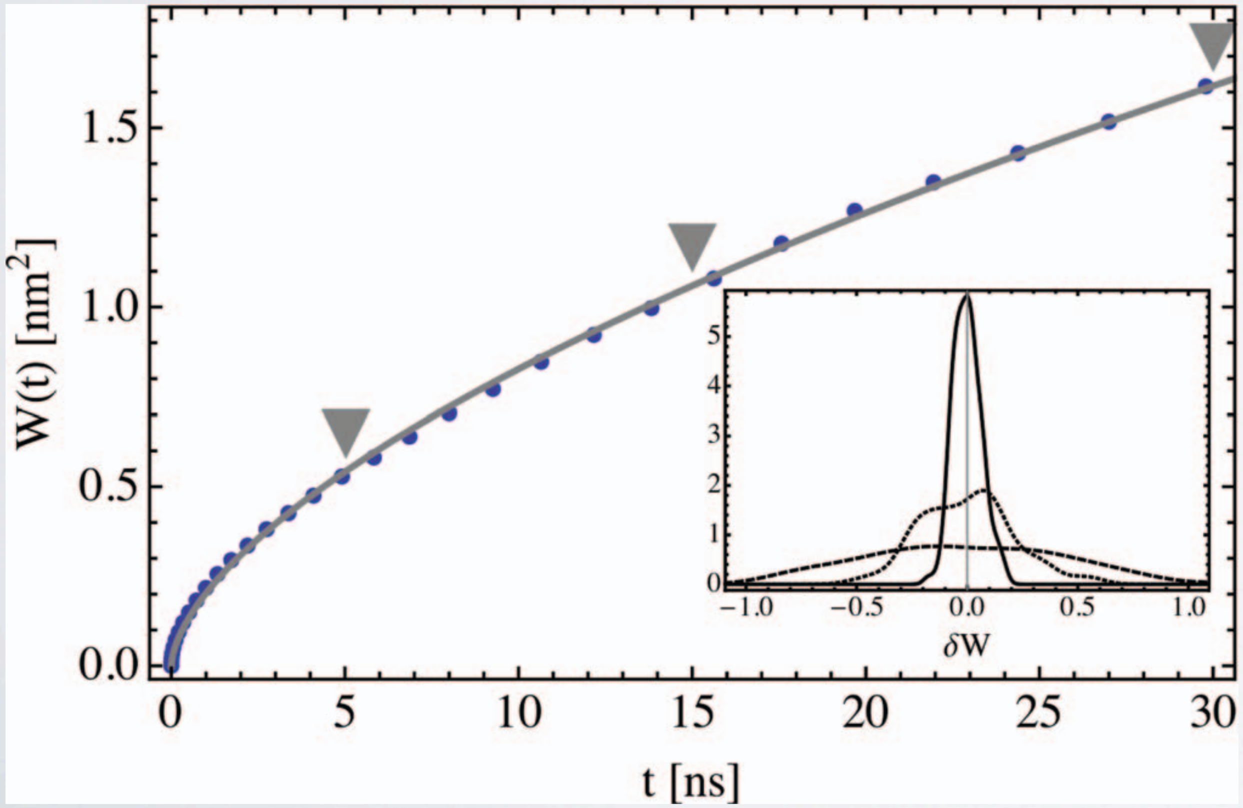
MD simulation of a DOPC bilayer



$D_\alpha = 0.107\ nm^2/ns^\alpha$ for $\alpha = 0.52$.



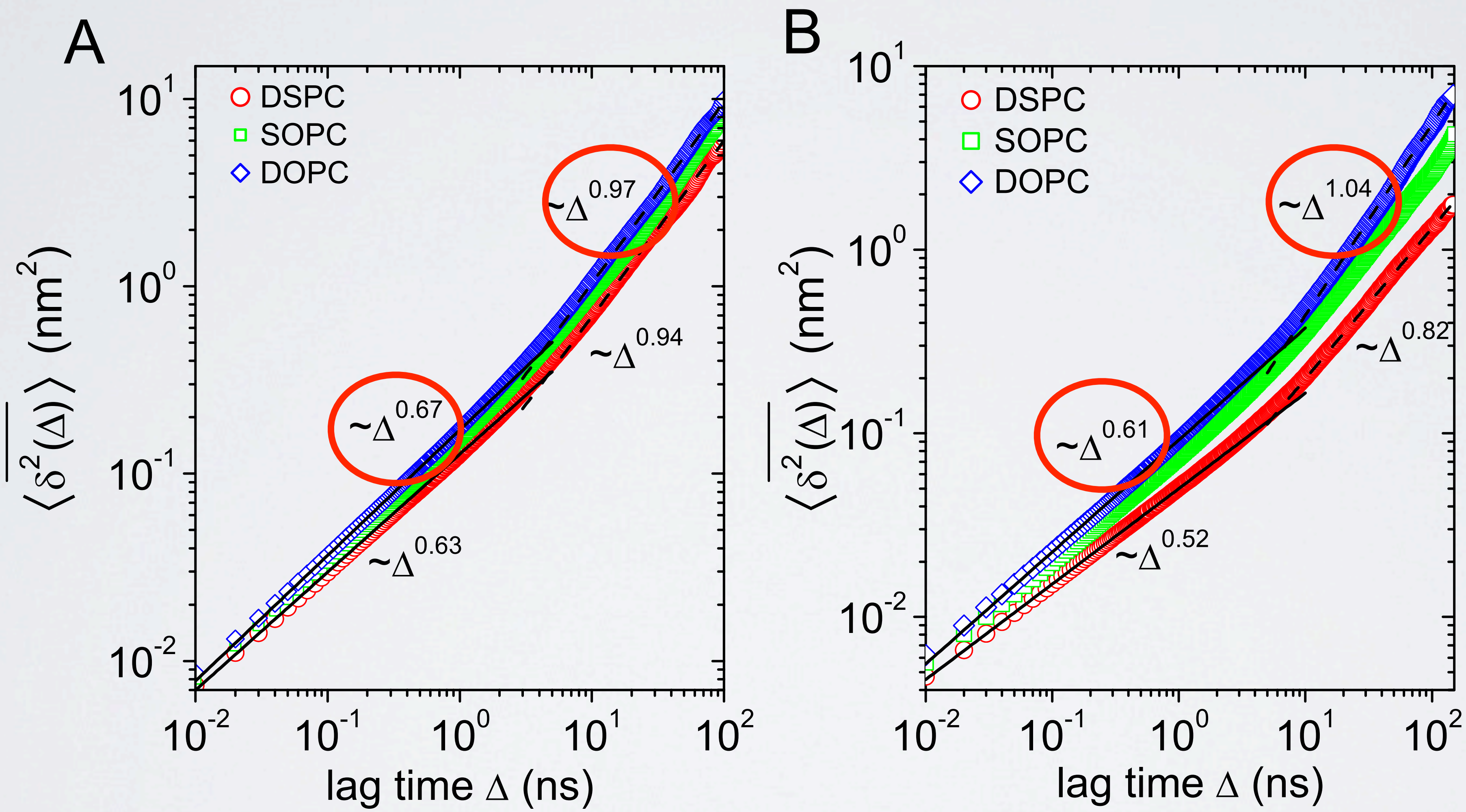
$D_\alpha = 0.101\ nm^2/ns^\alpha$ for $\alpha = 0.61$.



Experimental value for DLPC:
$D_\alpha = 0.088 \pm 0.007\ nm^2/ns^\alpha$
for $\alpha = 0.74 \pm 0.08$.

G. R. Kneller, K. Baczynski, and M. Pasenkiewicz-Gierula. *J. Chem. Phys.*, 135(14):141105, 2011.

Jeon, J. H., Monne, H., Javanainen, M. & Metzler, R. *Phys Rev Lett* 109, 188103 (2012)



Einstein's approach to diffusion

5. ***Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen;***
von A. Einstein.

In dieser Arbeit soll gezeigt werden, daß nach der molekularkinetischen Theorie der Wärme in Flüssigkeiten suspendierte Körper von mikroskopisch sichtbarer Größe infolge der Molekularbewegung der Wärme Bewegungen von solcher Größe ausführen müssen, daß diese Bewegungen leicht mit dem Mikroskop nachgewiesen werden können. Es ist möglich, daß die hier zu behandelnden Bewegungen mit der sogenannten „Brownschen Molekularbewegung" identisch sind; die mir erreichbaren Angaben über letztere sind jedoch so ungenau, daß ich mir hierüber kein Urteil bilden konnte.

A. Einstein, *Ann. Phys.*, vol. 322, no. 8, 1905.

$$f(x, t+\tau)\,dx = dx \cdot \int_{\Delta=-\infty}^{\Delta=+\infty} f(x+\Delta)\,\varphi(\Delta)\,d\Delta$$

→

$$\frac{\partial f}{\partial t} = D\,\frac{\partial^2 f}{\partial x^2}.$$

$$f(x,t) = \frac{n}{\sqrt{4\pi D}}\,\frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{t}}.$$

→

$$\lambda_x = \sqrt{\overline{x^2}} = \sqrt{2Dt}.$$

Diffusion in position space

$$\partial_t P(x,t|x_0,0) = D\frac{\partial^2}{\partial x^2}P(x,t|x_0,0)$$

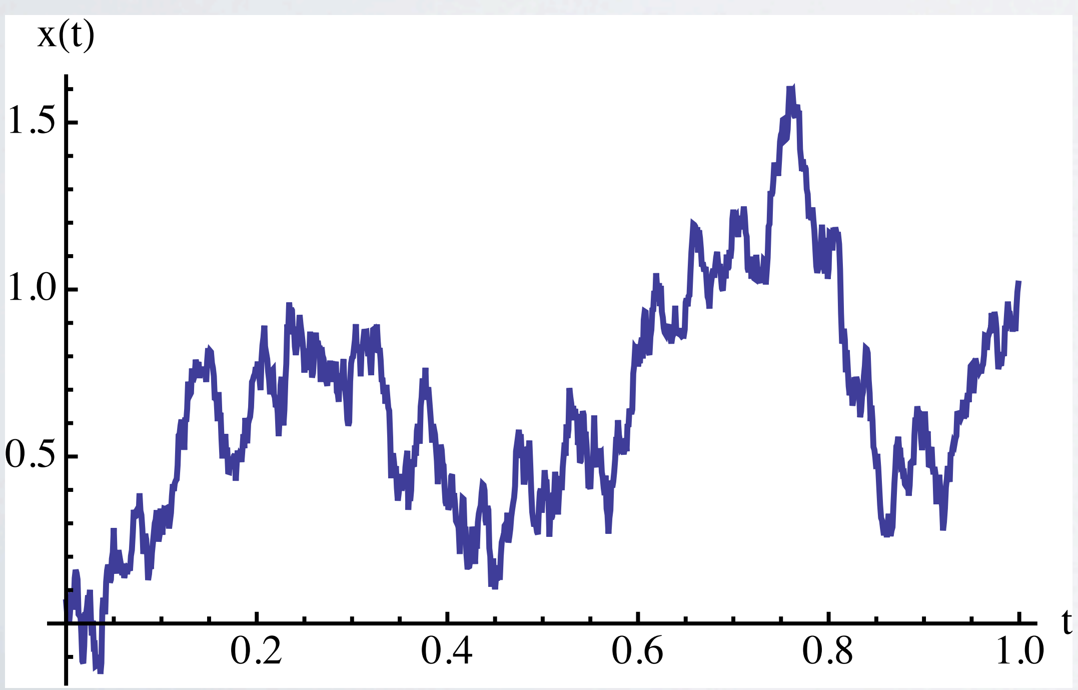
$$x(t_0+\Delta t) = x(t_0) + \xi$$

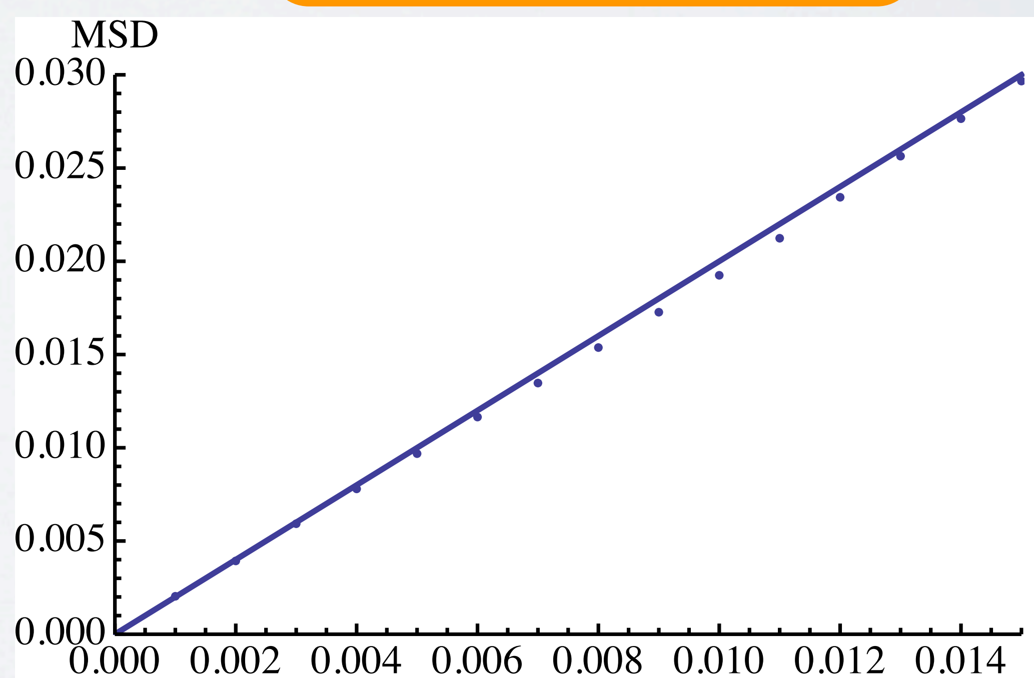
$$\overline{\xi} = 0$$
$$\overline{\xi^2} = 2D\Delta t$$

white noise

Trajectory

$$W(t) = 2Dt$$





Fractional diffusion equation

$$\partial_t P(\mathbf{x}, t|\mathbf{x}_0, 0) = {}_0\partial_t^{1-\alpha} \left\{ D_\alpha \frac{\partial^2}{\partial \mathbf{x}^2} \right\} P(\mathbf{x}, t|\mathbf{x}_0, 0) \quad (0 < \alpha < 2)$$

$${}_0\partial_t^{\rho} g(t) = \partial_t^{(-)n} \int_0^t dt' \, \frac{(t-t')^{\beta-1}}{\Gamma(\beta)} g(t').$$

Fractional Riemann-Liouville derivative of order ρ

Write $\rho = n - \beta$, where $n = 0, 1, 2, \ldots, \beta \geq 0$.

$$W(t) = 2D_\alpha t^\alpha$$

See e.g. Metzler and Klafter. Phys Rep (2000) vol. 339 (1) pp. 1-77

Self-similarity of Brownian motion

Consider a self-similar stochastic processes[1]

$$c^{-H}Y(ct) =_d Y(t)$$

such that $Y(t) =_d t^H Y(1), \quad (t > 0,\ 0 < H < 1)$

Assume zero mean average and stationary increments:

$$\langle Y(t) \rangle = 0$$

$$\langle [Y(t) - Y(t-1)]^2 \rangle = \langle Y^2(1) \rangle = \sigma^2$$

[1] Kolmogoroff, A. Wienersche Spiralen und einige andere interessante Kurven im Hilbertsche Raum. C. R. (Dokl.) Acad. Sci. URSS 26 (n. Ser.), 115–118 (1940).

[2] J. Beran, *Statistics for Long-Memory Processes*. Chapman and Hall, 1994.

Then the MSD is

$$\langle [Y(t) - Y(s)]^2 \rangle = \sigma^2 (t-s)^{2H}, \quad 0 < s < t$$

and the covariance is

$$\langle Y(t) Y(s) \rangle = \frac{\sigma^2}{2} \left(t^{2H} - (t-s)^{2H} + s^{2H} \right)$$

Setting $D_H = \sigma^2/2$, one recognizes "normal diffusion" for $H = 1/2$, subdiffusion for $0 < H < 1/2$, and superdiffusion for $1/2 < H < 1$.

Limits of self-similarity

$$W(t) = 2\int_0^t dt'\,(t-t')c_{vv}(t')$$

Velocity autocorrelation function

$$c_{vv}(t) = \langle \mathbf{v}(t)\cdot\mathbf{v}(0)\rangle$$

$$c_{vv}(t) = \sum_{k=0}^{\infty} c_{vv}^{(2k)}(0)\frac{t^{2k}}{(2k)!} \qquad \left(c_{vv}^{(2k)}(0) = (-1)^k\langle \mathbf{v}^{(k)}(0)\cdot\mathbf{v}^{(k)}(0)\rangle/3\right).$$

$$W(t) \overset{t\to 0}{\sim} \langle \mathbf{v}^2\rangle t^2$$

Ballistic regime

Self-similarity cannot be true on arbitrarily small time scales, but must be seen as a model which holds **asymptotically**.

$$W(t) \overset{t\to\infty}{\sim} 2D_\alpha t^\alpha$$

Asymptotic regime

Asymptotic analysis of anomalous diffusion

Generalized Langevin equation

$$\dot{\mathbf{v}}(t) = -\int_0^t dt'\, \kappa(t-t')\mathbf{v}(t') + \mathbf{f}^{(+)}(t)$$

Memory kernel

$$\langle \mathbf{v}(t)\cdot \mathbf{f}^{(+)}(t')\rangle = 0.$$

$$\Rightarrow \quad \partial_t c_{vv}(t) = -\int_0^t dt'\, c_{vv}(t-t')\kappa(t').$$

$$\kappa(t) \equiv \Omega^2 \Rightarrow c_{vv}(t) = \langle v^2\rangle \cos \Omega t$$

oscillatory «rattling» motions in the «cage» of nearest neighbors

R. Zwanzig, *Nonequilibrium statistical mechanics*. Oxford University Press, 2001.

Journal für die Reine und Angewandte Mathematik (Crelle's Journal) **1931,** 27–39 (1931).

Neuer Beweis und Verallgemeinerung der Tauberschen Sätze, welche die Laplacesche und Stieltjessche Transformation betreffen.

