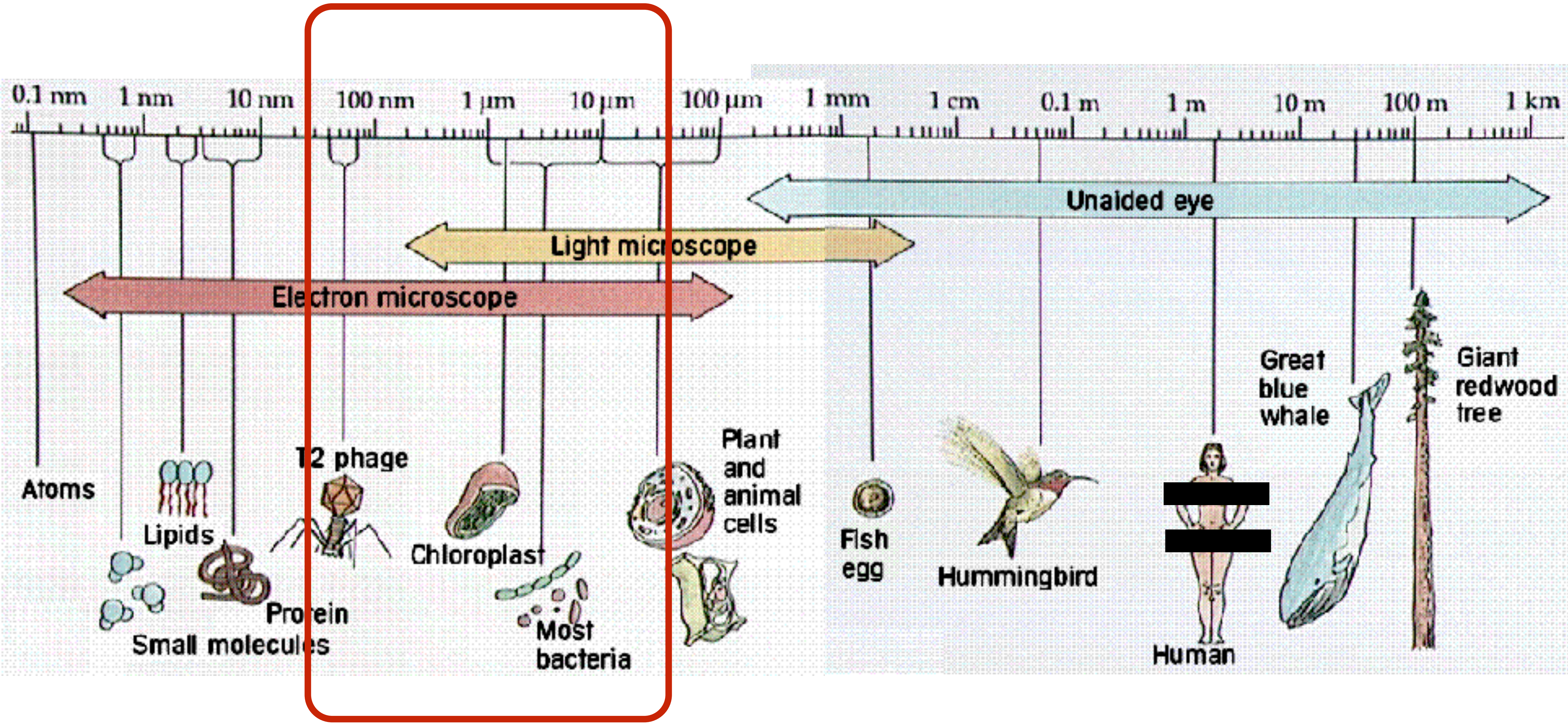
Brownian motion

18.S995 - L03 & 04

Typical length scales



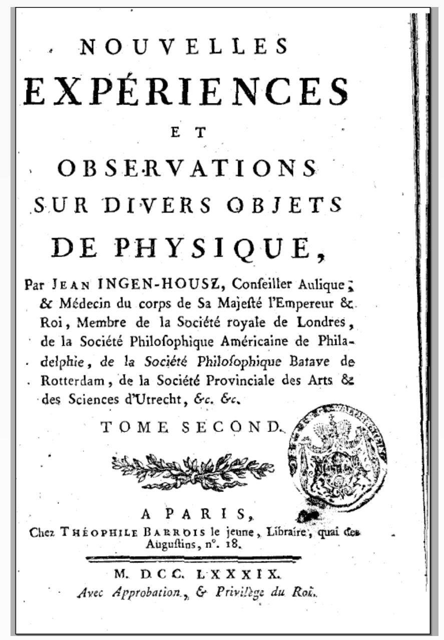
http://www2.estrellamountain.edu/faculty/farabee/BIOBK/biobookcell2.html

dunkel@math.mit.edu

Brownian motion

“Brownian” motion

Jan Ingen-Housz (1730-1799)



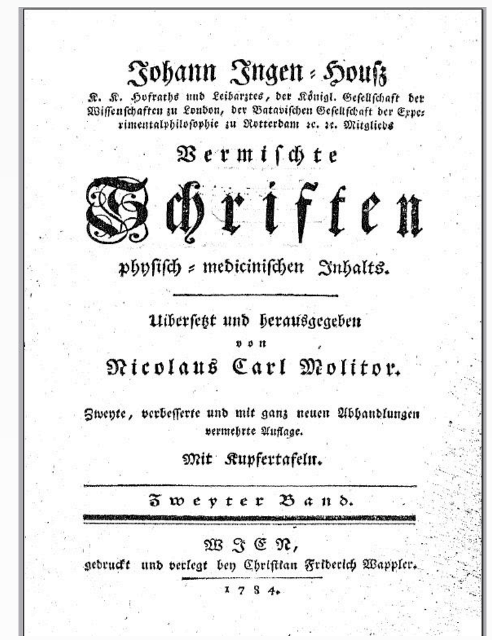
NOUVELLES
EXPÉRIENCES
ET
OBSERVATIONS
SUR DIVERS OBJETS
DE PHYSIQUE,

Par JEAN INGEN-HOUSZ, Conseiller Aulique, & Médecin du corps de Sa Majesté l'Empereur & Roi, Membre de la Société royale de Londres, de la Société Philosophique Américaine de Philadelphie, de la *Société Philosophique* Batave de Rotterdam, de la Société Provinciale des Arts & des Sciences d'Utrecht, *&c. &c.*

TOME SECOND.

A PARIS,
Chez THÉOPHILE BARROIS le jeune, Libraire, quai des Augustins, n°. 18.

M. DCC. LXXXIX.
Avec Approbation, & Privilège du Roi.



Johann Ingen-Housz
K. K. Hofraths und Leibarztes, der Königl. Gesellschaft der Wissenschaften zu London, der Batavischen Gesellschaft der Experimentalphilosophie zu Rotterdam rc. rc. Mitglieds

Vermischte
Schriften
physisch-medicinischen Inhalts.

Uibersetzt und herausgegeben
von
Nicolaus Carl Molitor.

Zweyte, verbesserte und mit ganz neuen Abhandlungen vermehrte Auflage.

Mit Kupfertafeln.

Zweyter Band.

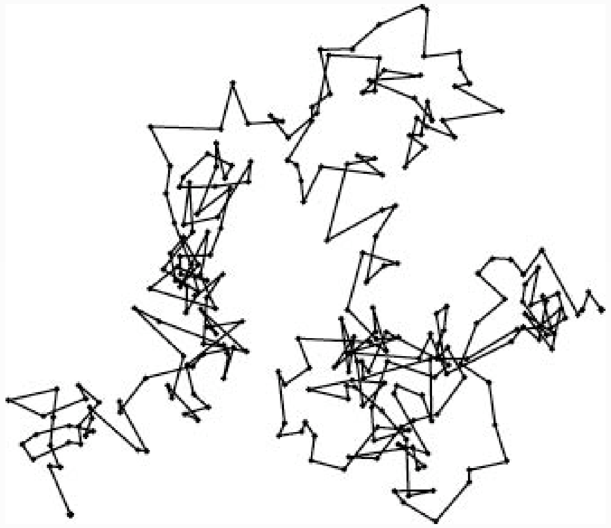
WIEN,
gedruckt und verlegt bey Christian Friderich Wappler.
1784.

