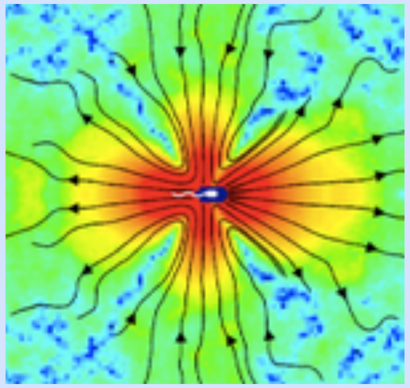
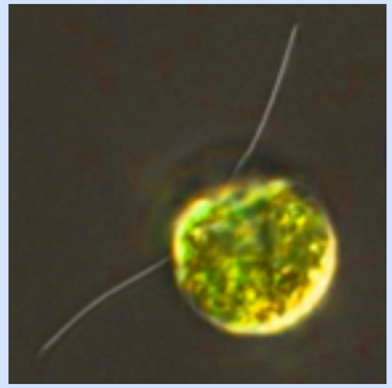
18.095 IAP Maths Lecture Series

Over-damped dynamics of small objects in fluids

Jörn Dunkel
Physical Applied Math

Fluid dynamics of microorganisms

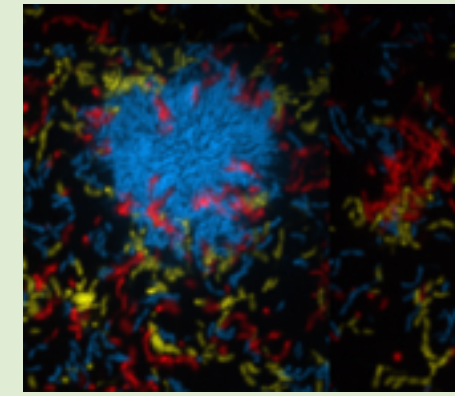




Goldstein group

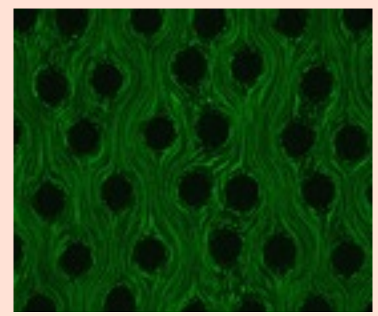
UNIVERSITY OF CAMBRIDGE

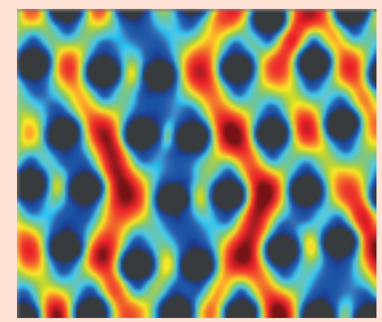
Biofilm formation



Drescher lab

Microbial transport in porous media





Guasto lab

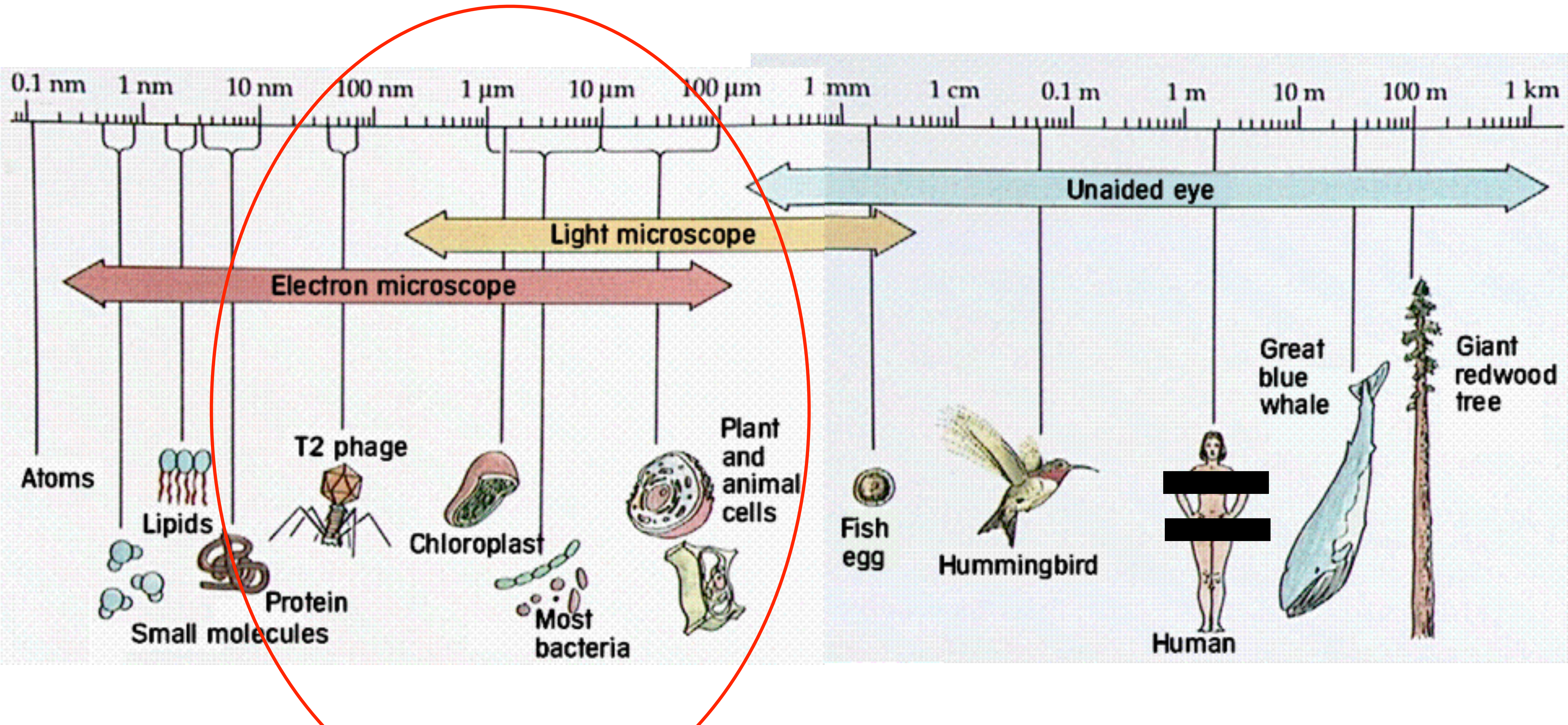
Surface wrinkling

Reis lab

Biological pattern formation

Gregor lab

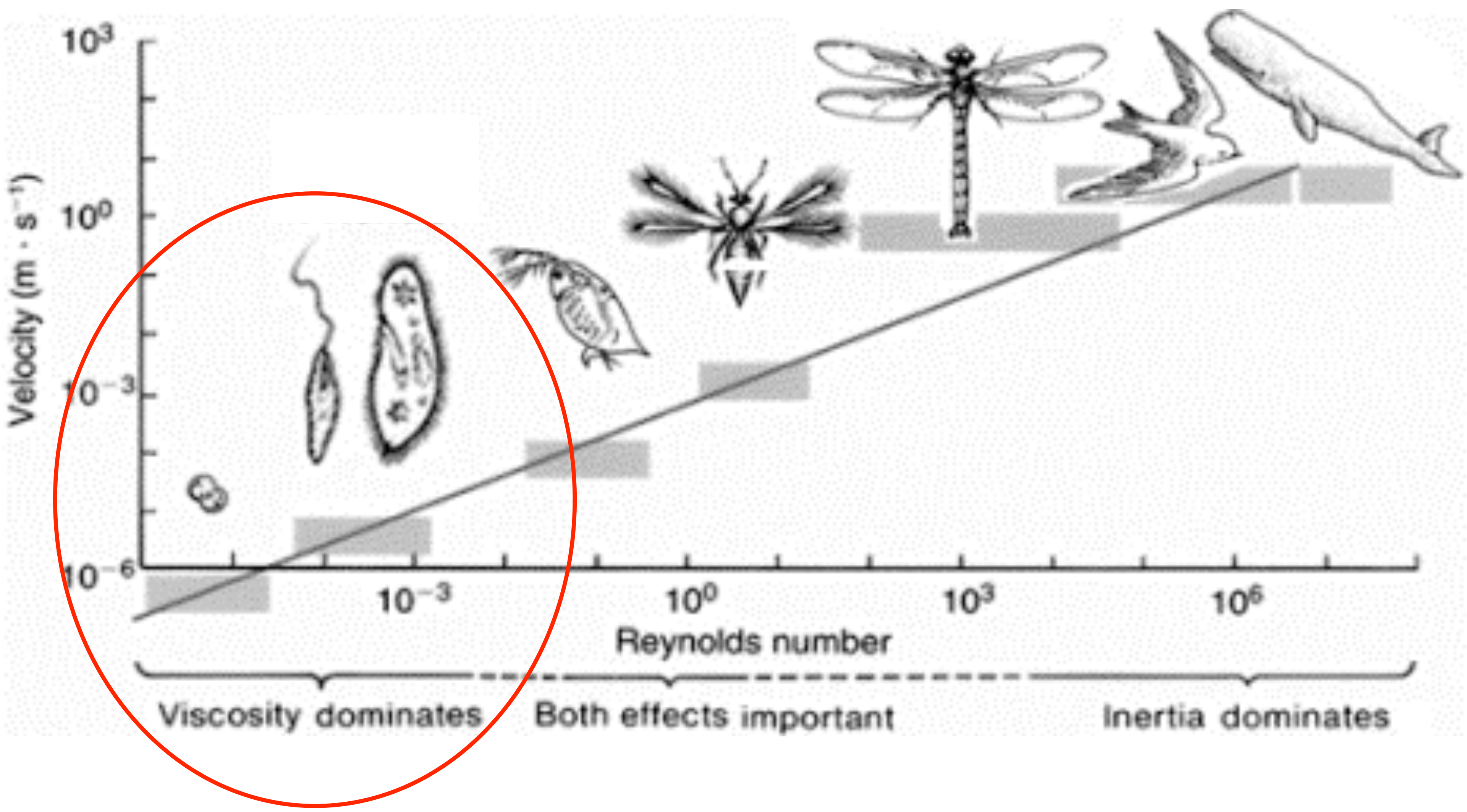
Typical length scales



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

Reynolds numbers

$$Re = \frac{\rho U L}{\mu} = \frac{U L}{\nu}$$



Laminar (low-Re) flow

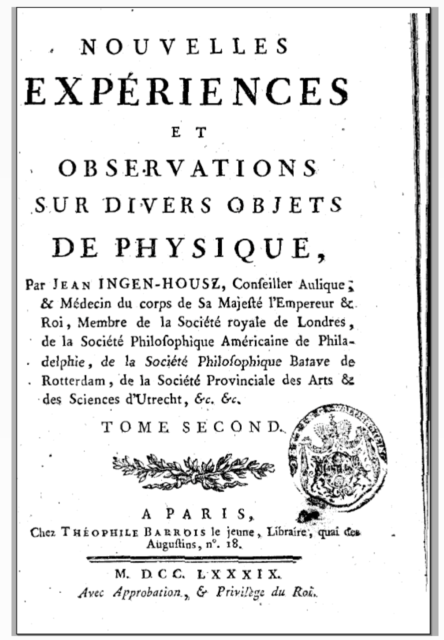
For $Re \rightarrow 0$
fluid flow becomes
reversible !

... except for thermal
fluctuations

Brownian motion

"Brownian" motion

Jan Ingen-Housz (1730-1799)



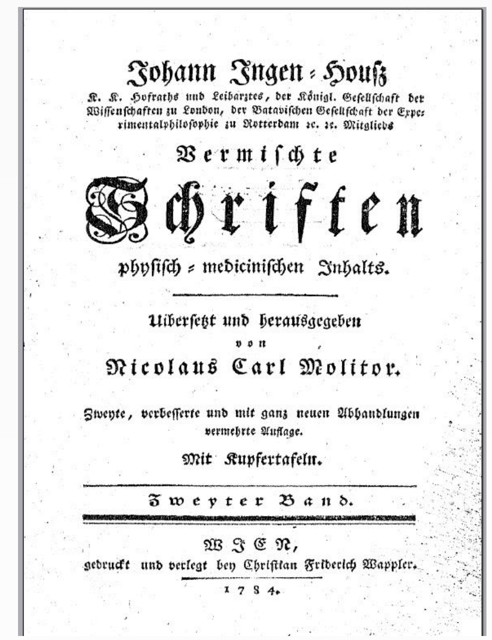
NOUVELLES
EXPÉRIENCES
ET
OBSERVATIONS
SUR DIVERS OBJETS
DE PHYSIQUE,

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.

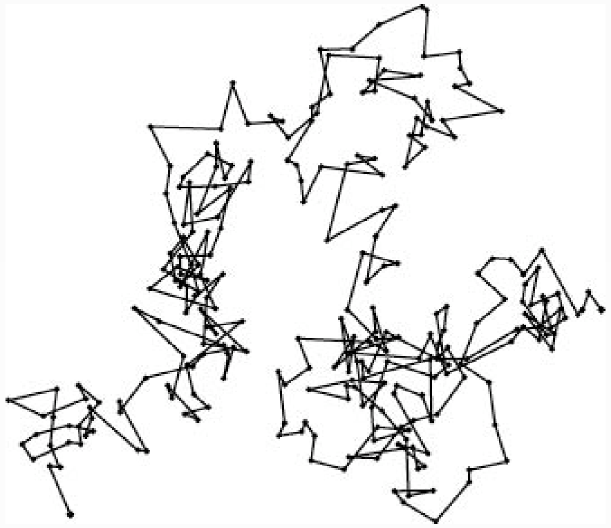
1784/1785:

> 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)

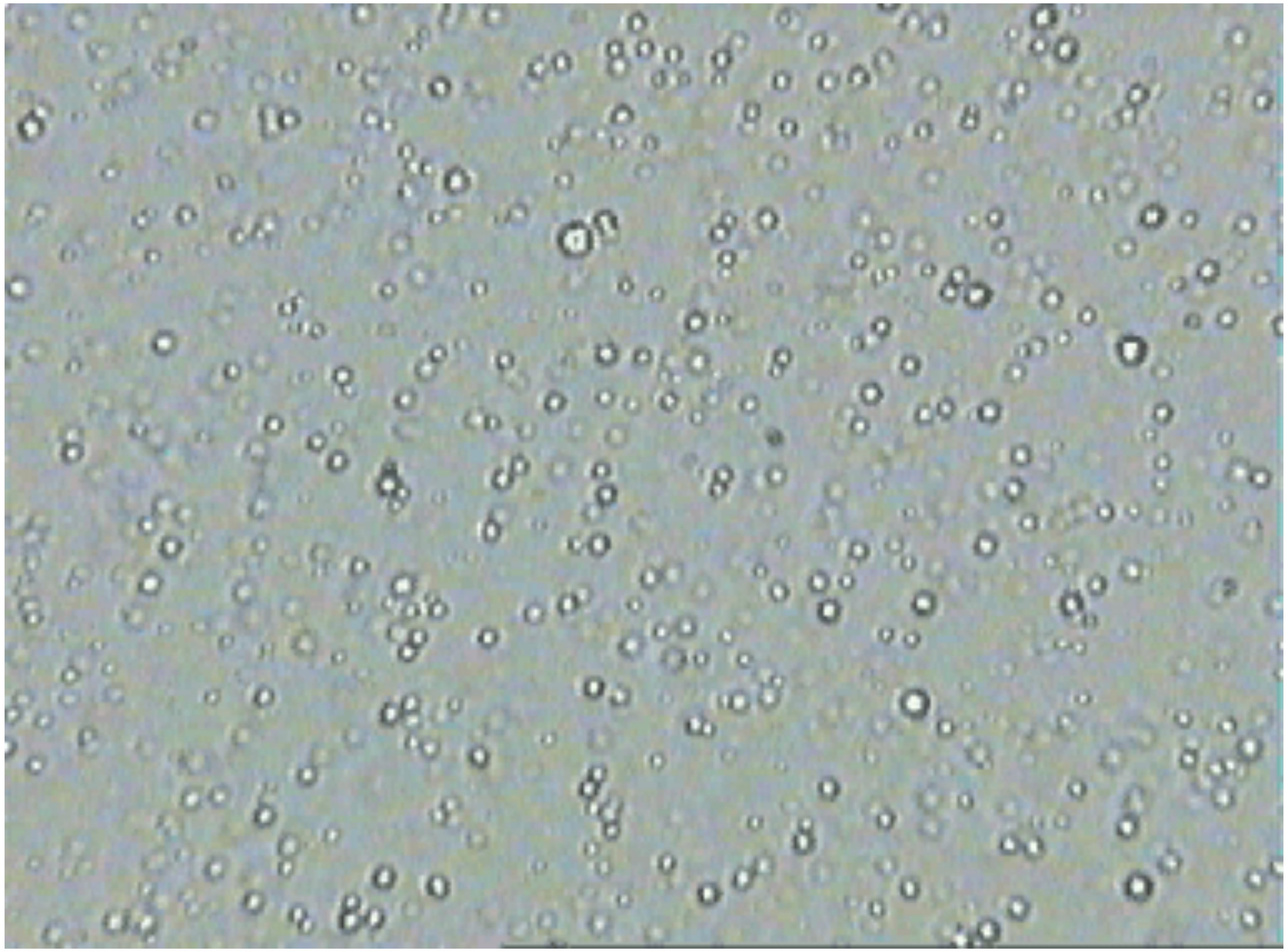
Linnean Society (London)



