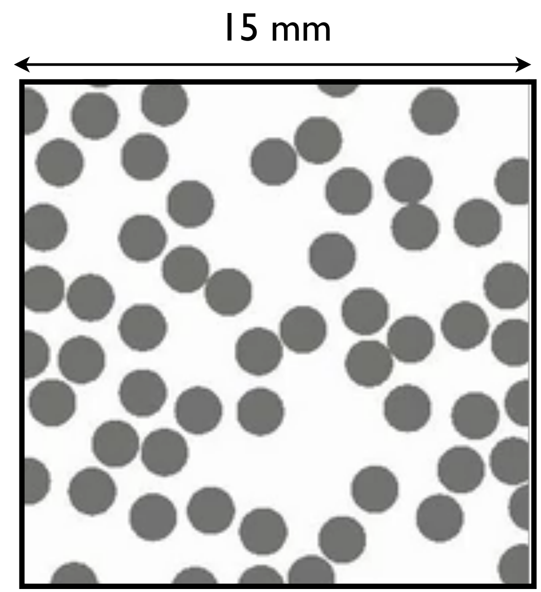
# L04:
# Continuum theory
# &
# diffusion

18.354

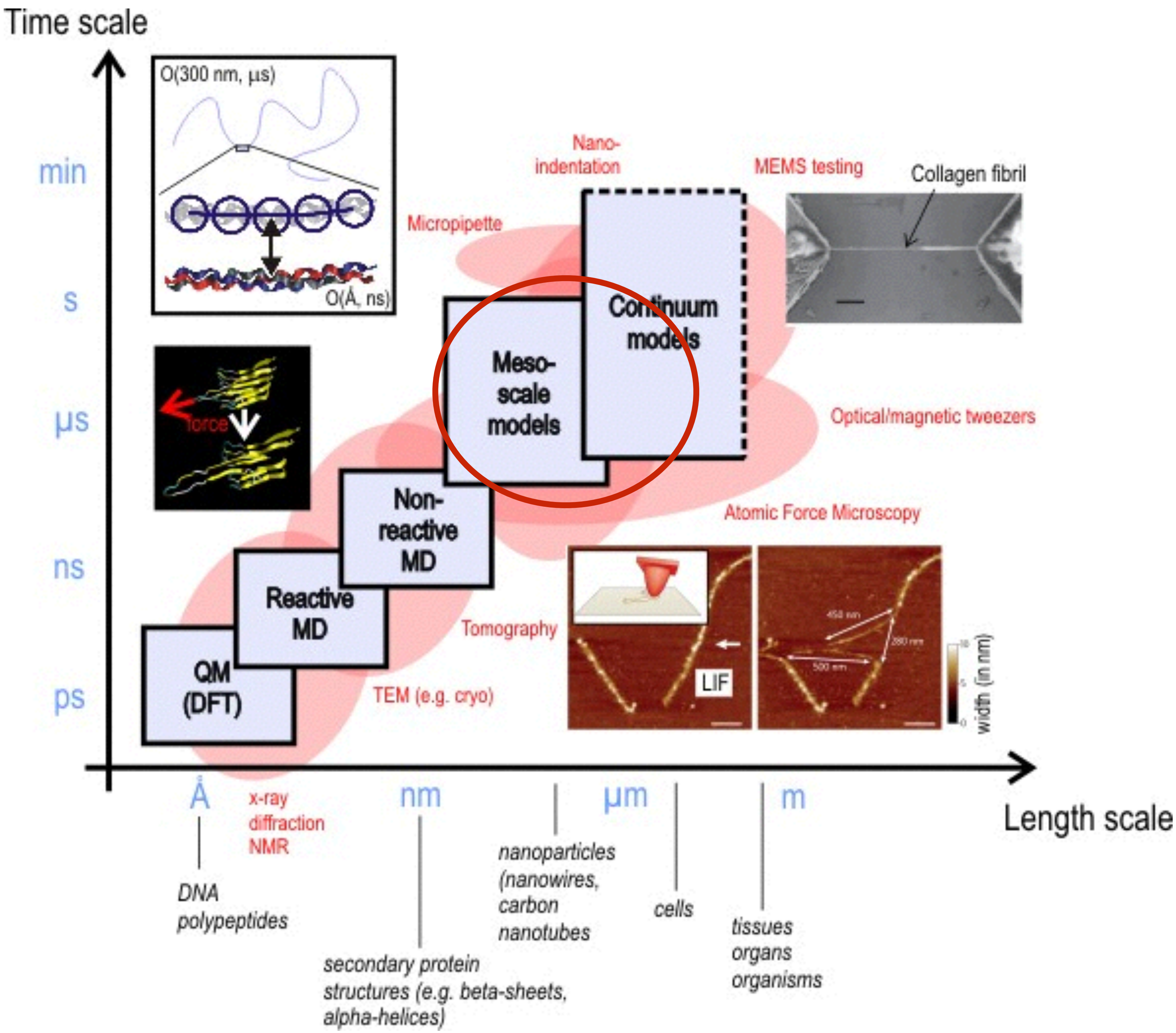
# Last class: Hamiltonian dynamics




Dilute Fluid

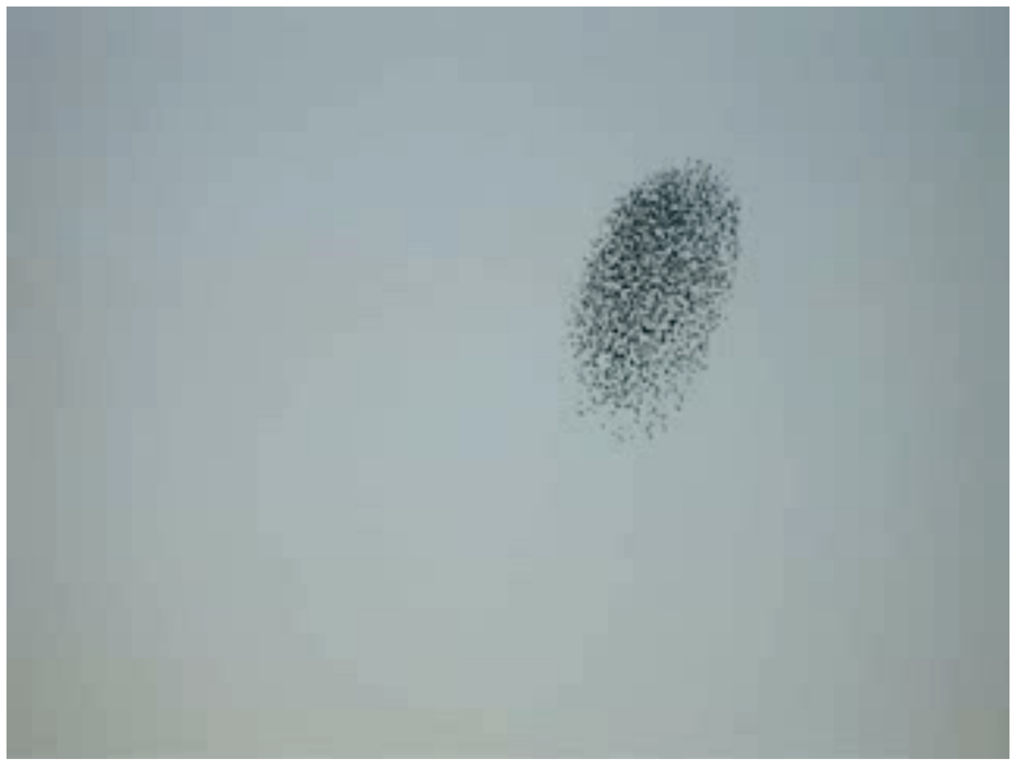
$\phi = 0.34$

## <u>Molecular Dynamics Simulations</u>




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

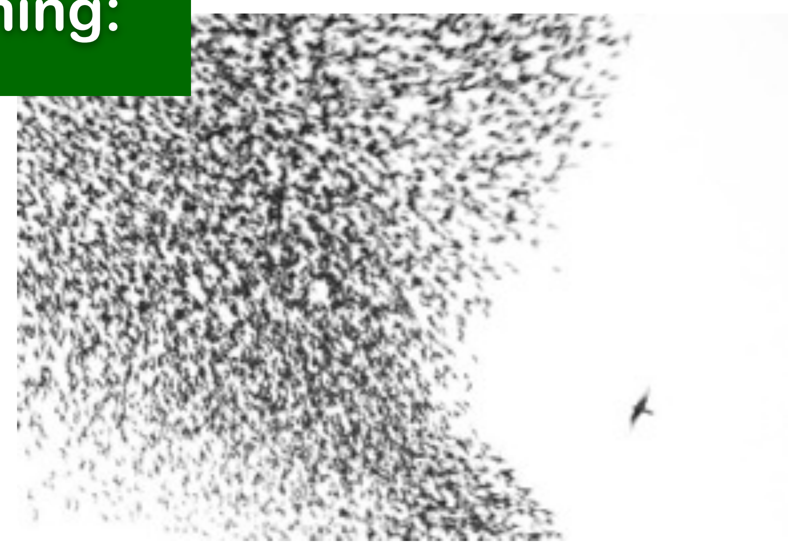
# How do we describe systems with large N of particles?



Falcon attacks a flock of starlings

## How do we describe systems with large N of particles?

**Swarming:**



# How do we describe systems with large N of particles?

**Traffic flow:**

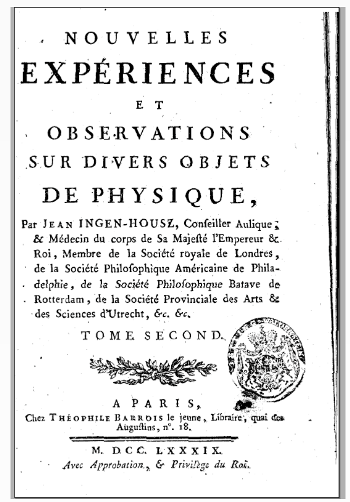
