Presse Lab

Pressé Lab
@LabPresse

CBP Summer School
Aug 5-16
Lecture 6

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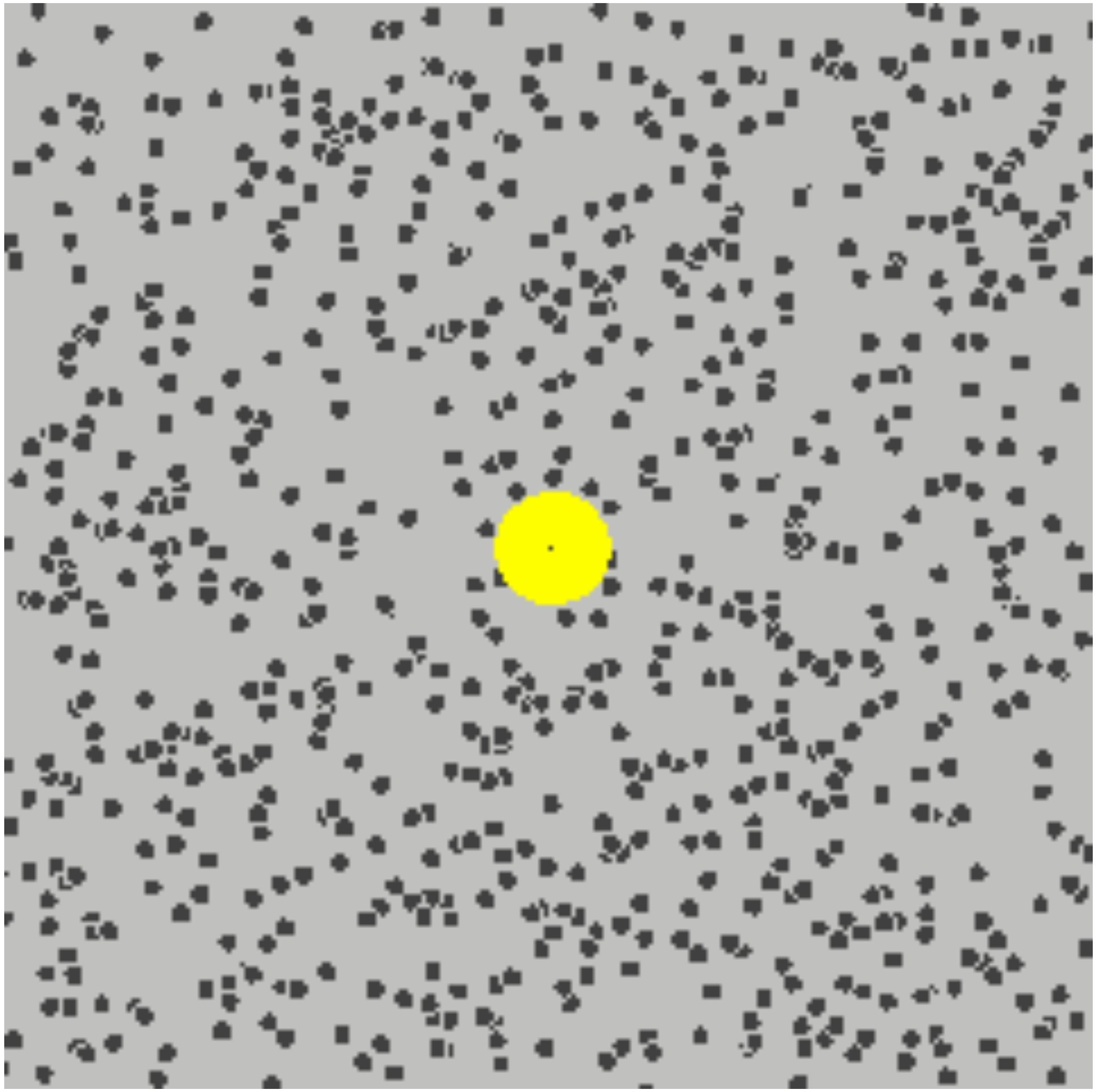
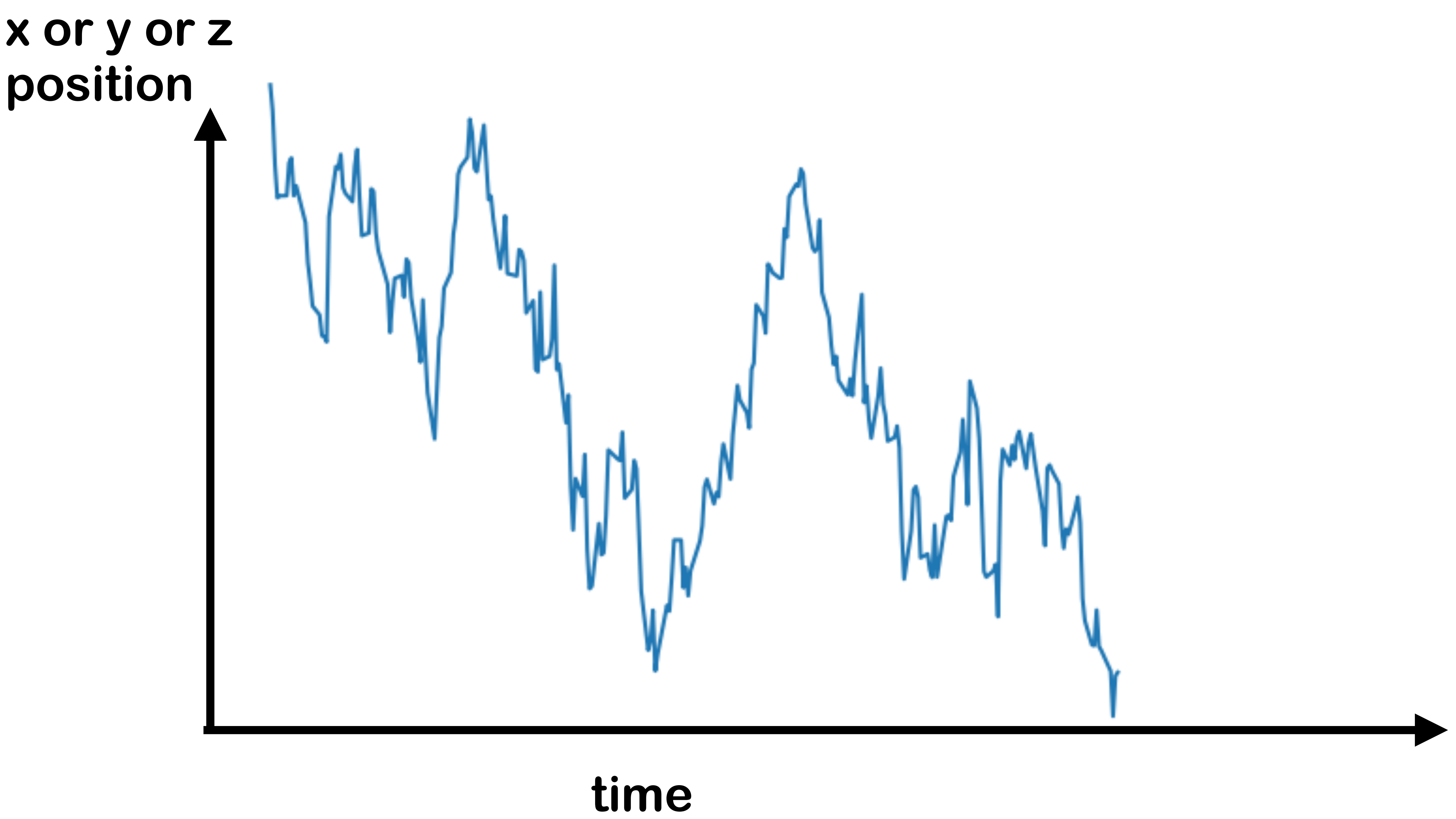
Recall from Lecture 2 & 5….