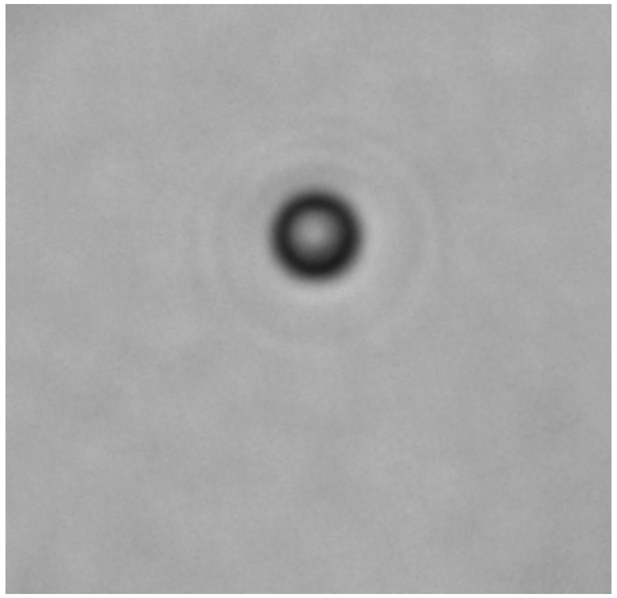
1827: irregular motion of pollen in fluid

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

Brownian motion



David Walker



Mark Haw

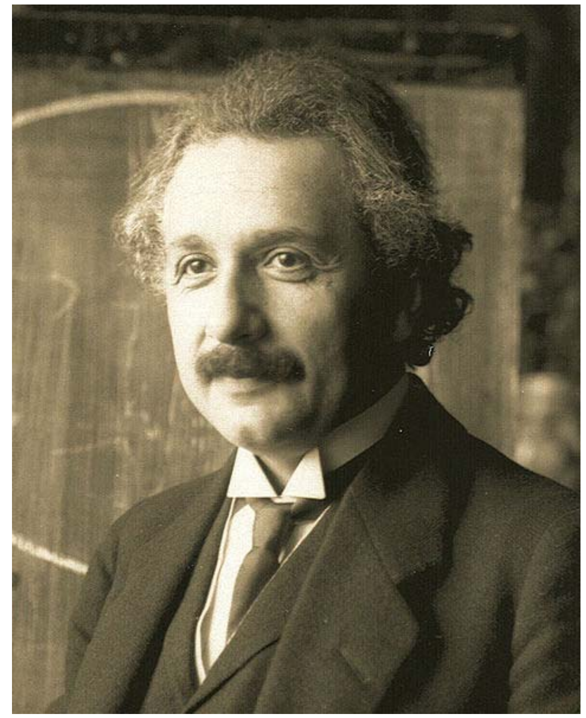
W. Sutherland (1858-1911)

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)

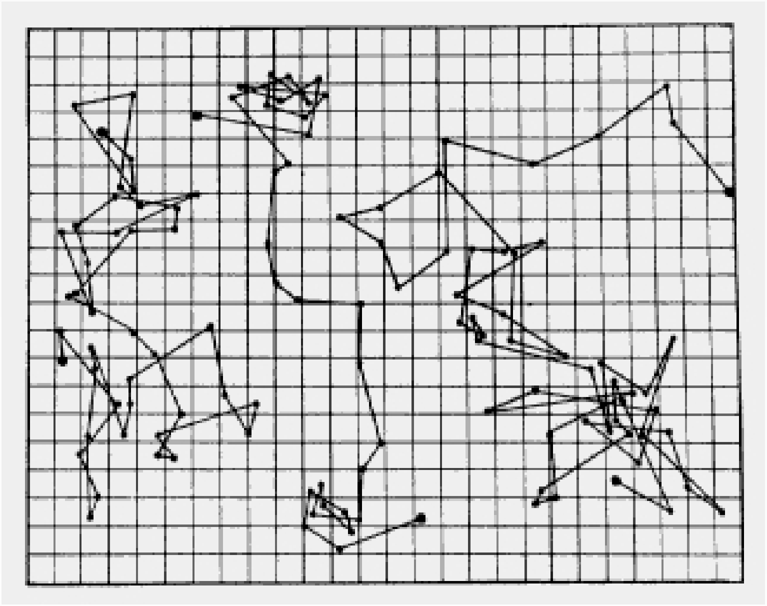
M. Smoluchowski (1872-1917)

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)

$$D = \frac{kT}{6\pi\eta_0 a}, \quad k = \frac{R}{N_A}$$

$$N_A = 6.56 \times 10^{23}$$

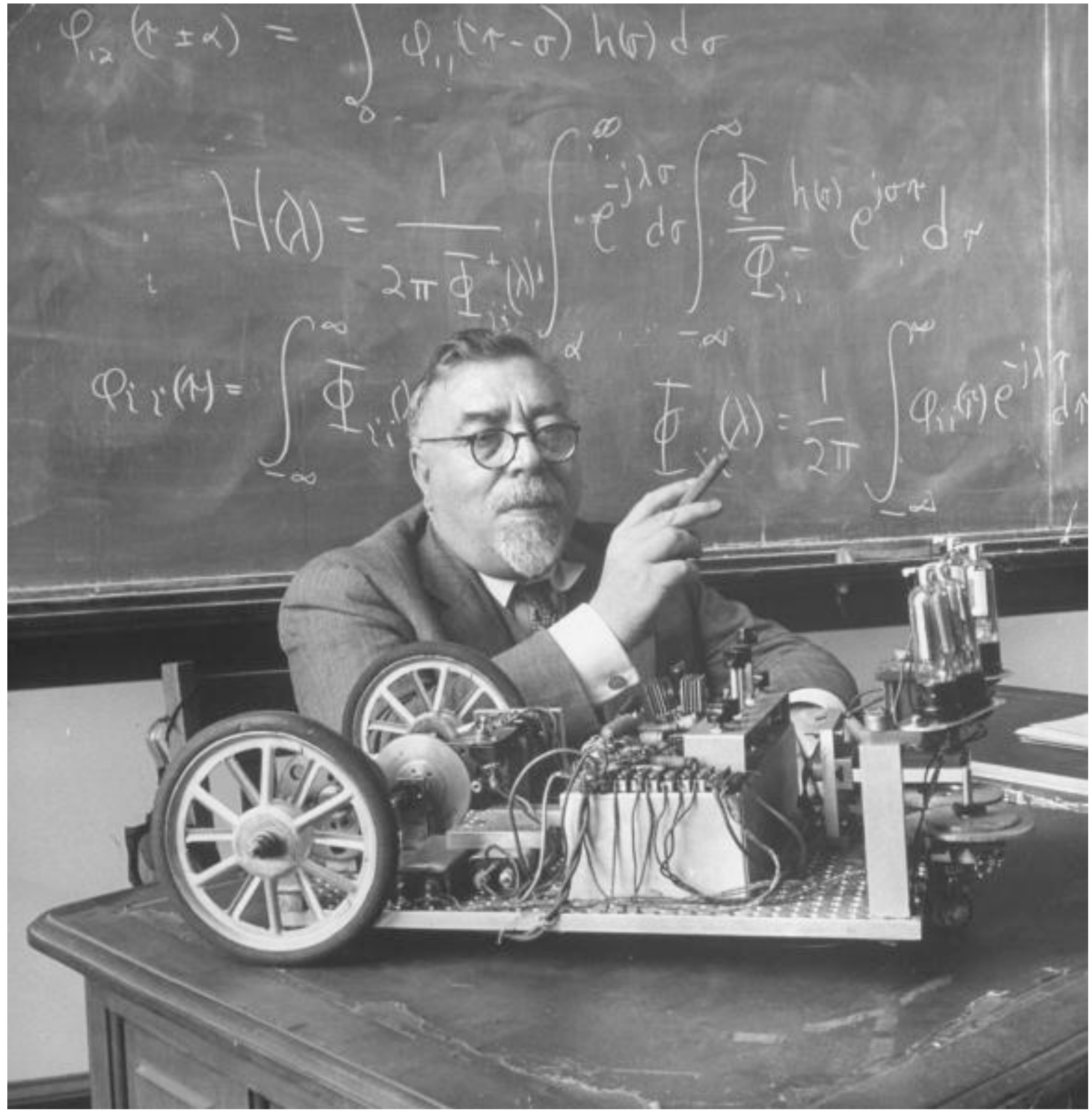
experimental evidence for atomistic structure of matter

Mathematical theory

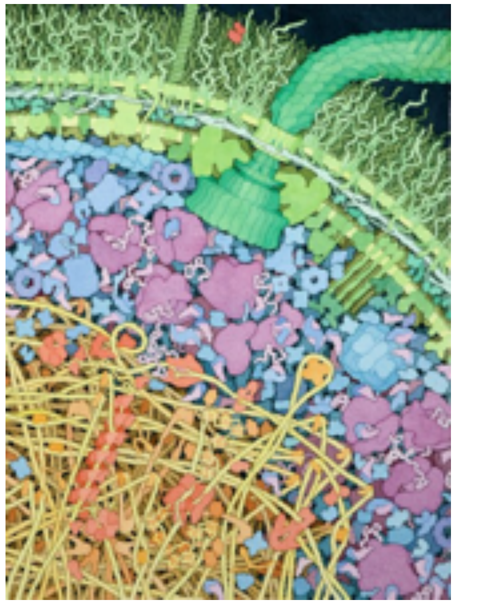
Norbert Wiener

(1894-1864)

MIT

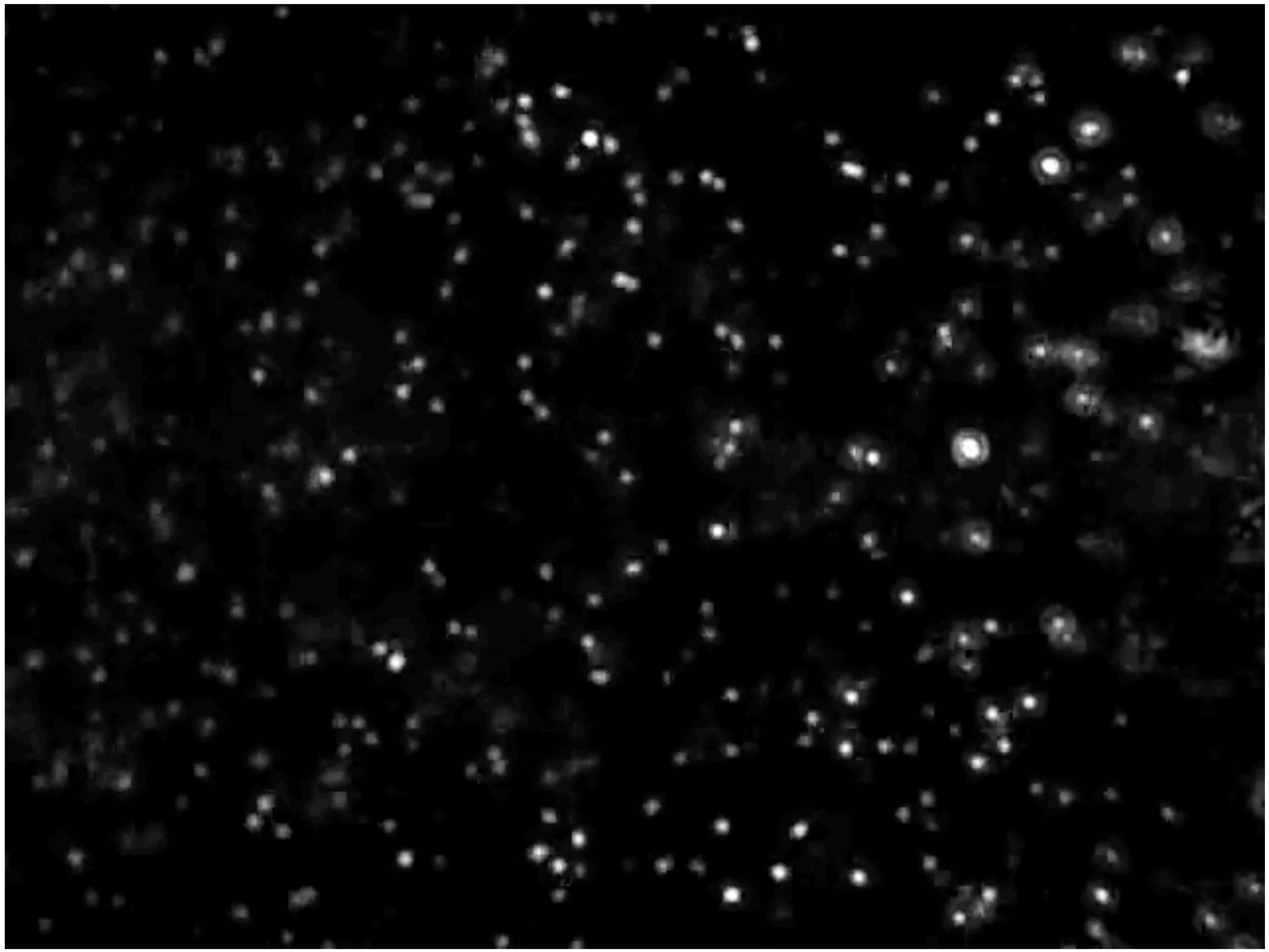


Relevance in biology



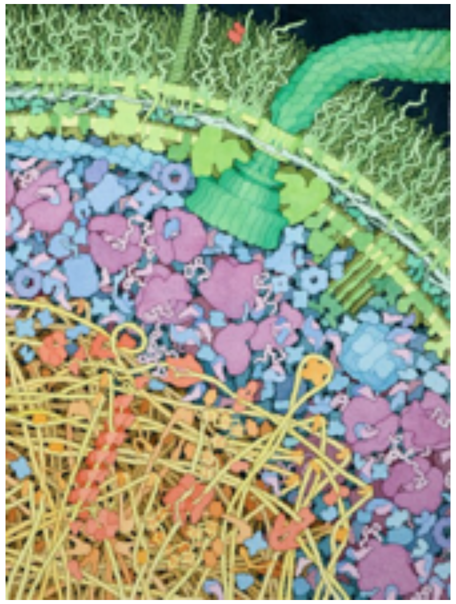
- intracellular transport
- intercellular transport
- microorganisms must beat BM to achieve directed locomotion
- tracer diffusion = important experimental “tool”
- generalized BMs (polymers, membranes, etc.)