## How do we describe systems with large N of particles?

# 1st example:
# Brownian motion

# Brownian motion

# “Brownian” motion

## Jan Ingen-Housz (1730-1799)



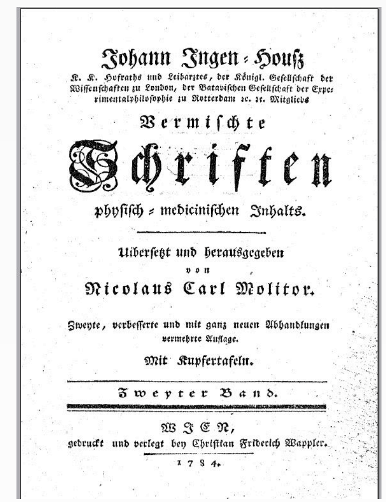
NOUVELLES
EXPÉRIENCES
ET
OBSERVATIONS
SUR DIVERS OBJETS
DE PHYSIQUE,

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 ꝛc. ꝛc. Mitglieds

Vermiſchte
Schriften
phyſiſch-mediciniſchen Inhalts.

Uiberſetzt und herausgegeben
von
Nicolaus Carl Molitor.

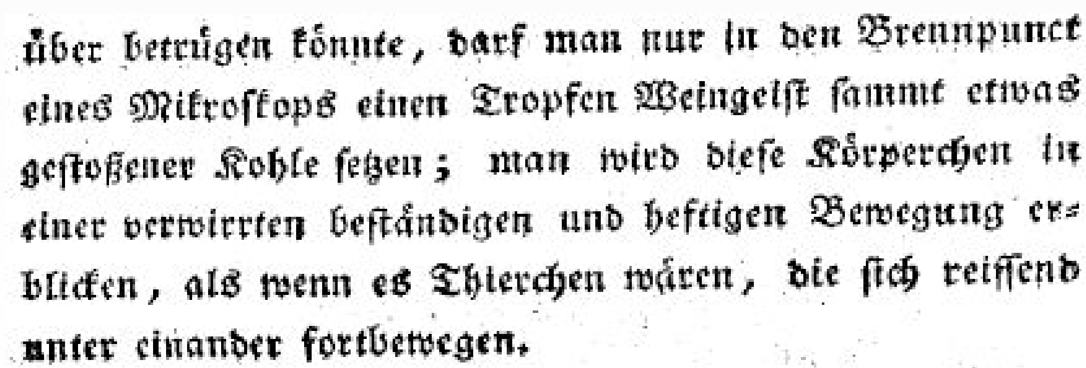
Zweyte, verbeſſerte und mit ganz neuen Abhandlungen vermehrte Auflage.