1784/1785:

über betrügen könnte, darf man nur in den Brennpunct eines Mikroskops einen Tropfen Weingeist sammt etwas gestoßener Kohle setzen; man wird diese Körperchen in einer verwirrten beständigen und heftigen Bewegung erblicken, als wenn es Thierchen wären, die sich reissend unter einander fortbewegen.

http://www.physik.uni-augsburg.de/theo1/hanggi/History/BM-History.html

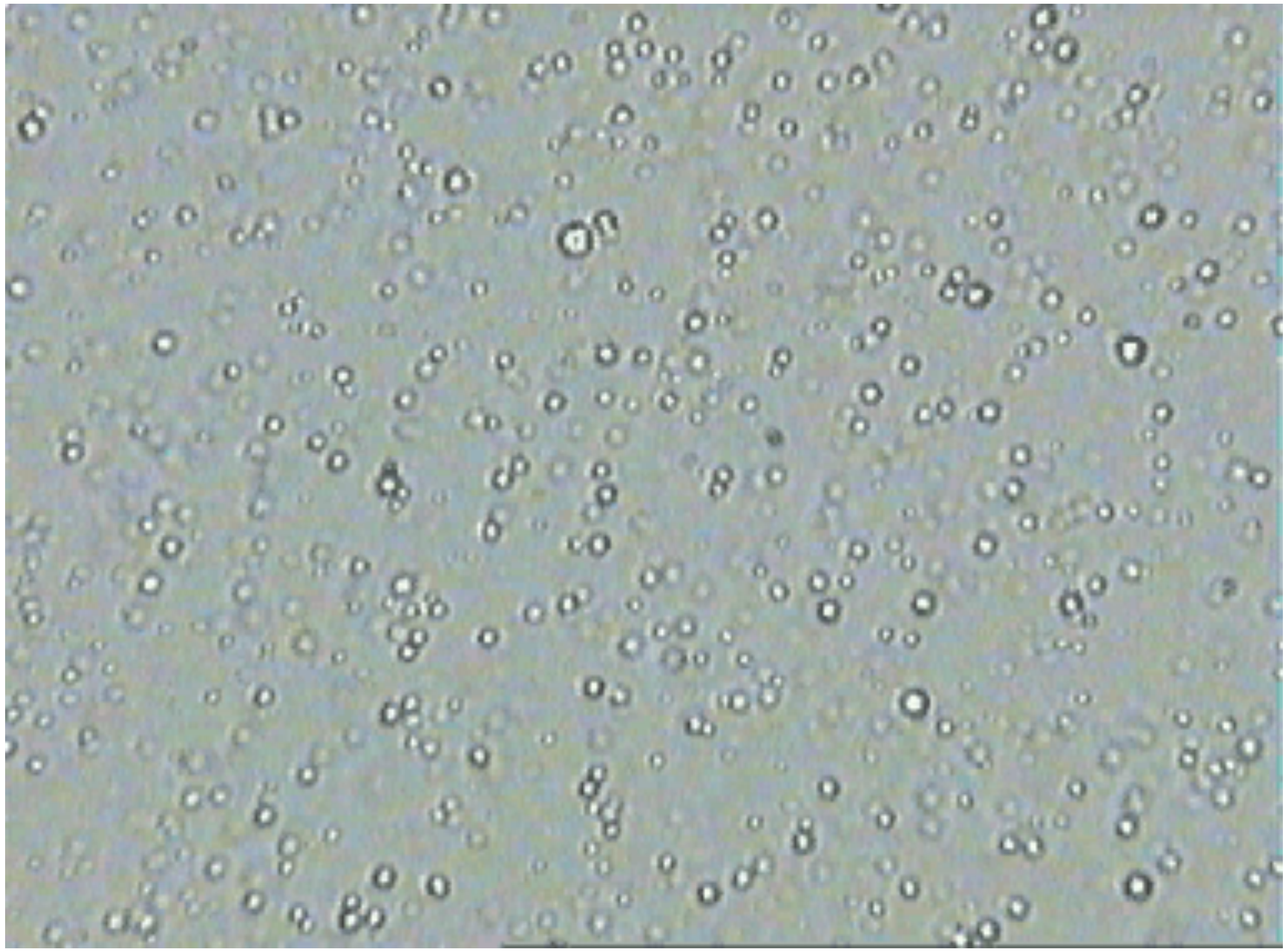
Robert Brown (1773-1858)



Linnean society, London

1827: irregular motion of pollen in fluid

http://www.brianjford.com/wbbrownc.htm



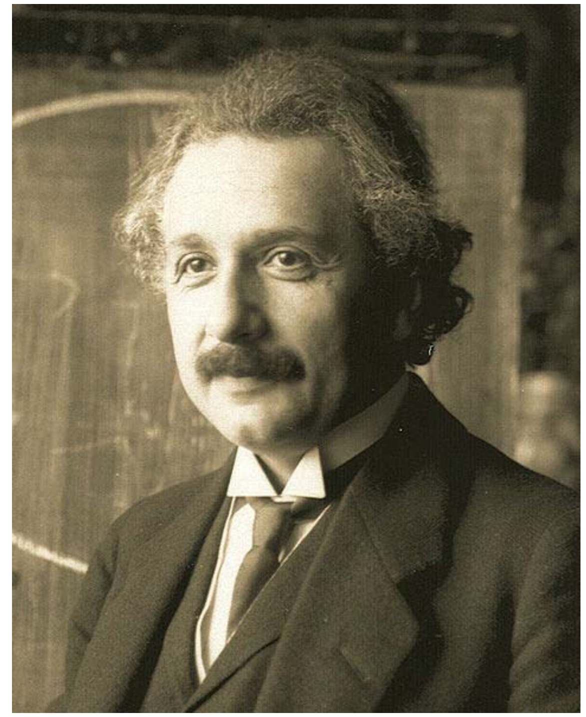
W. Sutherland (1858-1911)

Source: www.theage.com.au

$$D = \frac{RT}{6\pi\eta a C}$$

Phil. Mag. **9**, 781 (1905)

A. Einstein (1879-1955)



Source: wikipedia.org

$$\langle x^2(t) \rangle = 2Dt$$

$$D = \frac{RT}{N}\frac{1}{6\pi k P}$$

Ann. Phys. **17**, 549 (1905)

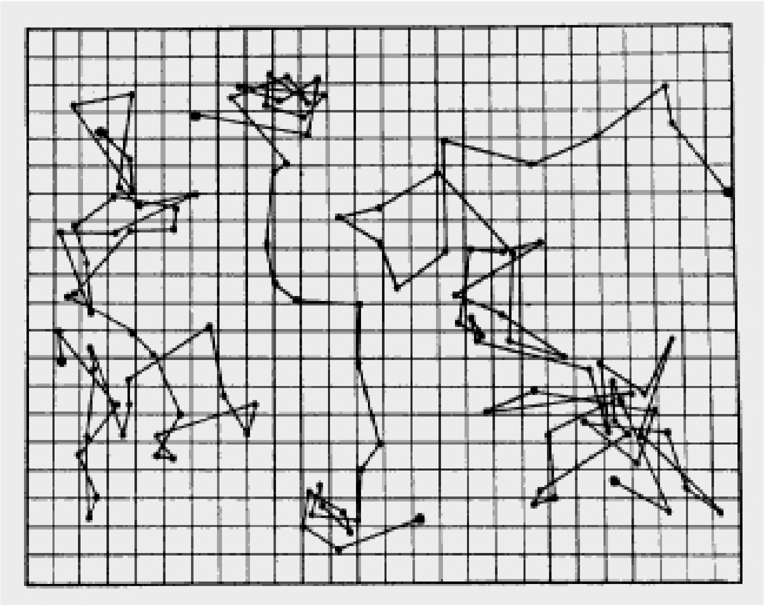
M. Smoluchowski (1872-1917)

Source: wikipedia.org

$$D = \frac{32}{243}\frac{mc^2}{\pi\mu R}$$

Ann. Phys. **21**, 756 (1906)

Jean Baptiste Perrin (1870-1942, Nobel prize 1926)



Mouvement brownien et réalité moléculaire, Annales de chimie et de physique VIII 18, 5-114 (1909)

- colloidal particles of radius 0.53μm
- successive positions every 30 seconds joined by straight line segments
- mesh size is 3.2μm