Von *J. Karamata* in Belgrad.

$$h(t) \overset{t\to\infty}{\sim} L(t)t^{\rho} \Leftrightarrow \hat{h}(s) \overset{s\to 0}{\sim} L(1/s)\frac{\Gamma(\rho+1)}{s^{\rho+1}} \quad (\rho > -1).$$

$\hat{h}(s) = \int_0^\infty dt\ \exp(-st)h(t) \quad (\Re\{s\} > 0)$ Laplace transform

$\lim_{t\to\infty} L(\lambda t)/L(t) = 1$, with $\lambda > 0$. Slowly growing function

Combining

1. Mathematics (Tauberian theorem)

$$W(t) \overset{t\to\infty}{\sim} 2D_\alpha L(t) t^\alpha \longleftrightarrow \hat{W}(s) \overset{s\to 0}{\sim} 2D_\alpha L(1/s)\frac{\Gamma(\alpha+1)}{s^{\alpha+1}}.$$

$$\lim_{t\to\infty} L(t) = 1 \qquad \lim_{t\to\infty} t\frac{dL(t)}{dt} = 0$$

$$\hat{W}(s) = \int_0^\infty dt\, \exp(-st) W(t)$$

2. Physics

$$W(t) = 2\int_0^t d\tau\,(t-\tau)c_{vv}(\tau)$$

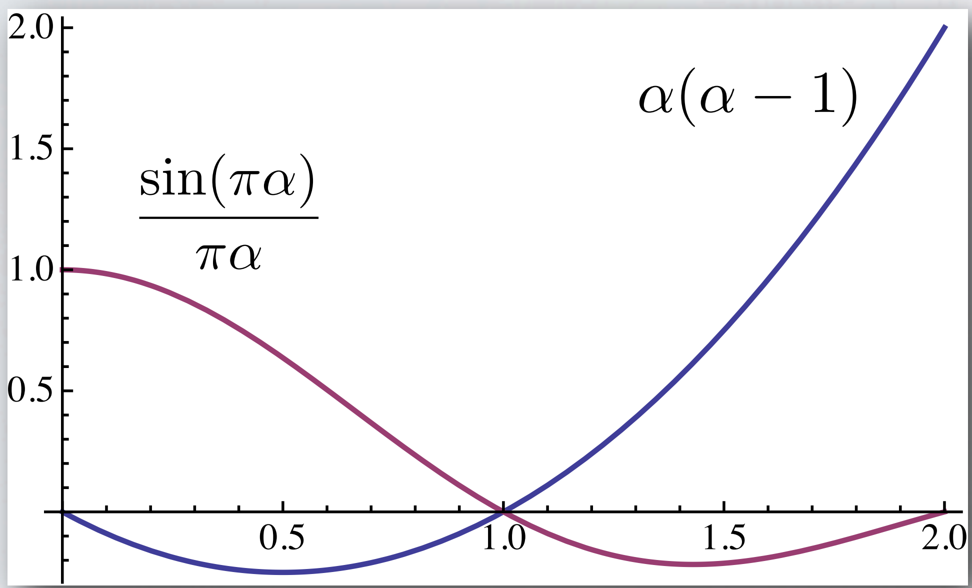
$$\frac{dc_{vv}(t)}{dt} = -\int_0^t d\tau\,\kappa(t-\tau)c_{vv}(\tau)$$

$$\hat{W}(s) = \frac{2\hat{c}_{vv}(s)}{s^2} = \frac{2\langle v^2\rangle}{s^2(s+\hat{\kappa}(s))}$$

leads to the **necessary conditions**

$$c_{vv}(t) \overset{t\to\infty}{\sim} D_\alpha \alpha(\alpha-1)L(t)t^{\alpha-2},$$ also sufficient for $1 < \alpha < 2$

$$\kappa(t) \overset{t\to\infty}{\sim} \frac{\langle \mathbf{v}^2\rangle}{D_\alpha}\frac{\sin(\pi\alpha)}{\pi\alpha}\frac{1}{L(t)}t^{-\alpha}.$$ also sufficient for $0 < \alpha < 1$



Signs of the long time tails

$$D_\alpha = \frac{1}{\Gamma(1+\alpha)}\int_0^\infty dt\ {}_0\partial_t^{\alpha-1} c_{vv}(t).$$

Generalized Kubo relation

Kneller, G. R., J Chem Phys 134, 224106 (2011).

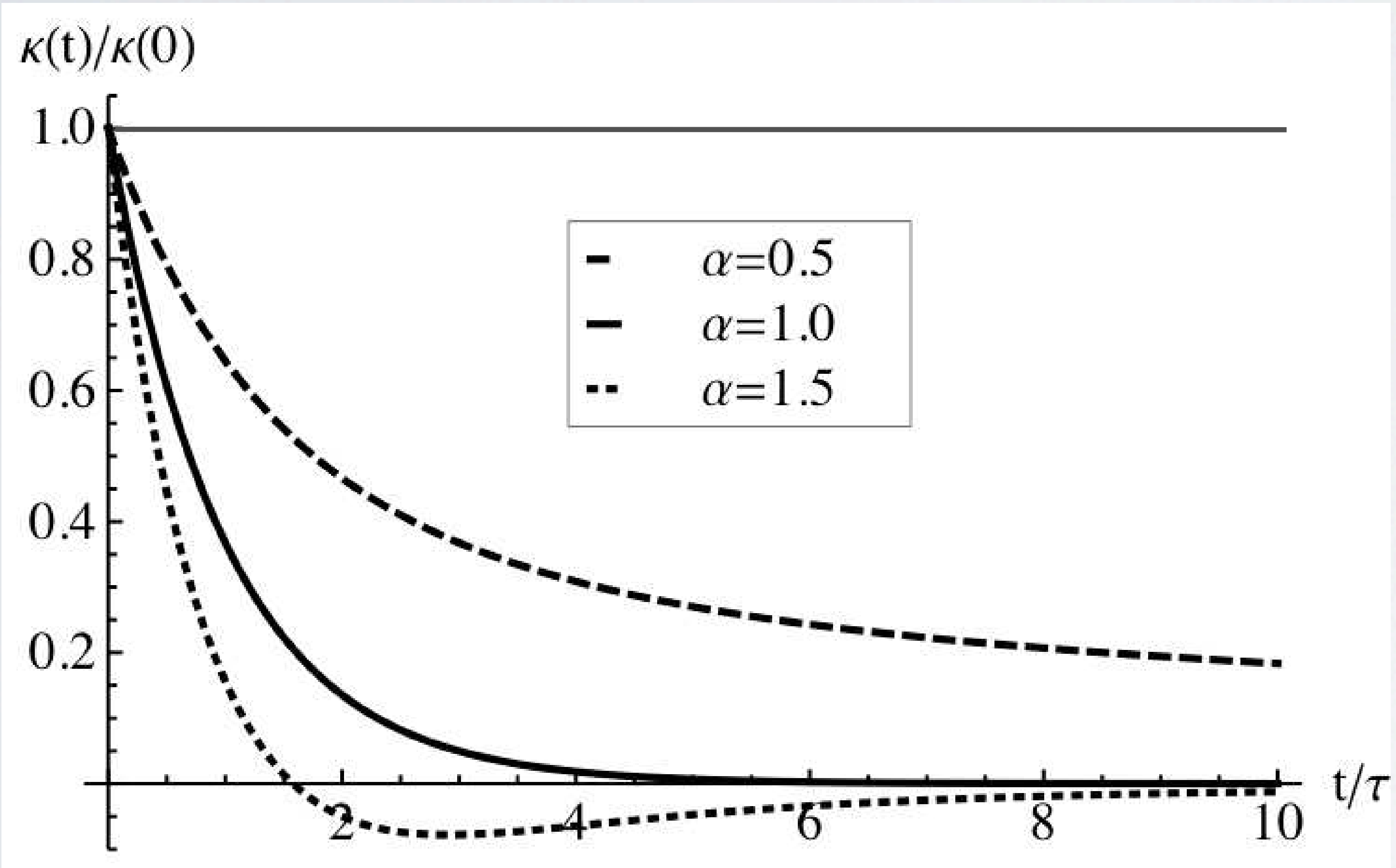
Simple model for free diffusion

model memory function

$$\kappa_f(t) = \Omega^2 M(\alpha, 1, -t/\tau)$$

Kummer function

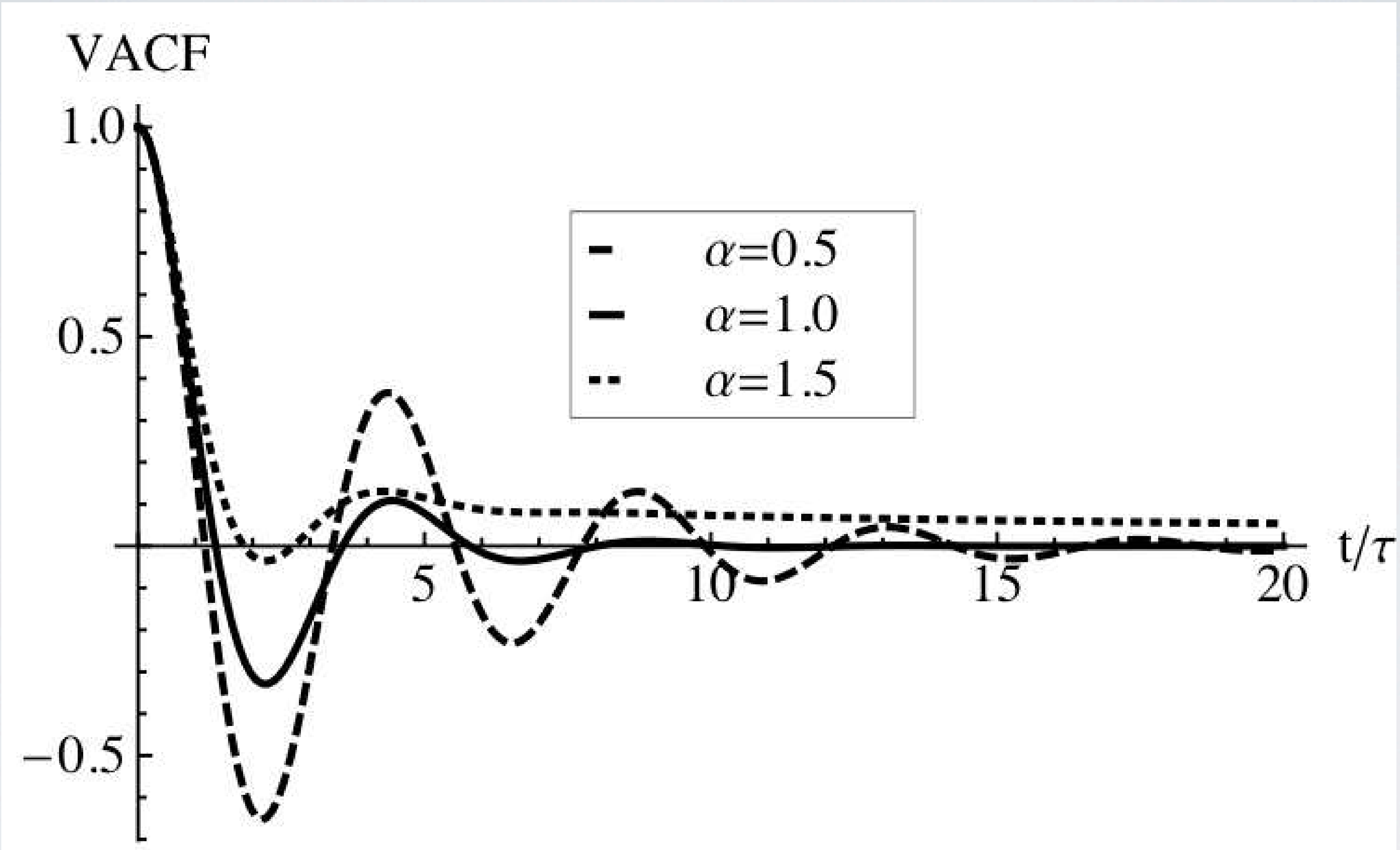
$$\hat{\kappa}_f(s) = \Omega^2 \left\{ \frac{\tau^\alpha}{s^{1-\alpha}} \frac{1}{(s\tau + 1)^\alpha} \right\}$$



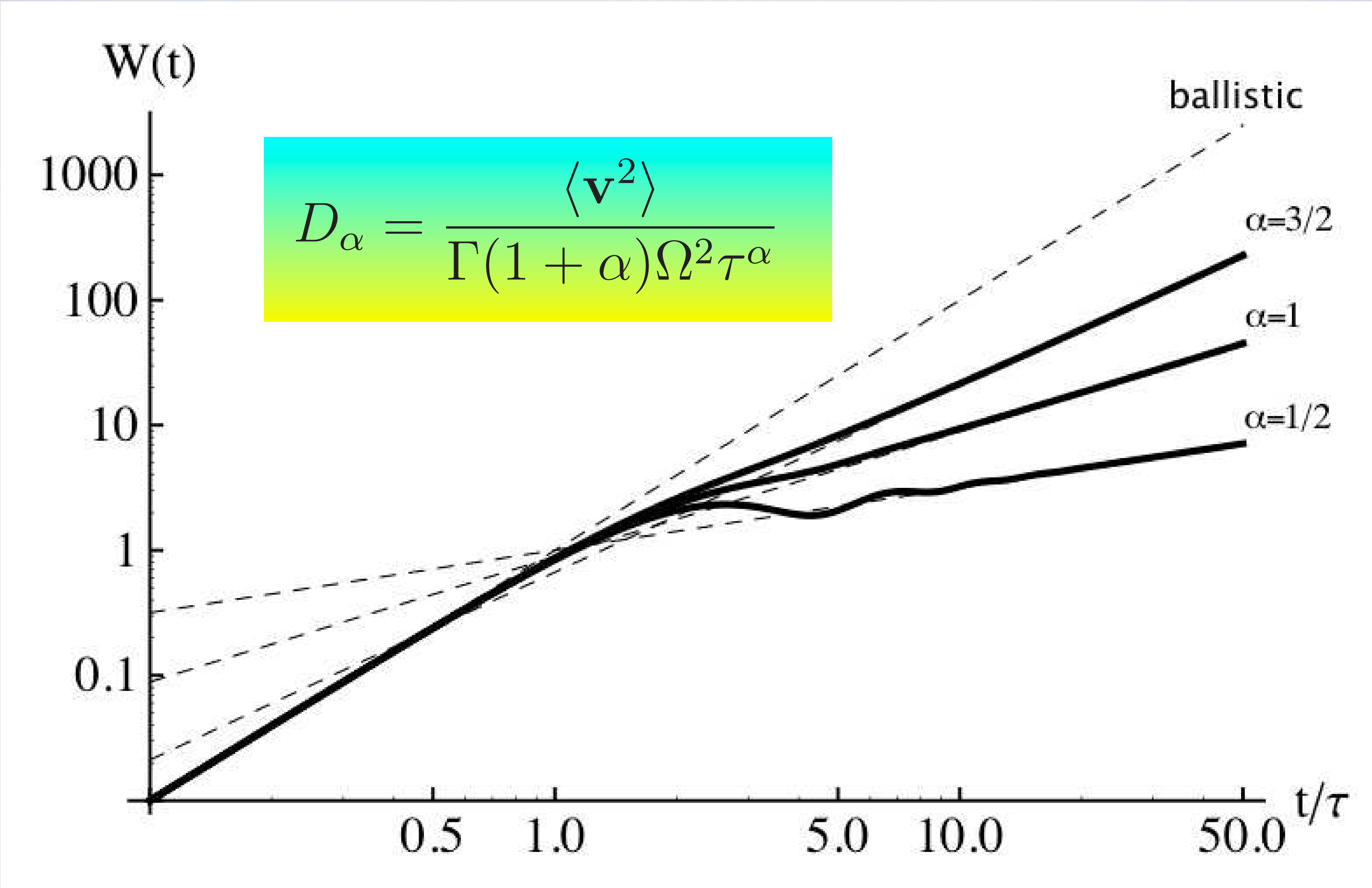
asymptotic form

$$\kappa_f(t) \overset{t\to\infty}{\sim} \begin{cases} \Omega^2 \frac{(t/\tau)^{-\alpha}}{\Gamma(1-\alpha)}, & \alpha \neq 1, \\ \Omega^2 \exp(-t/\tau), & \alpha = 1. \end{cases}$$