Mit Kupfertafeln.

Zweyter Band.

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

1784/1785:

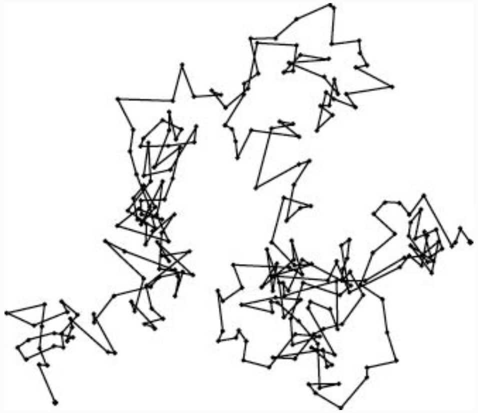


über betrügen könnte, darf man nur in den Brennpunct eines Mikroſkops einen Tropfen Weingeiſt ſammt etwas geſtoßener Kohle ſetzen; man wird dieſe Körperchen in einer verwirrten beſtändigen und heftigen Bewegung erblicken, als wenn es Thierchen wären, die ſich reiſſend unter einander fortbewegen.

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

## Robert Brown (1773-1858)

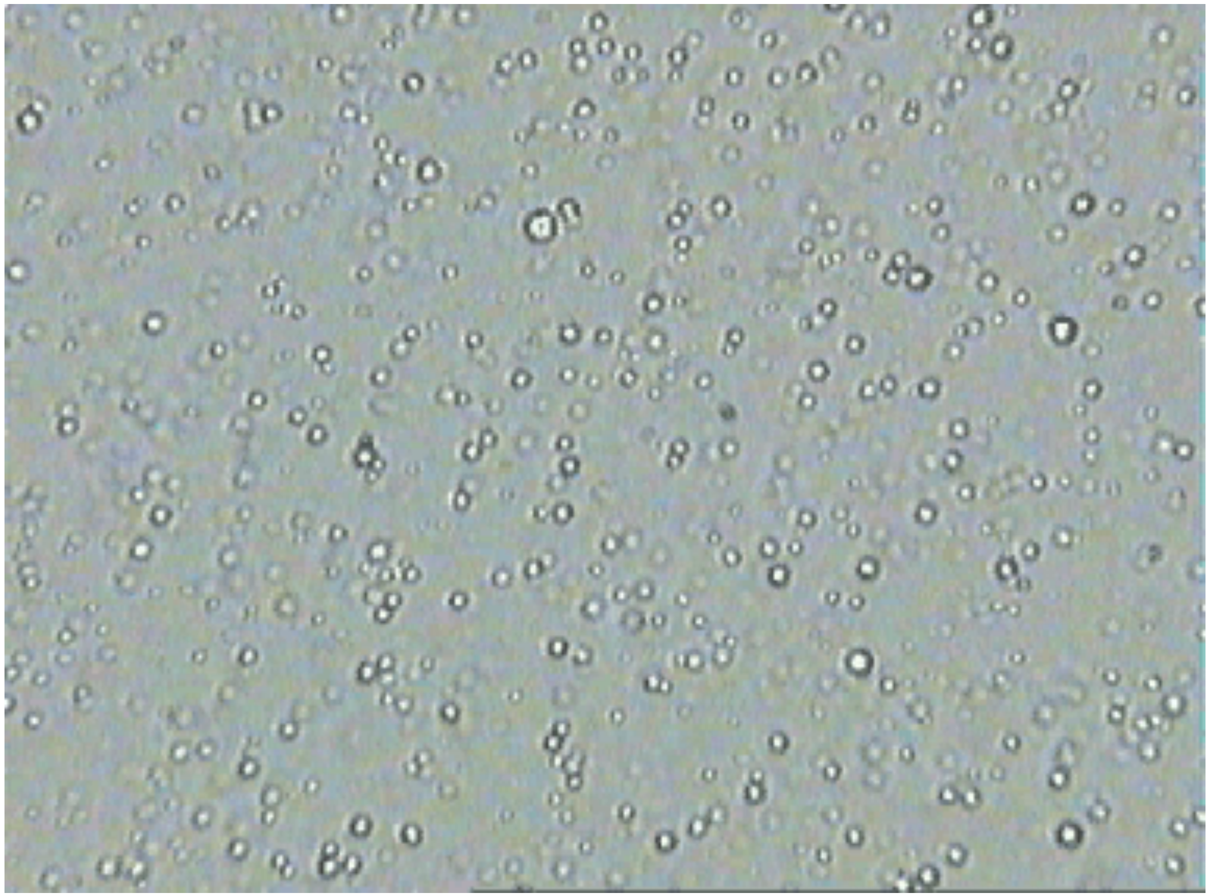
Linnean Society (London)



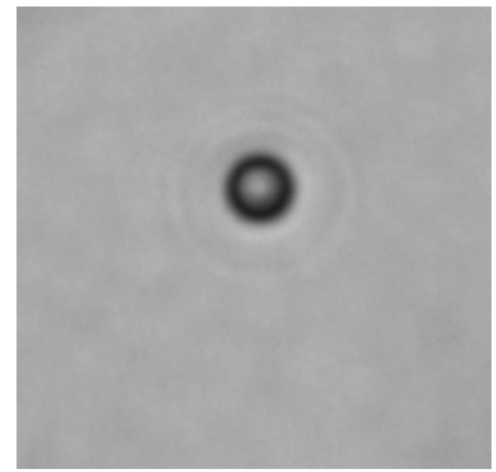
1827: irregular motion of pollen in fluid