Nano-spheres in water



Rutger Saly

Polymer in a fluid



Dogic lab
(Brandeis)

$< 1\mu m$

Ring-polymer in a fluid

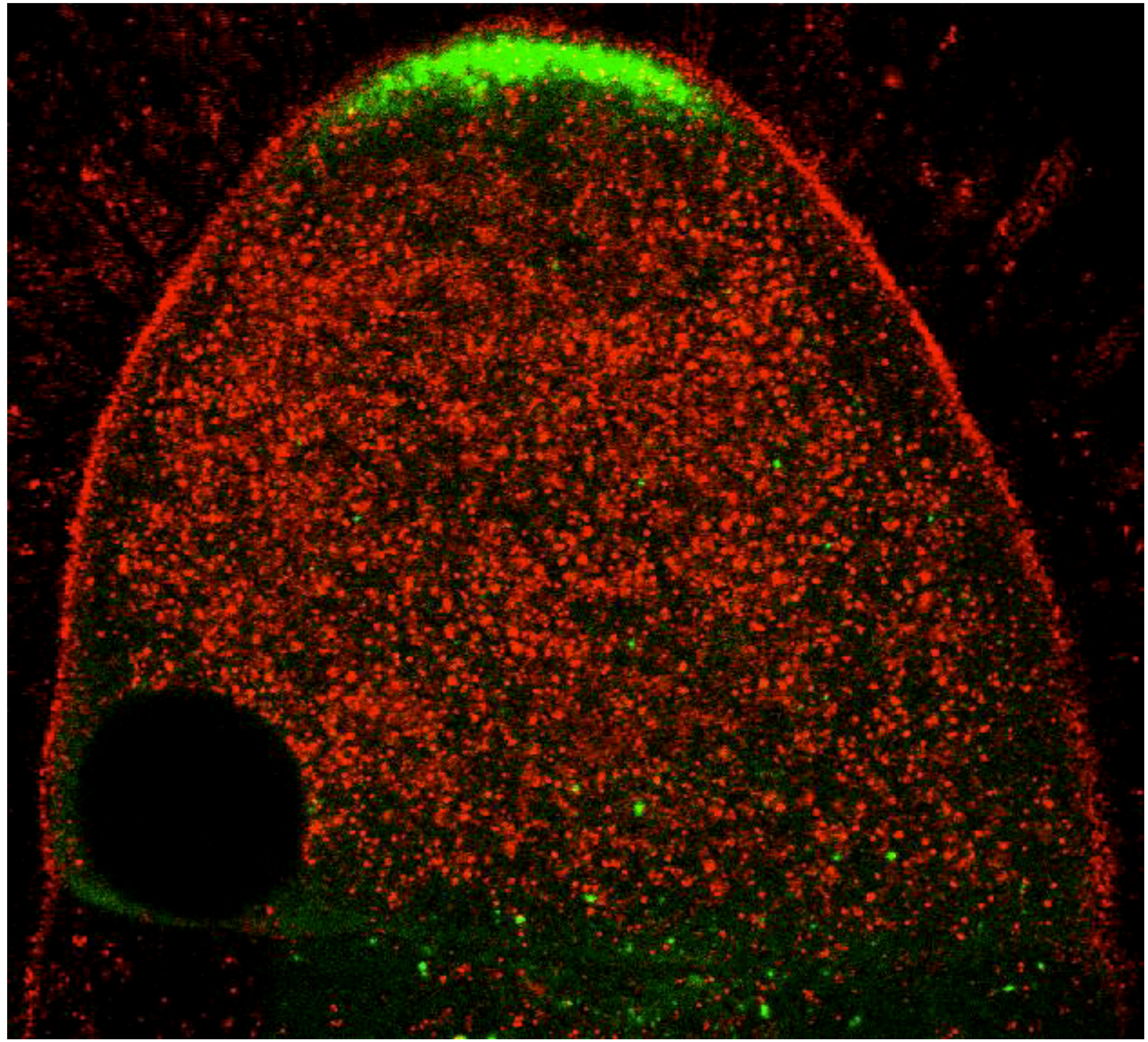
Dogic lab
(Brandeis)

$< 1\mu m$

Flow in cells

Flow & transport in cells

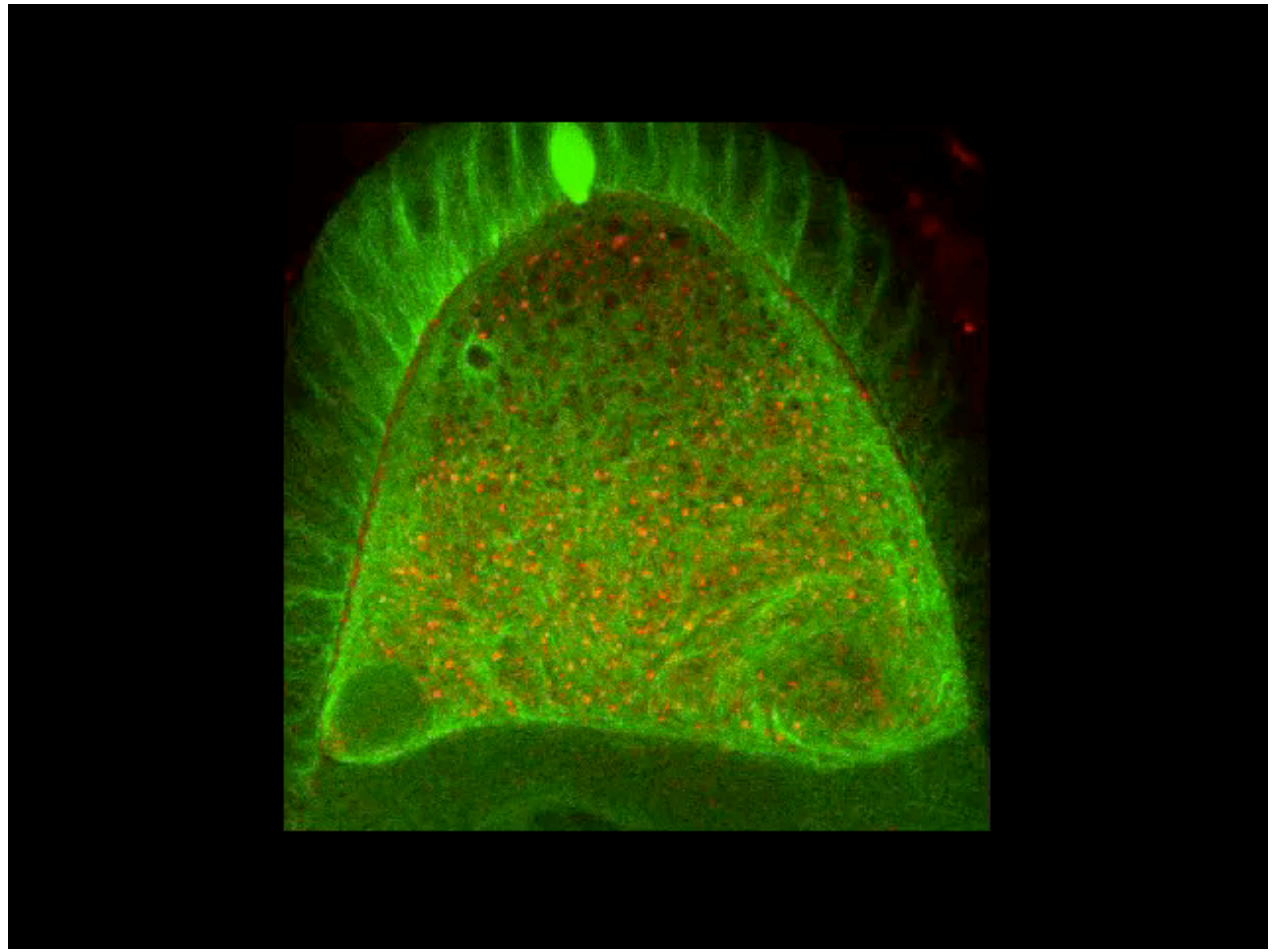
Drosophila
embryo



Goldstein lab (Cambridge)

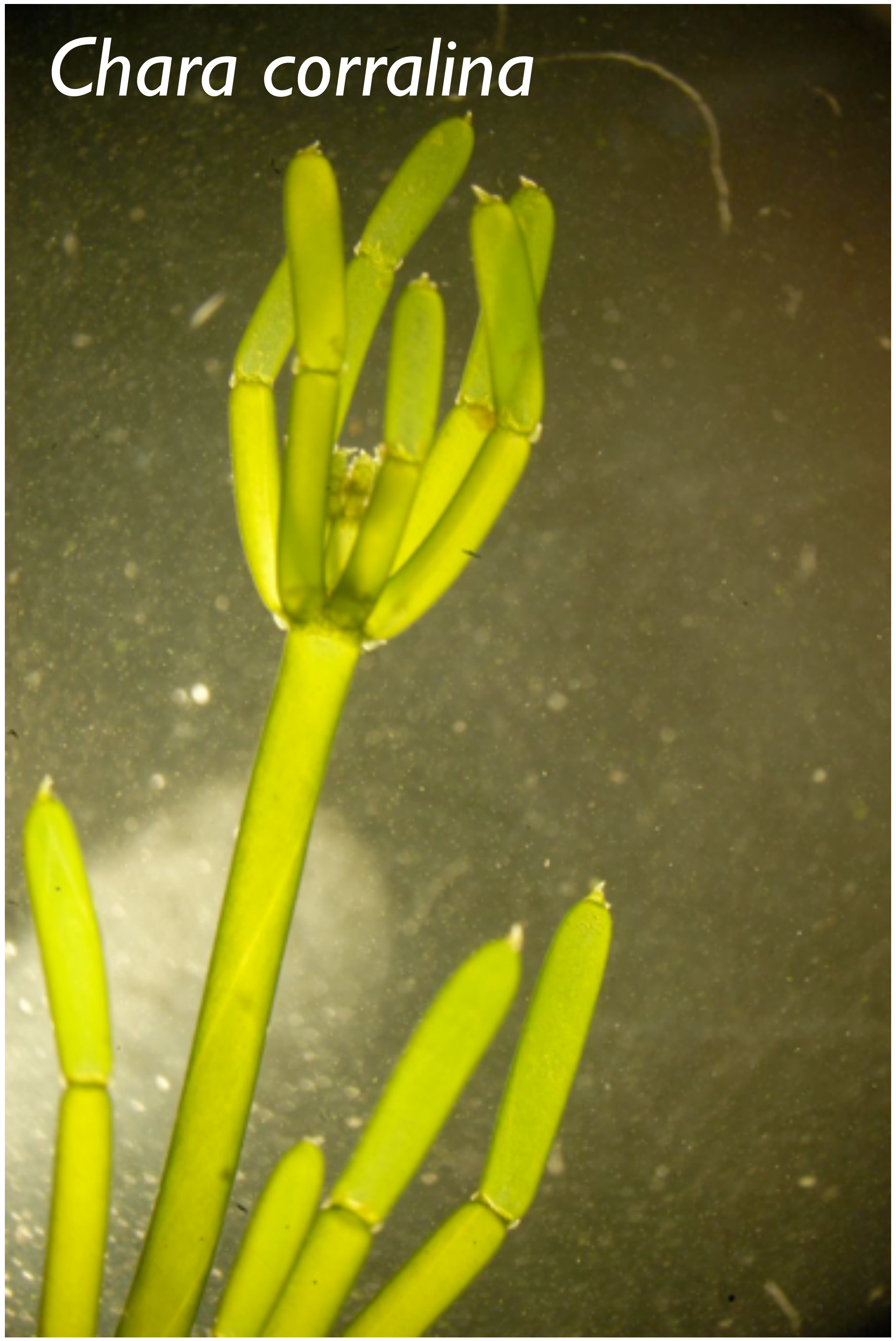
Flow & transport in cells

Drosophila
embryo



Goldstein lab (Cambridge)

Intracellular transport

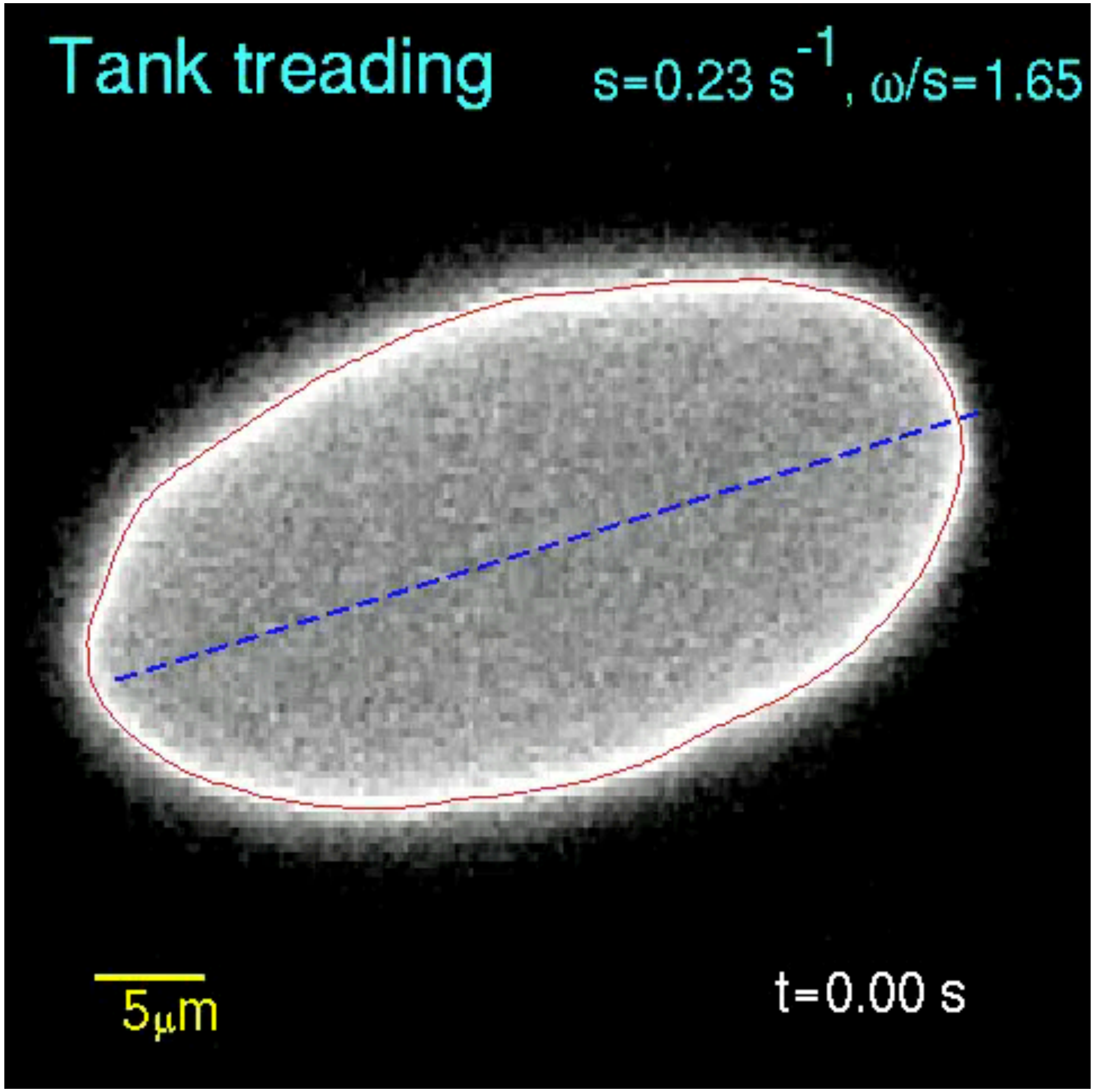


Giant cell

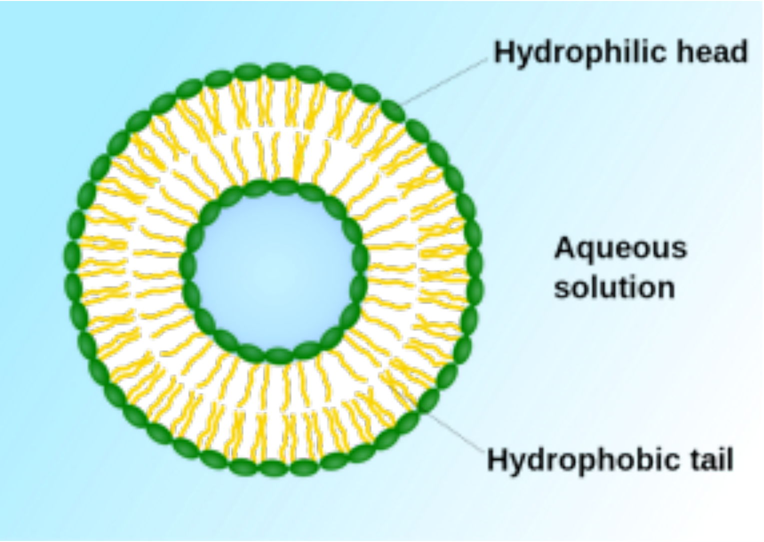
http://damtp.cam.ac.uk/user/gold/movies.html