G. Kneller, *J. Chem. Phys.*, vol. 134, p. 224106, 2011.

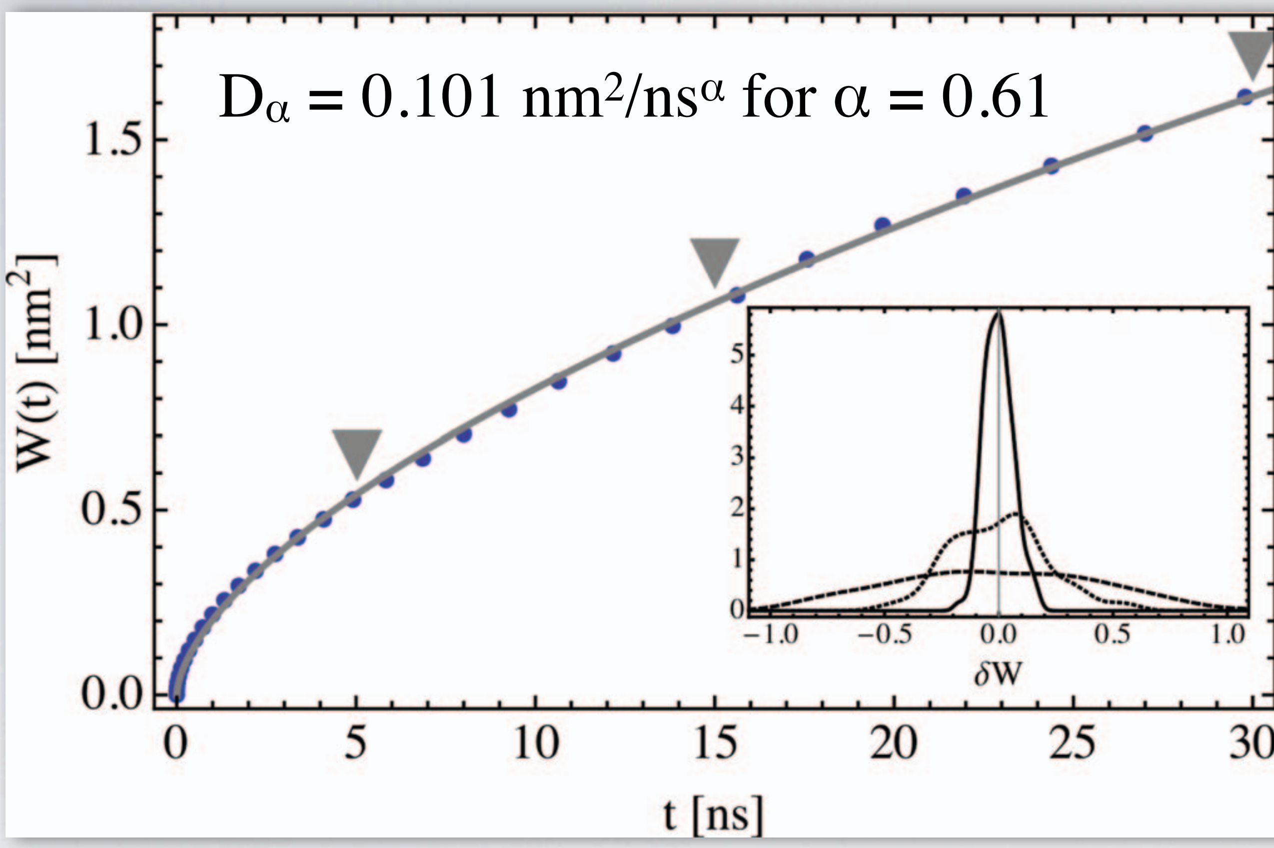


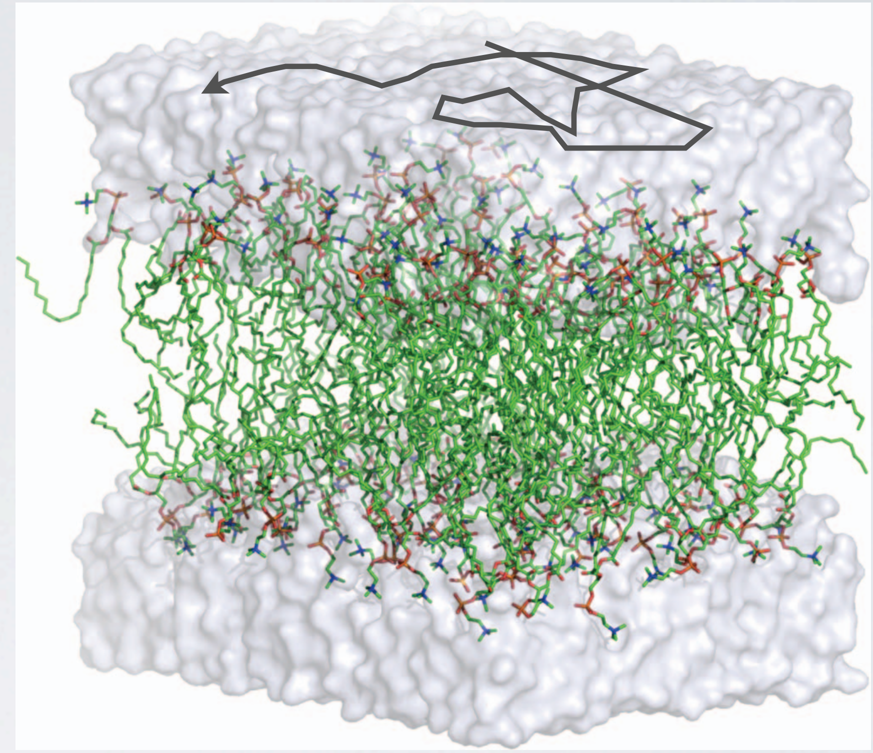
VACF
1.0
0.5
−0.5
α=0.5
α=1.0
α=1.5
5
10
15
20
t/τ

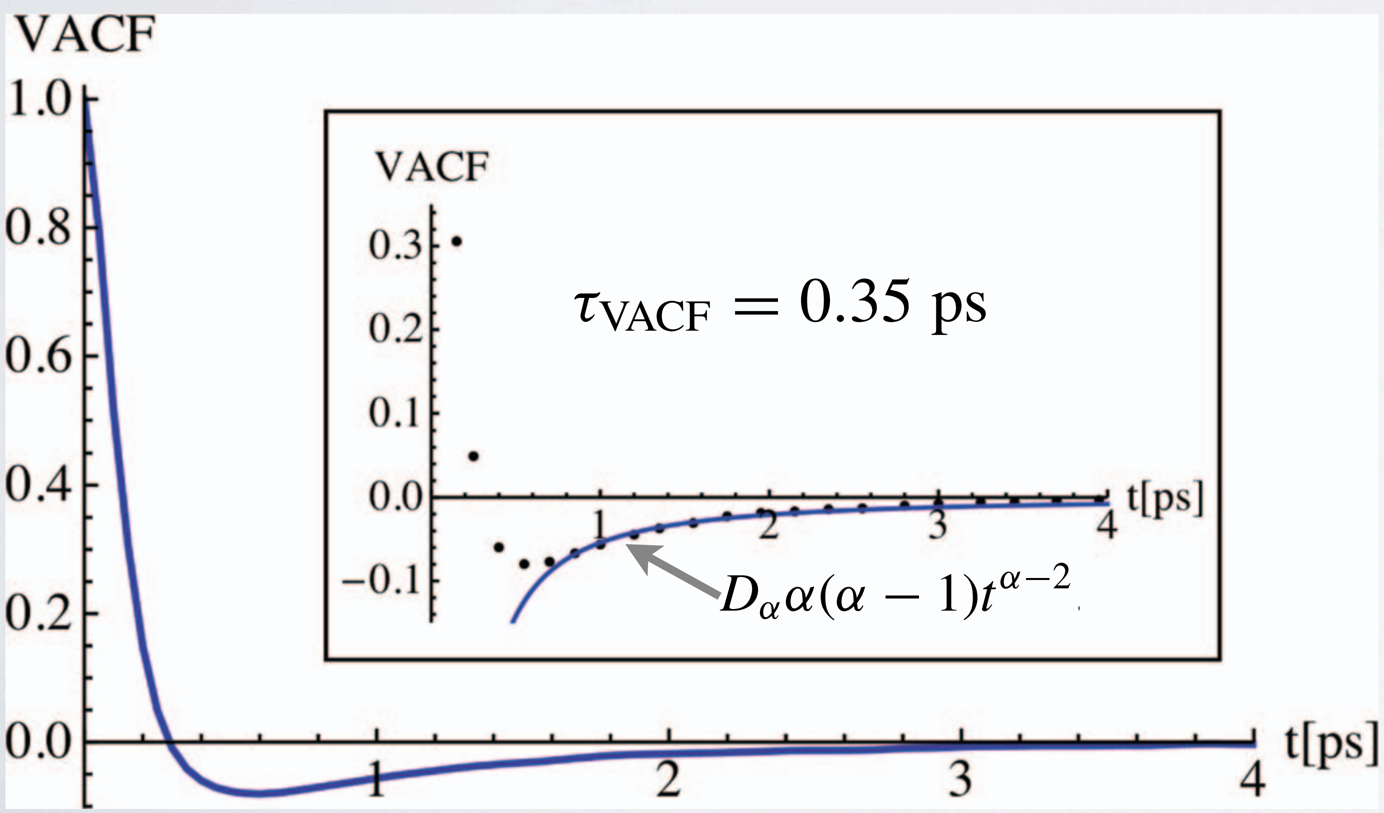


W(t)
ballistic
1000
100
10
1
0.1
$D_\alpha = \frac{\langle \mathbf{v}^2 \rangle}{\Gamma(1+\alpha)\Omega^2\tau^\alpha}$
α=3/2
α=1
α=1/2
0.5
1.0
5.0
10.0
50.0
t/τ

Back to DOPC





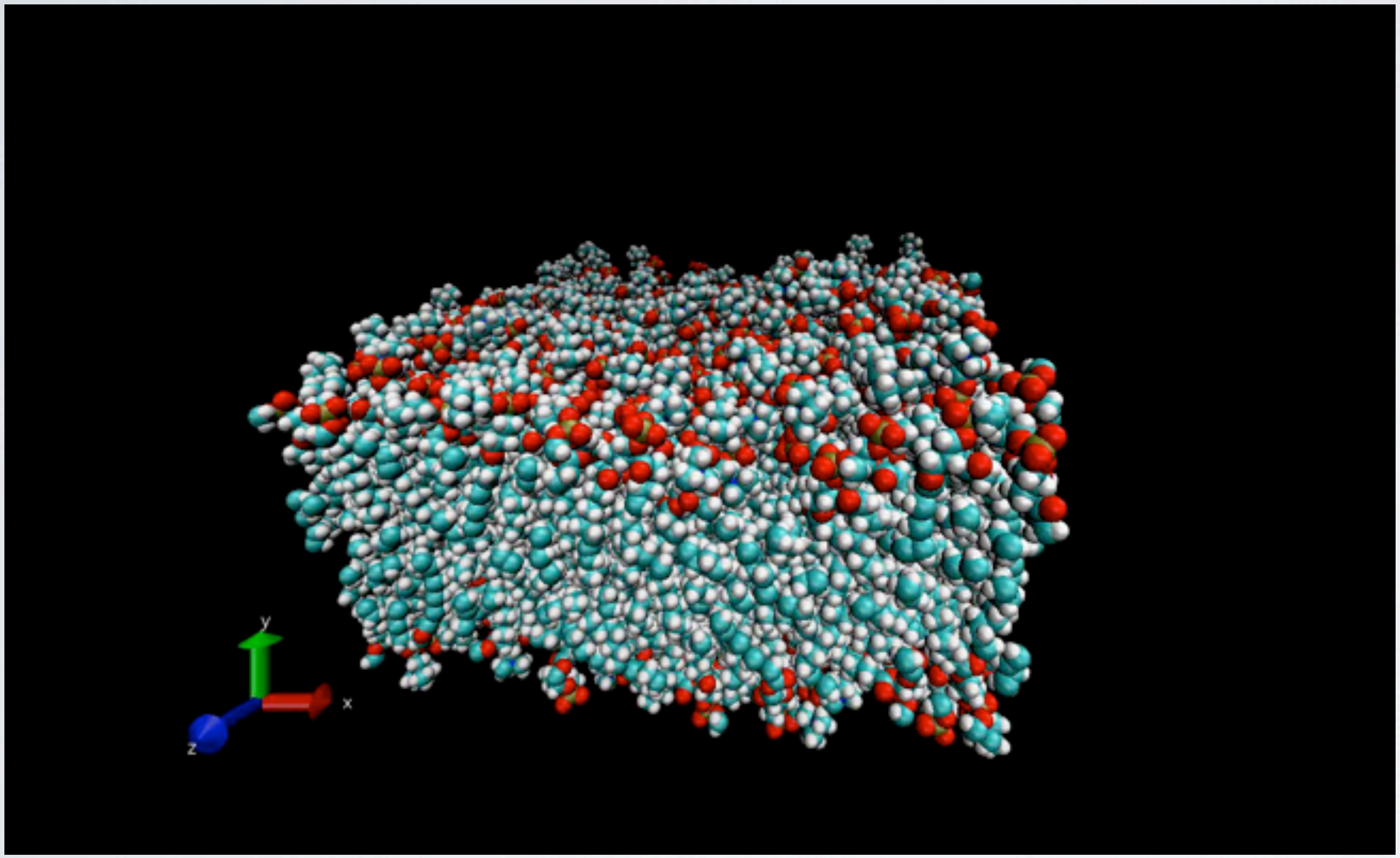


Characteristic time scale:

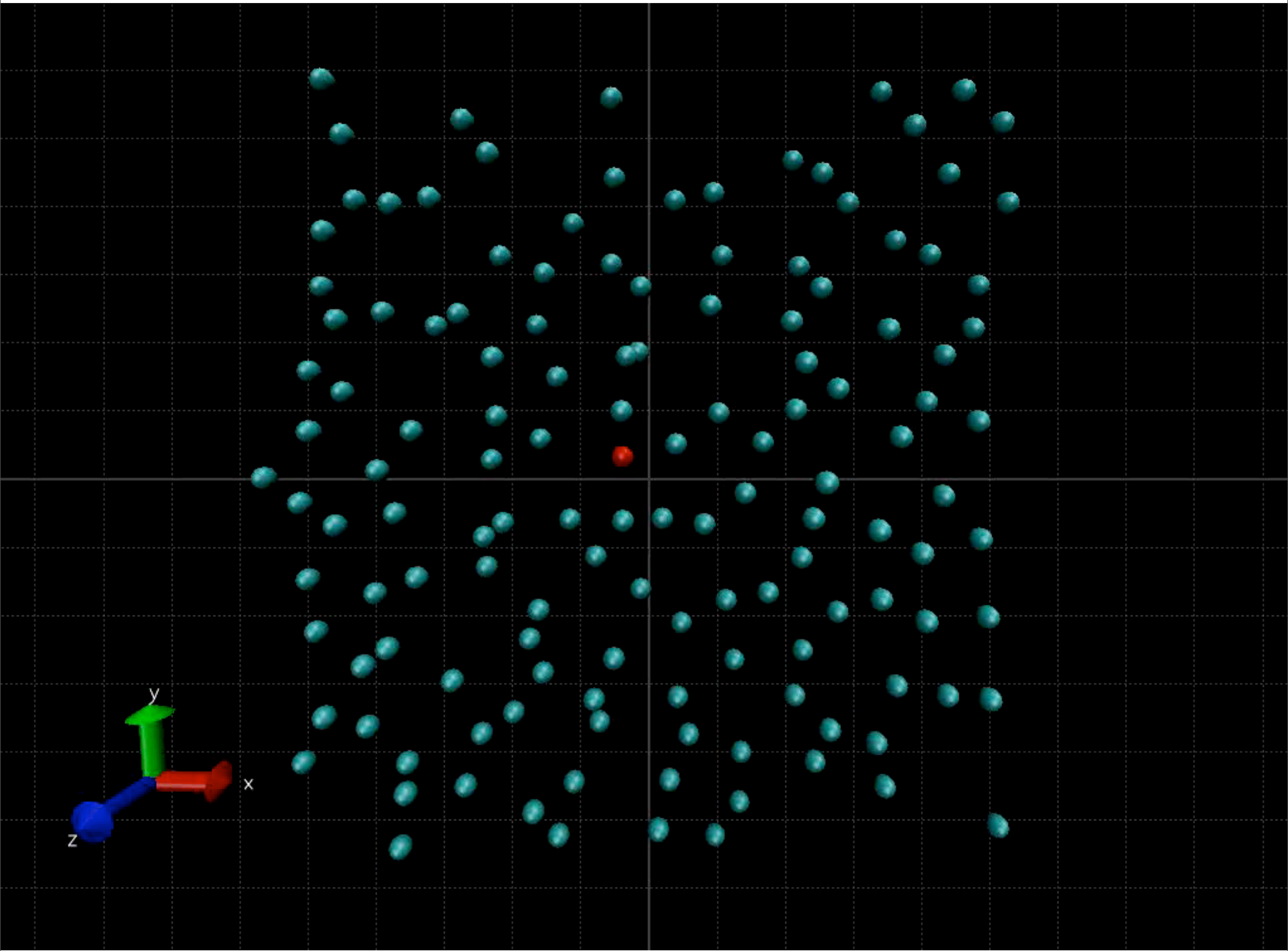
$$\tau_{VACF} = \left(\frac{D_\alpha}{\langle \mathbf{v}^2 \rangle}\right)^{1/(2-\alpha)}$$

G. R. Kneller, K. Baczynski, and M. Pasenkiewicz-Gierula. *J. Chem. Phys.*, 135(14):141105, 2011.

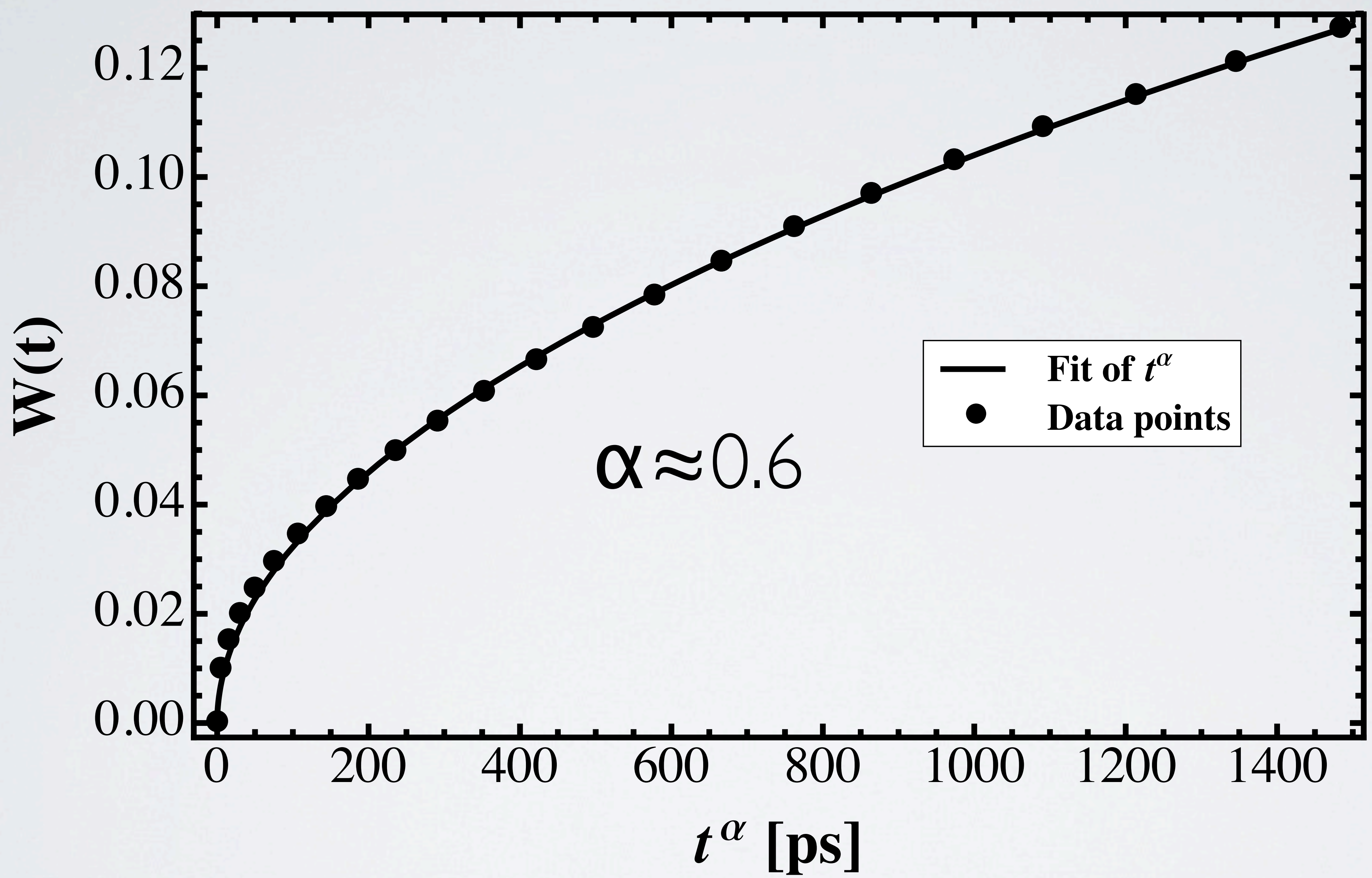
Visualizing the cage effect in a POPC bilayer



- 2x137 POPC molecules (10 nm ✕ 10 nm in the XY-plane)
- 10471 water molecules (fully hydrated)
- OPLS force field
- T=310 K


y
x
z

The average lateral MSD



Mean Square Displacement of POPC lipids after 15ns simulation (dots) and fit of the model for anomalous diffusion (thick line).