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

# Brownian motion

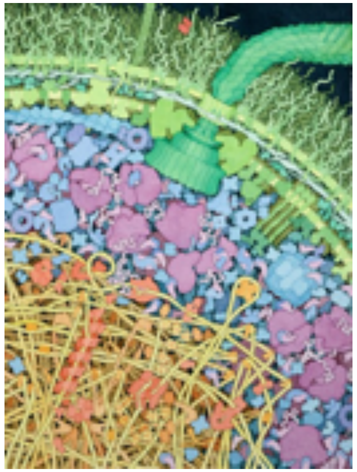


David Walker

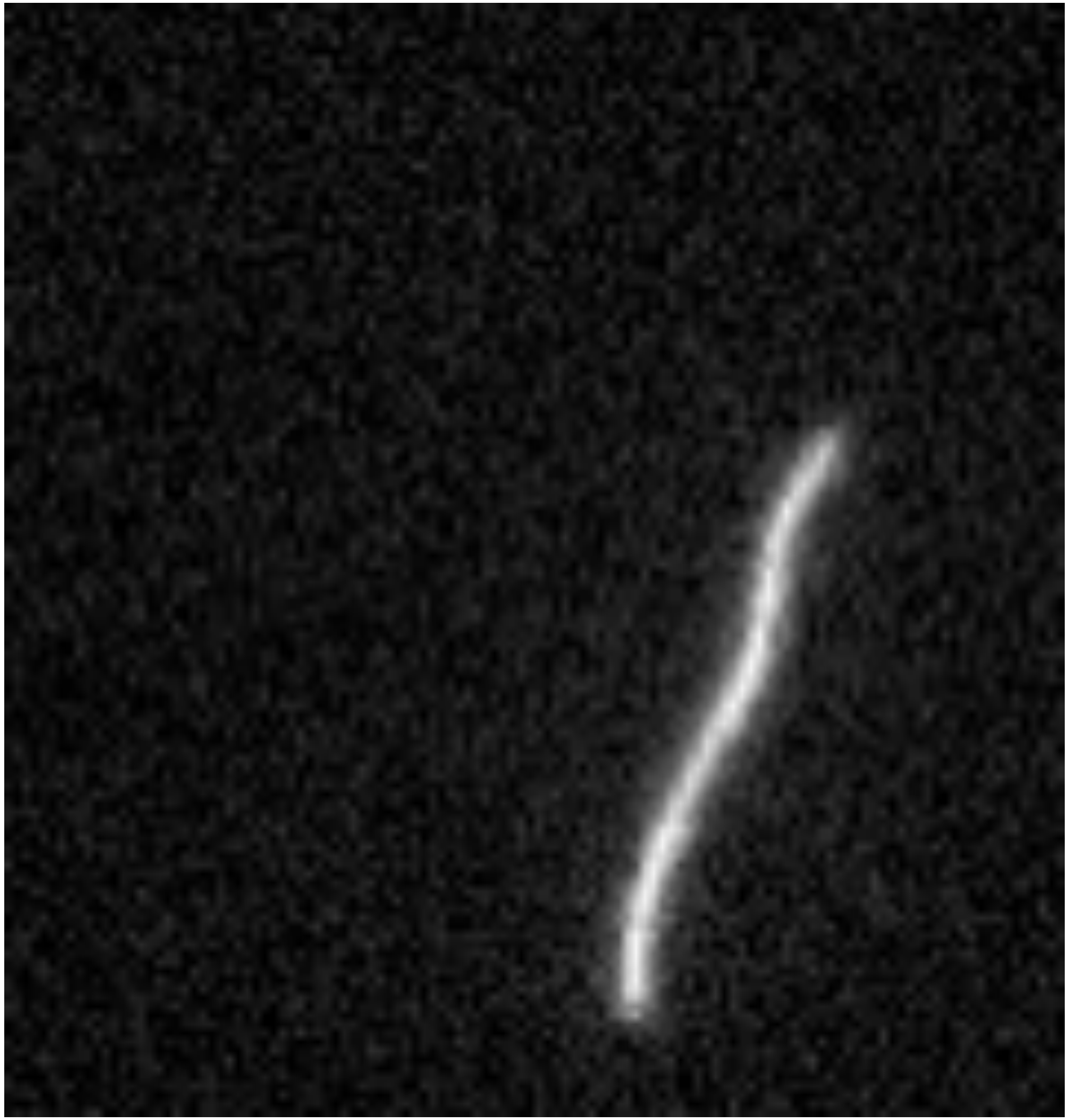


Mark Haw

# Polymer in a fluid



Dogic lab (Brandeis)