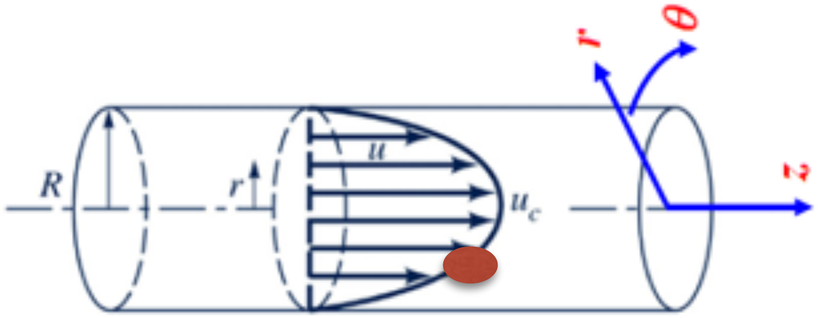
Flow around cells

Vesicles in a shear flow



Vasily Kantsler

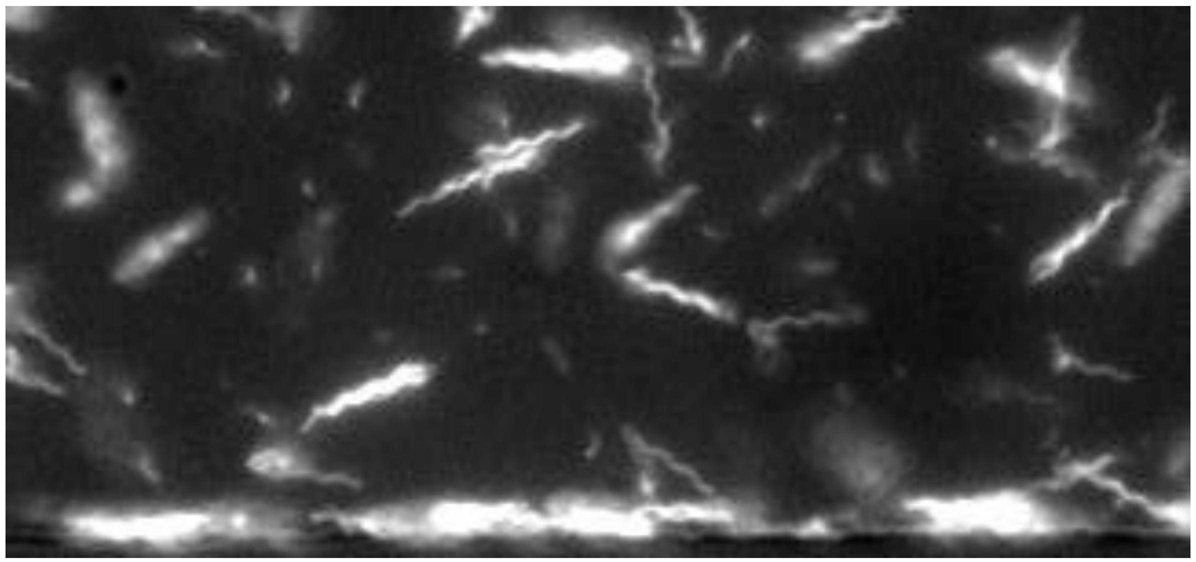




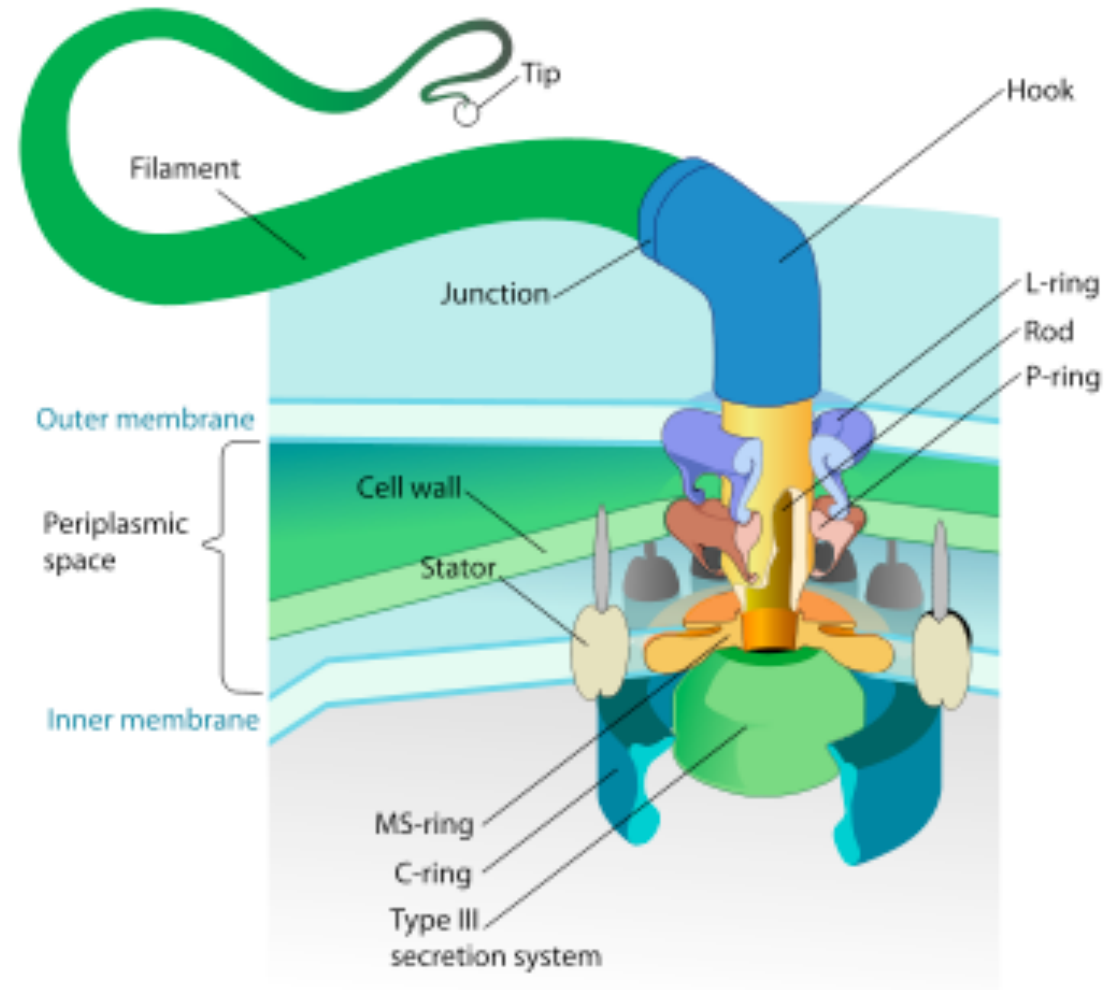
model for blood cells dynamics

Swimming bacteria

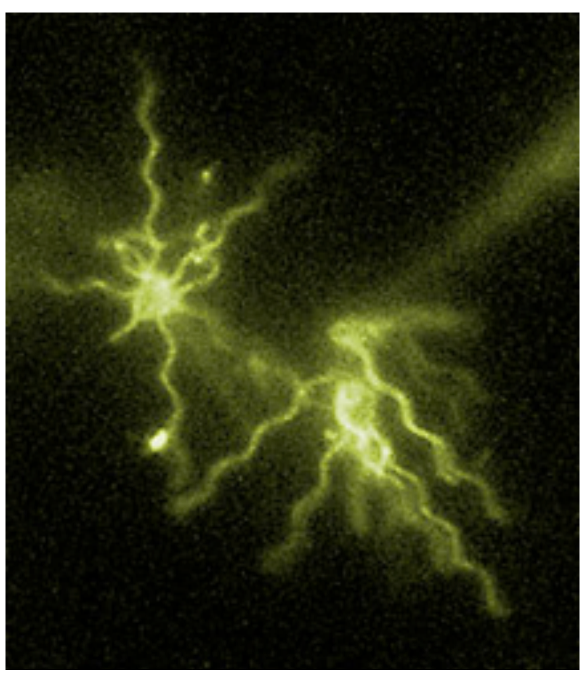
movie: V. Kantsler



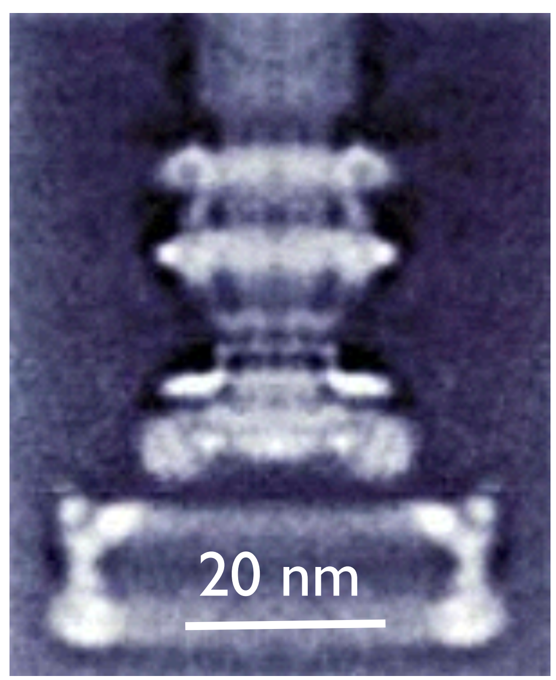
~20 parts



source: wiki



Berg (1999) Physics Today



Chen et al (2011) EMBO Journal

dunkel@math.mit.edu

How fast must a cell swim to beat Brownian motion?

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

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

$$kT = 4 \times 10^{-21}\,\mathrm{J}$$

$$a \sim 1\mu m$$

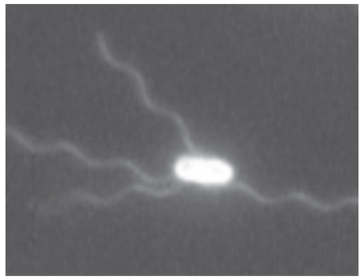
$$\gamma_S = 6\pi\eta a \sim 2 \times 10^{-8}\,\mathrm{kg/s}$$

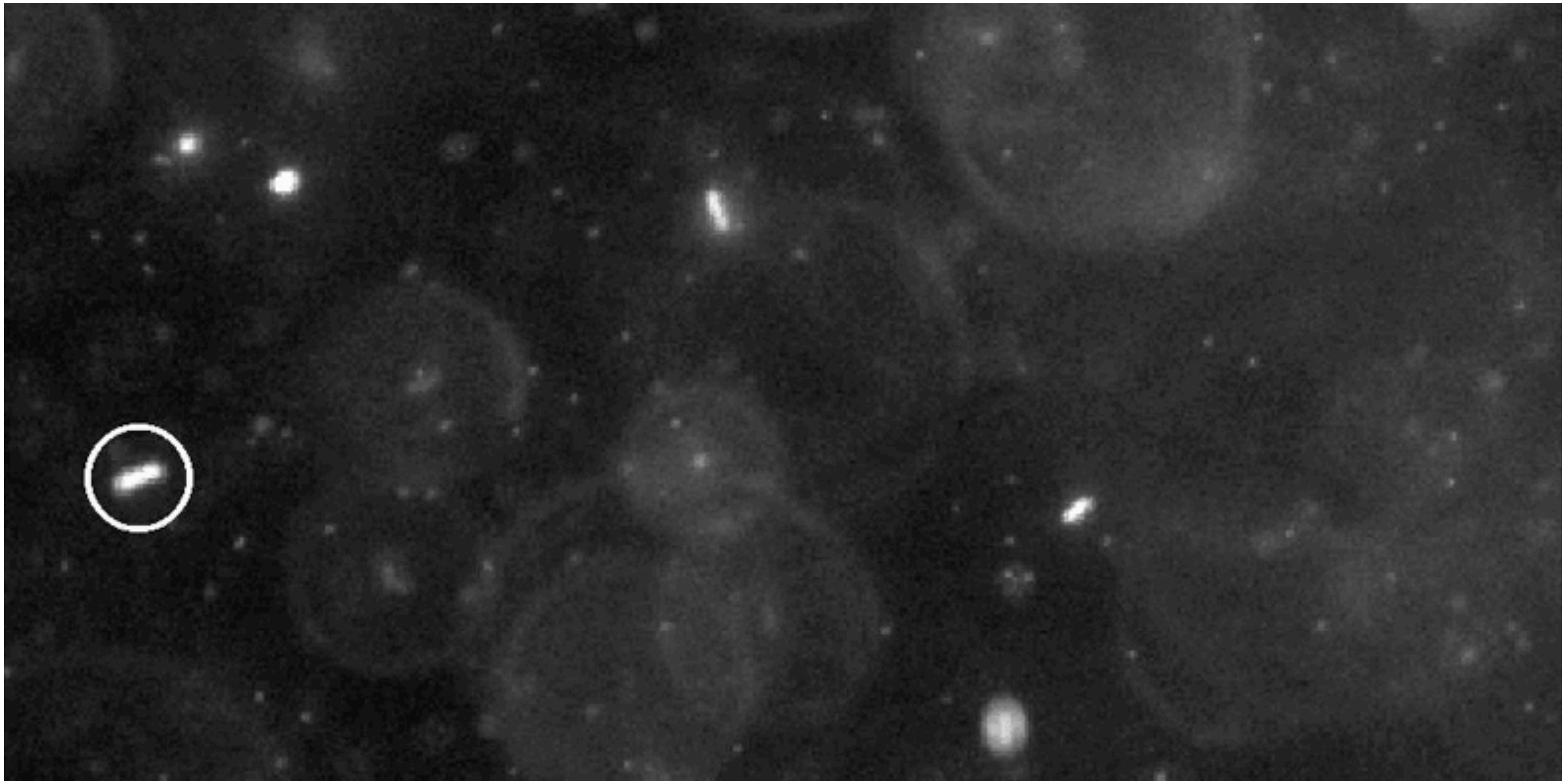
Hence, we find for the diffusion constant

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

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 μm/s, which is close to typical swim bacterial speeds.

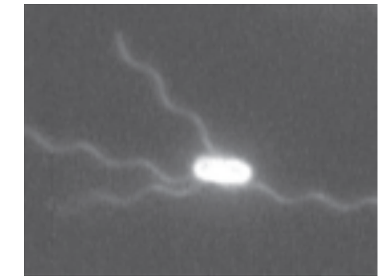
E.coli (non-tumbling HCB 437)

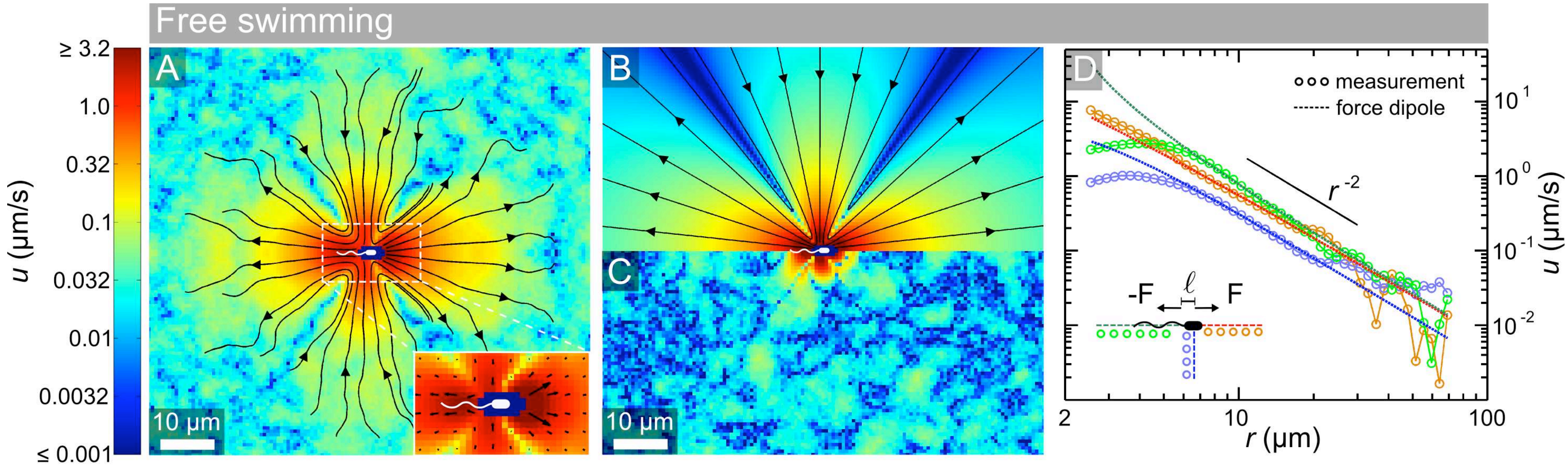




Drescher, Dunkel, Ganguly, Cisneros, Goldstein (2011) PNAS

E.coli (non-tumbling HCB 437)





$$\boldsymbol{u}(\boldsymbol{r}) = \frac{A}{|\boldsymbol{r}|^2}\left[3(\hat{\boldsymbol{r}}.\hat{\boldsymbol{d}})^2 - 1\right]\hat{\boldsymbol{r}}, \quad A = \frac{\ell F}{8\pi\eta}, \quad \hat{\boldsymbol{r}} = \frac{\boldsymbol{r}}{|\boldsymbol{r}|}$$