Van Hove correlation function and the „cage" of nearest neighbours

- The pair Distribution Function (PDF), g(r), is proportional to the probability of finding a particle between distances „r+dr", from a tagged central particle in a liquid.
- Time-dependent PDFs (van Hove PDFs), $G_D(r,t)$, display the dynamic structure in a liquid.

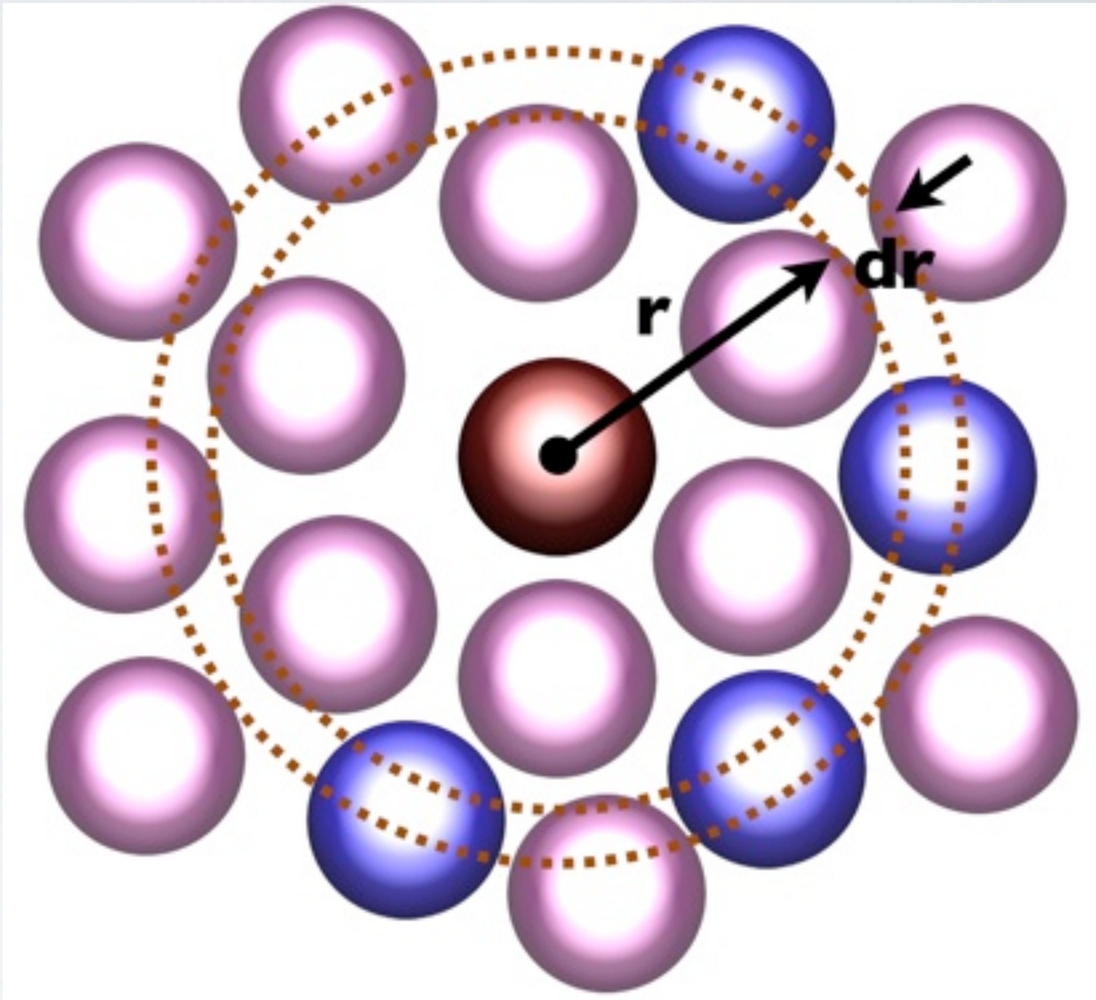
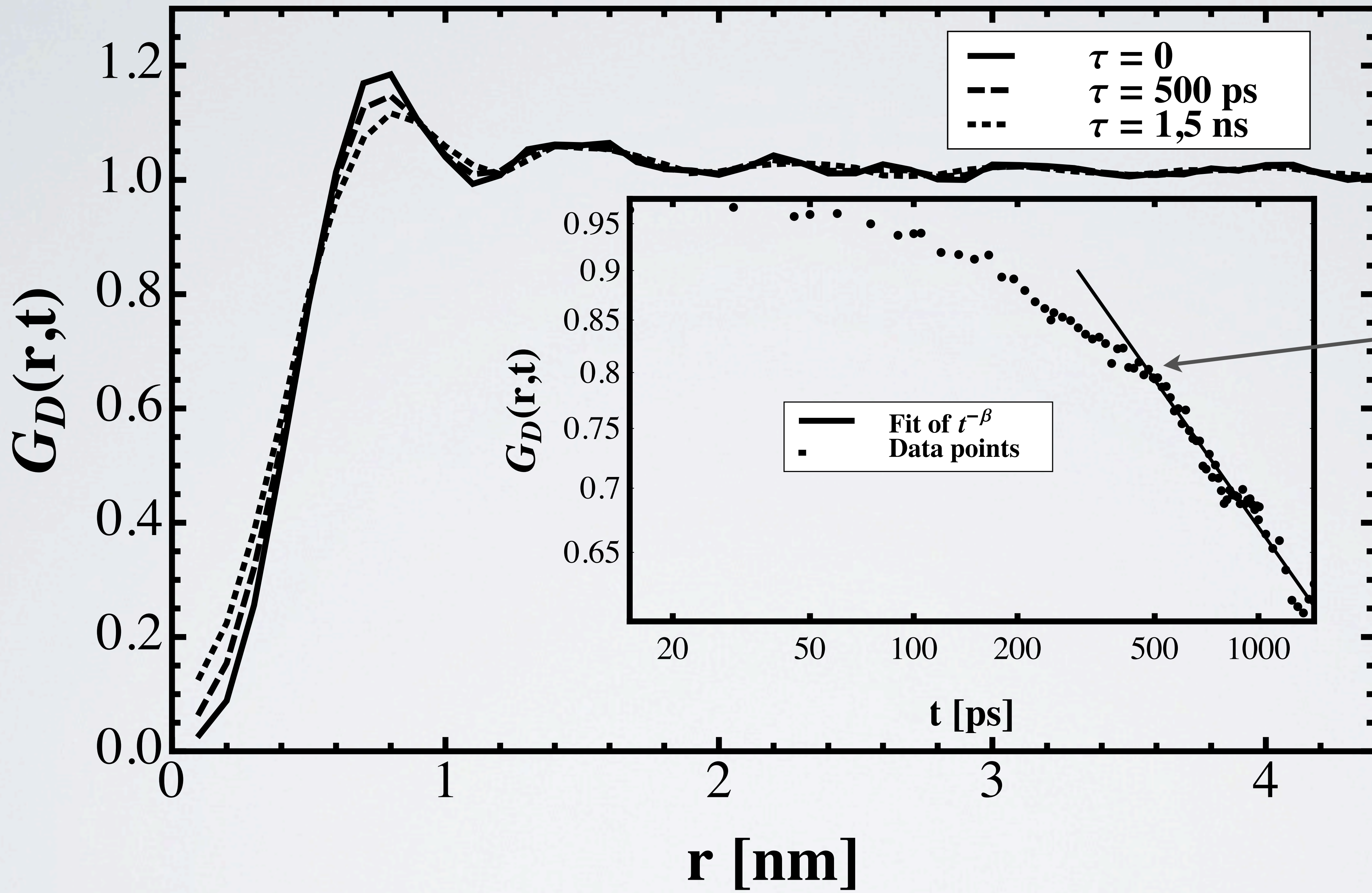


Image: "The structure of the cytoplasm" from Molecular Biology of the Cell. Adapted from D.S. Goodsell, Trends Biochem. Sci. 16:203-206, 1991.

- (Van Hove) PDFs can be obtained from scattering experiments (neutron scttering, inelastic X-ray scattering)

Time-dependent pair correlation function for POPC

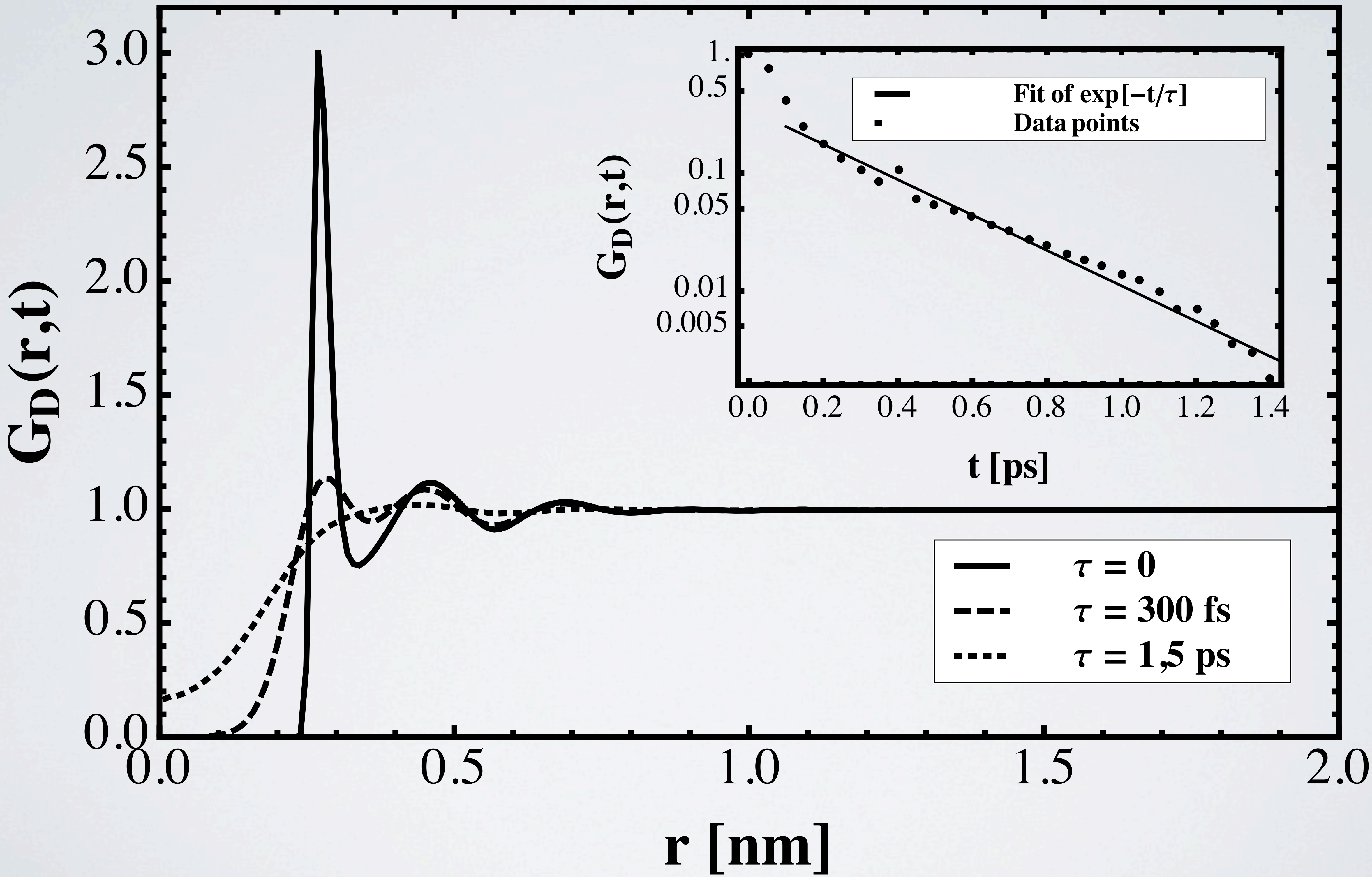


$\propto t^{-\beta}$

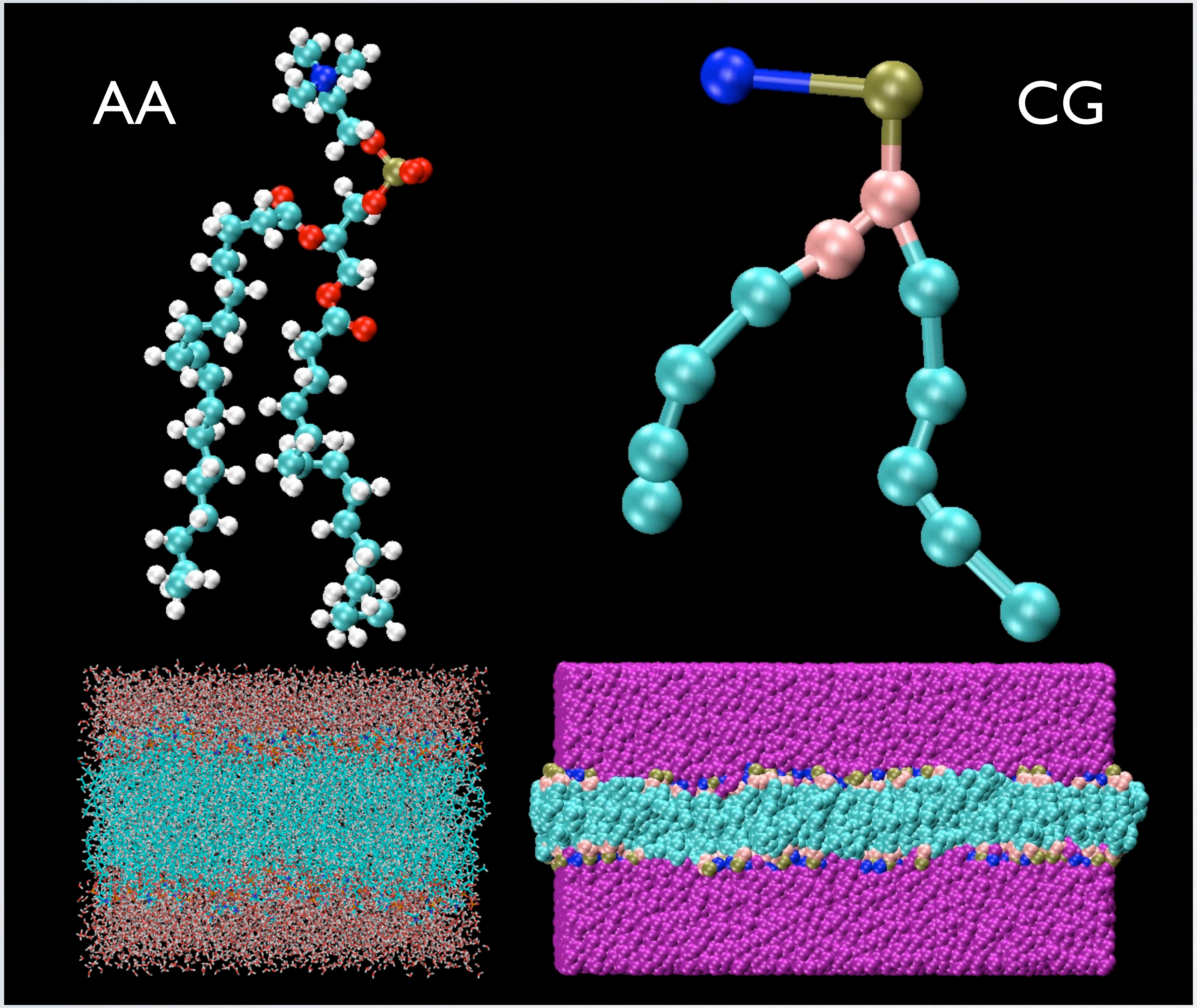
$\beta = 0.34$

Time-dependent Pair Correlation Function G_d(r,t) of POPC lipids (CM) for three time slices : t=0 (thick line), t=500 ps (dashed line) and for t=1.5 ns (dotted line). **Inset:** Log-log plot for the decay of Gd(r,t) as a function of time for r =0.8 nm.

Bulk water for comparison....