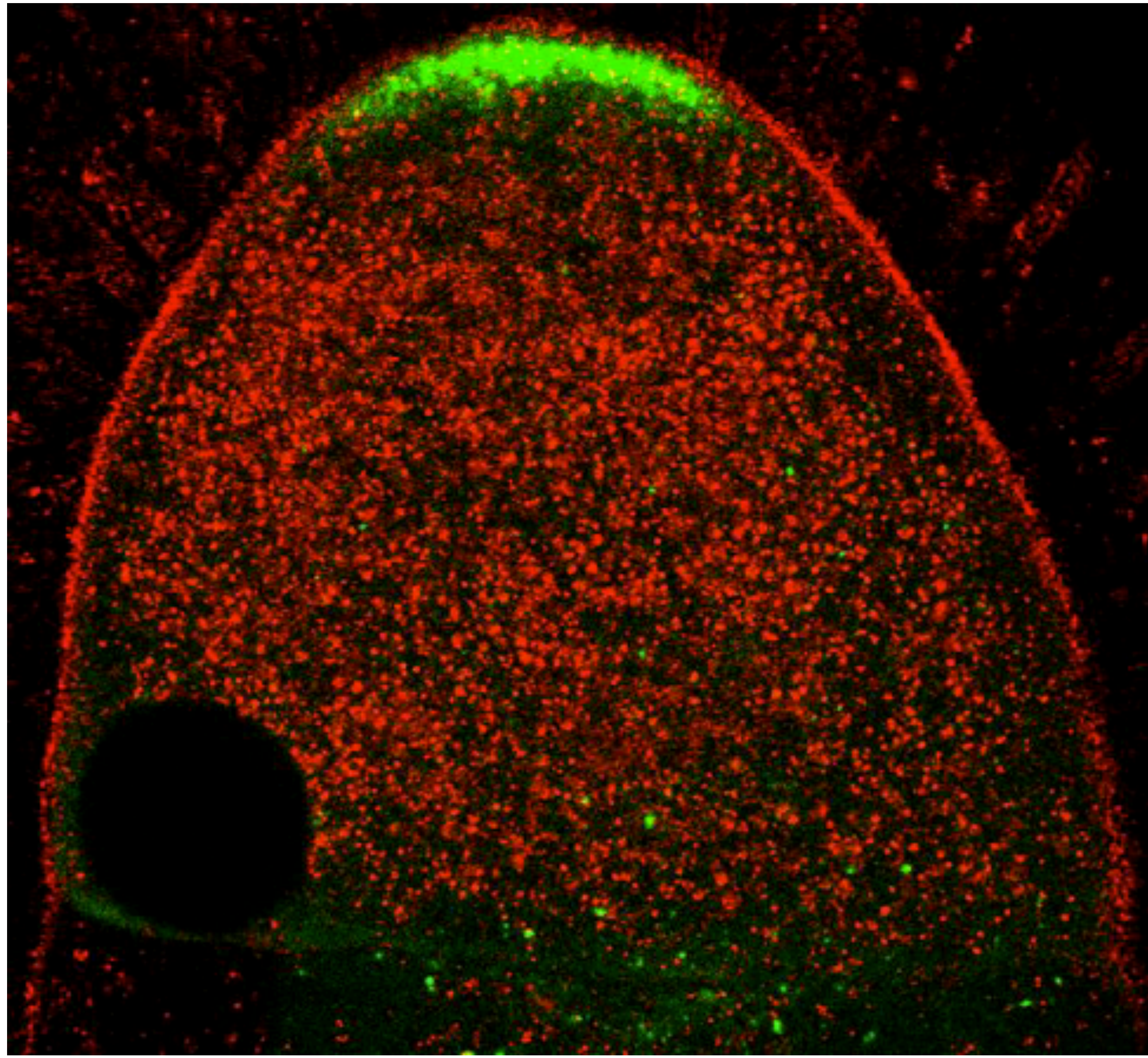


$< 1\mu m$

18.S995

# Flow & transport in cells

Drosophila embryo



Goldstein lab (Cambridge)

# Mathematical description of standard BM

Louis Bachelier, Theorie de la speculation,

*Ann. Sci. l'École Norm. Sup.* **3** (17): 21–86 (1900)

**Adolf Eugen Fick (1829-1901)**

first law

$$\frac{\partial}{\partial t}\varrho(t,x) = -\nabla J(t,x)$$

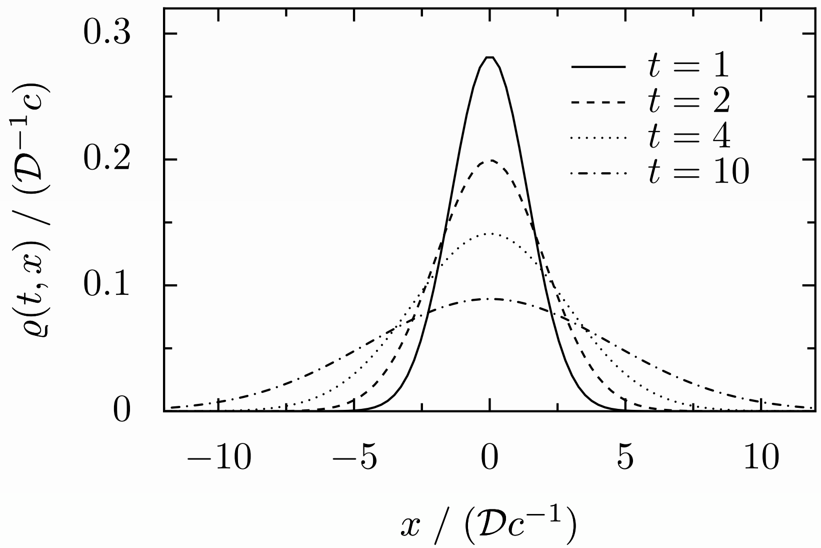
second law

$$J(t,x) = -\mathcal{D}\,\nabla\varrho(t,x)$$

$$\Rightarrow \quad \frac{\partial}{\partial t}\varrho = \mathcal{D}\,\nabla^2\varrho$$

Phil. Mag. **10**: 30 (1855)

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

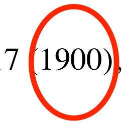



Goal: *D=f(microscopic parameters)*

1870 – 1946

Louis Bachelier, aged 15

*Annales scientifiques de l'É.N.S. 3e série*, tome 17 (1900), p. 21-86.