https://upload.wikimedia.org/wikipedia/commons/c/c2/Brownian_motion_large.gif

The position versus time looks like



What is the “diffusion coefficient”?

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$$D = \frac{k_B T}{6\pi\eta r}$$

Remember from Lecture 2 that energy is conserved: so the energy provided from the kicks on average must be dissipated by friction

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"kicks"

$$\zeta = \frac{k_B T}{D}$$

friction coeff

Langevin equation

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$$v_{\mathrm{new}} \approx v_{\mathrm{old}} + \frac{F(x_{\mathrm{old}})}{m}\Delta t \; - \text{friction term} \; + \text{force kick term}$$

Langevin equation

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"kicks"

$$\zeta = \frac{k_B T}{D}$$

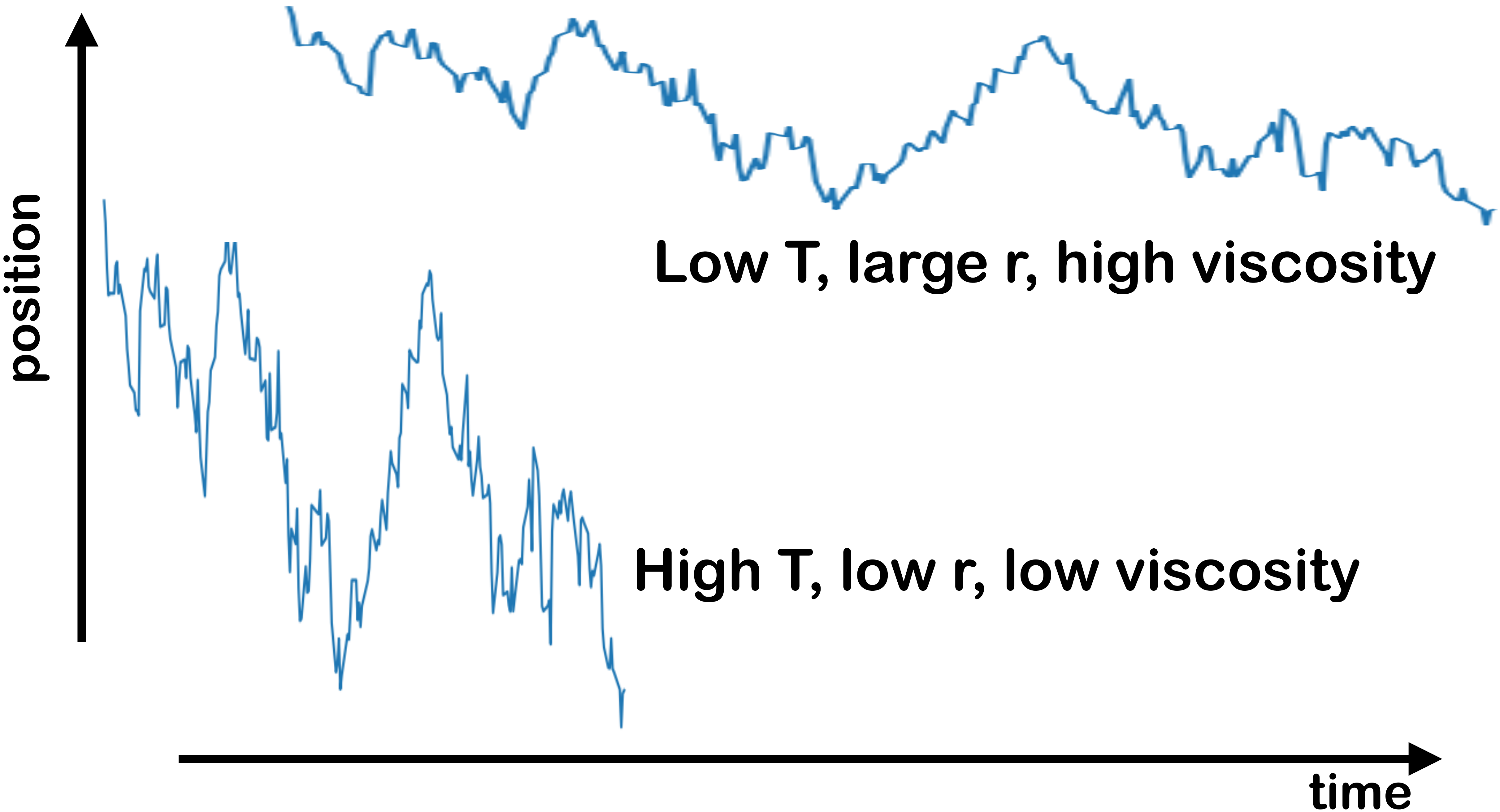
friction coeff

$$v_{\text{new}} \approx v_{\text{old}} + \frac{F(x_{\text{old}})}{m}\Delta t \quad -\frac{\zeta}{m} v_{\text{old}}\Delta t \quad +\sqrt{2D/\Delta t}\xi$$