Comparing all-atom (OPLS) and coarse-grained (MARTINI) force field for POPC



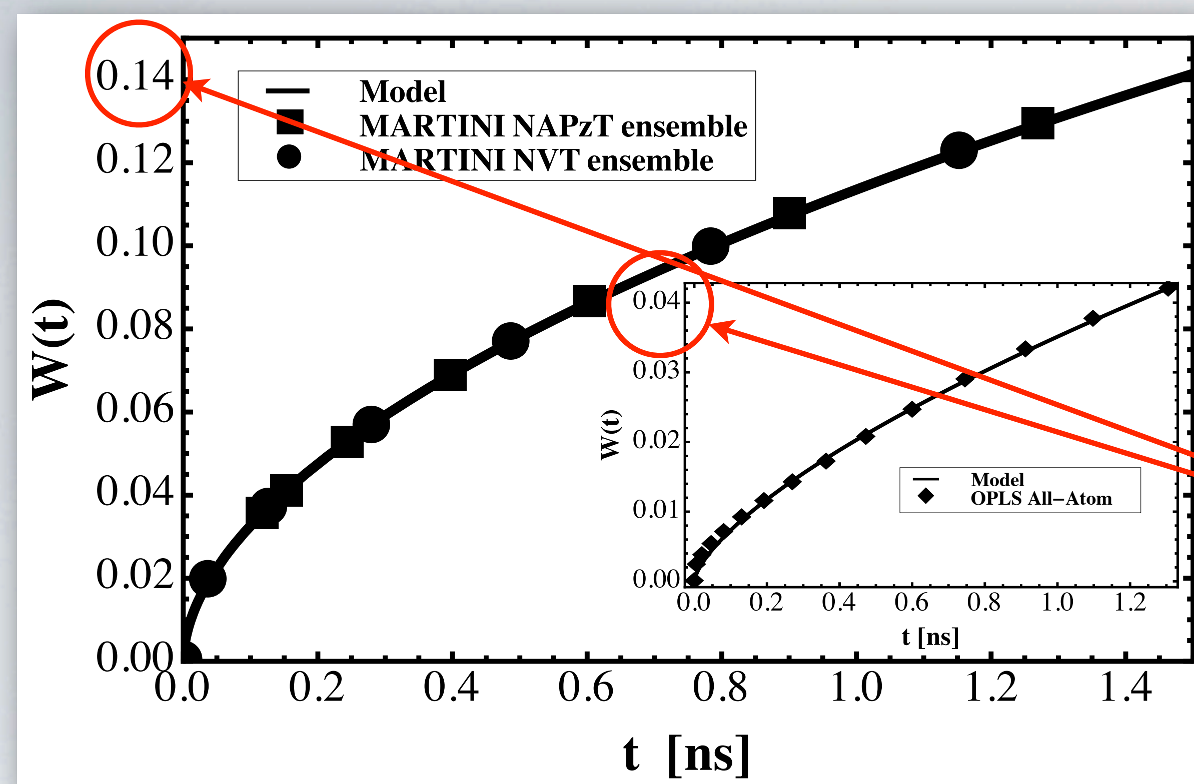
All atom (AA):

274 POPC lipids in 10 471 water molecules (OPLS)

Coarse Grained (CG):

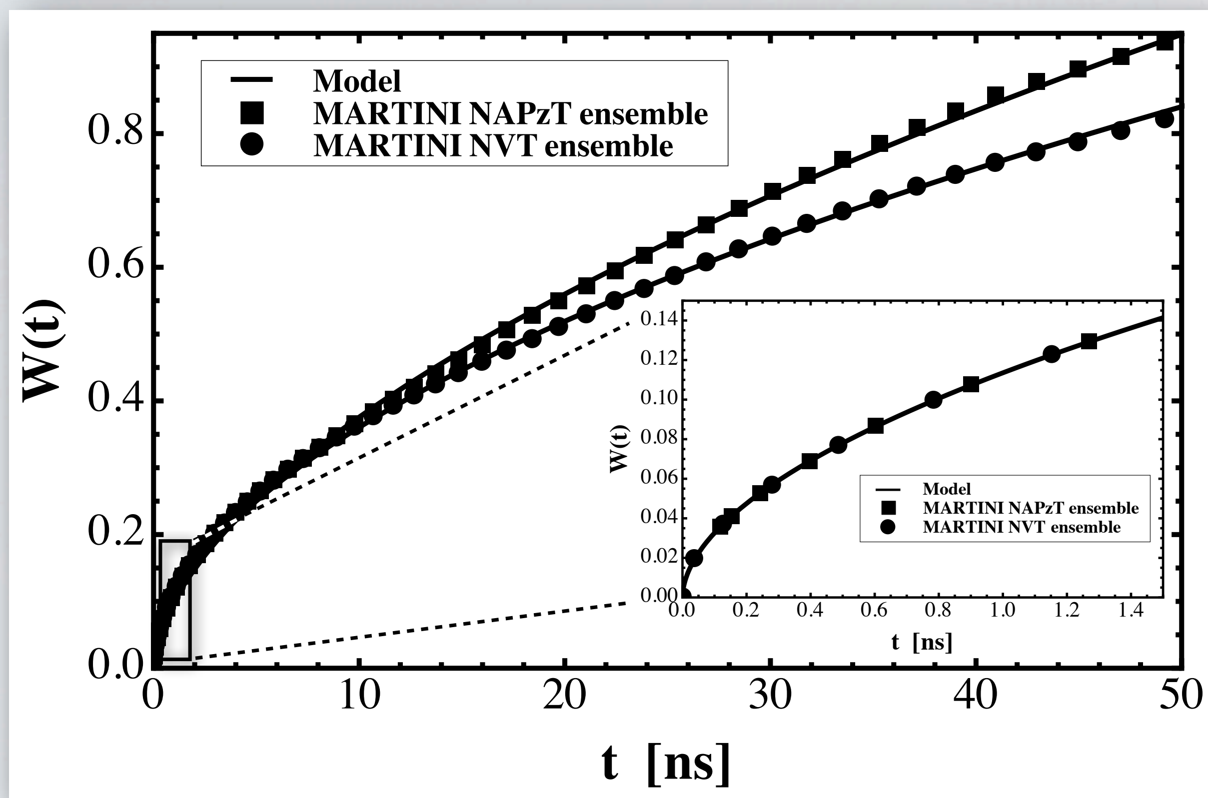
2033 POPC lipids in 231 808 water molecules (MARTINI)

1. Marrink, et al. J Phys Chem B 111, 7812–7824 (2007).
2. de Jong, D. H. et al. JCTC 9, 687–697 (2012).



Short time scale (OPLS and MARTINI)

☛ MARTINI is 3 x faster than OPLS

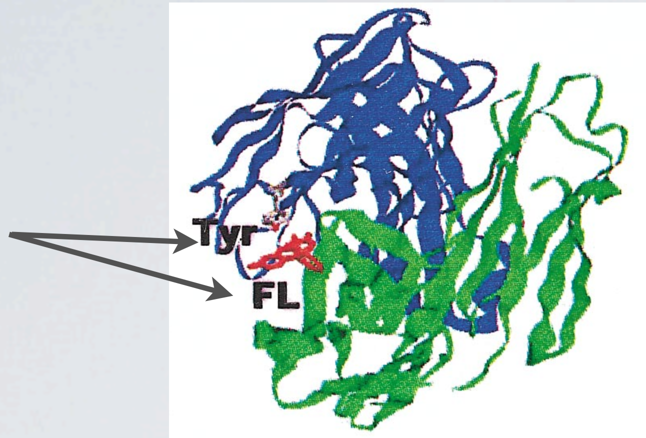


Long time scale (only MARTINI)

S. Stachura & G. R. Kneller, Mol. Simul., in press

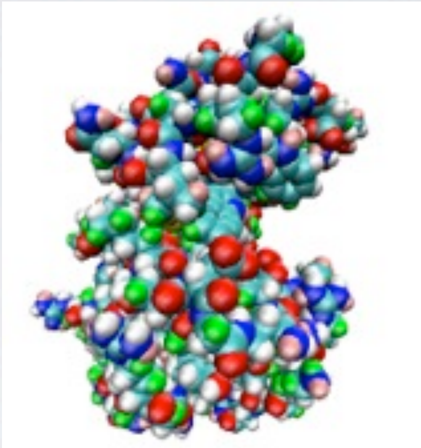
	AA 1.5 ns	CG(1) 1.5 ns	CG(2) 1.5 ns	$CG(1)$ 50 ns	$CG(2)$ 50 ns
α	0.668	0.515	0.508	0.571	0.558
$D_\alpha[\mathrm{nm}^2/\mathrm{ns}]$	0.018	0.057	0.058	0.051	0.051

Self-similar protein dynamics - anomalous confined diffusional motion



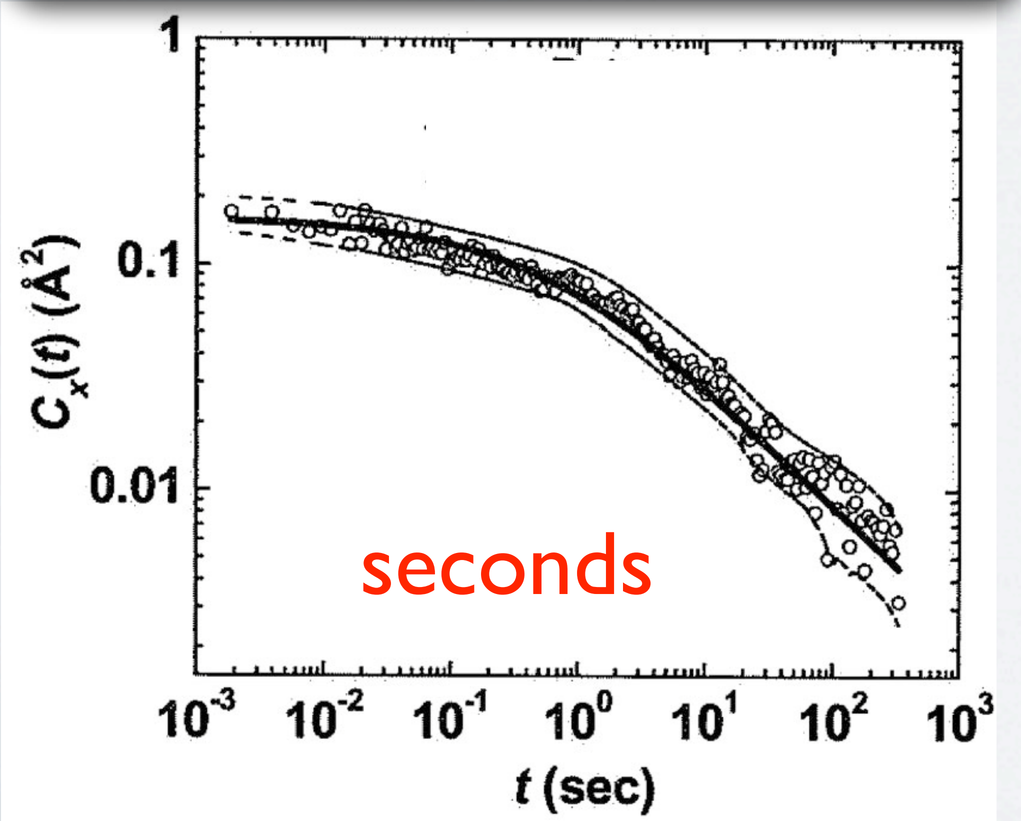
FL/Anti-FL complex

Min et al. PRL 94, 198302

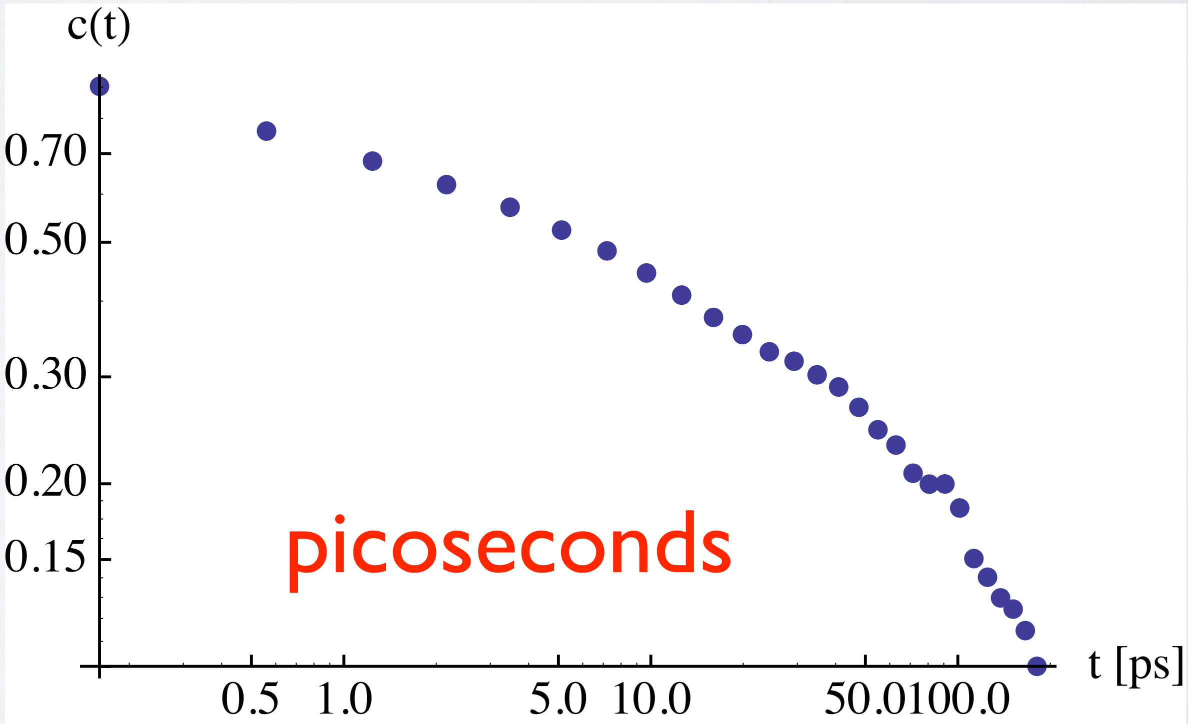


Lysozyme

Distance autocorrelation by single moleculefluorescence spectrocopy



auto-corrélation <x(0)x(t)> de positions par simulation MD

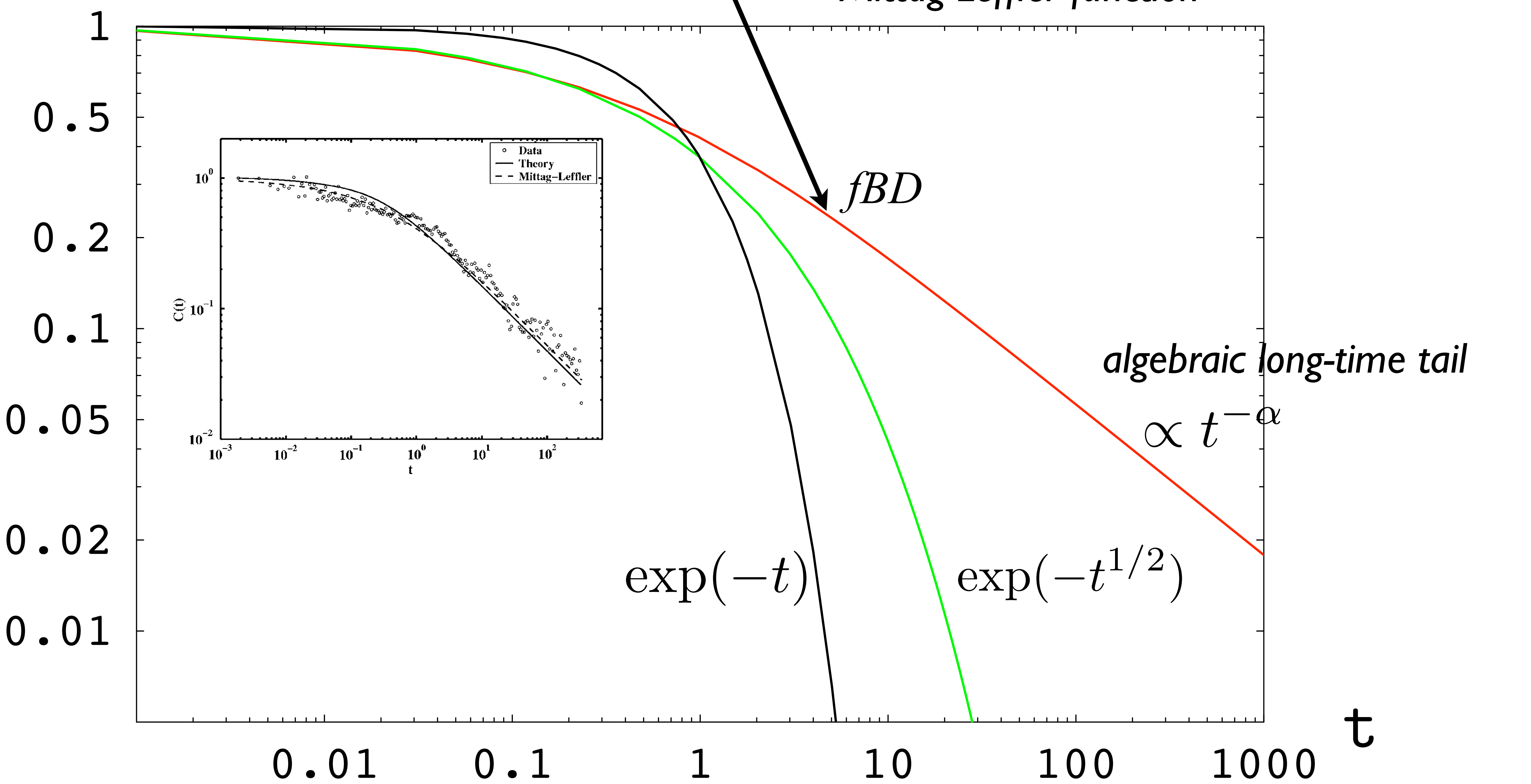


Model correlation function (α=0.5)

$$c_{xx}(t) = \langle x^2 \rangle E_\alpha(-[t/\tau]^\alpha)$$

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+\alpha k)}.$$

Mittag-Leffler function



Fractional reaction kinetics

46 Biophysical Journal Volume 68 January 1995 46–53

A Fractional Calculus Approach to Self-Similar Protein Dynamics

Walter G. Glöckle and Theo F. Nonnenmacher
Department of Mathematical Physics, University of Ulm, D-89069 Ulm, Germany