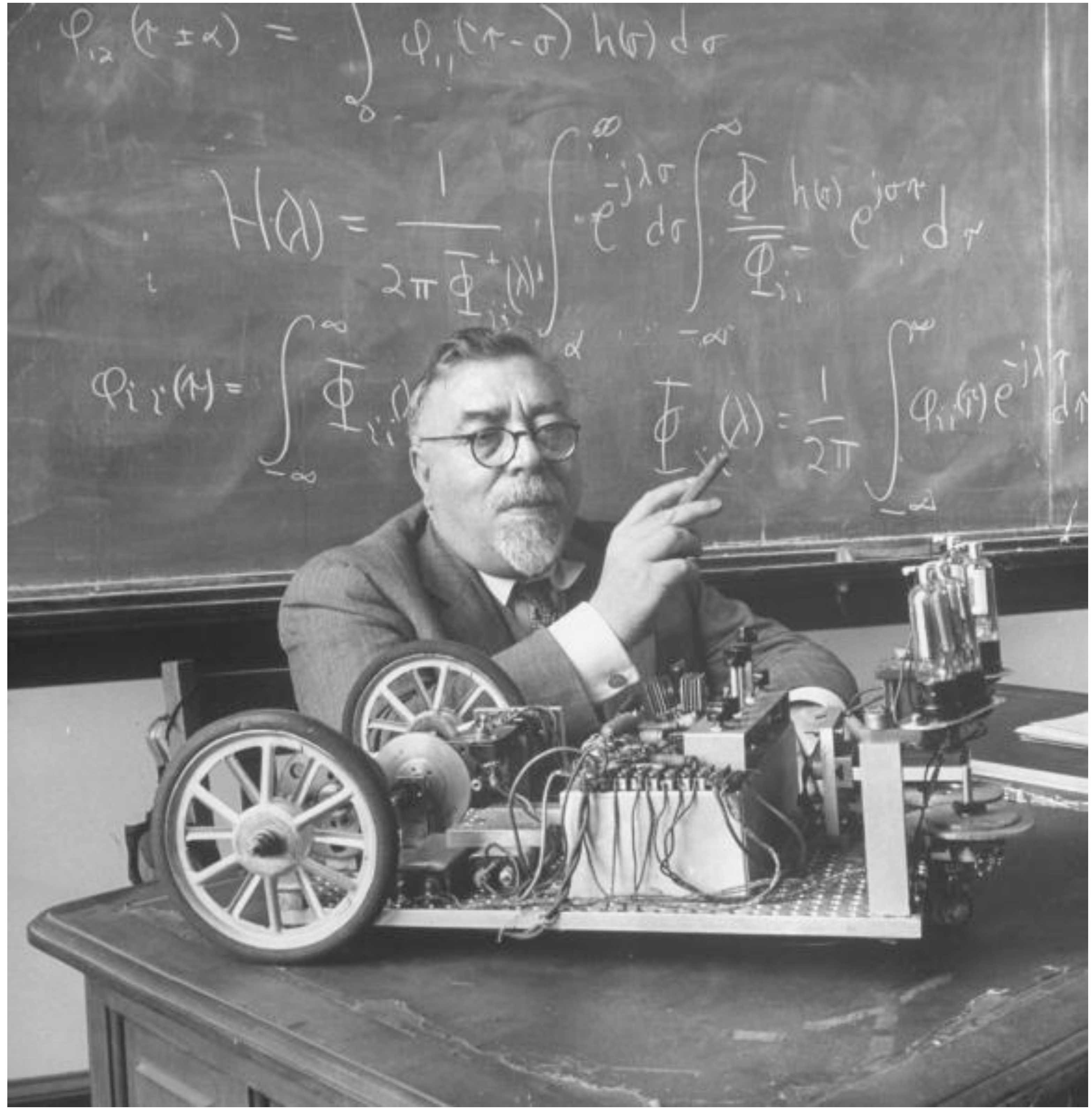
Les Atomes, Paris, Alcan (1913)

experimental evidence for
atomistic structure of matter

Norbert Wiener

(1894-1864)

MIT



Relevance in biology

- intracellular transport
- intercellular transport
- microorganisms must beat BM to achieve directed locomotion
- tracer diffusion = important experimental "tool"
- generalized BMs (polymers, membranes, etc.)

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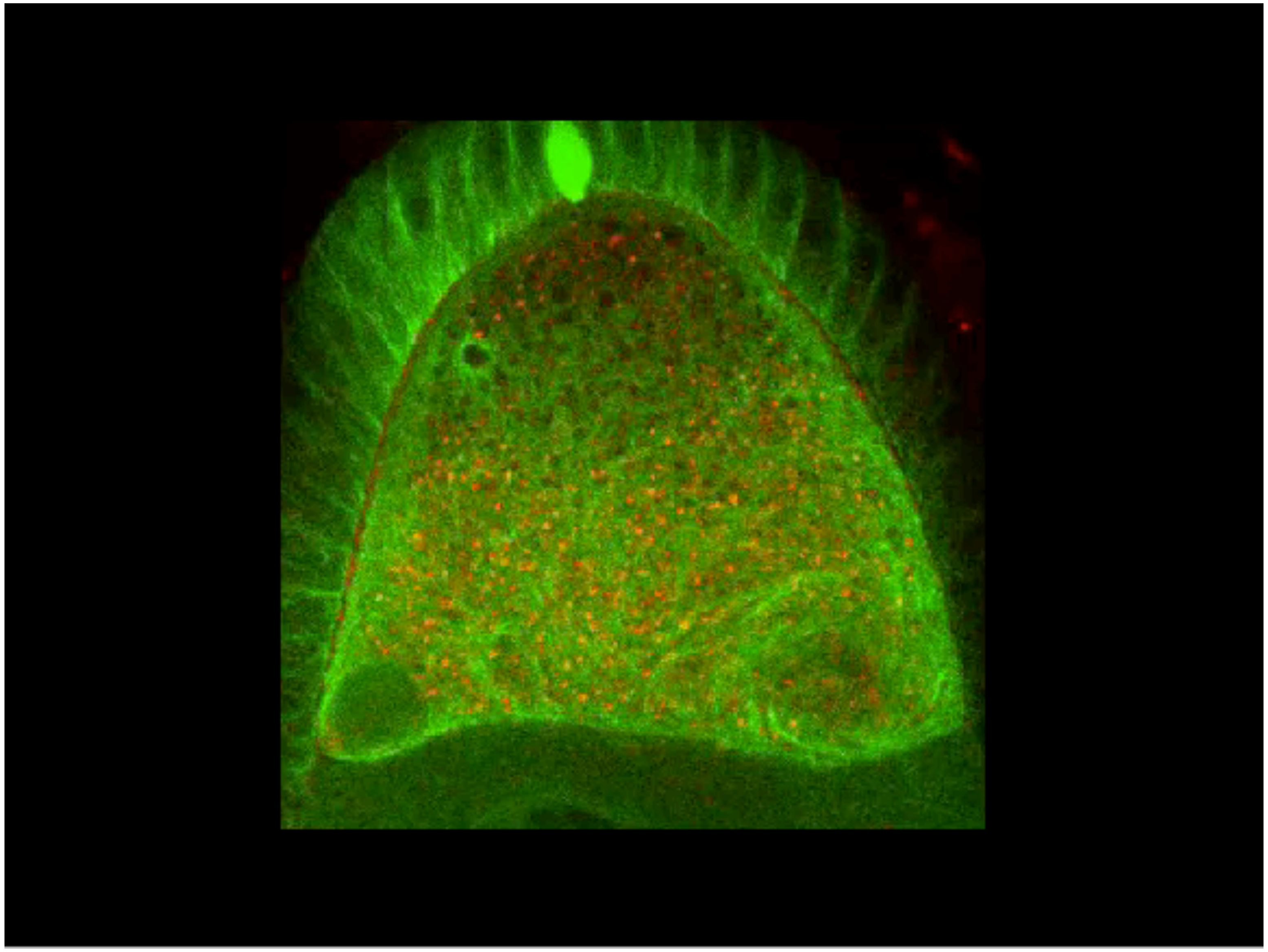
Polymers & filaments (D=1)