THÉORIE

DE

LA SPÉCULATION,

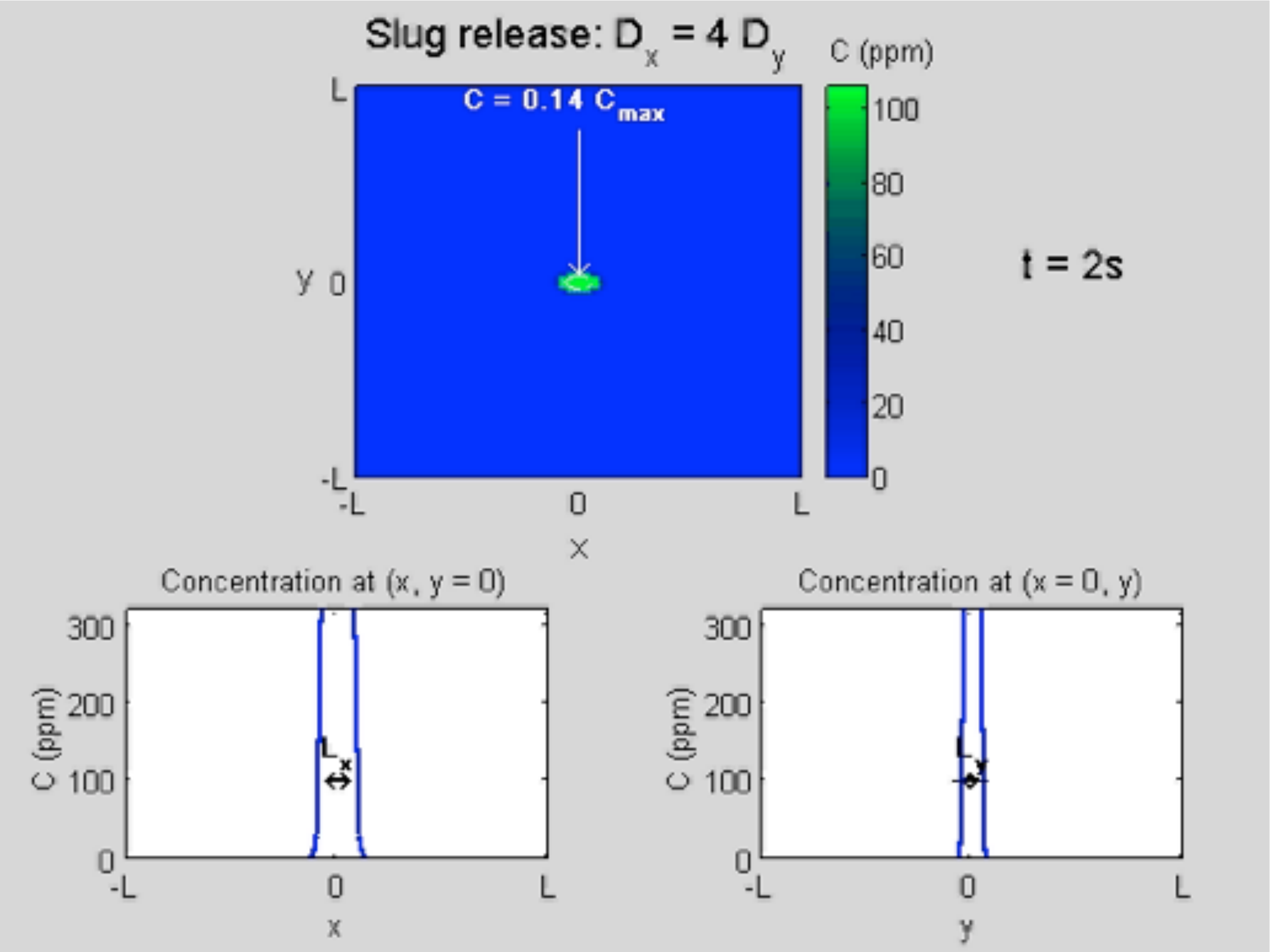
PAR M. L. BACHELIER.

38 L. BACHELIER.

Nous avons donc pour expression de la probabilité

$$p = \frac{H}{\sqrt{t}} e^{-\frac{\pi H^2 x^2}{t}}.$$

# Diffusion of an Instantaneous Point Source




This animation depicts the diffusion of a discrete mass released at (x = 0, y = 0, t = 0). The diffusion is anisotropic, Dx = 4 Dy. The length scales grow in proportion to the square root of the diffusion, such that the dimensions of the cloud are anisotropic, with Lx = 2 Ly. Note that the profiles of concentration along the x- and y-axes are Gaussian in shape.

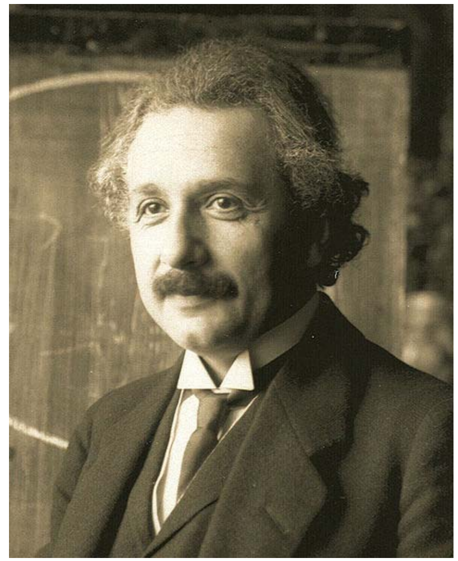
W. Sutherland (1858-1911)

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

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

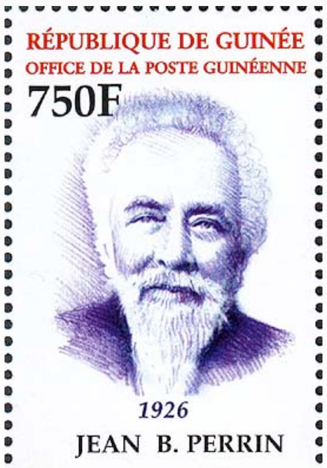
Ann. Phys. **21**, 756 (1906)

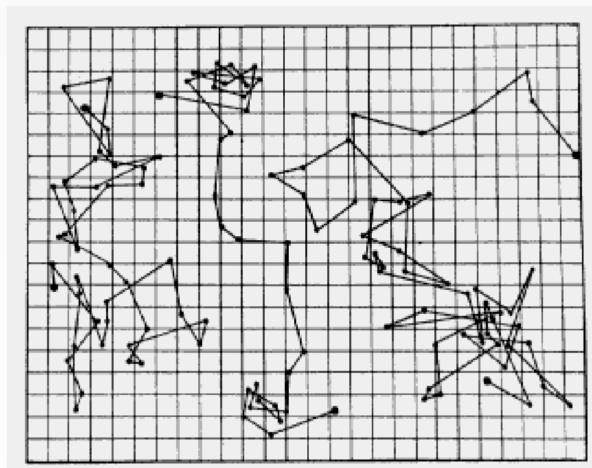
*R* : molar gas constant
*k* : viscosity