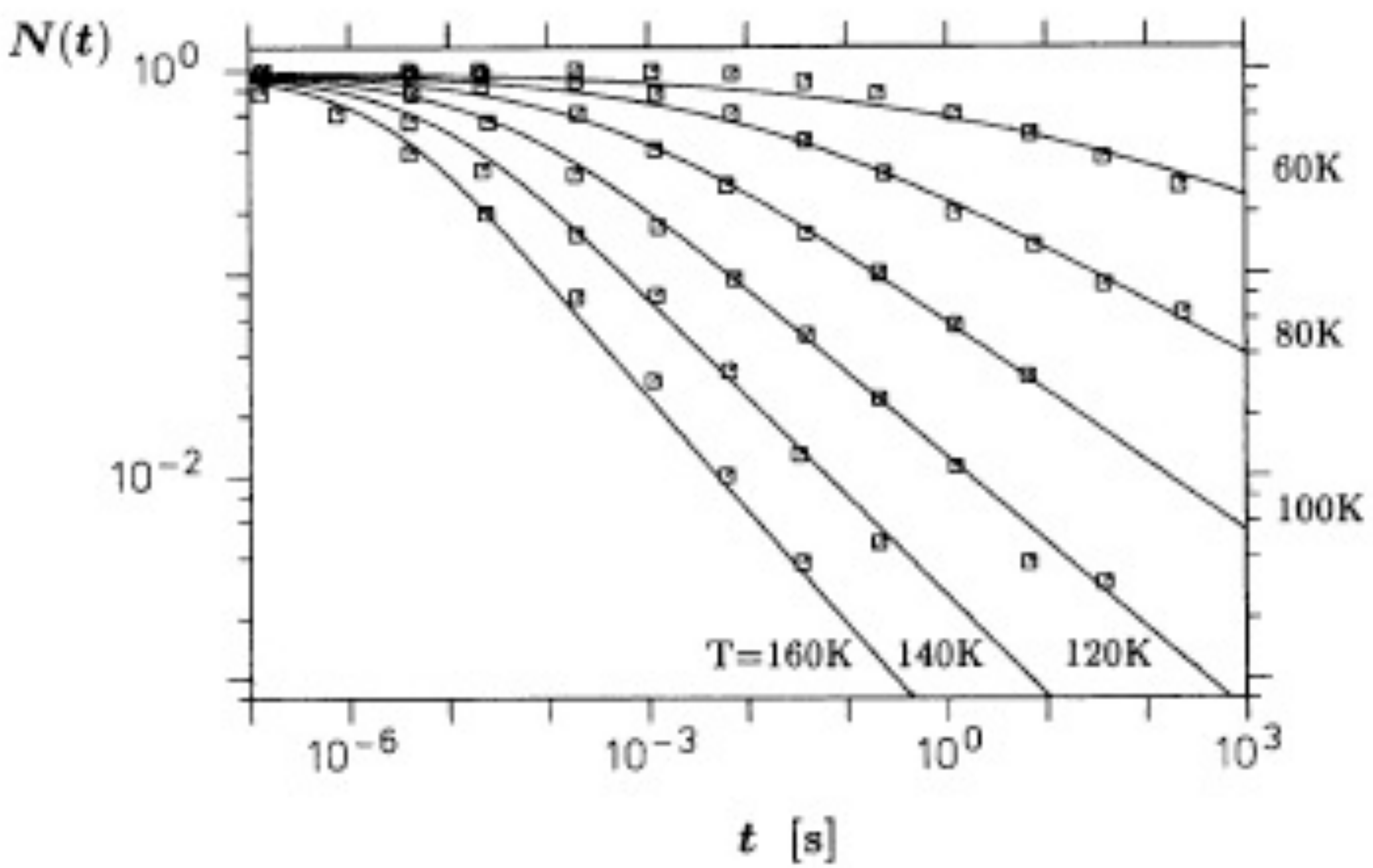
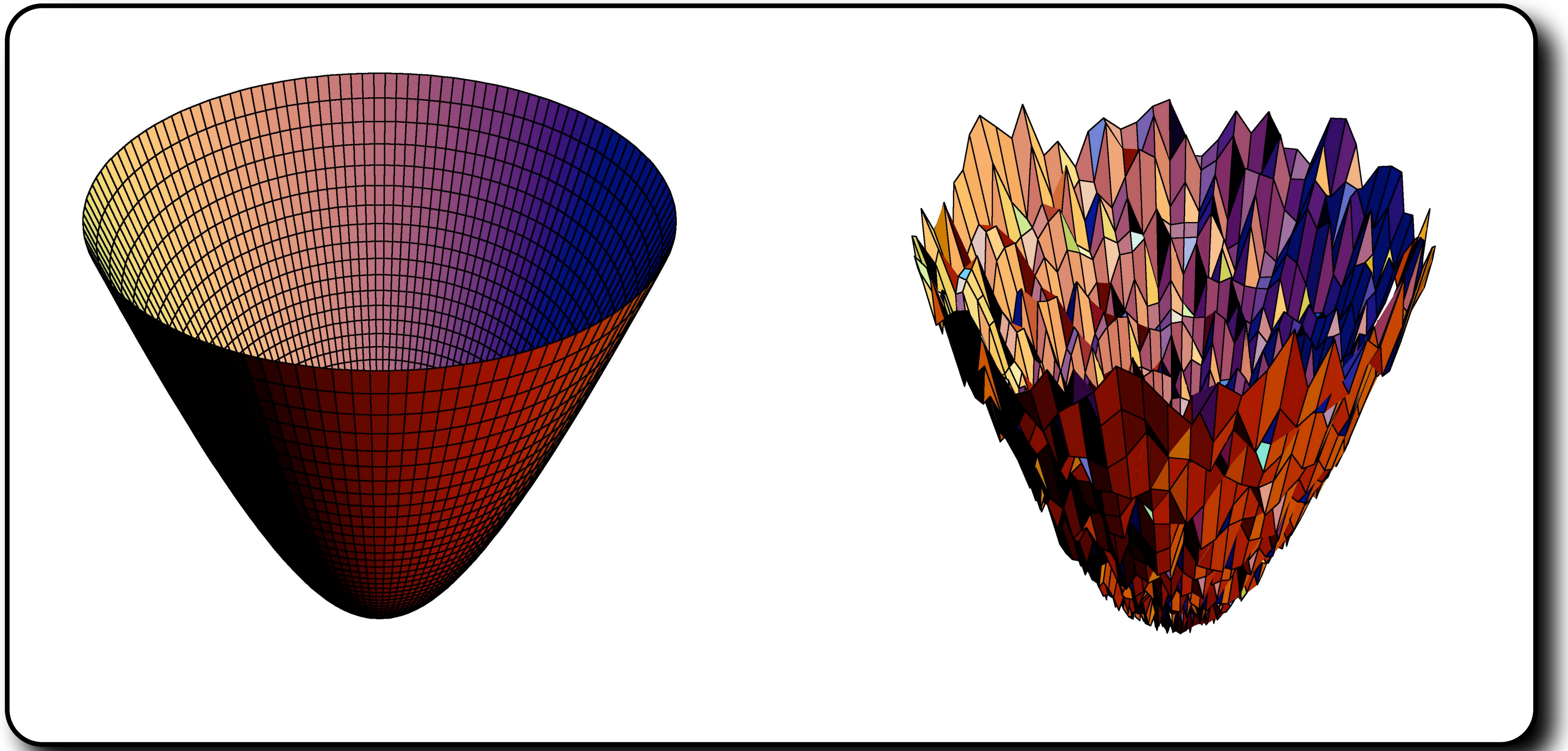
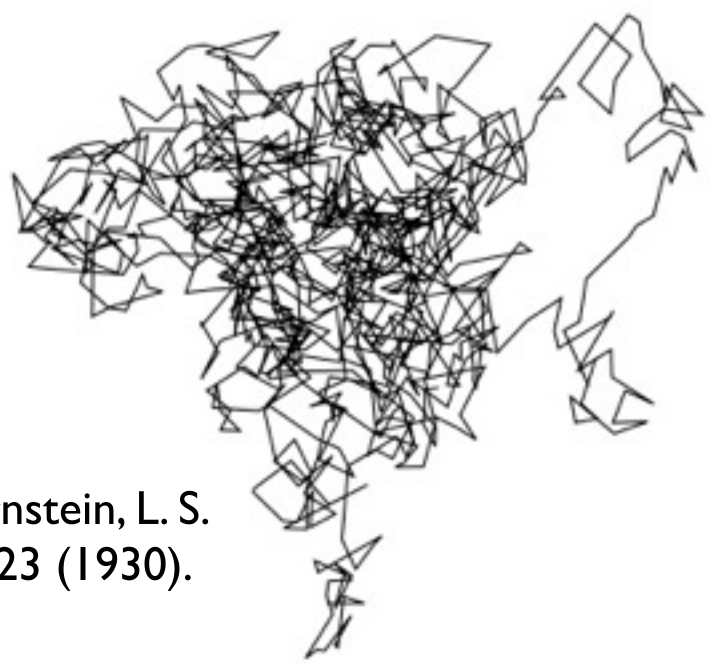


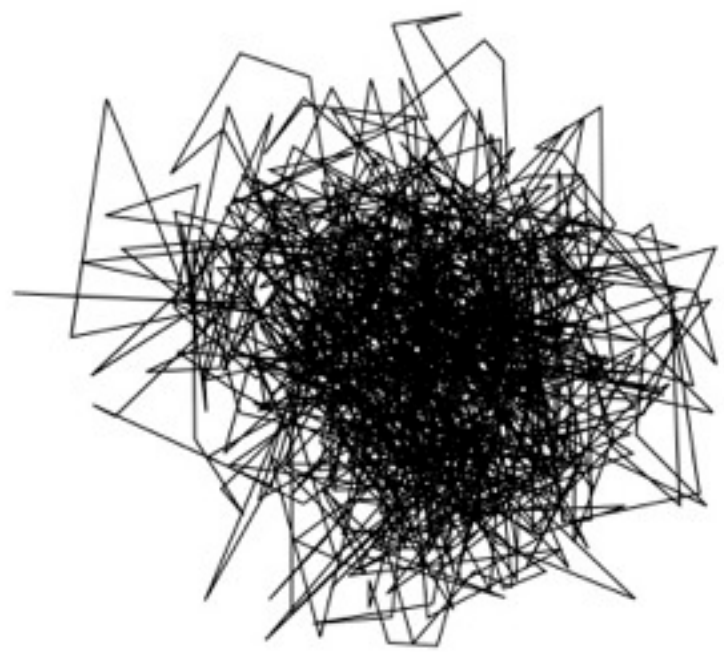
FIGURE 2 Three-parameter model Eq. 32 for rebinding of CO to Mb after photo dissociation. The parameters are $\tau_m = 8.4 \times 10^{-10}$s, $\alpha = 3.5 \times 10^{-3}\ K^{-1}$ and $k = 130$, the data points are from Austin et al. (1975).

$$N(t) = N(0) E_\alpha(-[t/\tau]^\alpha)$$

Self-similar fractional Brownian dynamics







Uhlenbeck, G. E. & Ornstein, L. S. Physical Review 36, 823 (1930).

1. Shao, Y. Physica D: Nonlinear Phenomena 83, 461–477 (1995).
2. Metzler, R. & Klafter, J. Phys Rep 339, 1–77 (2000).

Ornstein-Uhlenbeck process

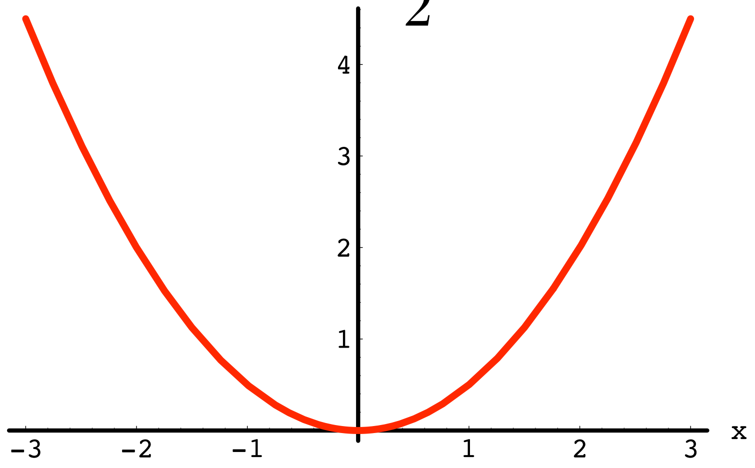
Fractional Ornstein-Uhlenbeck process

Fractional Smoluchowski equation

$$\partial_t P(\mathbf{x}, t|\mathbf{x}_0, 0) = {}_0\partial_t^{1-\alpha} \left\{ D_\alpha \frac{\partial}{\partial \mathbf{x}} \cdot \left(\frac{\partial}{\partial \mathbf{x}} + \frac{1}{k_B T} \frac{\partial U(\mathbf{x})}{\partial \mathbf{x}} \right) \right\} P(\mathbf{x}, t|\mathbf{x}_0, 0)$$

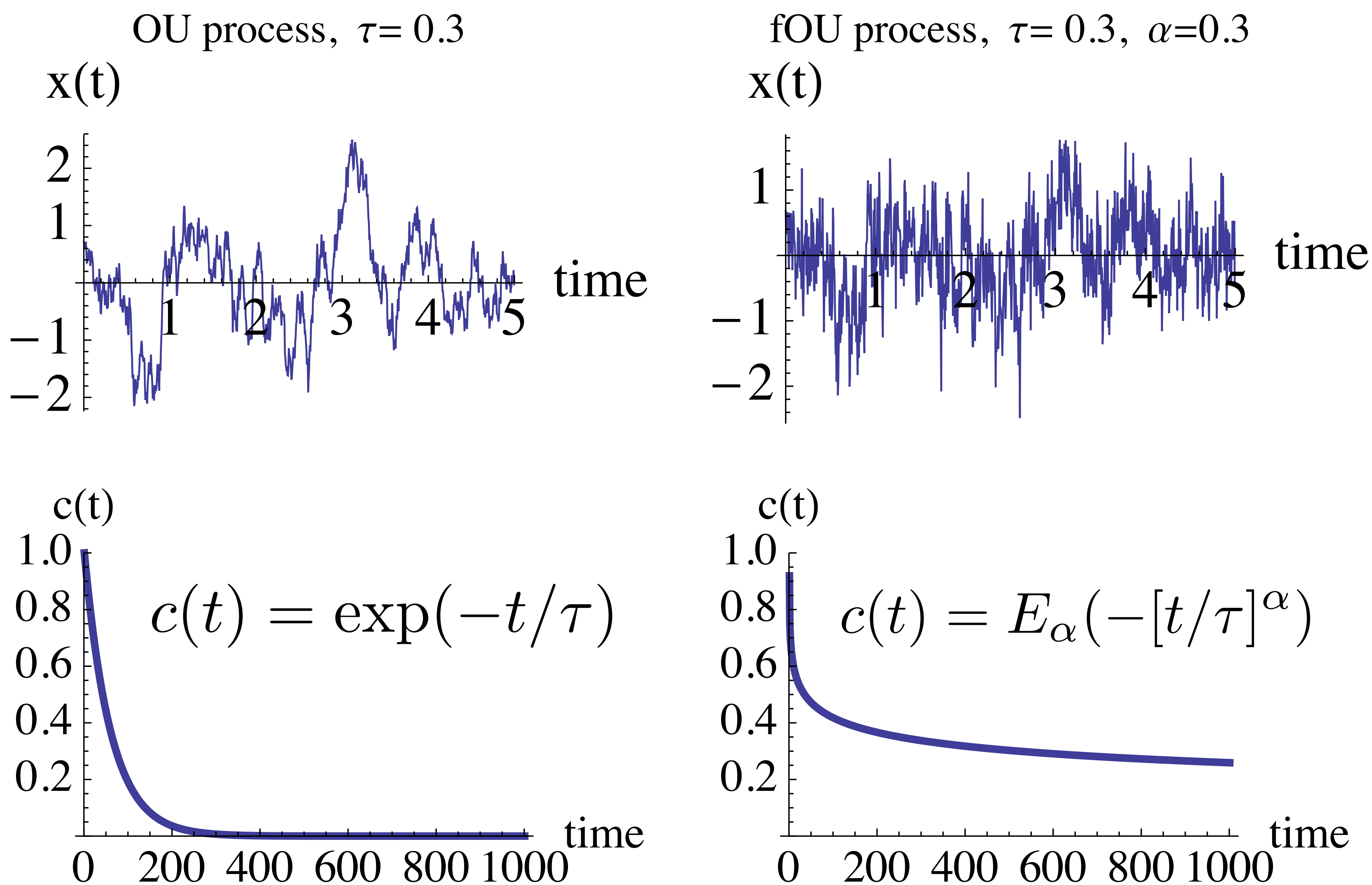
$$U(x) = \frac{1}{2} K x^2$$

Harmonic potential



$$W(t) = 2\langle (\mathbf{x} - \langle \mathbf{x} \rangle)^2 \rangle E_\alpha(-[t/\tau]^\alpha)$$

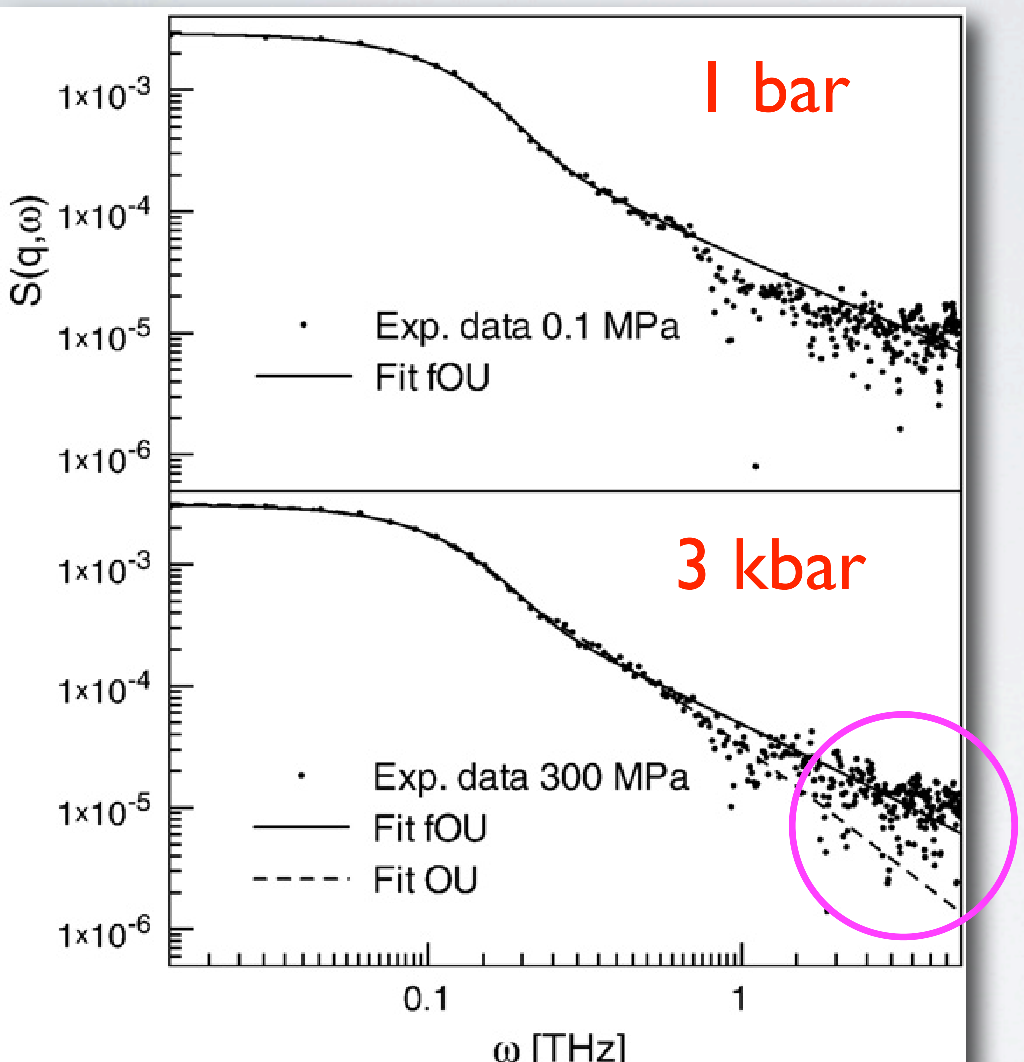
Time series and autocorrelation functions