Drosophila oocyte

Physical parameters (e.g. bending rigidity) from fluctuation analysis

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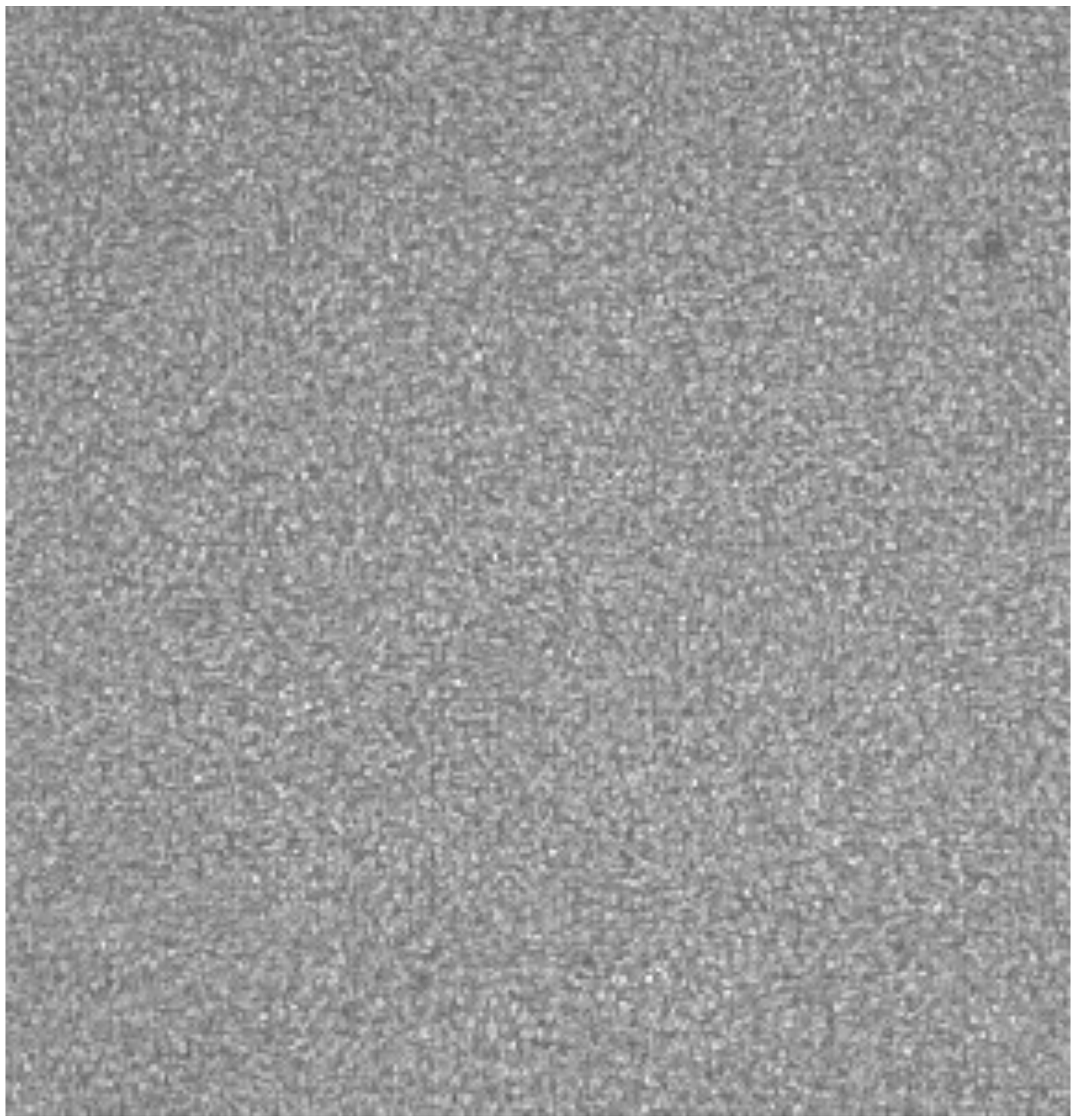
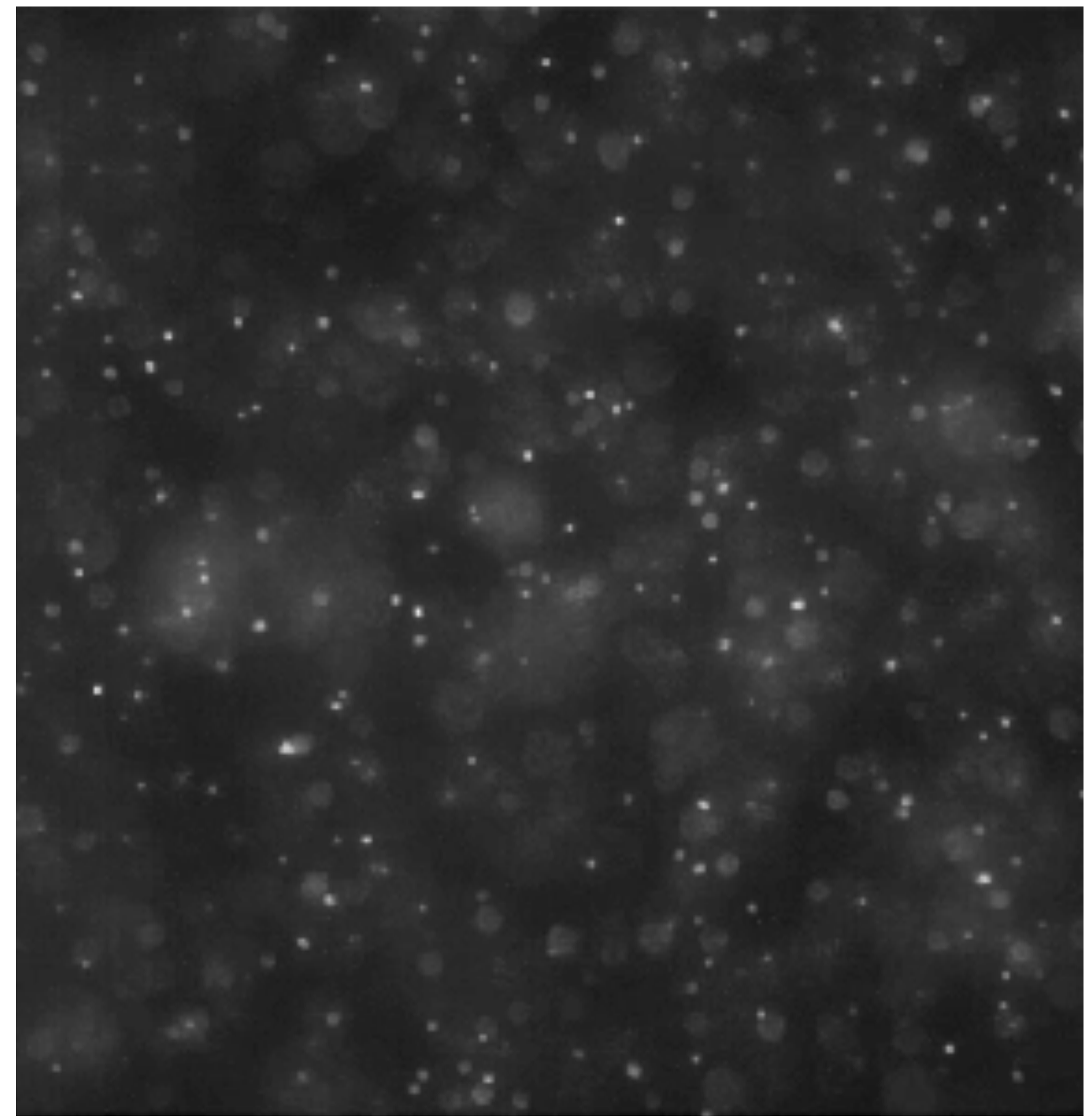
Brownian tracer particles in a bacterial suspension