*T* : Temperature
*P* : ParticleRadius

*N*: Avogadro's number

## 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 0.53$\mu$m
- successive positions every 30 seconds joined by straight line segments
- mesh size is 3.2$\mu$m

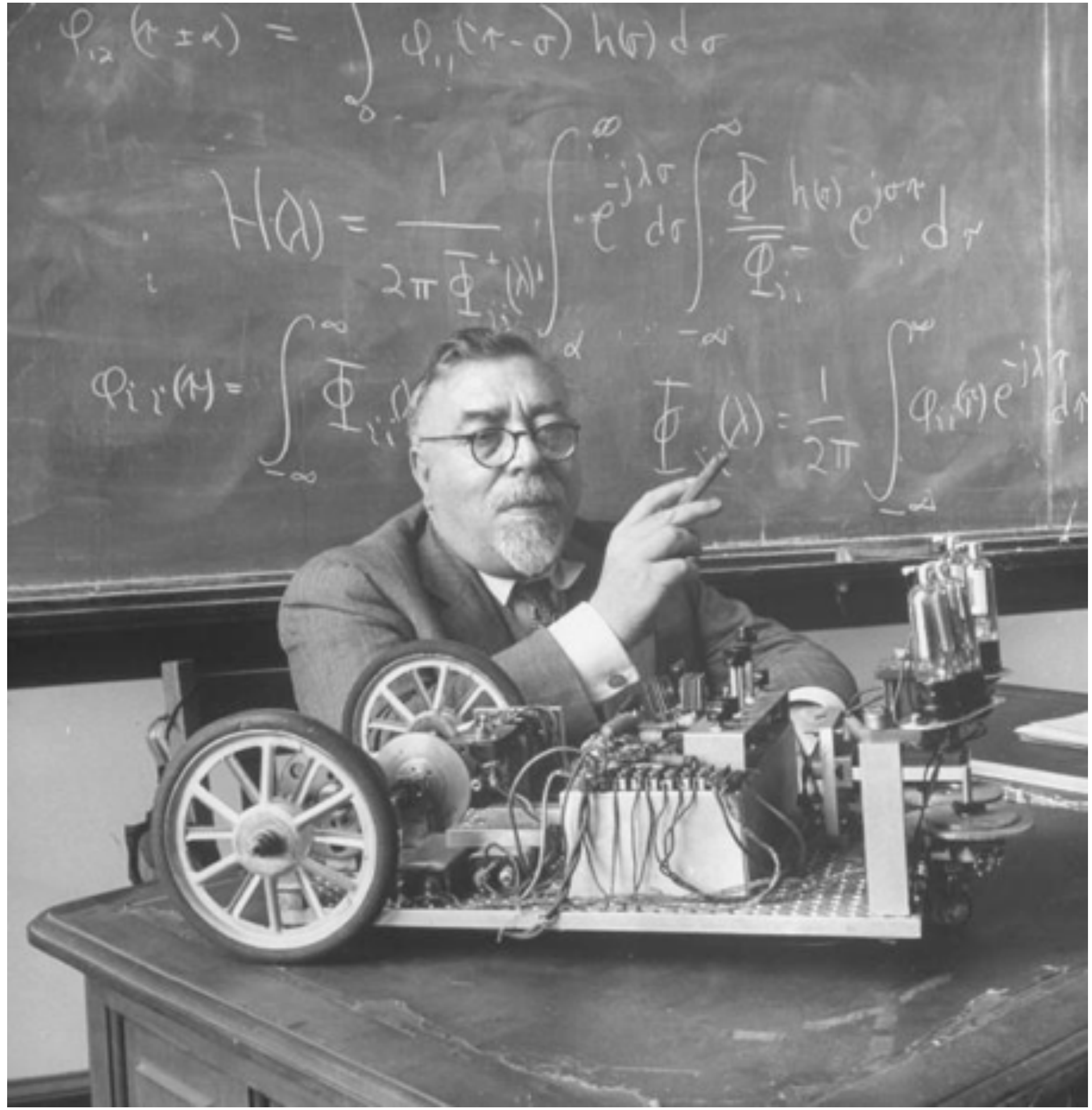
*Les Atomes*, Paris, Alcan (1913)

experimental evidence for
atomistic structure of matter

# Norbert Wiener

(1894-1864)

MIT



# How fast must a cell swim to beat Brownian motion?

$$\langle x^2 \rangle = 2Dt$$

$$D = \frac{kT}{6\pi\eta_0 a}$$

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$$a \sim 1\mu m$$

$$\gamma_S = 6\pi\eta a \sim 2 \times 10^{-8}\,\mathrm{kg/s}$$

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Hence, we find for the diffusion constant