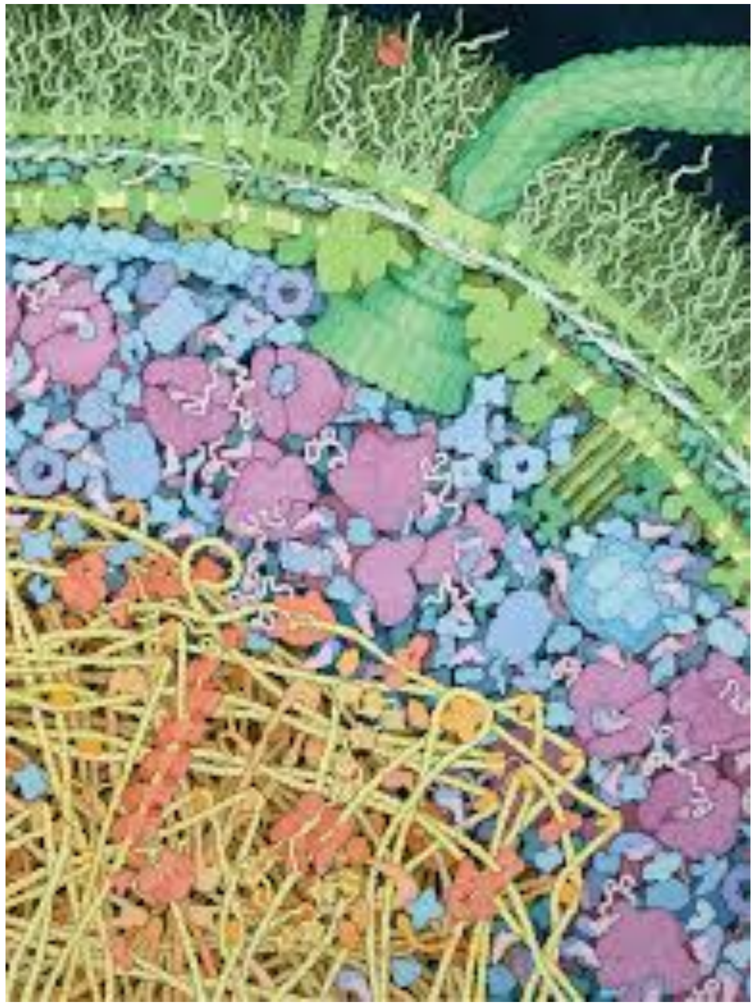
$$\xi \sim \text{Gaussian}$$

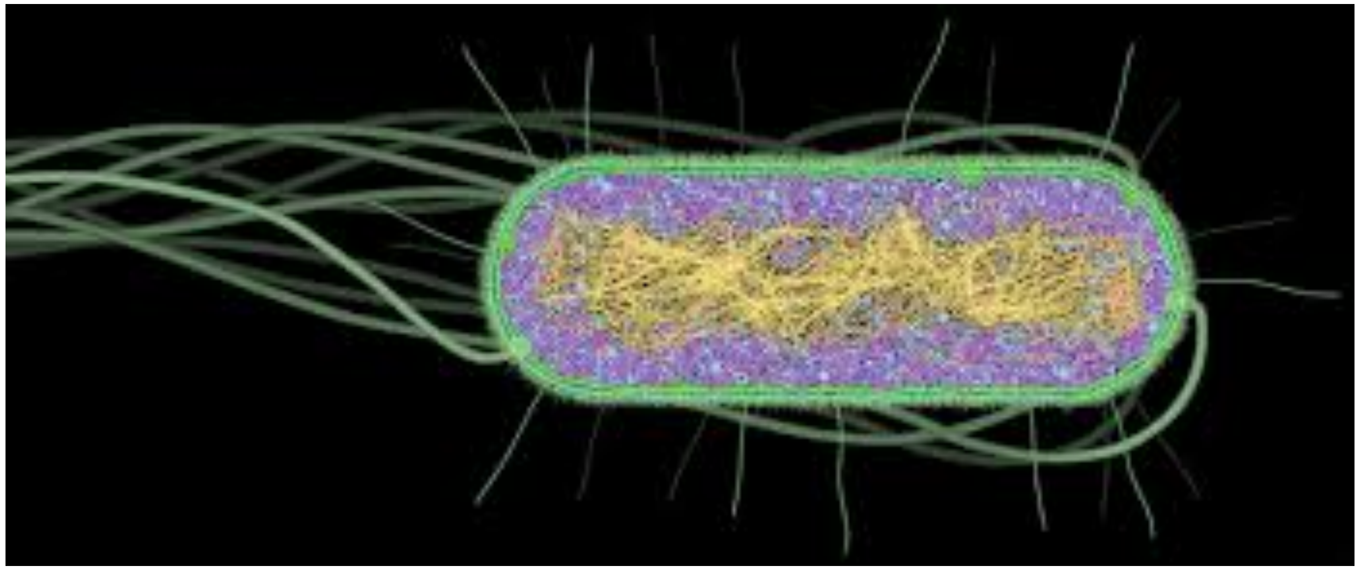
What is the “diffusion coefficient”?

$$D = \frac{k_B T}{6\pi\eta r}$$



What is a typical area spanned by a protein inside a bacterium in 1 second?





David Goodsell

If a protein covers about the area of a cell (1 micron^2) in 1 sec, then how many “body-lengths” is that?

Protein is about 1nm^2. So that’s about an area whose length and width is a thousand times its size. Btw there are about 1 million proteins covering that rough area.

That’s like you covering every corner of the area the size of the ASU campus in 1 second!