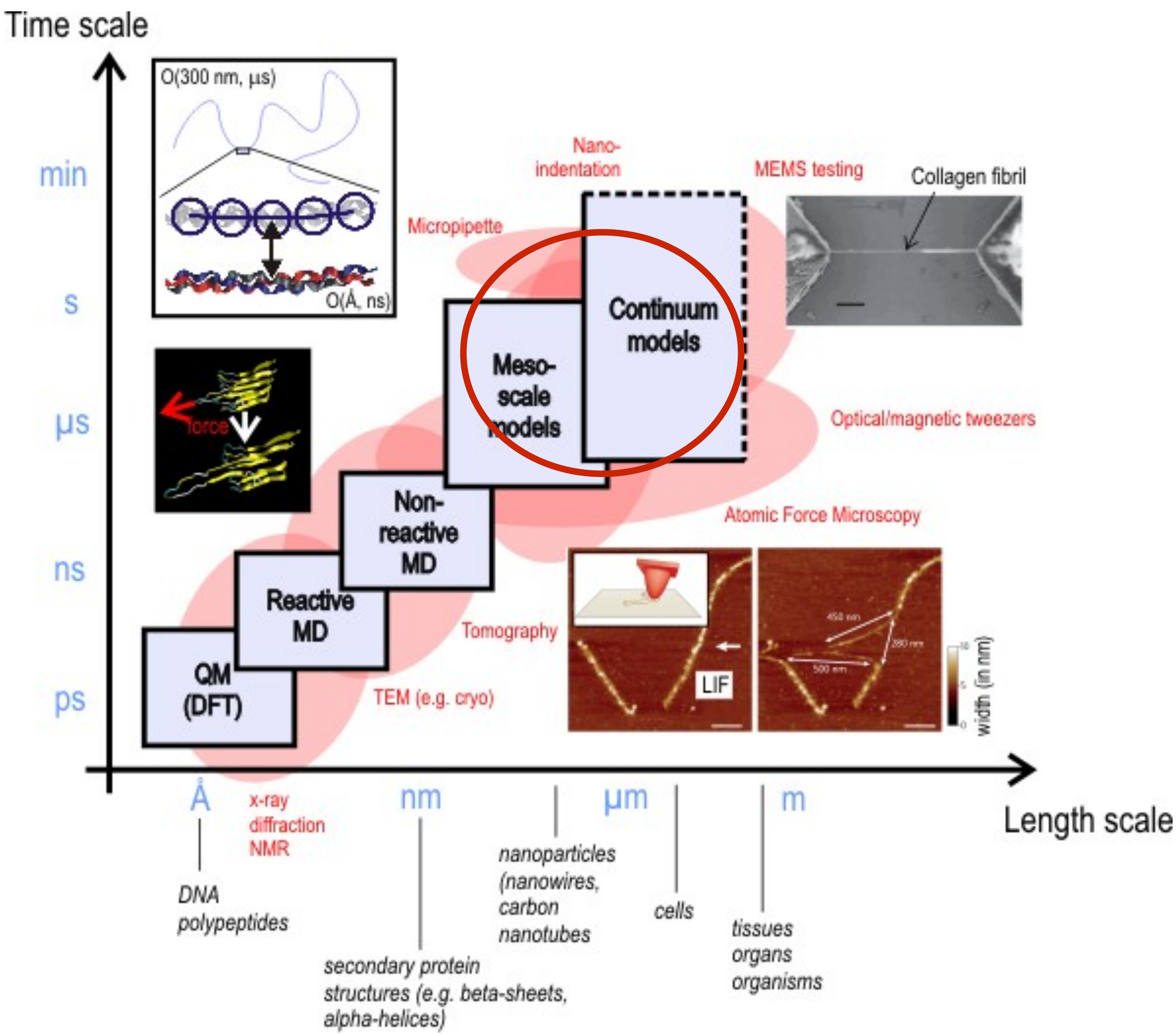


Bacillus subtilis



Tracer colloids

PRL 2013



http://web.mit.edu/mbuehler/www/research/f103.jpg

Basic idea

Split dynamics into

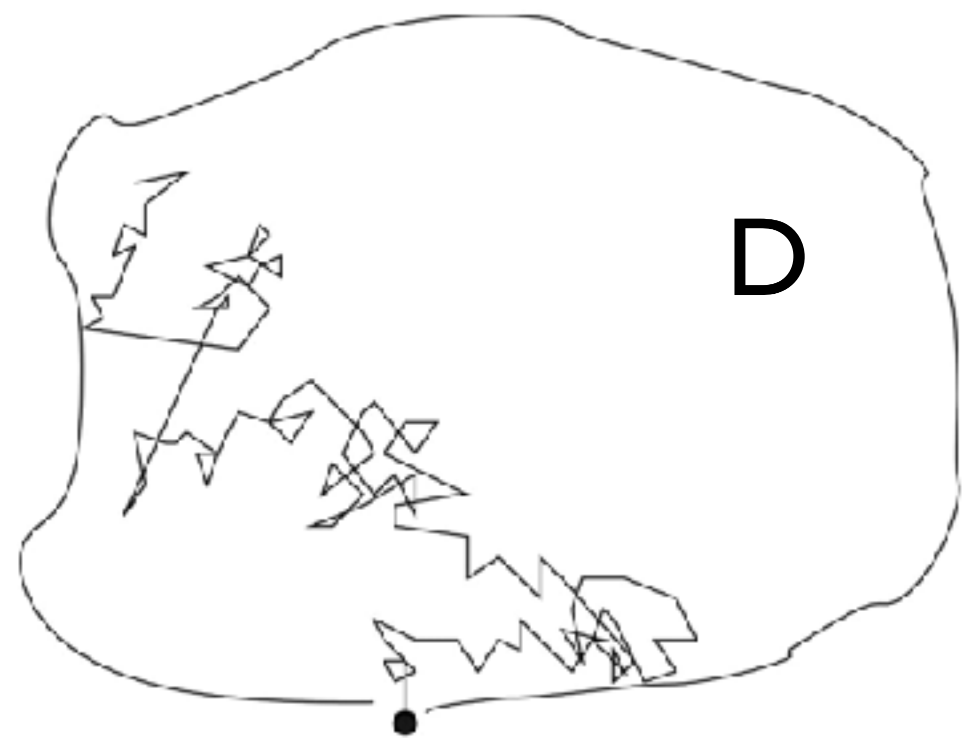
- deterministic part (drift)
- random part (diffusion)

$$\dot{x} = f(t, x(t)) + \text{noise}$$

Typical problems

Determine

- noise ‘structure’
- transport coefficients
- first passage (escape) times

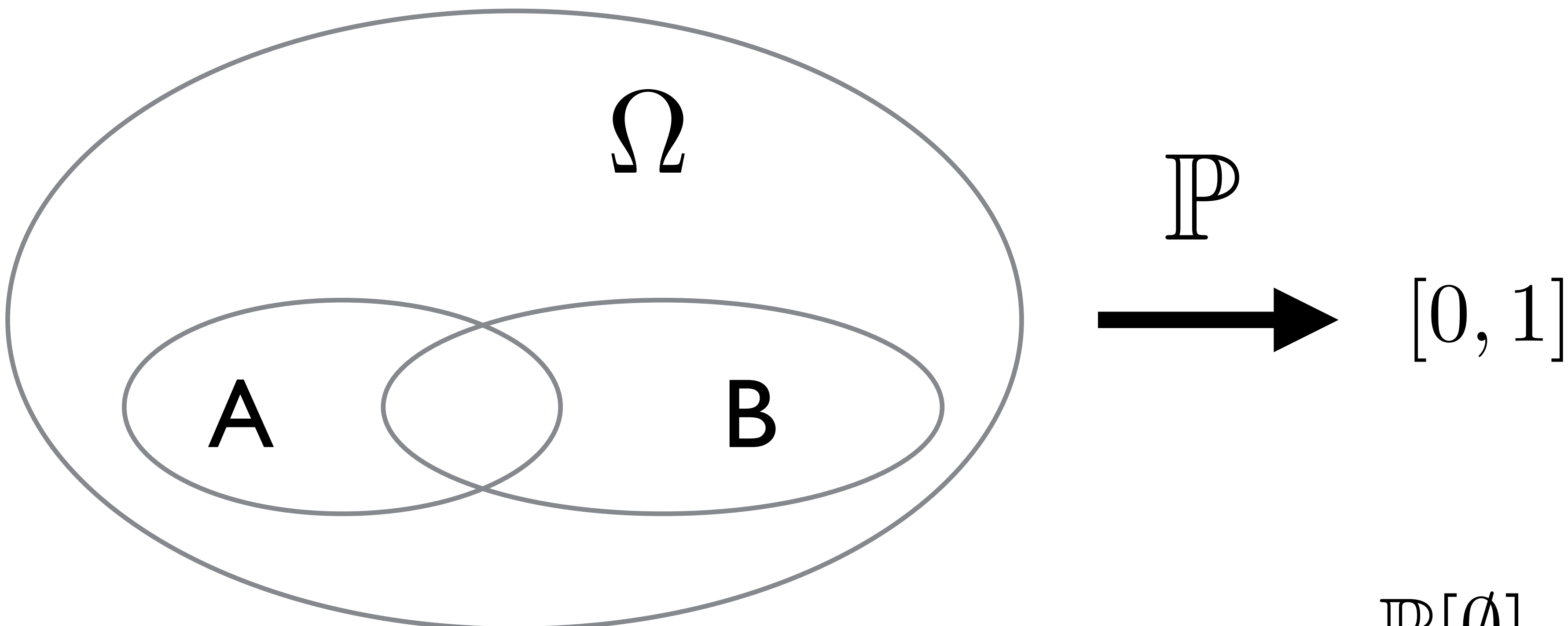


http://www.pnas.org/content/104/41/16098/F1.expansion.html

$$\dot{x} = f(t, x(t)) + \text{noise}$$

Probability space $(\Omega, \mathcal{F}, \mathbb{P})$

$$\mathcal{F} = \{\emptyset, \quad A, \quad \Omega/A, \quad B, \quad A \cap B, \quad A \cup B, \quad \ldots, \quad \Omega\}$$



$$\mathbb{P}[\emptyset] = 0$$

$$\mathbb{P}[\Omega] = 1$$

$$\mathbb{P}[A \cup B] = \mathbb{P}[A] + \mathbb{P}[B] - \mathbb{P}[A \cap B]$$

Expectation values of discrete random variables

$$X \; : \; \Omega \to \{x_1, \ldots, x_N\}$$

$$p_i \geq 0, \qquad \sum_{i=1}^{N} p_i = 1$$

$$\mathbb{E}[f(X)] = \sum_{i=1}^{N} p_i \, f(x_i)$$

$$\mathbb{E}[\alpha f(X) + \beta g(X)] = \alpha \mathbb{E}[f(X)] + \beta \mathbb{E}[g(X)]$$

Expectation values of continuous random variables

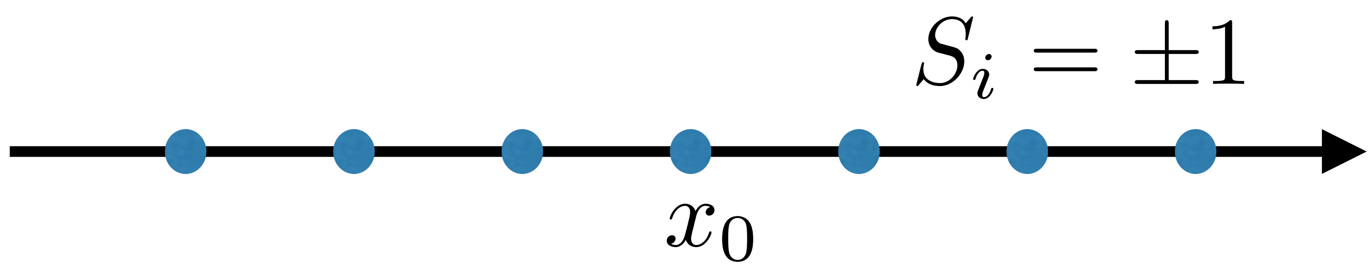
$$X : \Omega \to \mathbb{R}^n$$

$$p(x) \geq 0, \qquad \int dx\, p(x) = 1$$

$$\mathbb{E}[f(X)] = \int d\mathbb{P} f(x) = \int dx\, p(x) f(x)$$

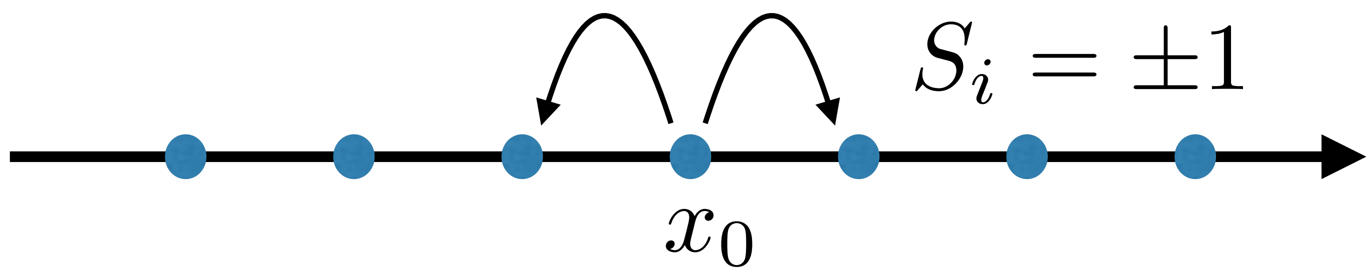
$$\mathbb{E}[\alpha f(X) + \beta g(X)] = \alpha \mathbb{E}[f(X)] + \beta \mathbb{E}[g(X)]$$