$$D \sim 0.2\,\mu\mathrm{m}^2/\mathrm{s}$$

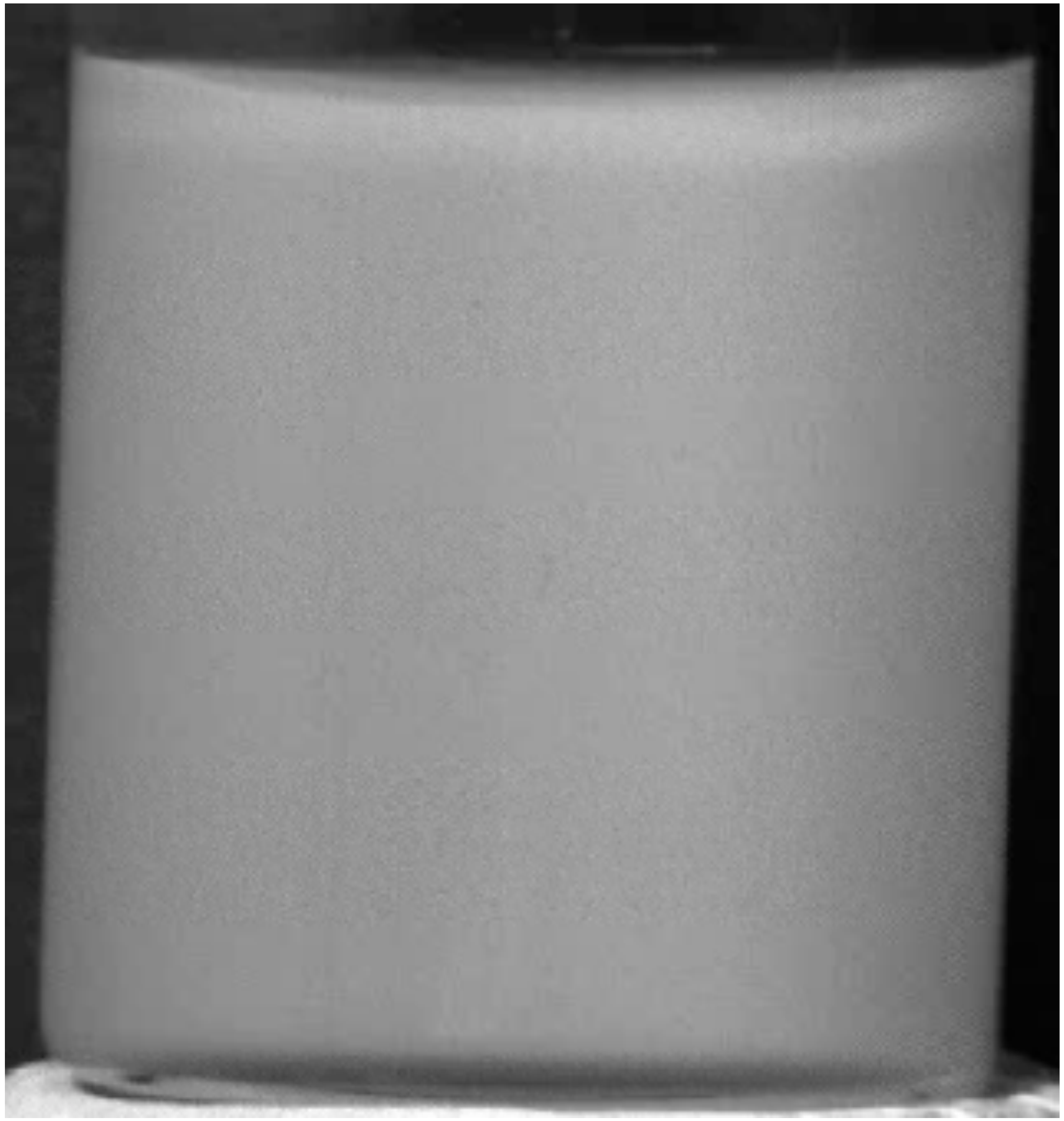
Assuming a run length $\sim 1\,\mathrm{s}$, Brownian motion would move a micron-sized bacterium by approximately $0.5\,\mu$m per second. Thus a bacterium should swim at last 5-10 $\mu$m/s, which is close to typical bacterial swimming speeds.

# Sedimentation

Mississippi

NASA Earth Observatory

# Sedimentation

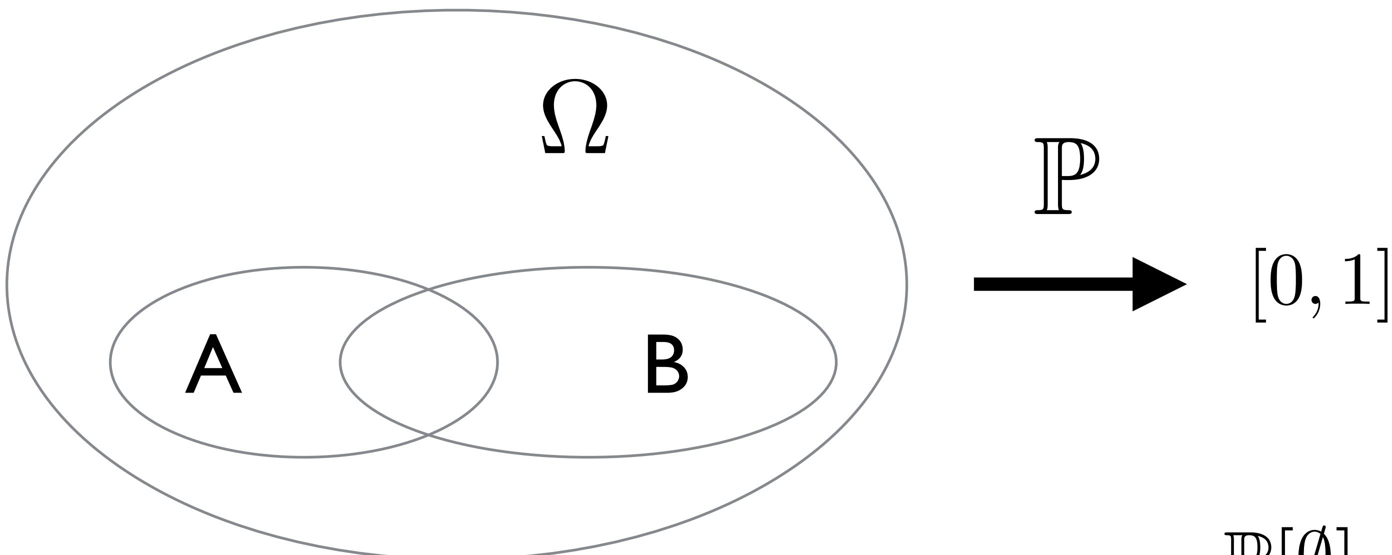


Particle separation

Falk Renth

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

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




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

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

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

# Expectation values of random variables

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

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

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

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

# This course simply:

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

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

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