$$V_0 = 22 \pm 5 \ \ \mu\text{m/s}$$

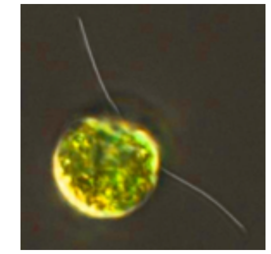
$$\ell = 1.9 \ \mu\text{m}$$

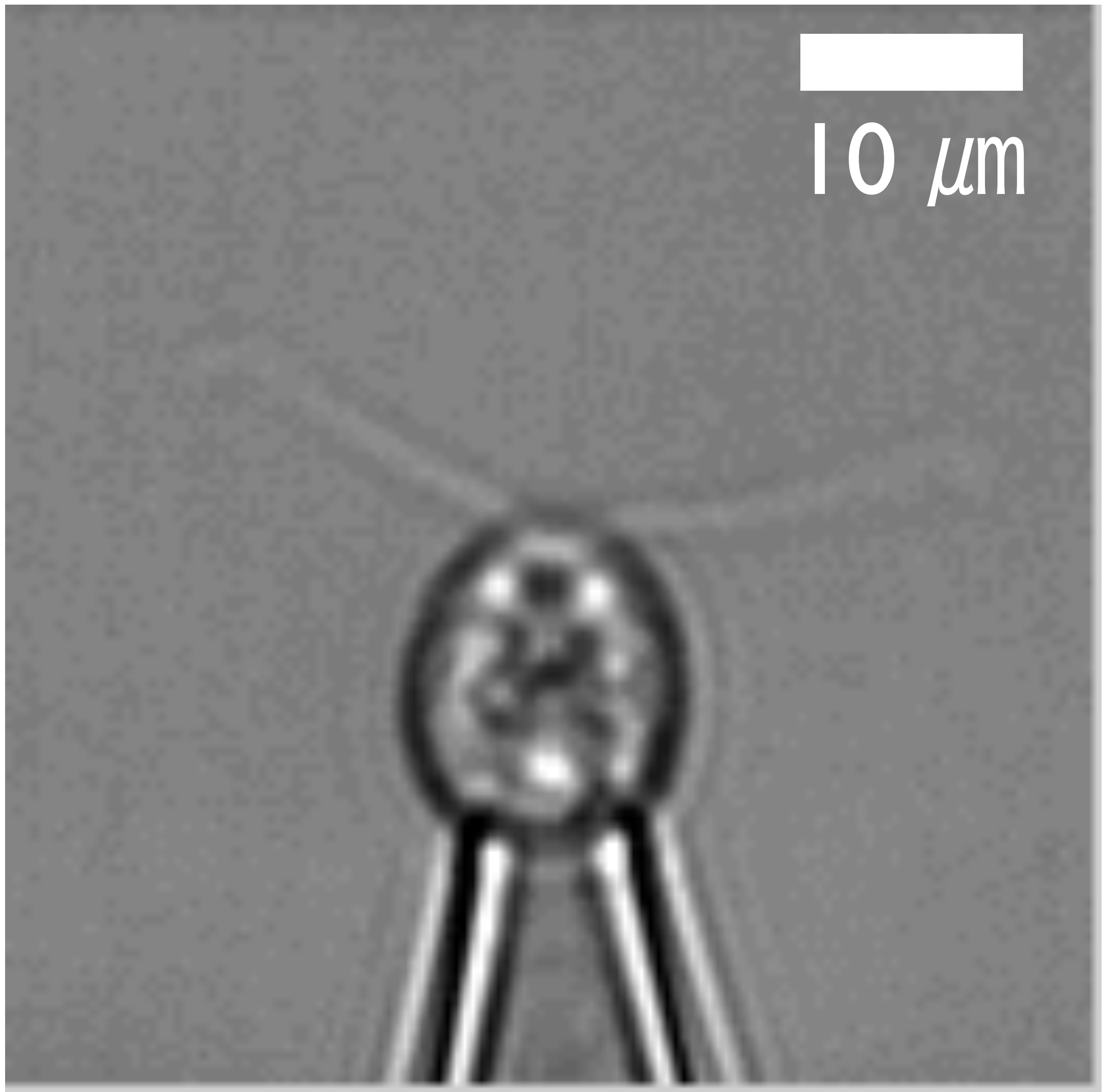
$$F = 0.42 \ \text{pN}$$

weak 'pusher' dipole

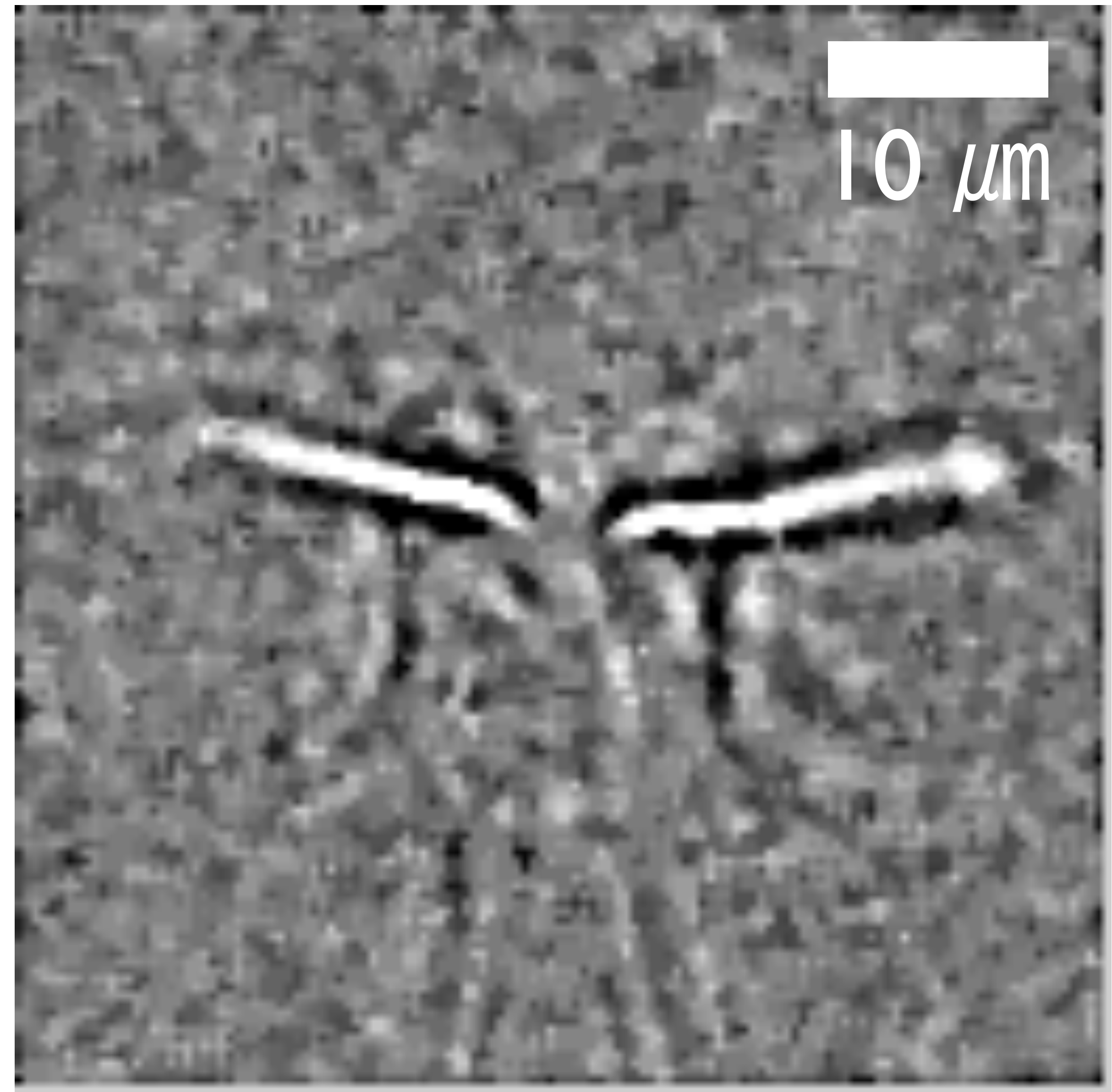
Drescher, Dunkel, Ganguly, Cisneros, Goldstein (2011) PNAS

Chlamydomonas alga





~ 50 beats / sec



speed ~100 μm/s

Goldstein et al (2011) PRL

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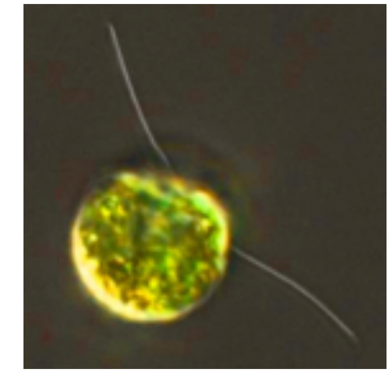
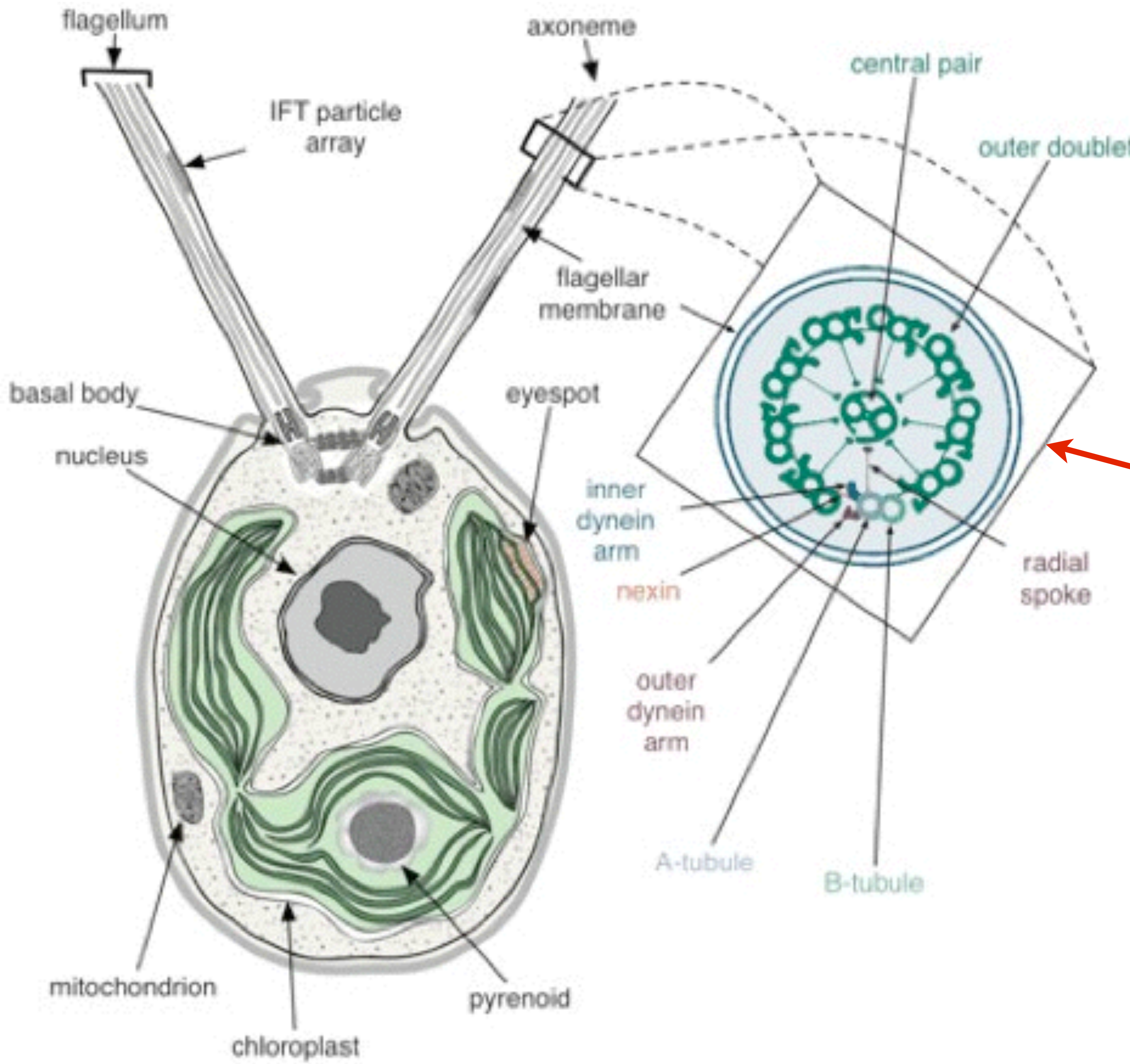
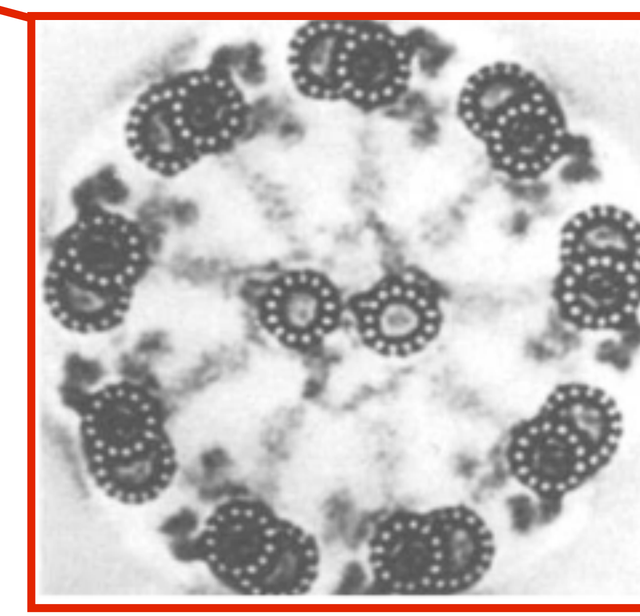
Chlamydomonas







Merchant et al (2007) Science

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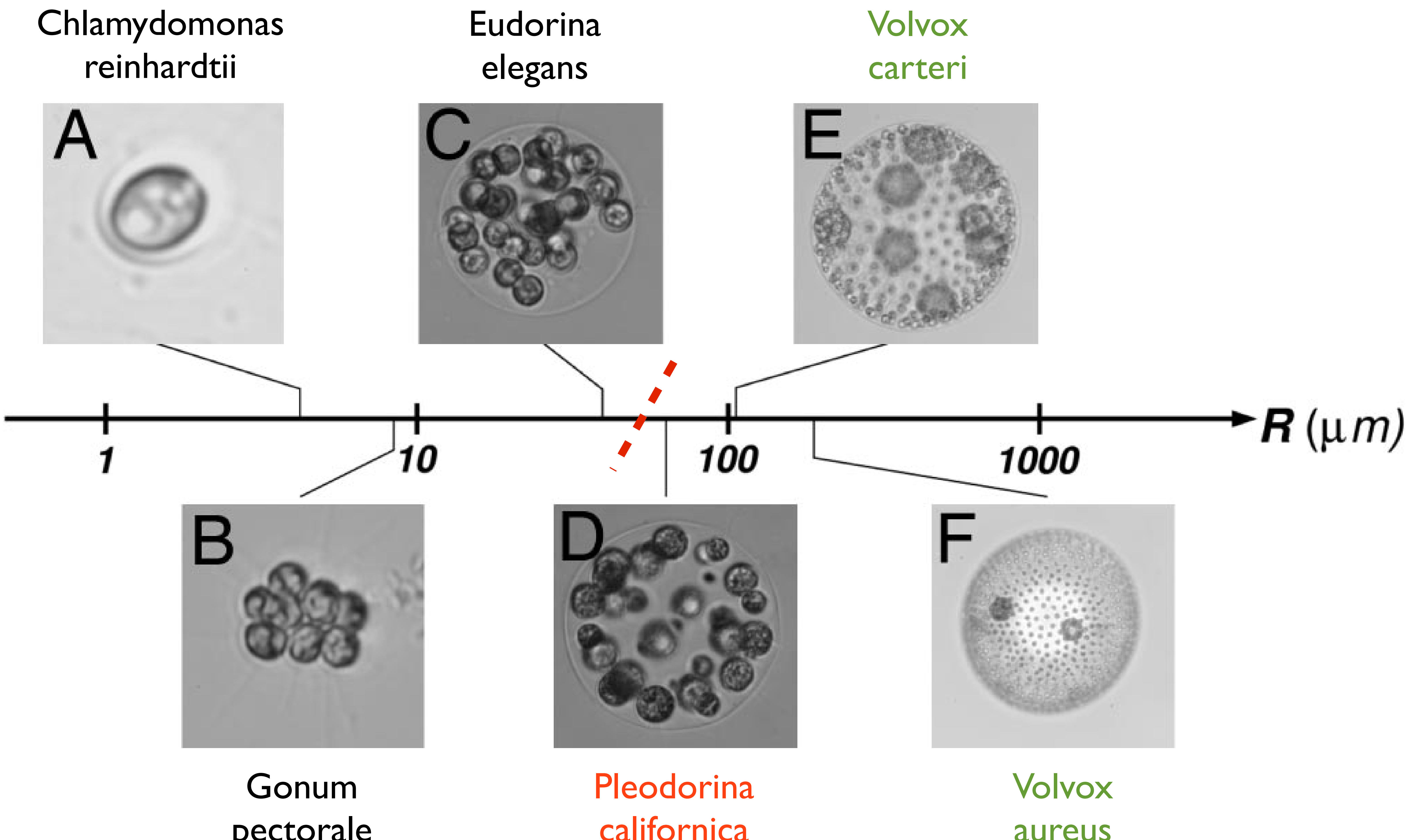
Evolution of multicellularity