Random walk model



$$X_N = x_0 + \ell \sum_{i=1}^{N} S_i$$

$$\mathbb{E}[f(S)] = \sum_{a=1}^{2} p_a \, f(s_a)$$



1.1 Random walks

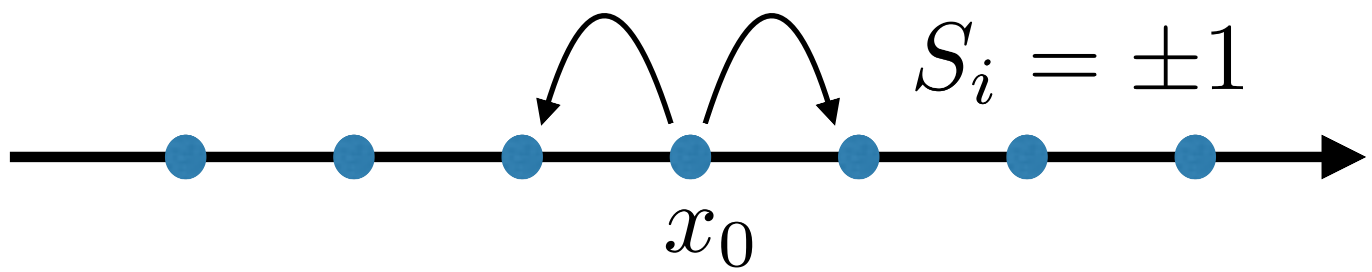
1.1.1 Unbiased random walk (RW)

Consider the one-dimensional unbiased RW (fixed initial position $X_0 = x_0$, N steps of length ℓ)

$$X_N = x_0 + \ell \sum_{i=1}^{N} S_i \tag{1.1}$$

where $S_i \in \{\pm 1\}$ are iid. random variables (RVs) with $\mathbb{P}[S_i = \pm 1] = 1/2$. Noting that [1]

$$\mathbb{E}[S_i] \;=\; -1 \cdot \frac{1}{2} + 1 \cdot \frac{1}{2} = 0, \tag{1.2}$$



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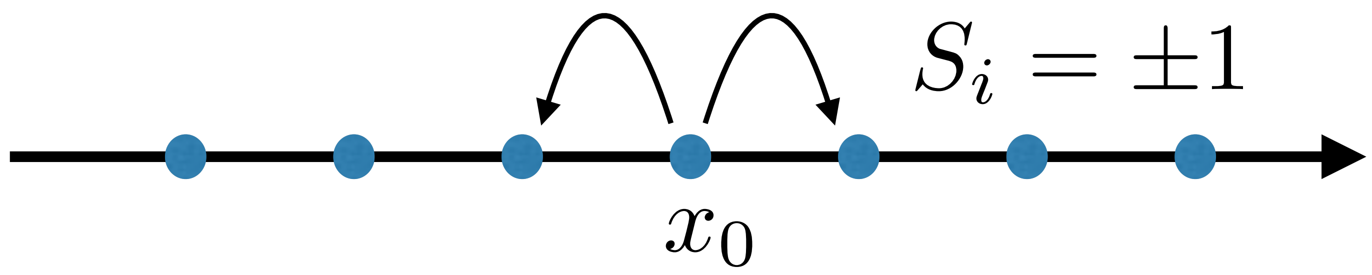
$$\mathbb{E}[S_i S_j] = \delta_{ij}\, \mathbb{E}[S_i^2] = \delta_{ij} \left[(-1)^2 \cdot \frac{1}{2} + (1)^2 \cdot \frac{1}{2} \right] = \delta_{ij}, \tag{1.3}$$



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we find for the first moment of the RW

$$\mathbb{E}[X_N] = x_0 + \ell \sum_{i=1}^{N} \mathbb{E}[S_i] = x_0 \tag{1.4}$$

Second moment (uncentered)

$$\mathbb{E}[X_N^2] \quad = \quad \mathbb{E}[(x_0 + \ell \sum_{i=1}^{N} S_i)^2]$$

Second moment (uncentered)

$$\begin{aligned}
\mathbb{E}[X_N^2] &= \mathbb{E}[(x_0 + \ell \sum_{i=1}^{N} S_i)^2] \\
&= \mathbb{E}[x_0^2 + 2x_0\ell \sum_{i=1}^{N} S_i + \ell^2 \sum_{i=1}^{N} \sum_{j=1}^{N} S_i S_j]
\end{aligned}$$

Second moment (uncentered)

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\mathbb{E}[X_N^2] &= \mathbb{E}[(x_0 + \ell \sum_{i=1}^{N} S_i)^2] \\
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&= x_0^2 + 2x_0 \cdot 0 + \ell^2 \sum_{i=1}^{N} \sum_{j=1}^{N} \mathbb{E}[S_i S_j]
\end{aligned}
$$

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&= x_0^2 + 2x_0 \cdot 0 + \ell^2 \sum_{i=1}^{N} \sum_{j=1}^{N} \mathbb{E}[S_i S_j] \\
&= x_0^2 + 2x_0 \cdot 0 + \ell^2 \sum_{i=1}^{N} \sum_{j=1}^{N} \delta_{ij}
\end{aligned}
$$

Second moment (uncentered)

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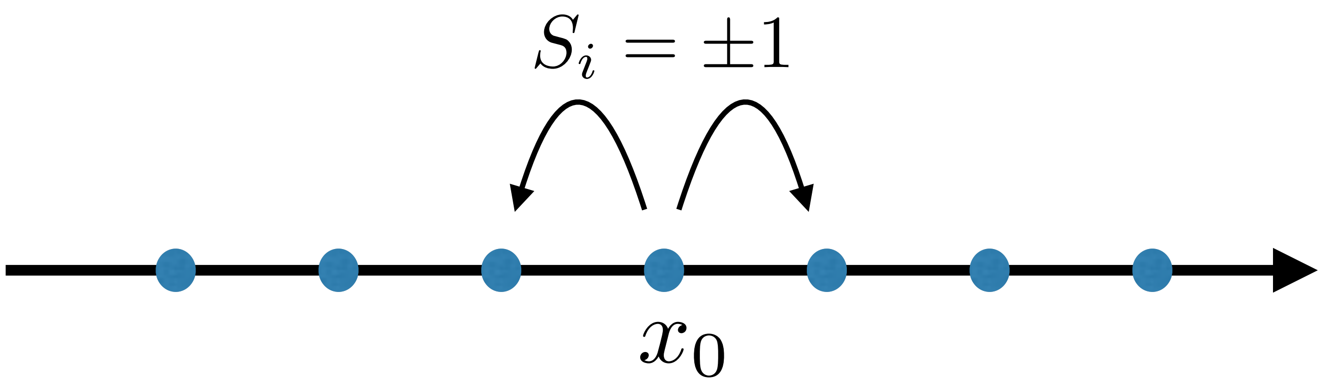
&= x_0^2 + 2x_0 \cdot 0 + \ell^2 \sum_{i=1}^{N}\sum_{j=1}^{N} \mathbb{E}[S_i S_j] \\
&= x_0^2 + 2x_0 \cdot 0 + \ell^2 \sum_{i=1}^{N}\sum_{j=1}^{N} \delta_{ij} \\
&= x_0^2 + \ell^2 N. \qquad (1.5)
\end{aligned}
$$