Life is very agitated (dare I say violent!) at the protein scale

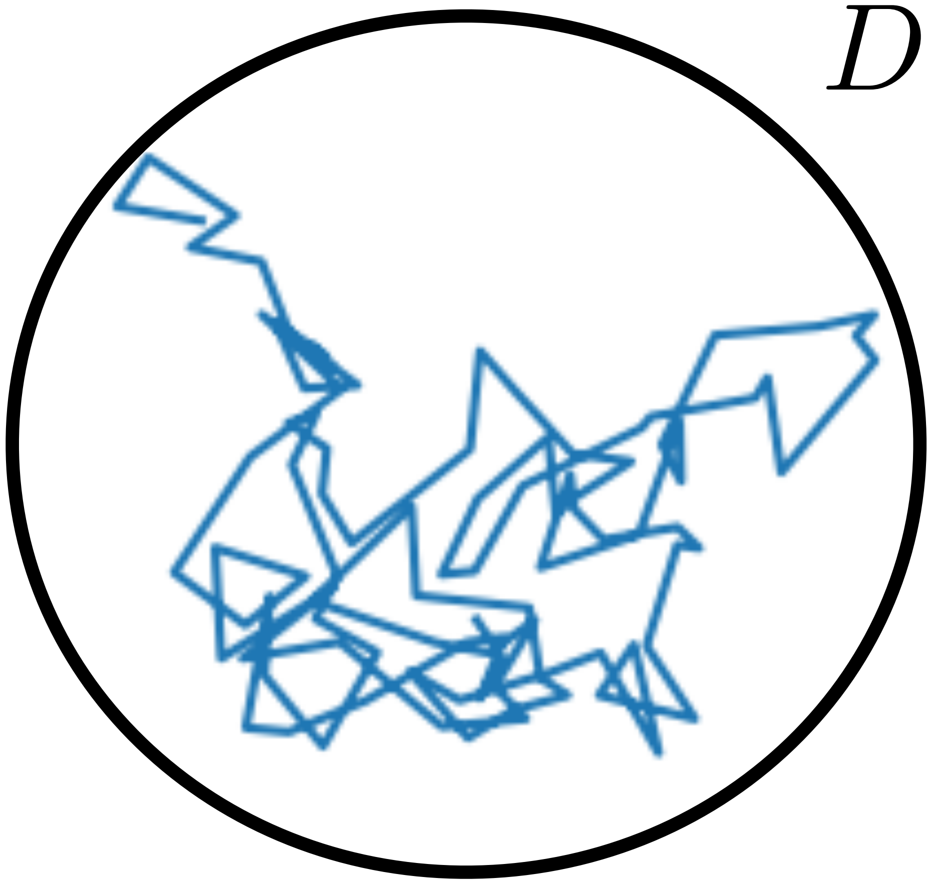
This is equivalent to having 1 million people in the area of the ASU campus and you shaking everyone's hand in 1 second!!

Protein motion, and having proteins interact with all other proteins quickly, is therefore an inherent part of internal cell communication, signaling and function!

$$D = \frac{\text{Area spanned}}{6 \times \text{time elapsed}}$$

$$D = \frac{\langle \mathbf{x}(t)^2 \rangle}{6t}$$

What is the “diffusion coefficient”?



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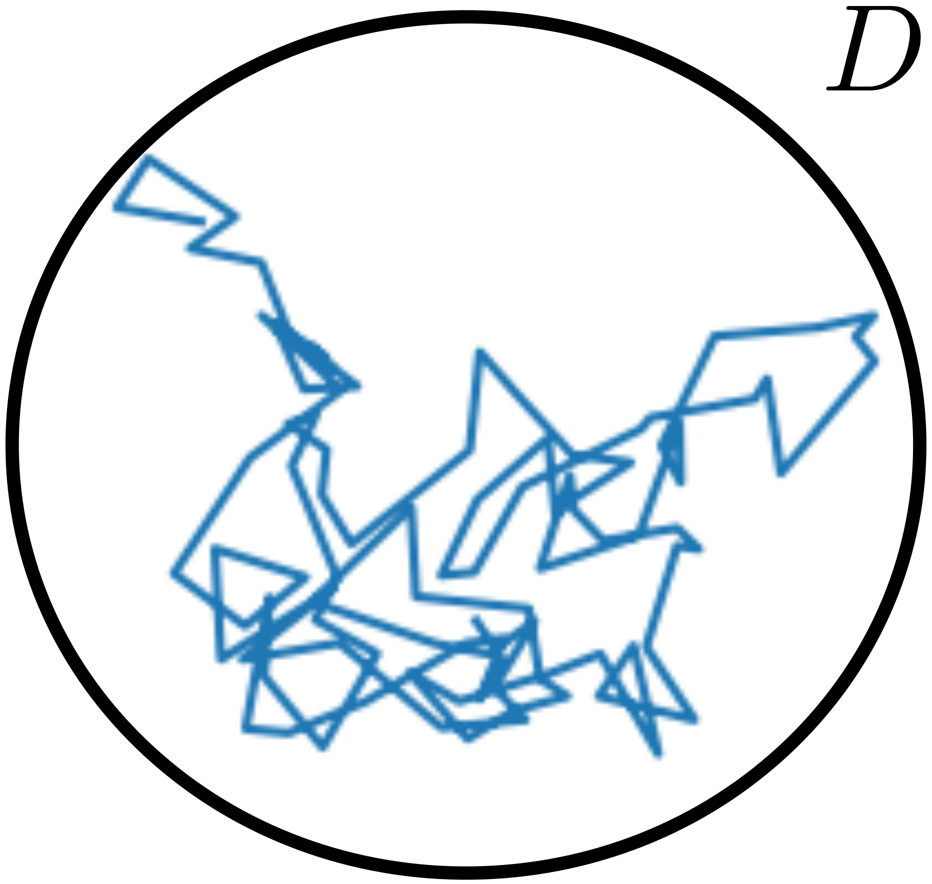