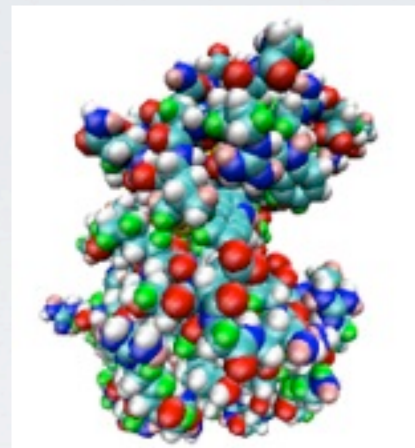


Proteins under pressure

Neutron scattering

QENS dynamic structure factor

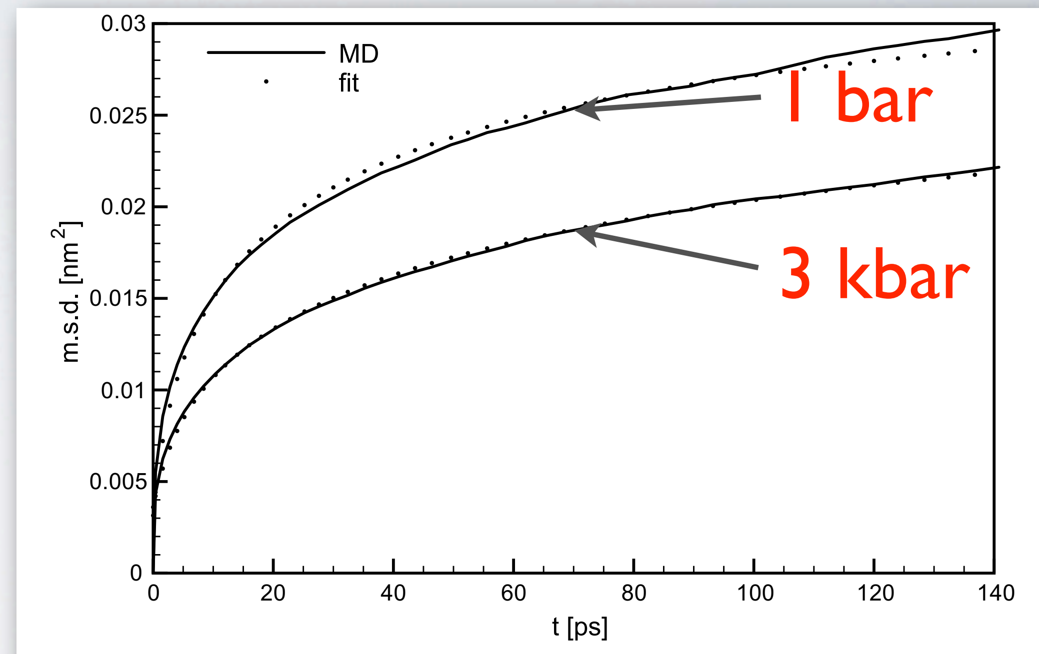




Lysozyme

MD simulation

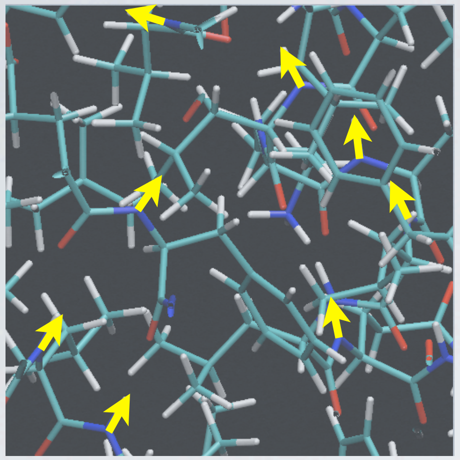
Mean square displacement <[x(t)-x(0)]²> of the H atoms in lysozyme MD simulation



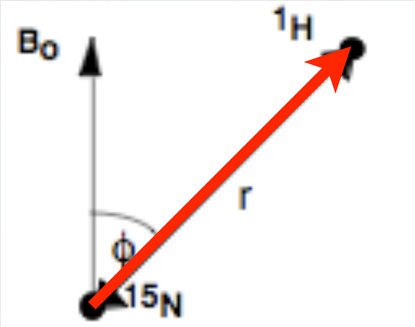
	0.1 MPa			300 MPa		
	$\langle x^2 \rangle$ (nm^2)	α	τ (ps)	$\langle x^2 \rangle$ (nm^2)	α	τ (ps)
MSD	6.17×10^{-3}	0.54	31.75	4.74×10^{-3}	0.54	39.08

- Calandrini, Kneller, *J. Chem. Phys.*, vol. 128, no. 6, p. 065102, 2008.
- Calandrini et al,, *Chem. Phys.*, vol. 345, pp. 289–297, 2008.
- Kneller, Calandrini, *Biochimica et Biophysica Acta,* vol. 1804, pp. 56–62, 2010.

Protein dynamics & NMR



Relaxation $^{15}N - {}^{1}H$



$$C_{ii}(t) = \langle P_2(\boldsymbol{\mu}_i(t) \cdot \boldsymbol{\mu}_i(0))\rangle,$$

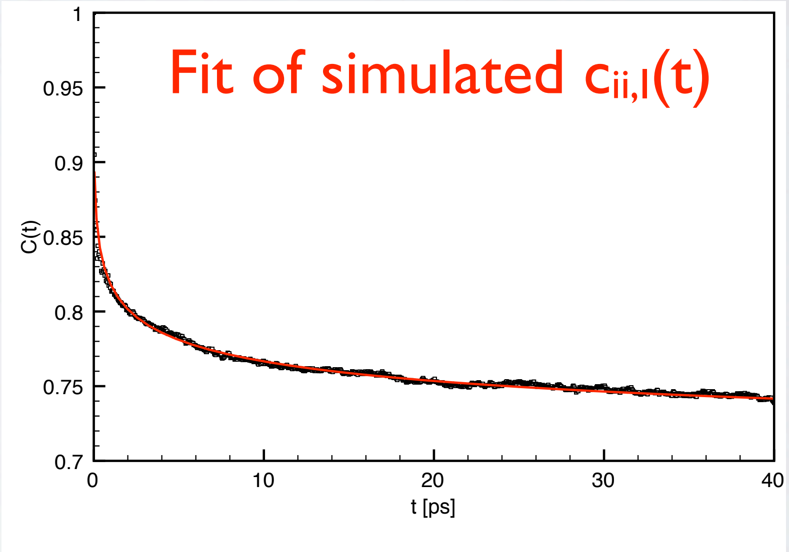
$$c_{ii}(t) = C_{ii,R}(t) C_{ii,I}(t)$$

Global rotation — Internal dynamics

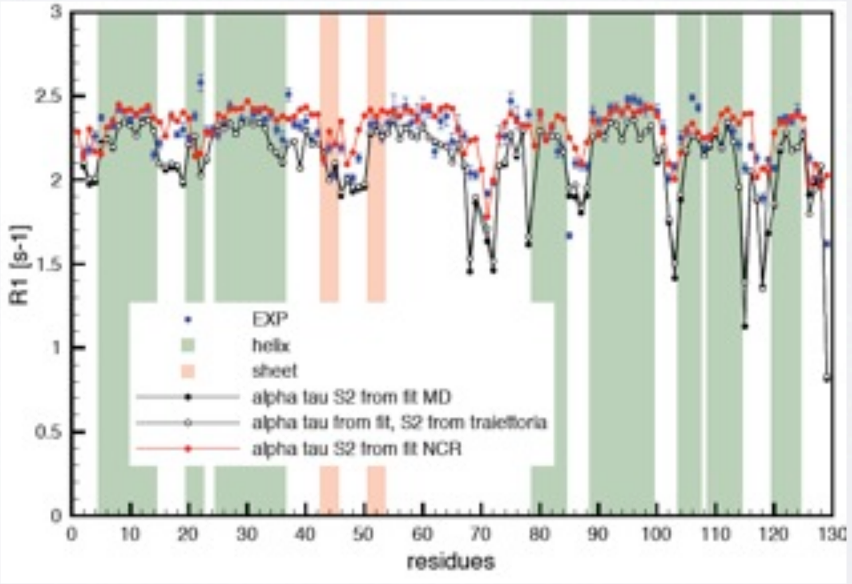
Model pour $c_{ii,I}(t)$:

$$c_{ii,I}(t) = S_{ii}^2 + (1 - S_{ii}^2) E_\alpha(-[t/\tau]^\alpha)$$

Mittag-Leffler function



Prediction of Expérimental data (T1, T2, NOE)



- Calandrini, Abergel, Kneller, *J. Chem. Phys.*, vol. 128, p. 145102, 2008.
- Calandrini, Abergel, Kneller, *J. Chem. Phys.*, vol. 133, p. 145101, 2010.

Limits of fractional Brownian dynamics

The model correlation functions have the experimentally observed power law decay, but they are not analytic and thus unphysical at t=0.

$$\left.\frac{d^n c(t)}{dt^n}\right|_{t=0} = (-1)^n \infty$$

Asymptotic model for Confined anomalous diffusion (α=0)

$$W(t) \overset{t\to\infty}{\sim} 2D_0 L(t), \quad \text{with} \quad D_0 = \langle (\mathbf{x} - \langle \mathbf{x} \rangle)^2 \rangle$$

$$c_{vv}(t) \overset{t\to\infty}{\sim} D_\alpha \alpha(\alpha-1) L(t) t^{\alpha-2},$$

$$\kappa(t) \overset{t\to\infty}{\sim} \frac{\langle \mathbf{v}^2 \rangle}{D_\alpha} \frac{\sin(\pi\alpha)}{\pi\alpha} \frac{1}{L(t)} t^{-\alpha}.$$

α=0 ⇒

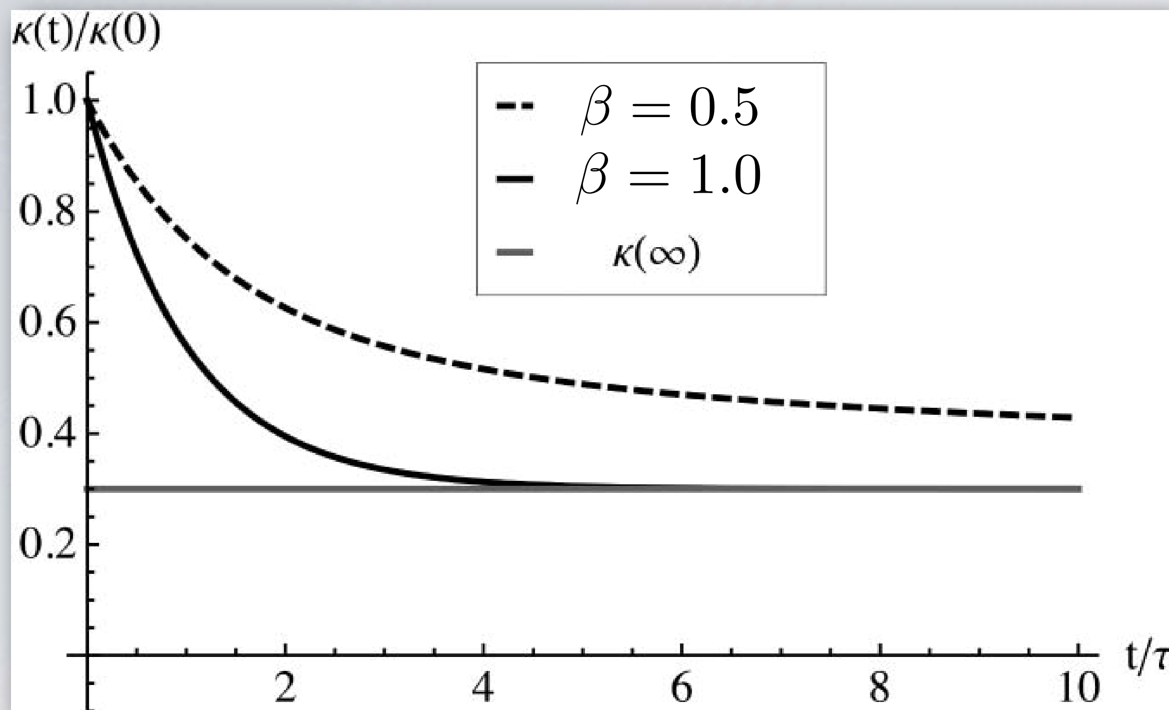
$$c_{vv}(t) \overset{t\to\infty}{\sim} 0,$$

$$\kappa(t) \overset{t\to\infty}{\sim} \frac{\langle \mathbf{v}^2 \rangle}{D_0} \frac{1}{L(t)}$$

No long time tail

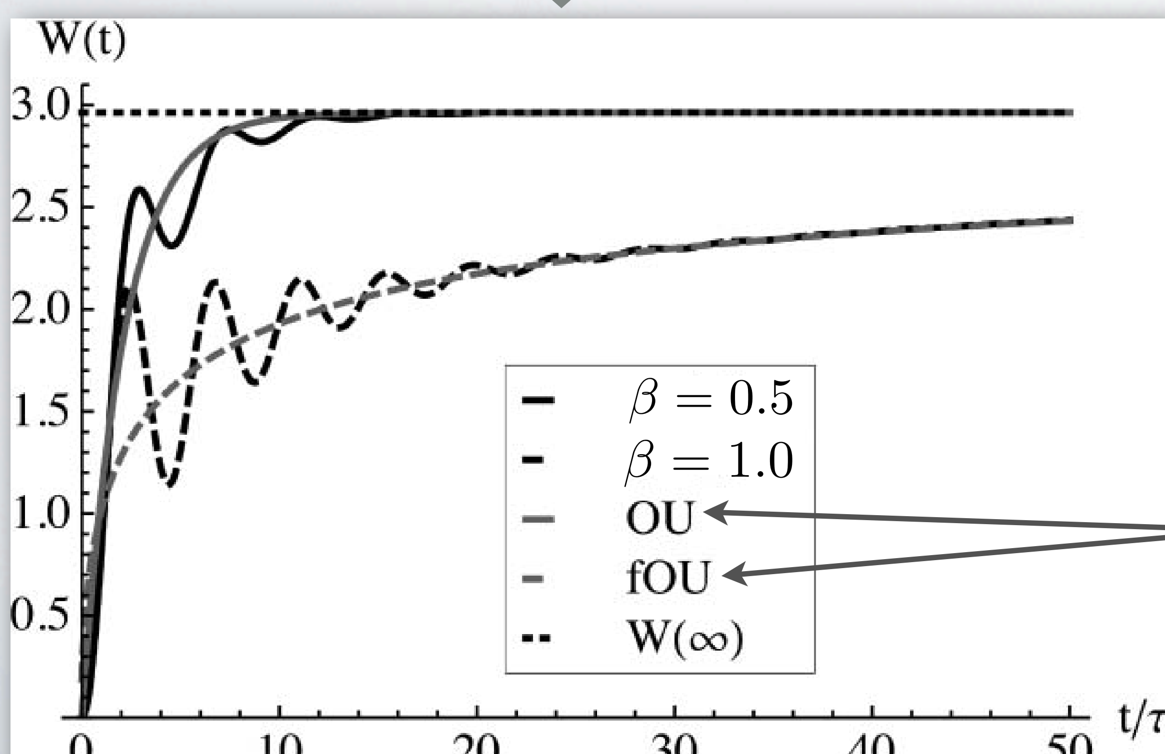
The memory function tends to a plateau value

A memory functio for confined anomalous diffusion



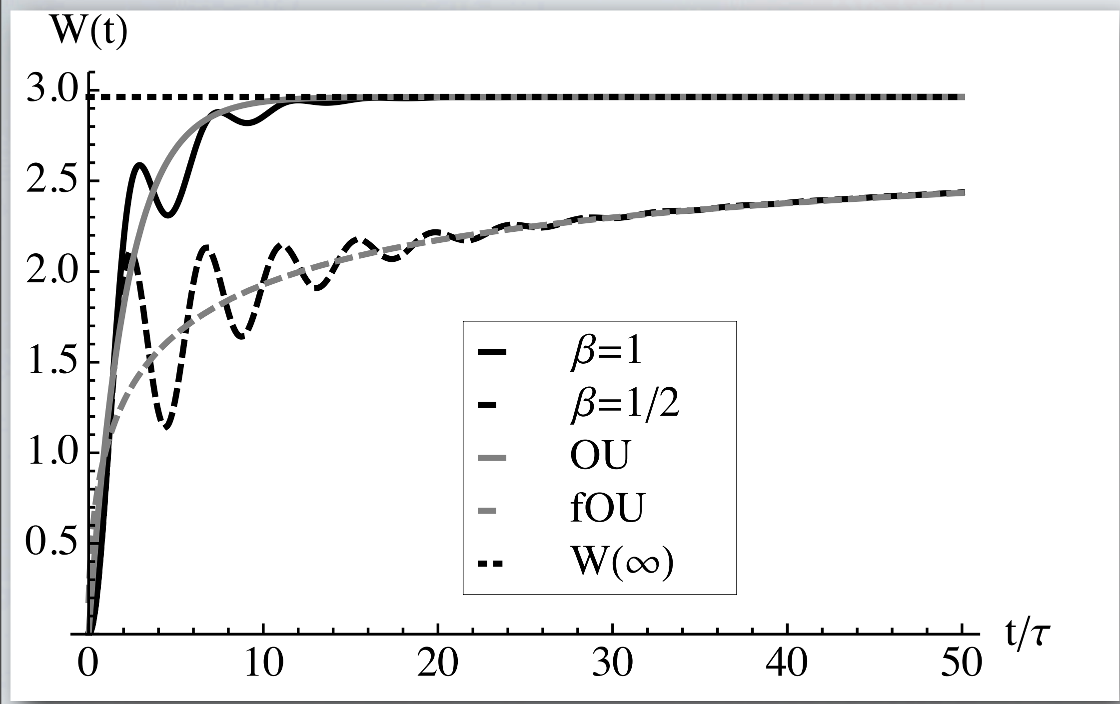
$$\kappa_c(t) = \Omega^2 \{r + (1-r)M(\beta, 1, -t/\tau)\}$$