Short et al, PNAS 2013

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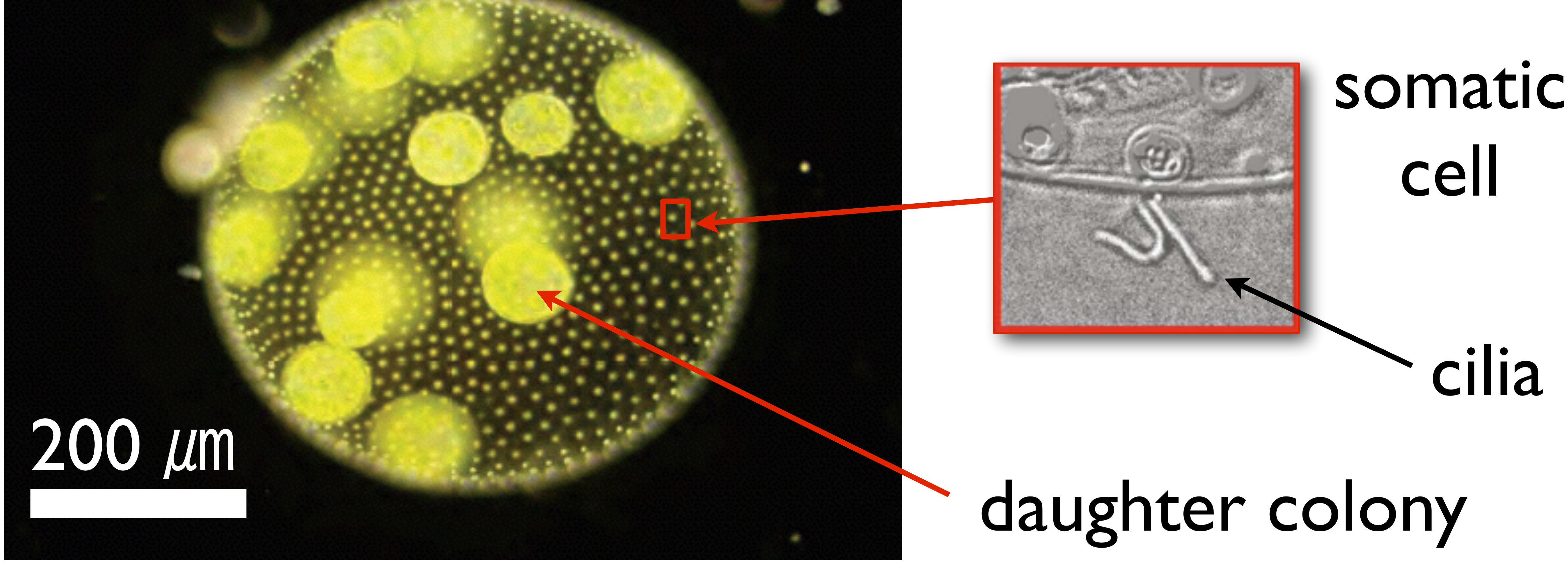
Volvox carteri



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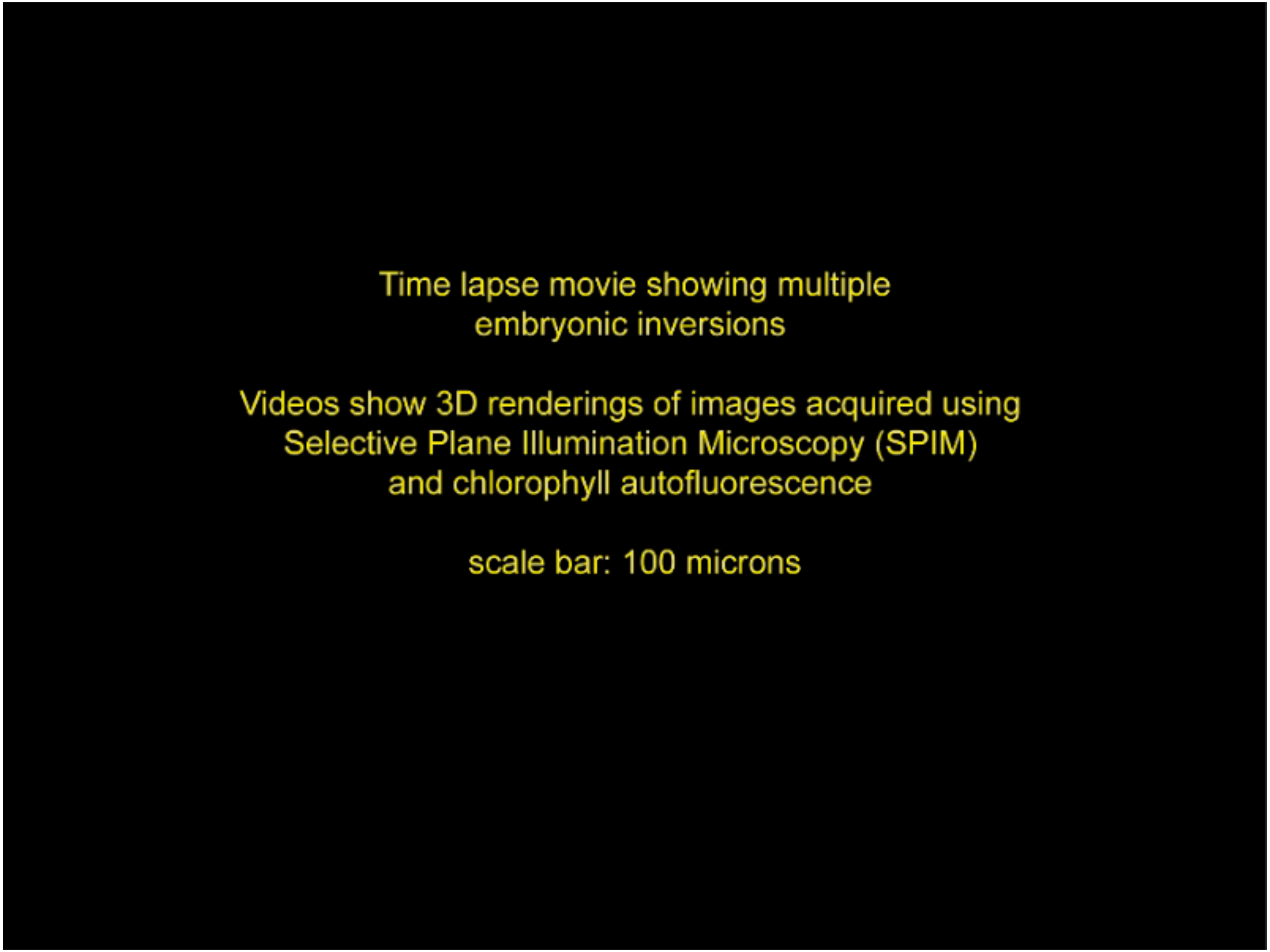
Asexual reproduction & inversion



2014 Goldstein lab

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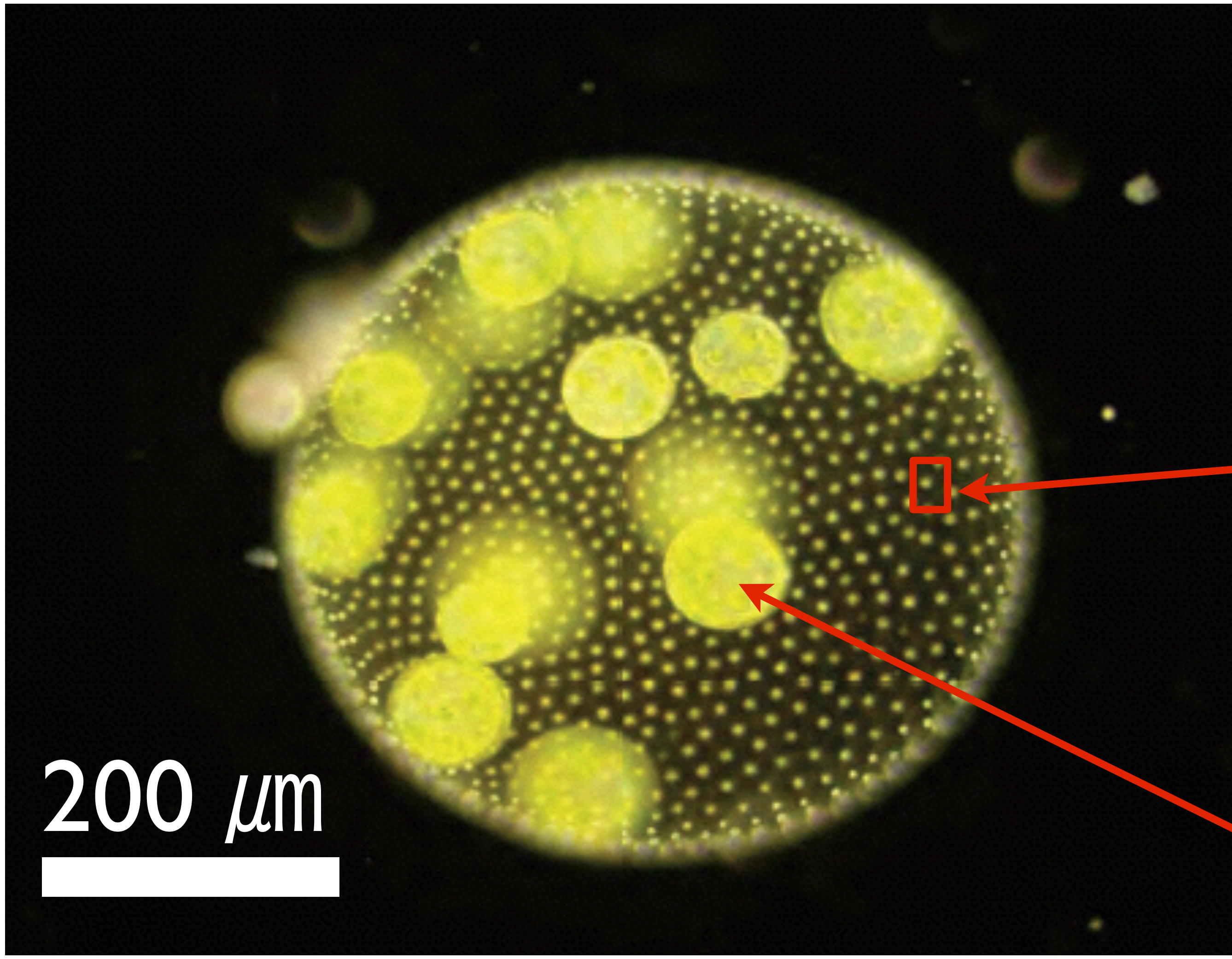
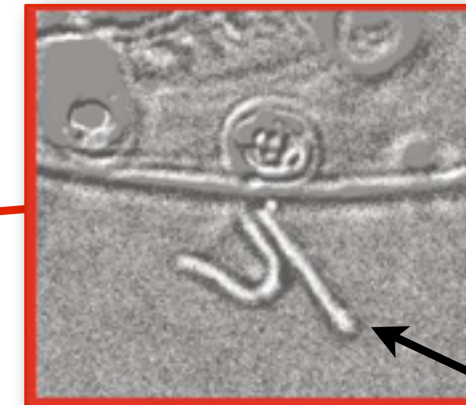
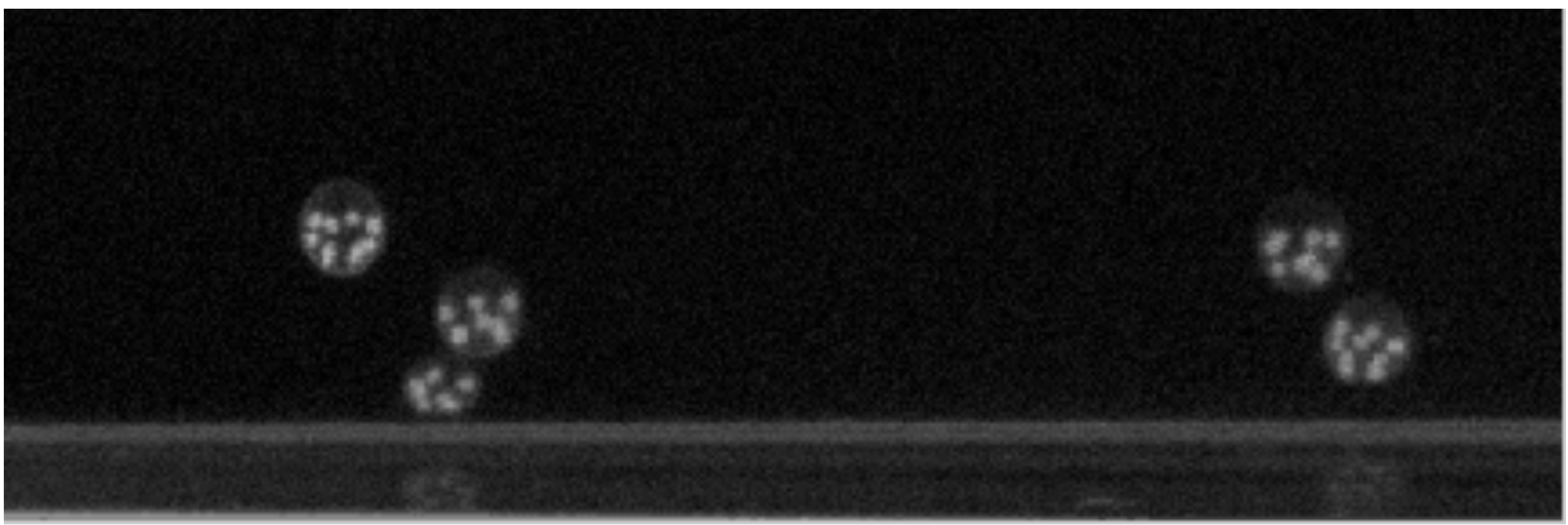
Volvox carteri