$$D = \frac{\langle \mathbf{x}(t)^2 \rangle}{6t}$$

$6Dt = \langle \mathbf{x}(t)^2 \rangle = \text{mean square displacement}$

Another intuitive way to calculate the diffusion coefficient is from "velocity time correlations"

$$D = \frac{1}{3}\left(\mathbf{v}(0)\cdot\mathbf{v}(0) + \mathbf{v}(\Delta t)\cdot\mathbf{v}(0) + \mathbf{v}(2\Delta t)\cdot\mathbf{v}(0) + \ldots\right)$$

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$$D = \frac{1}{3}\int_0^\infty \langle\mathbf{v}(t)\cdot\mathbf{v}(0)\rangle\, dt$$

Another intuitive way to calculate the diffusion coefficient is from “velocity time correlations”

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

This tells me how particle velocities are aligned on average from 0 to t.

When my D is greater, the velocities are aligned longer.

So the average alignment is larger for longer.

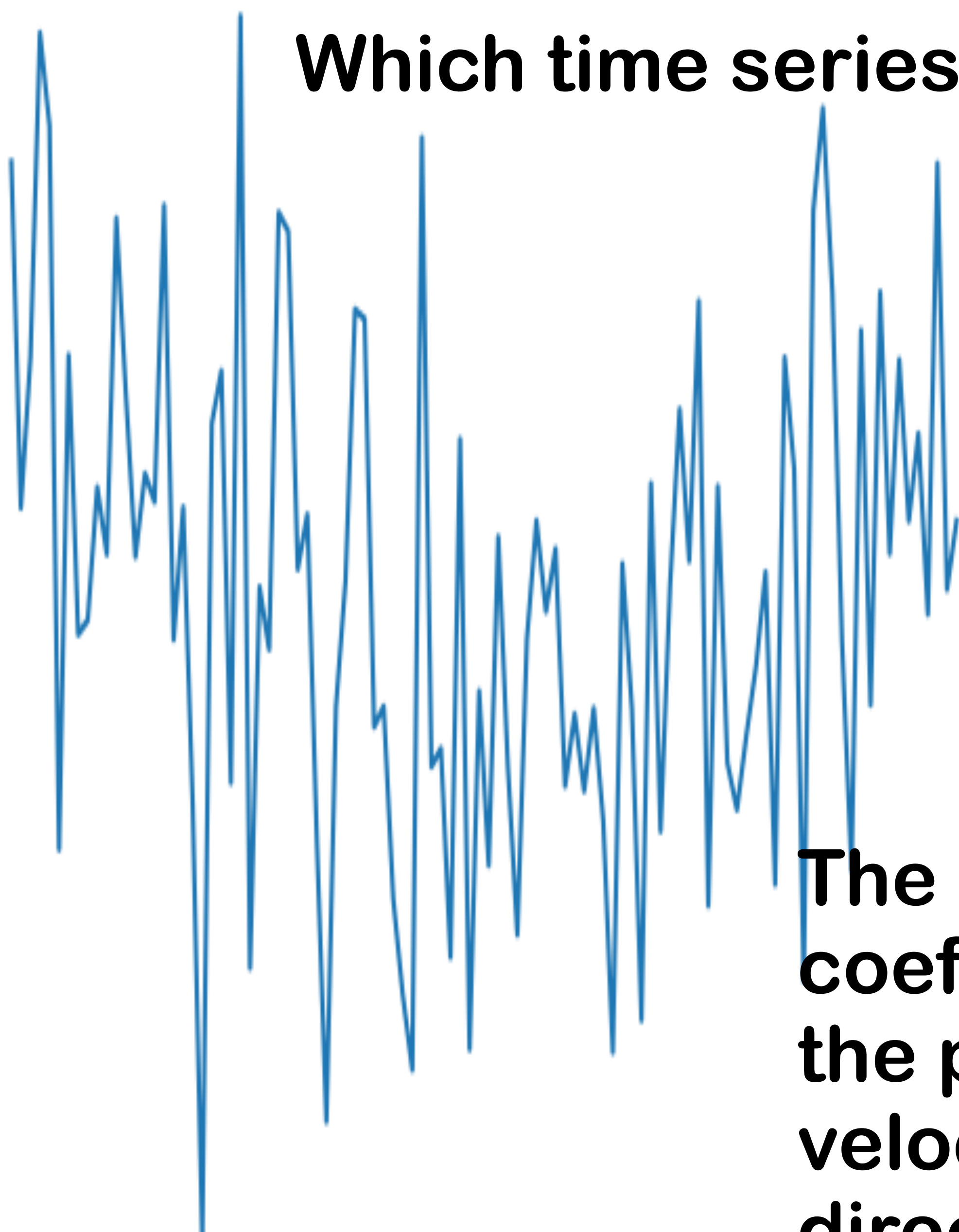
Another intuitive way to calculate the diffusion coefficient is from "velocity time correlations"