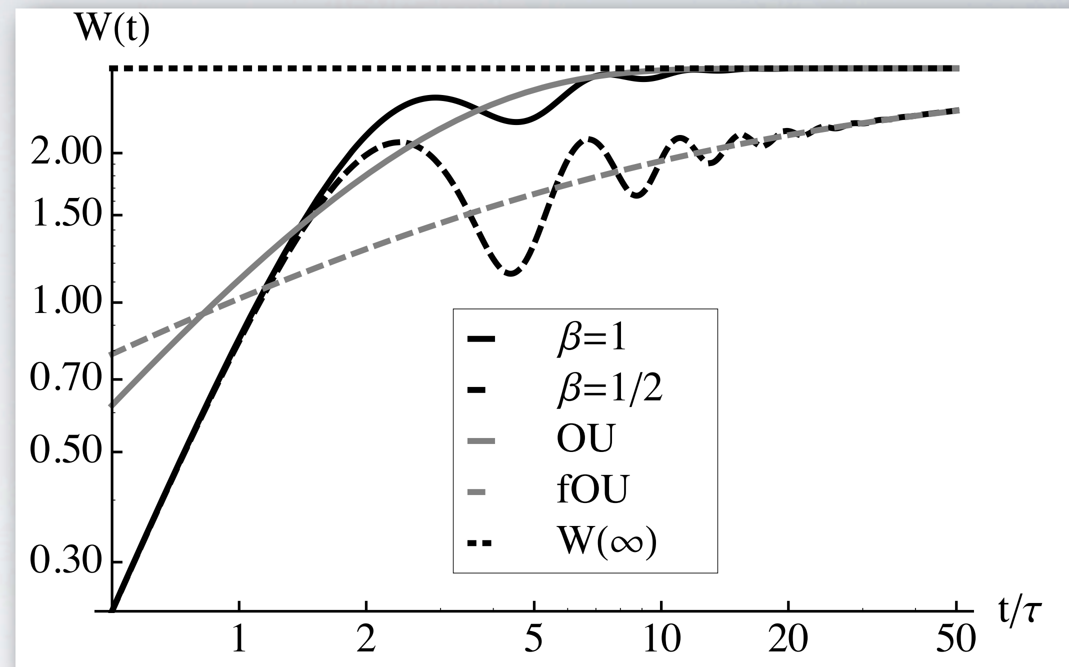
$$\kappa_c(t) - \kappa_c(\infty) \overset{t\to\infty}{\sim} \begin{cases} \Omega^2(1-r)\frac{(t/\tau)^{-\beta}}{\Gamma(1-\beta)}, & 0 < \beta < 1, \\ \Omega^2(1-r)\exp(-t/\tau), & \beta = 1. \end{cases}$$

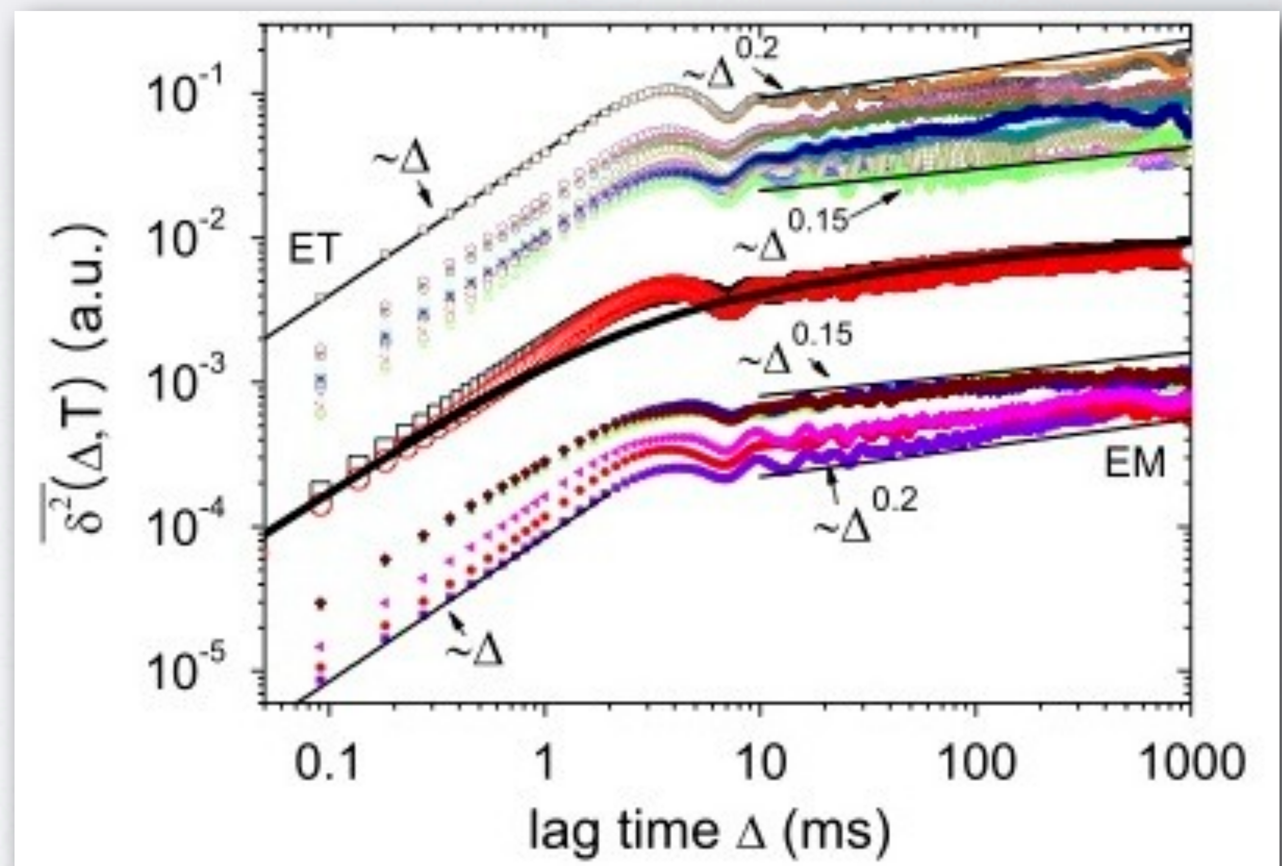


GLE versus fractional brownian motion

$$W_{\mathrm{(f)OU}}(t) = 2\langle \mathbf{u}^2 \rangle (1 - E_b(-[t/t_0]^b)), \quad 0 < b \leq 1.$$







Jeon et al. PRL 106, 048103 (2011)

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Communication: A minimal model for the diffusion-relaxation backbone dynamics of proteins

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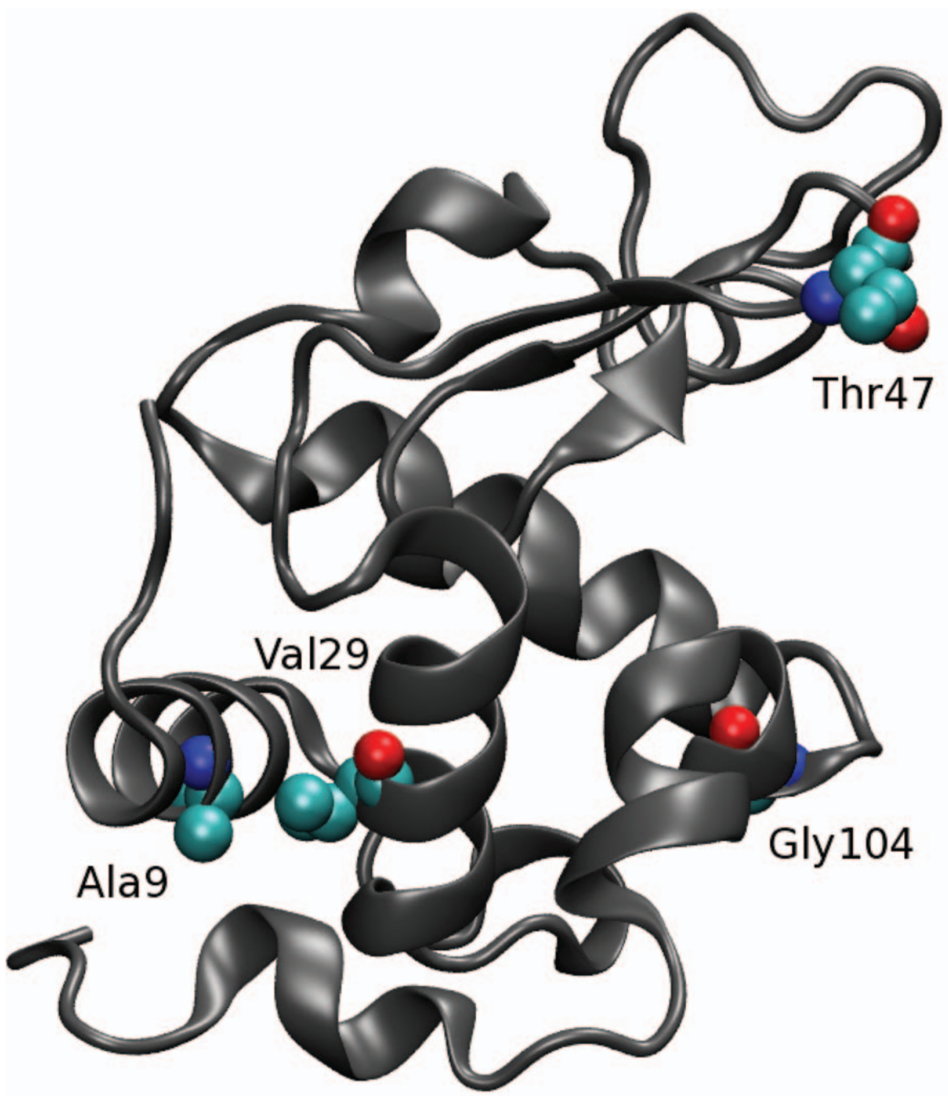


FIG. 1. Four selected residues in the lysozyme molecule.

Position autocorrelation functions

$$\frac{c(t)}{c(0)} \approx \psi(t/\tau;\alpha,\beta).$$

$$\psi(t;\alpha,\beta) = \frac{\exp(-\alpha t)}{(1+t/\beta)^\beta}$$

- Acommodates exponential and power-law decay

$$\lim_{\beta\to\infty} \psi(t;\alpha,\beta) = \exp(-[1+\alpha]t)$$

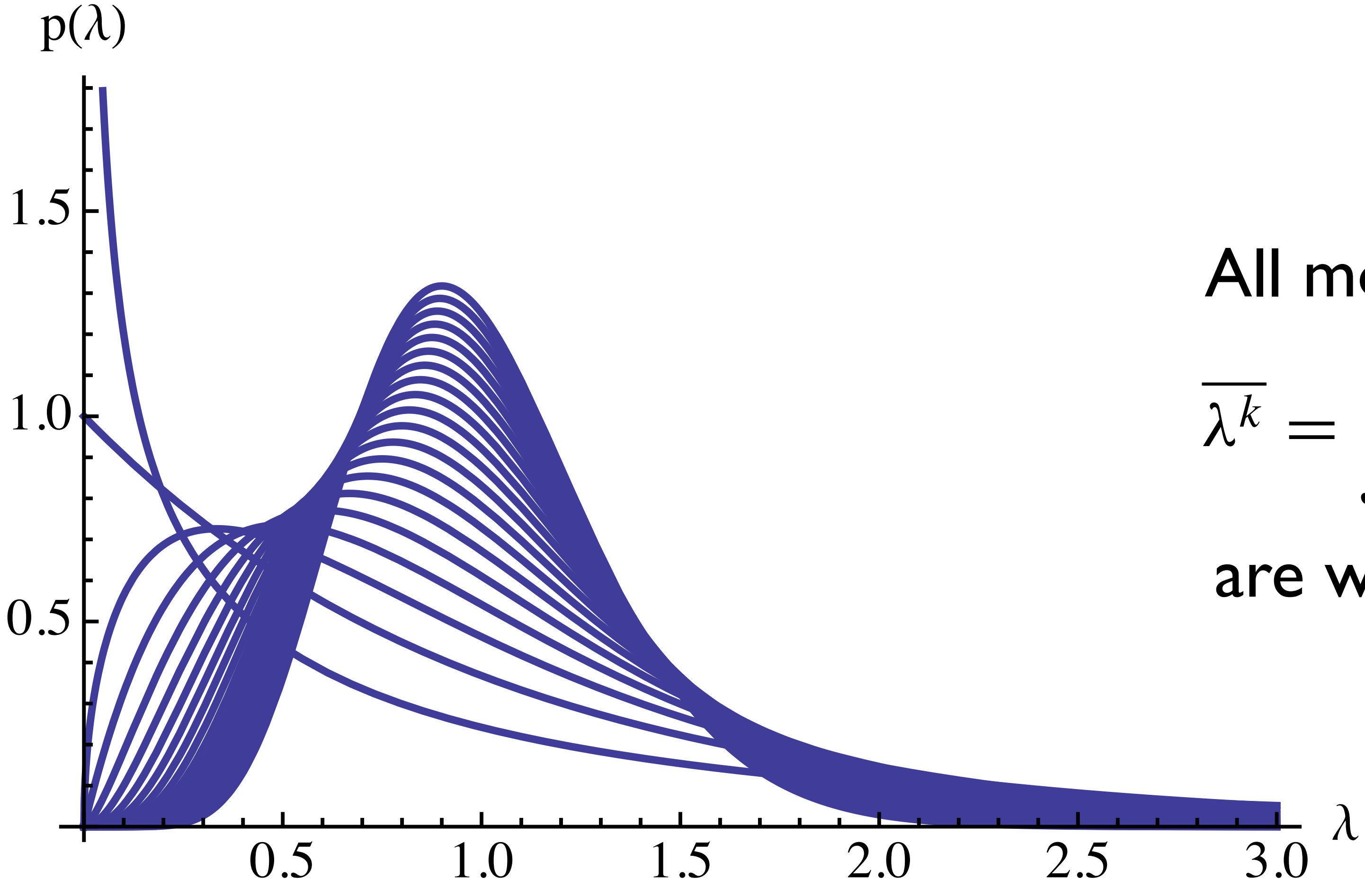
- Is analytical <u>everywhere</u>.

$$\psi(t) = \int_0^\infty d\lambda\, p(\lambda) \exp(-\lambda t),$$

$$p(\lambda;\alpha,\beta) = \theta(\lambda-\alpha)\, p(\lambda-\alpha;\beta)$$

$$p(\lambda;\beta) = \frac{\lambda^{\beta-1}\beta^{\beta}\exp(-\beta\lambda)}{\Gamma(\beta)},$$

$$\psi(t;\alpha,\beta) = \frac{\exp(-\alpha t)}{(1+t/\beta)^{\beta}}.$$

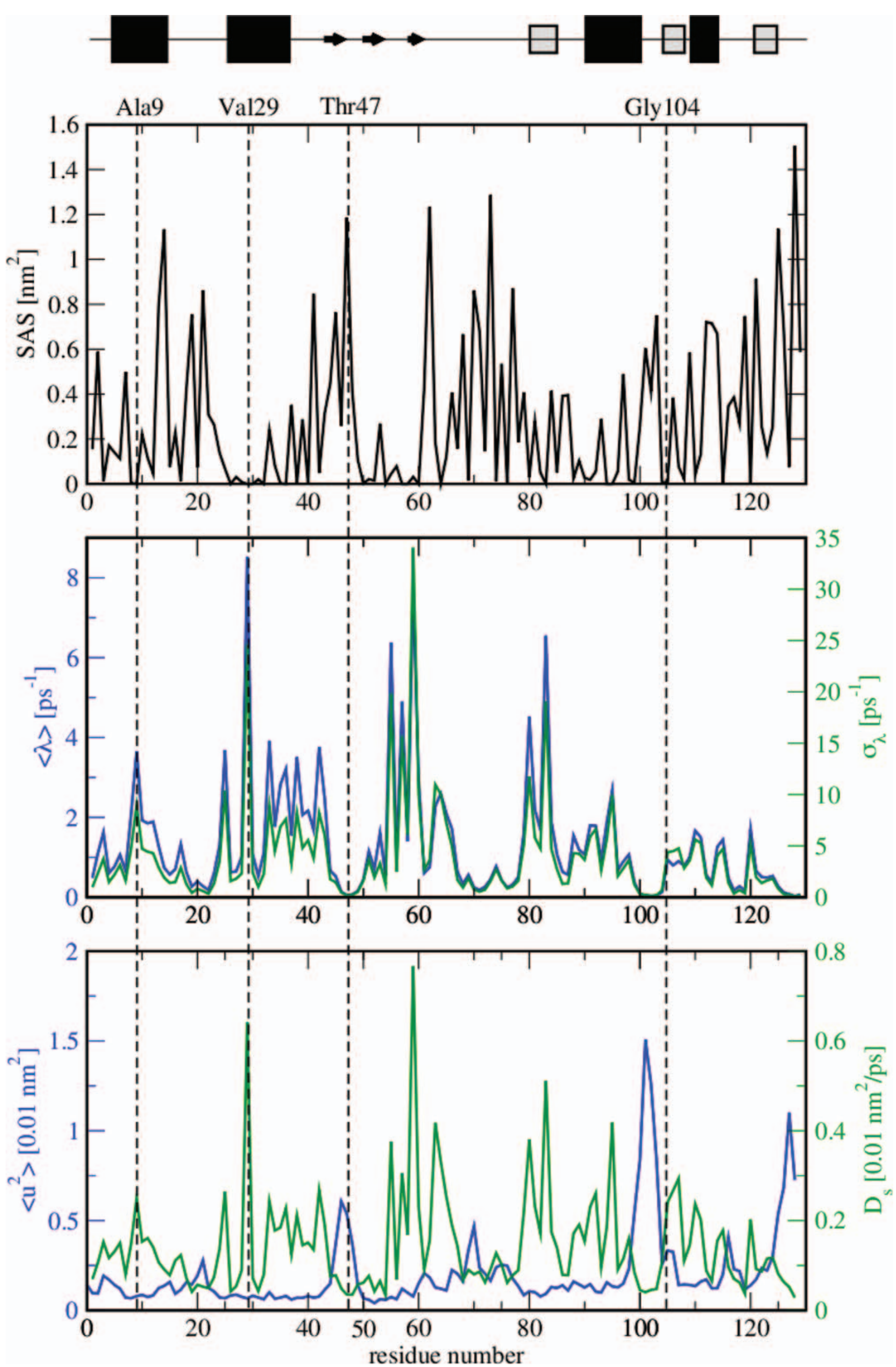


All moments

$$\overline{\lambda^k} = \int_0^\infty d\lambda\, \lambda^k p(\lambda) = (-1)^k \psi^{(k)}(0)$$

are well defined

FIG. 3: Relaxation rate spactrum $p(\lambda;\beta)$ for $\beta = k/2$, with $k = 1, 20$.



Helices (black) and beta-sheets (grey).

Solvent-accessible surfaces.

Mean relaxation rates, $\overline{\lambda}$, and corresponding spreads (green).

Mean square position fluctuations, $\langle \mathbf{u}^2 \rangle$, and short-time diffusion coefficients, D_s (green).

CONCLUSIONS

- The combination of physical models (GLE) and mathematics (asymptotic analysis) yields insight into the origin anomalous diffusion : The decay of the local cage of neighbors represented by a memory function defines the type of diffusion.
- Free and confined diffusion can be handled
- Develop simple models to interpolate between the (known) short time and the long time regime of time correlation functions.

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