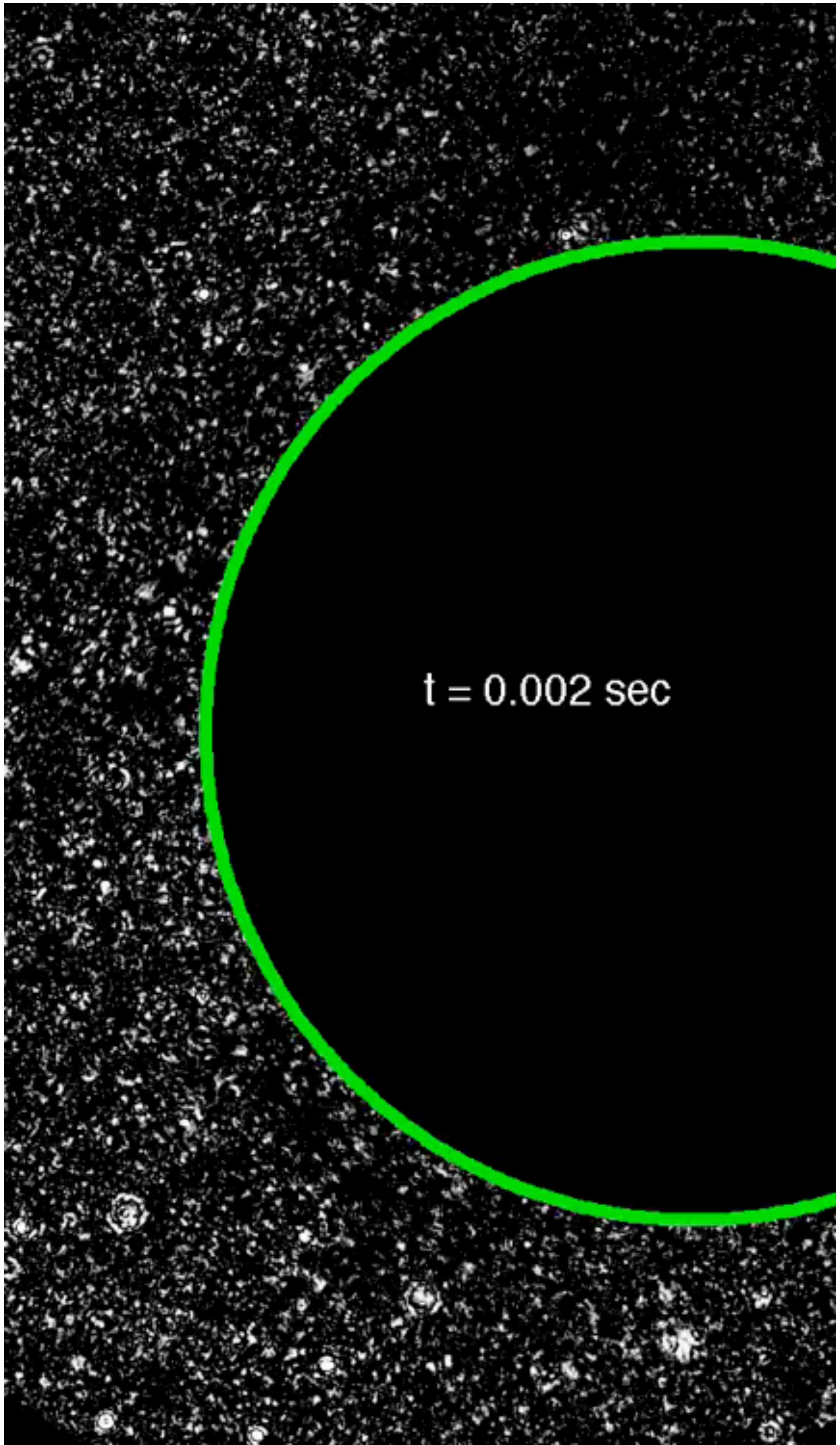






Drescher et al (2010) PRL

dunkel@math.mit.edu



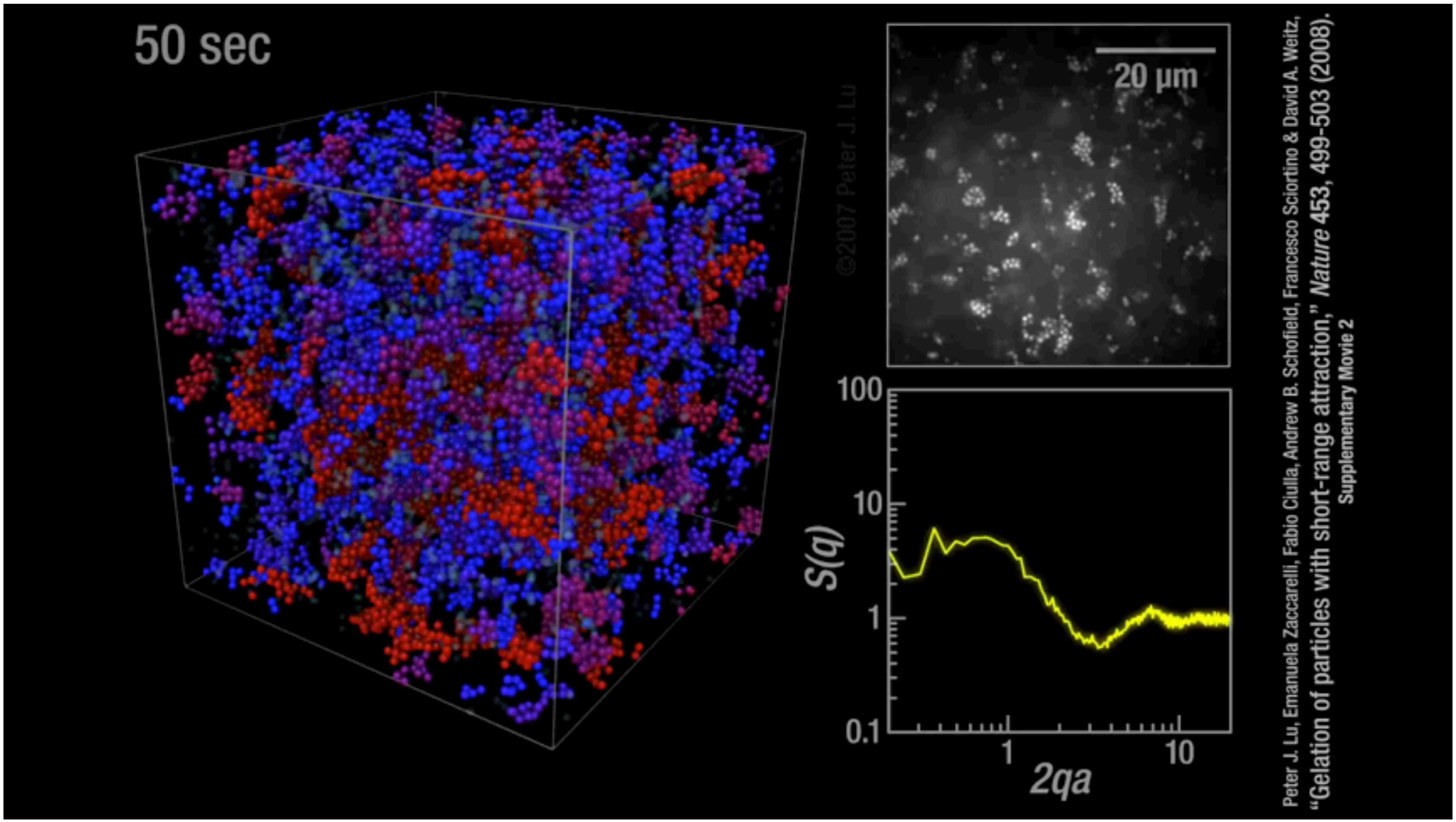
Volvox

Meta-chronal waves

Brumley et al (2012) PRL

Ecological implications
&
technical applications

Colloidal gel formation via spinodal decomposition (rapid demixing)



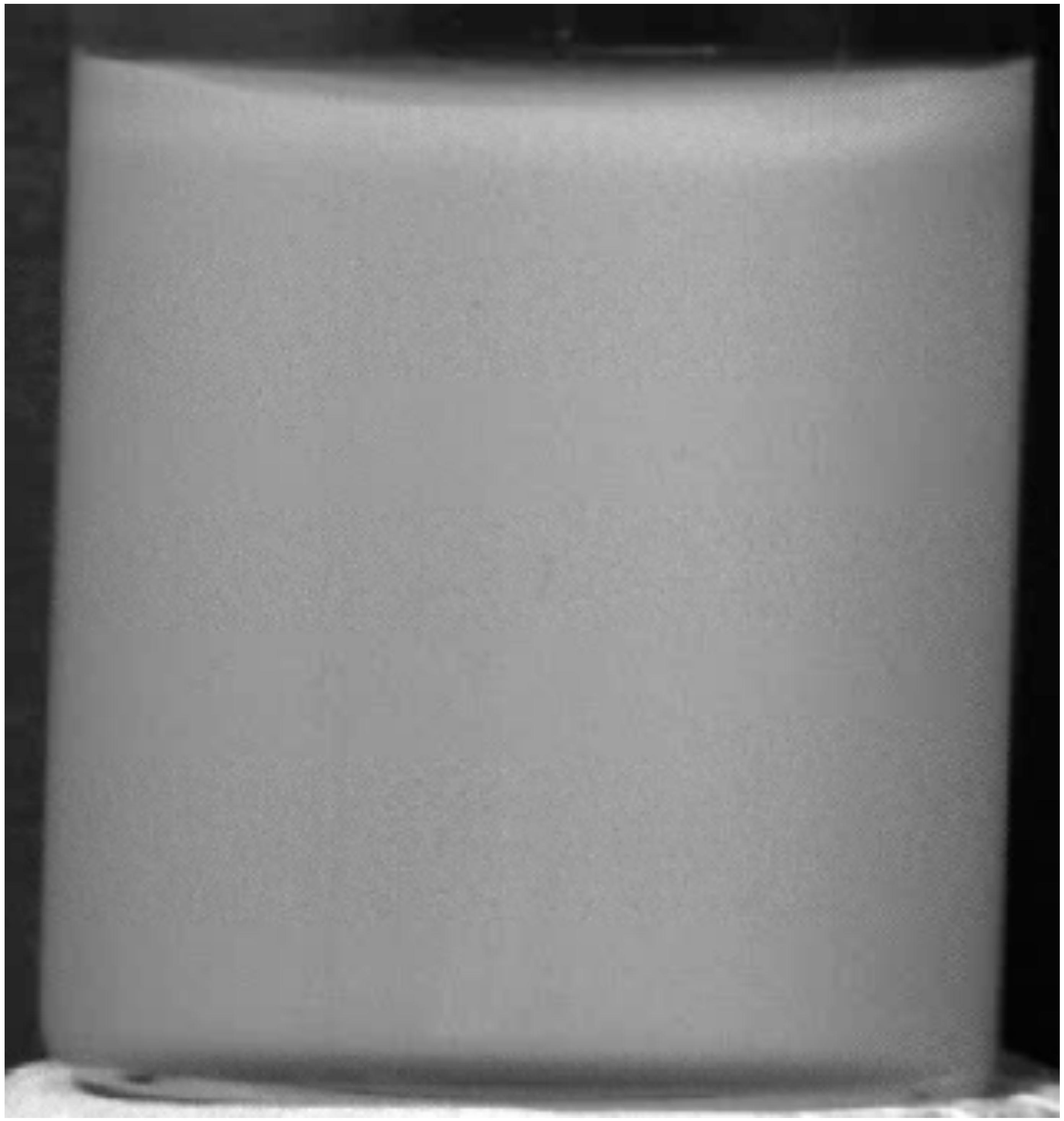
Peter Lu

Sedimentation

Mississippi

NASA Earth Observatory

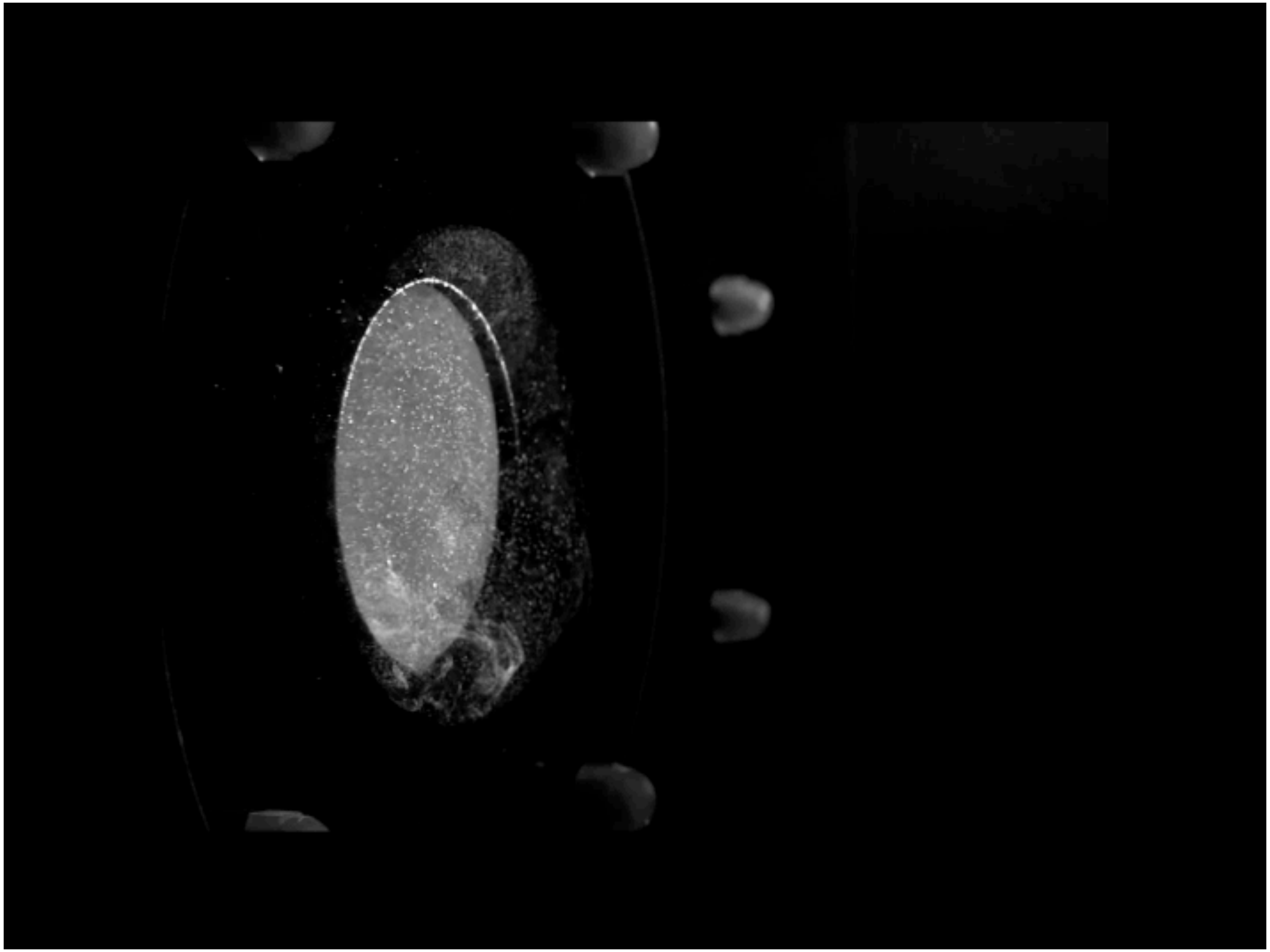
Sedimentation



Particle separation

Falk Renth

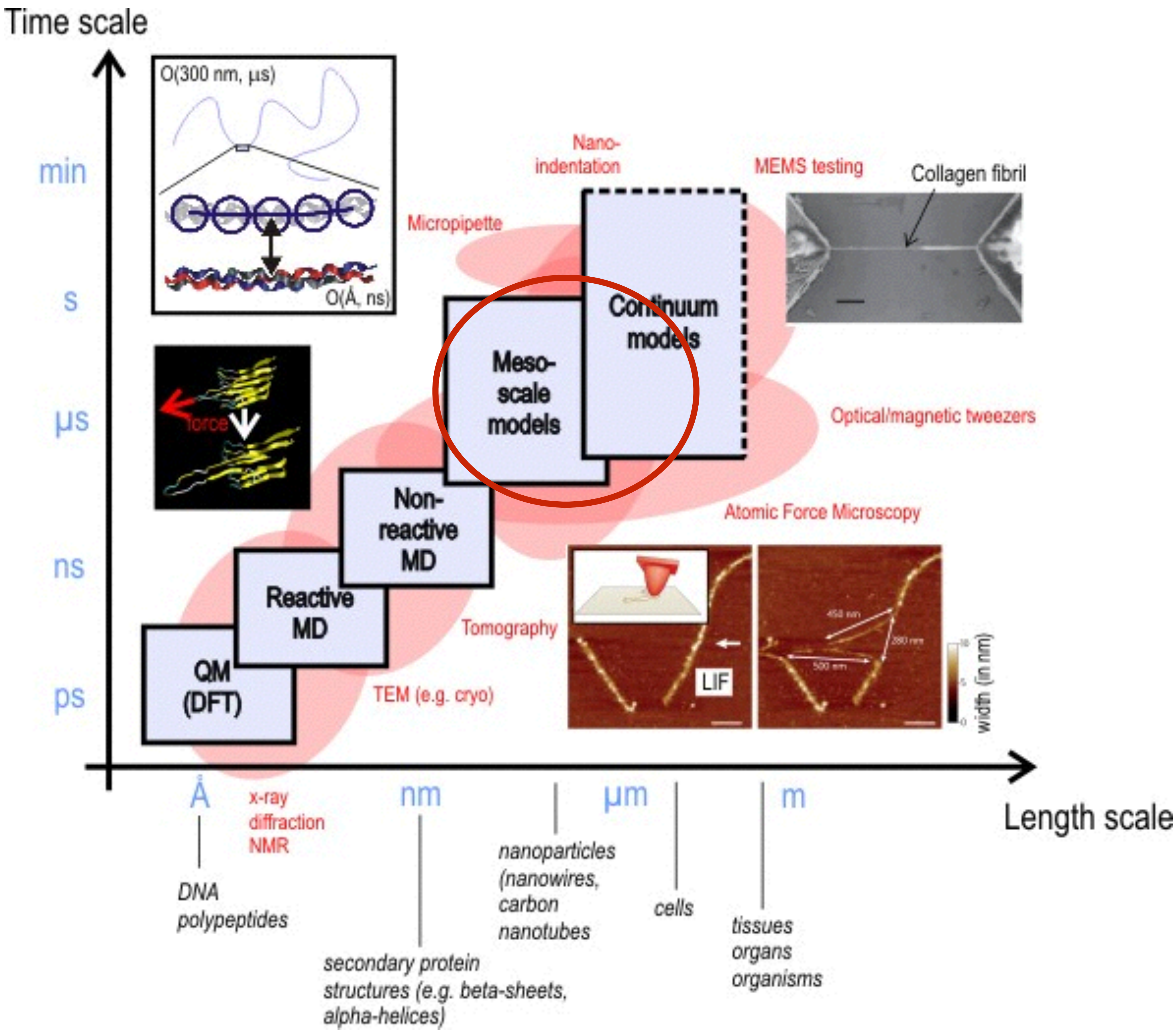
Knotted water



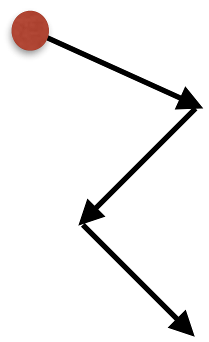
Irvine lab (Chicago)

Brownian motion of small objects in fluids
is biologically and technologically relevant
(and interesting)

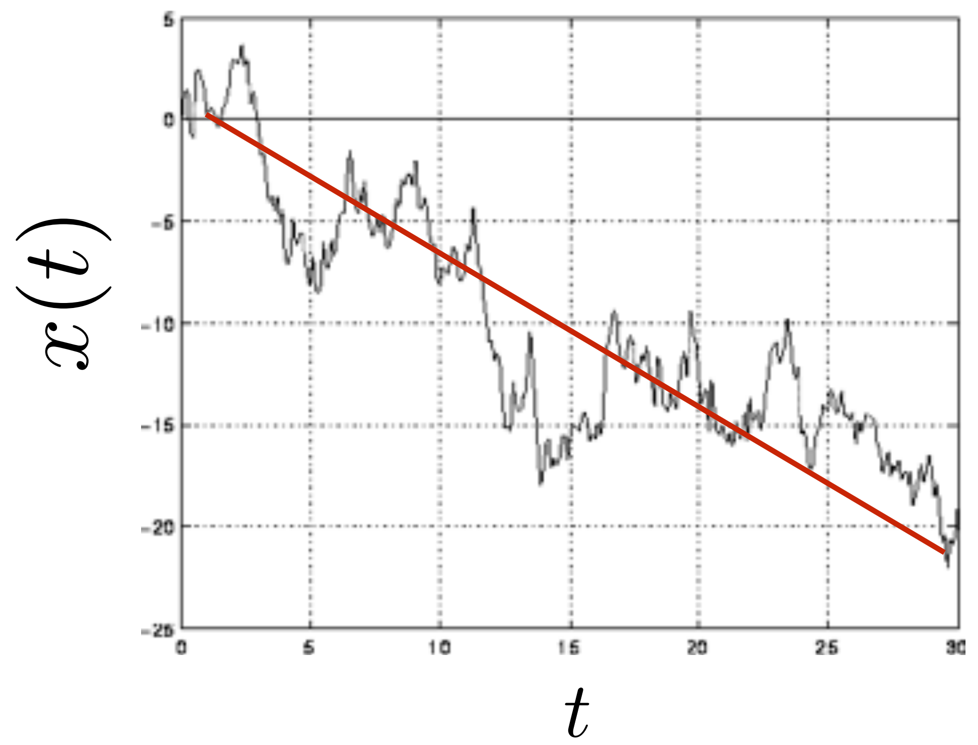
How can we describe these phenomena
mathematically ?