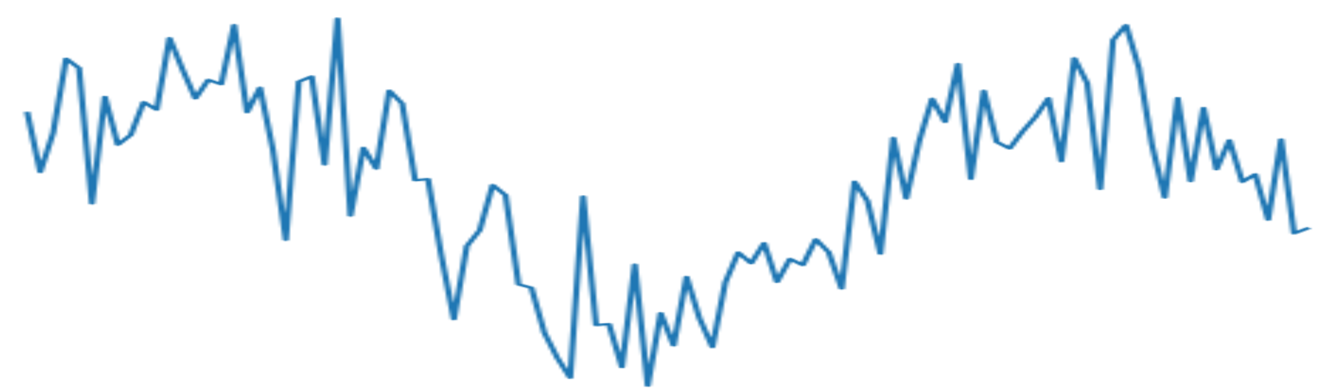
$$D = \frac{1}{3}\int_0^\infty \langle \mathbf{v}(t) \cdot \mathbf{v}(0) \rangle \, dt$$

If the average alignment is bigger for longer, then the time integral over the correlation is larger.

Where does this equation mean and where does it come from?

Which time series has more “correlated” velocity?





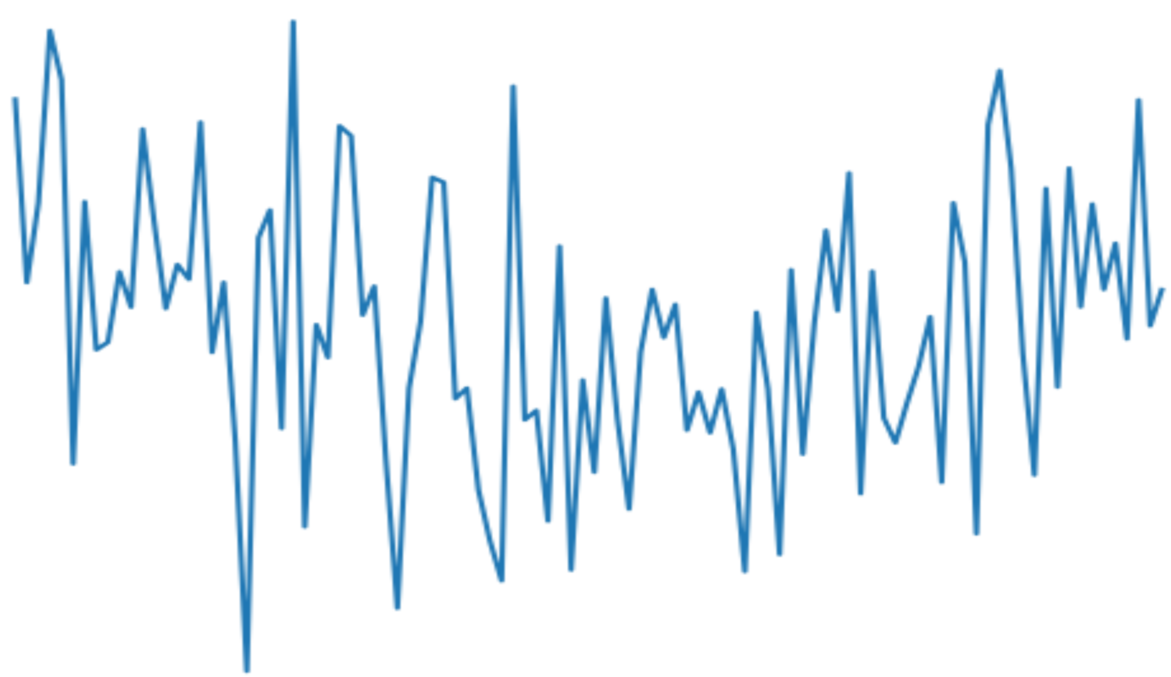
The larger the diffusion coefficient, the longer the particle retains its velocity in the same direction.