Continuum limit

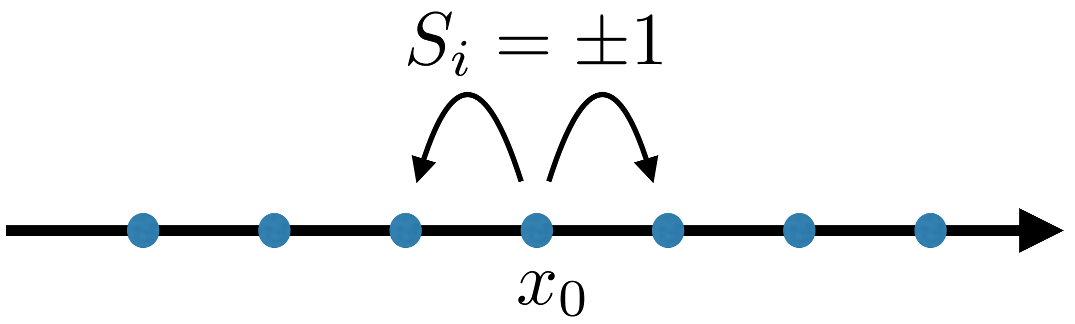


$$X_N = x_0 + \ell \sum_{i=1}^{N} S_i$$

Let $x_0 = 0, \qquad N = t/\tau$

$$P(N, K) := \mathbb{P}[X_N/\ell = K]$$

Continuum limit



$$
\begin{aligned}
P(N,K) &= \left(\frac{1}{2}\right)^N \binom{N}{\frac{N-K}{2}} \\
&= \left(\frac{1}{2}\right)^N \frac{N!}{((N+K)/2)!\,((N-K)/2)!}.
\end{aligned}
\tag{1.8}
$$

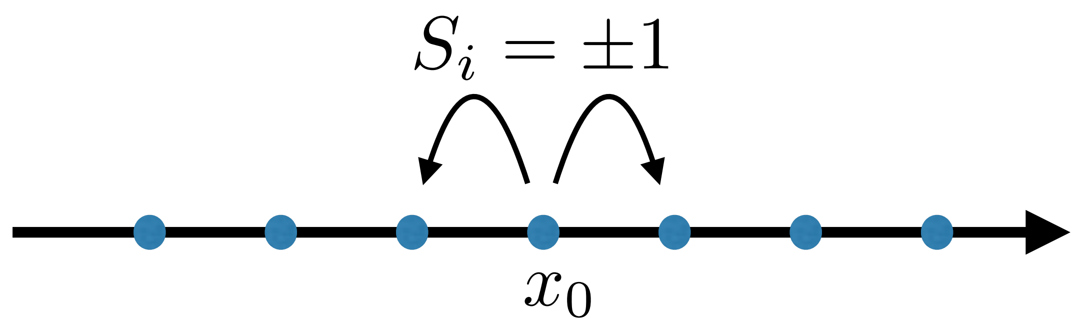
The associated probability density function (PDF) can be found by defining

$$p(t,x) := \frac{P(N,K)}{2\ell} = \frac{P(t/\tau, x/\ell)}{2\ell} \tag{1.9}$$

and considering limit $\tau, \ell \to 0$ such that

$$D := \frac{\ell^2}{2\tau} = const, \tag{1.10}$$

Continuum limit



(pset1)

yielding the Gaussian

$$p(t,x) \simeq \sqrt{\frac{1}{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right) \tag{1.11}$$

Eq. (1.11) is the fundamental solution to the diffusion equation,

$$\partial_t p \; = D\partial_{xx} p, \tag{1.12}$$

where $\partial_t, \partial_x, \partial_{xx}, \ldots$ denote partial derivatives. The mean square displacement of the continuous process described by Eq. (1.11) is

$$\mathbb{E}[X(t)^2] = \int dx \; x^2 \, p(t,x) = 2Dt, \tag{1.13}$$

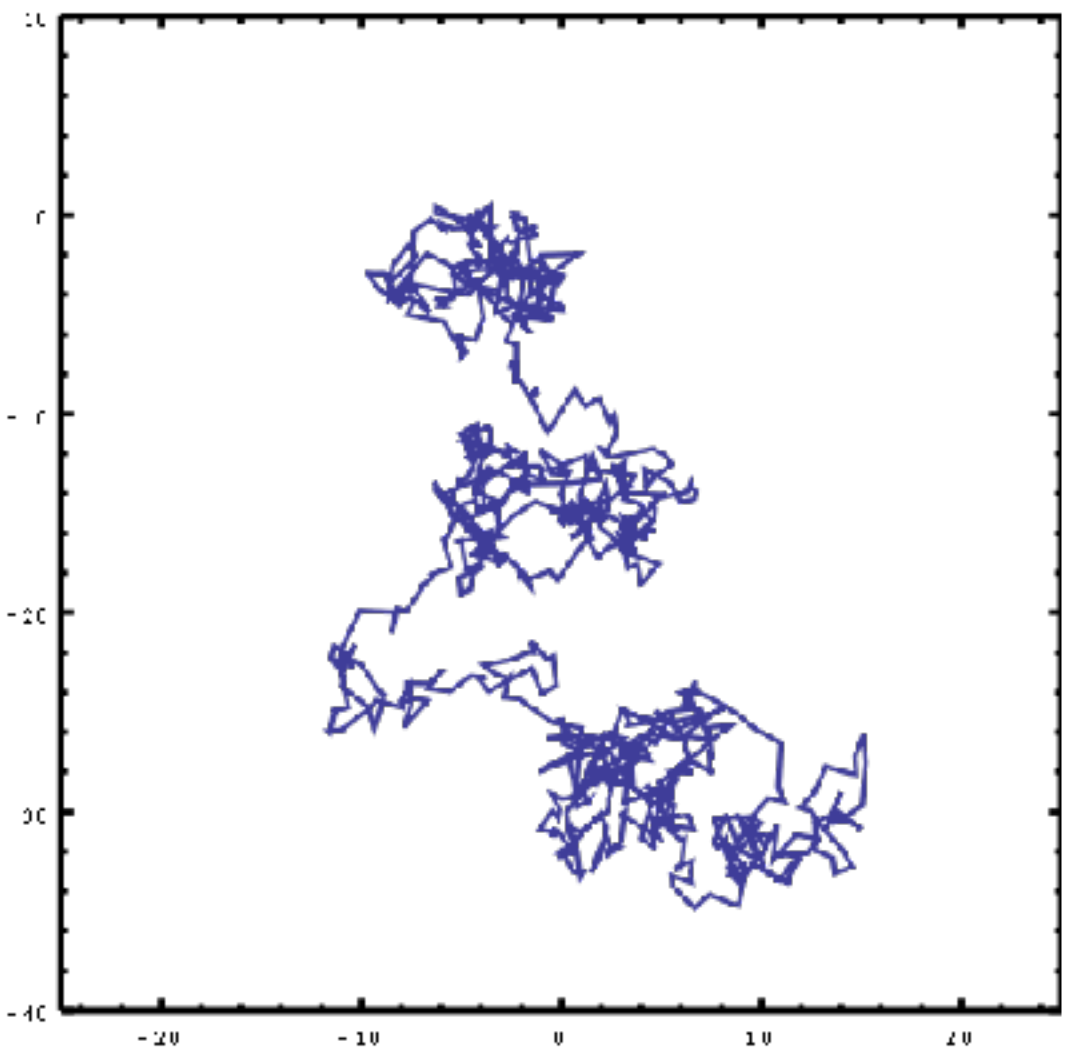
in agreement with Eq. (1.7).

Remark One often classifies diffusion processes by the (asymptotic) power-law growth of the mean square displacement,

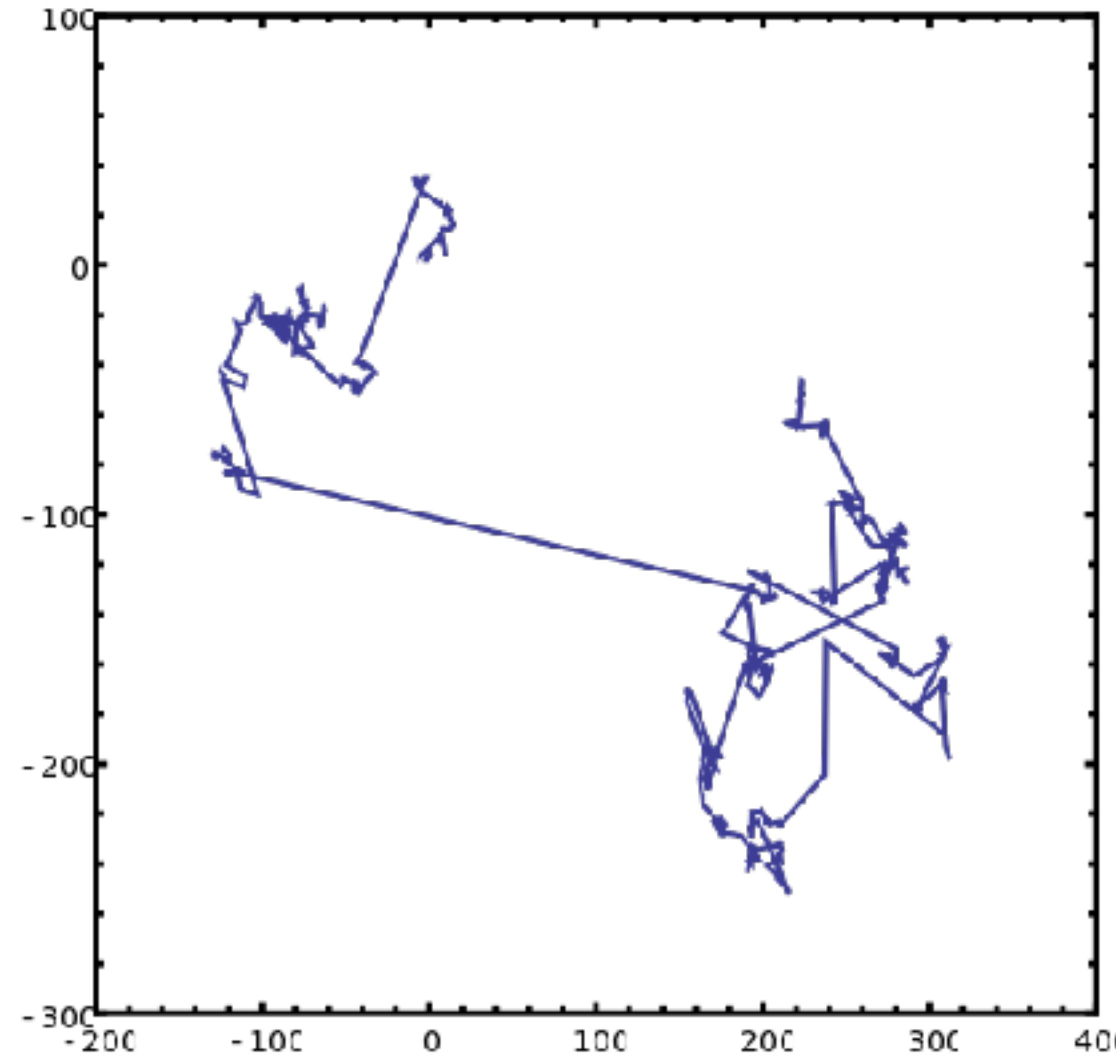
$$\mathbb{E}[(X(t) - X(0))^2] \sim t^\mu. \tag{1.14}$$