Thought-provoking question:

How is the diffusion coefficient related to the following?

$$\int \langle \mathbf{x}(t) \cdot \mathbf{x}(0) \rangle dt$$

Try to get a hint from looking at picture below



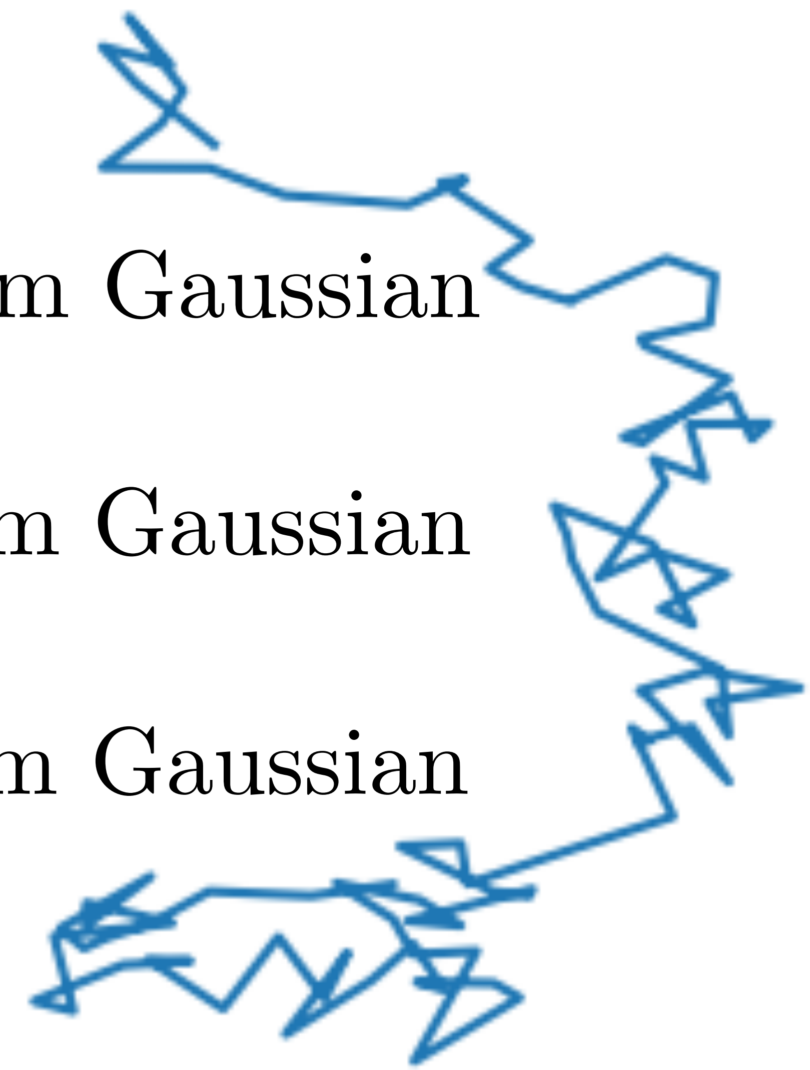
A Langevin equation is a type of random walk

A random walk is another name for this equation:

$$x_{\text{new}} = x_{\text{old}} + \text{random term draw from Gaussian}$$

$$y_{\text{new}} = y_{\text{old}} + \text{random term draw from Gaussian}$$

$$z_{\text{new}} = z_{\text{old}} + \text{random term draw from Gaussian}$$



The big difference between the Langevin equation and the equations below is that, in the Langevin equation we saw earlier, the velocities had a random term drawn from a Gaussian. Here we assume that the position is the quantity that has a random term drawn from a Gaussian. This is another type of Langevin equation.

$$x_{\mathrm{new}} = x_{\mathrm{old}} + \text{random term draw from Gaussian}$$

$$y_{\mathrm{new}} = y_{\mathrm{old}} + \text{random term draw from Gaussian}$$

$$z_{\mathrm{new}} = z_{\mathrm{old}} + \text{random term draw from Gaussian}$$

Deep physics and the difference in timescale at which it takes water as compared to the protein to diffuse an area about its own size allows us to replace the more exact Langevin equations we previously wrote with the more approximate Langevin equations below.

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$$z_{\text{new}} = z_{\text{old}} + \text{random term draw from Gaussian}$$

In a random walk, the new position is centered on the old position

Many things are well modeled as random walks:

- Positions of a protein in solution
- Stock price
- End-to-end distance of a polymer (a string molecule)
- Insect motion