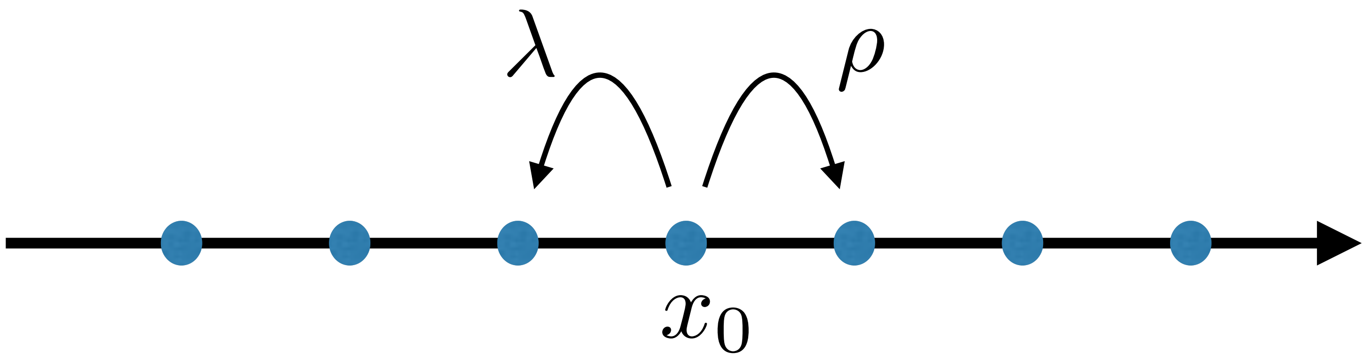
- $\mu = 0$: Static process with no movement.
- $0 < \mu < 1$: Sub-diffusion, arises typically when waiting times between subsequent jumps can be long and/or in the presence of a sufficiently large number of obstacles (e.g. slow diffusion of molecules in crowded cells).
- $\mu = 1$: Normal diffusion, corresponds to the regime governed by the standard Central Limit Theorem (CLT).
- $1 < \mu < 2$: Super-diffusion, occurs when step-lengths are drawn from distributions with infinite variance (Lévy walks; considered as models of bird or insect movements).
- $\mu = 2$: Ballistic propagation (deterministic wave-like process).

Brownian motion



non-Brownian
Levy-flight





1.1.2 Biased random walk (BRW)

Consider a one-dimensional hopping process on a discrete lattice (spacing ℓ), defined such that during a time-step τ a particle at position $X(t) = \ell j \in \ell\mathbb{Z}$ can either

(i) jump a fixed distance ℓ to the left with probability λ, or

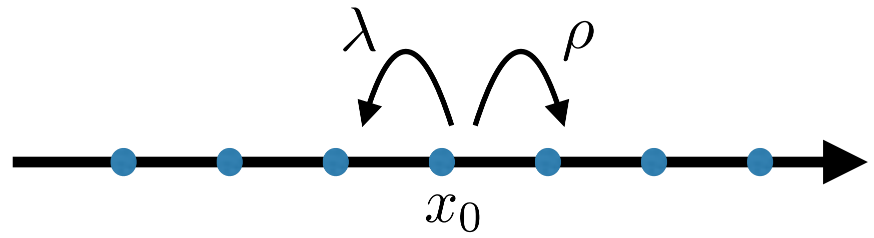
(ii) jump a fixed distance ℓ to the right with probability ρ, or

(iii) remain at its position x with probability $(1 - \lambda - \rho)$.

Assuming that the process is Markovian (does not depend on the past), the evolution of the associated probability vector $P(t) = (P(t,x)) = (P_j(t))$, where $x = \ell j$, is governed by the master equation

$$P(t+\tau, x) = (1 - \lambda - \rho)\, P(t,x) + \rho\, P(t, x-\ell) + \lambda\, P(t, x+\ell). \tag{1.15}$$

Master equations



$$P(t+\tau, x) = (1-\lambda-\rho)\, P(t,x) + \rho\, P(t, x-\ell) + \lambda\, P(t, x+\ell). \tag{1.15}$$

Technically, ρ, λ and $(1-\lambda-\rho)$ are the non-zero-elements of the corresponding transition matrix $W = (W_{ij})$ with $W_{ij} > 0$ that governs the evolution of the column probability vector $P(t) = (P_j(t)) = (P(t,y))$ by

$$P_i(t+\tau) = W_{ij} P_j(t) \tag{1.16a}$$

or, more generally, for n steps

$$P(t+n\tau) = W^n P(t). \tag{1.16b}$$

The stationary solutions are the eigenvectors of W with eigenvalue 1. To preserve normalization, one requires $\sum_i W_{ij} = 1$.

Continuum limit Define the density $p(t,x) = P(t,x)/\ell$. Assume τ, ℓ are small, so that we can Taylor-expand

$$p(t+\tau, x) \simeq p(t,x) + \tau \partial_t p(t,x) \tag{1.17a}$$

$$p(t, x \pm \ell) \simeq p(t,x) \pm \ell \partial_x p(t,x) + \frac{\ell^2}{2} \partial_{xx} p(t,x) \tag{1.17b}$$

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Neglecting the higher-order terms, it follows from Eq. (1.15) that

$$\begin{aligned} p(t,x) + \tau\partial_t p(t,x) \simeq\; & (1-\lambda-\rho)\, p(t,x) + \\ & \rho\left[p(t,x) - \ell\partial_x p(t,x) + \frac{\ell^2}{2}\partial_{xx}p(t,x)\right] + \\ & \lambda\left[p(t,x) + \ell\partial_x p(t,x) + \frac{\ell^2}{2}\partial_{xx}p(t,x)\right]. \end{aligned} \tag{1.18}$$

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Dividing by τ, one obtains the advection-diffusion equation

$$\partial_t p = -u\, \partial_x p + D\, \partial_{xx} p \tag{1.19a}$$

with drift velocity u and diffusion constant D given by[2]

$$u := (\rho - \lambda)\frac{\ell}{\tau}\,, \qquad D := (\rho + \lambda)\frac{\ell^2}{2\tau}. \tag{1.19b}$$

Time-dependent solution

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with drift velocity u and diffusion constant D given by[2]

$$u := (\rho - \lambda)\frac{\ell}{\tau}\;, \qquad D := (\rho + \lambda)\frac{\ell^2}{2\tau}. \tag{1.19b}$$

We recover the classical diffusion equation (1.12) from Eq. (1.19a) for $\rho = \lambda = 0.5$. The time-dependent fundamental solution of Eq. (1.19a) reads

$$p(t,x) = \sqrt{\frac{1}{4\pi D t}}\exp\left(-\frac{(x-ut)^2}{4Dt}\right) \tag{1.20}$$

Remarks Note that Eqs. (1.12) and Eq. (1.19a) can both be written in the current-form

$$\partial_t p + \partial_x j_x = 0 \tag{1.21}$$

with

$$j_x = up - D\partial_x p, \tag{1.22}$$

reflecting conservation of probability. Another commonly-used representation is

$$\partial_t p = \mathcal{L}p, \tag{1.23}$$

where $\mathcal{L}$ is a linear differential operator; in the above example (1.19b)

$$\mathcal{L} := -u\,\partial_x + D\,\partial_{xx}. \tag{1.24}$$

Stationary solutions, if they exist, are eigenfunctions of $\mathcal{L}$ with eigenvalue 0.

(useful later when discussing Brownian motors)