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



Basic idea



Split dynamics into

- deterministic part (drift)
- random part (diffusion, "noise")

$$\dot{x}(t) = f(x(t)) + \sqrt{2D}\,\xi(t)$$

Stochastic Differential Equation

Over-damped dynamics

Newton: $$m\ddot{x}(t) = F(x(t)) + S(\dot{x}(t)) + L(t)$$

Stokes: $$m\ddot{x}(t) = F(x(t)) - \gamma\dot{x}(t) + L(t)$$

Neglect inertia (*Re=0*): $$m\ddot{x}(t) \to 0$$

$$0 = F(x(t)) - \gamma\dot{x}(t) + L(t)$$

$$\dot{x}(t) = f(x(t)) + \sqrt{2D}\,\xi(t)$$

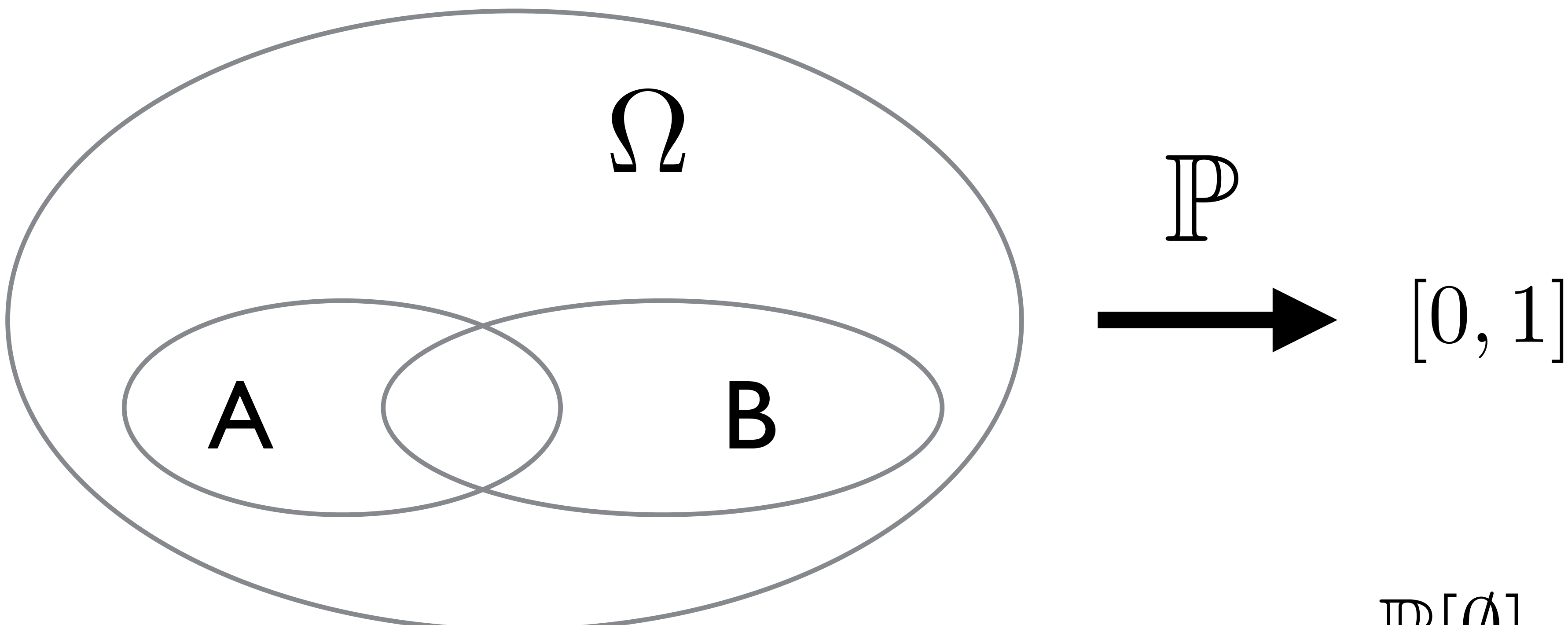
$$\dot{x}(t) = f(x(t)) + \sqrt{2D}\,\xi(t)$$

↑

How can we characterize randomness?

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

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



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

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

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

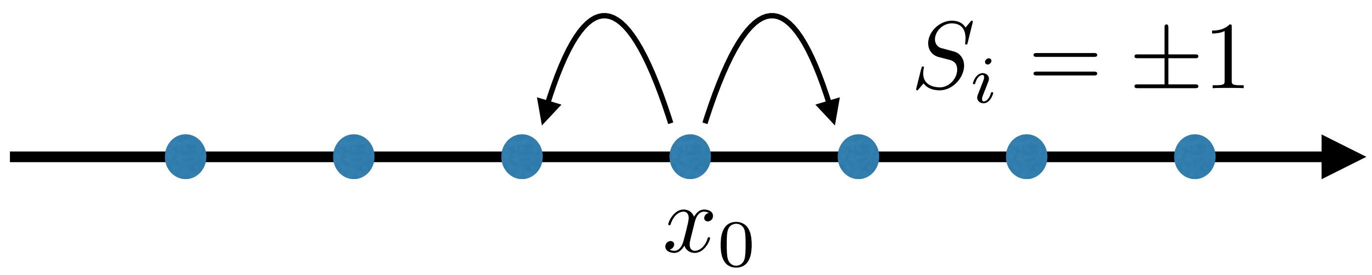
Expectation values of random variables

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

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

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

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



1.1 Random walk

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]

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

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

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)

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

Variance

The variance (second centered moment)

$$\begin{aligned}\mathbb{E}\left[(X_N - \mathbb{E}[X_N])^2\right] &= \mathbb{E}[X_N^2 - 2X_N\mathbb{E}[X_N] + \mathbb{E}[X_N]^2] \\ &= \mathbb{E}[X_N^2] - 2\mathbb{E}[X_N]\mathbb{E}[X_N] + \mathbb{E}[X_N]^2] \\ &= \mathbb{E}[X_N^2] - \mathbb{E}[X_N]^2 \end{aligned} \tag{1.6}$$

therefore grows linearly with the number of steps:

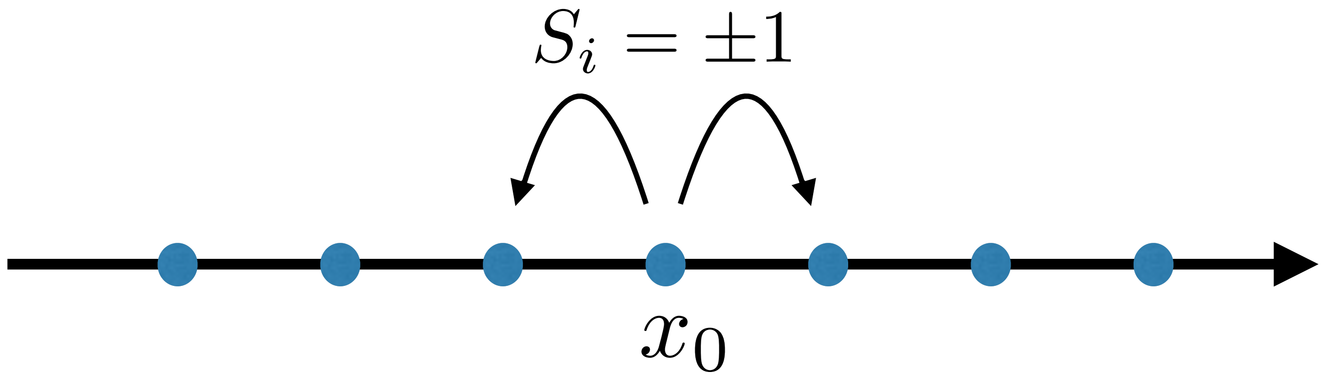
$$\mathbb{E}\left[(X_N - \mathbb{E}[X_N])^2\right] = \ell^2 N. \tag{1.7}$$

Let

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

$$\mathbb{E}[X_N^2] = 2Dt, \qquad D := \frac{\ell^2}{2\tau}$$

Continuum limit

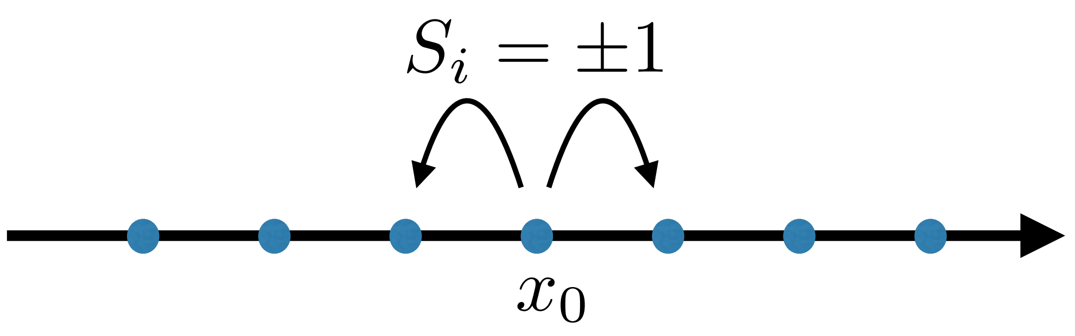


$$X_N = x_0 + \ell \sum_{i=1}^{N} S_i$$

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

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

Continuum limit



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

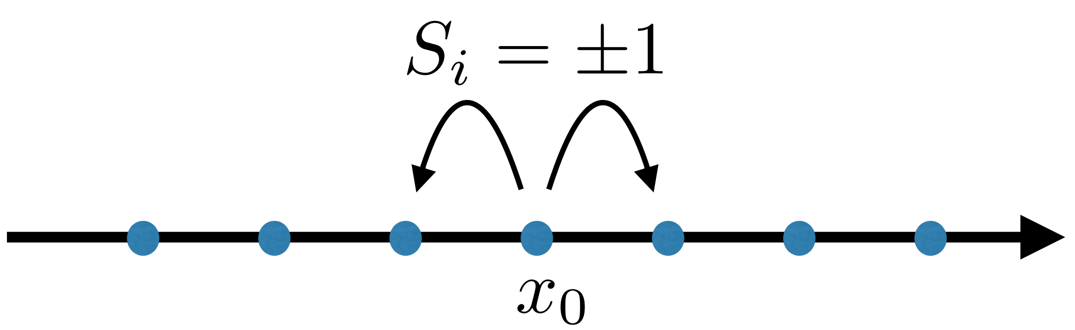
The associated probability density function (PDF) can be found by defining

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

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

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

Continuum limit



yielding the Gaussian

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

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

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

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).

Different types of "diffusion"

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

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

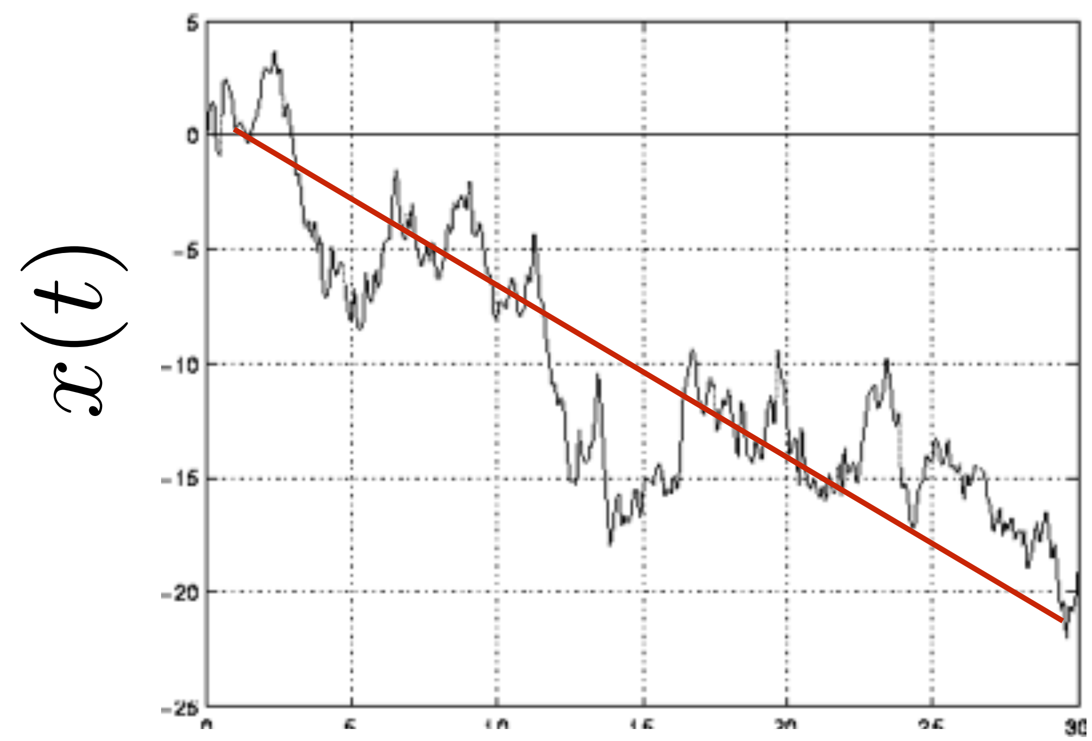
- $\mu = 0$: Static process with no movement.
- $0 < \mu < 1$: Sub-diffusion, arises typically when waiting times between subsequent jumps can be long and/or in the presence of a sufficiently large number of obstacles (e.g. slow diffusion of molecules in crowded cells).
- $\mu = 1$: Normal diffusion, 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).

Continuous representation of Brownian trajectories ?

1.2 Brownian motion (constant drift)

$$\dot{X}(t) = u + \sqrt{2D}\,\xi(t)$$

$$dB(t) = \xi(t)\,dt$$



$$dX(t) = u\,dt + \sqrt{2D}\,dB(t)$$

SDE

Wiener process

$$dX(t) = u\,dt + \sqrt{2D}\,dB(t). \tag{1.25}$$

Here, $dX(t) = X(t+dt) - X(t)$ is increment of the stochastic particle trajectory $X(t)$, whilst $dB(t) = B(t+dt) - B(t)$ denotes an increment of the standard Brownian motion (or Wiener) process $B(t)$, uniquely defined by the following properties[3]:

(i) $B(0) = 0$ with probability 1.

(ii) $B(t)$ is stationary, i.e., for $t > s \geq 0$ the increment $B(t) - B(s)$ has the same distribution as $B(t-s)$.

(iii) $B(t)$ has independent increments. That is, for all $t_n > t_{n-1} > \ldots > t_2 > t_1$, the random variables $B(t_n) - B(t_{n-1}), \ldots, B(t_2) - B(t_1)$, $B(t_1)$ are independently distributed (i.e., their joint distribution factorizes).

(iv) $B(t)$ has Gaussian distribution with variance t for all $t \in (0, \infty)$.

(v) $B(t)$ is continuous with probability 1.

The probability distribution $\mathbb{P}$ governing the driving process $B(t)$ is commonly known as the Wiener measure.

Langevin equation

$$dX(t) = u\,dt + \sqrt{2D}\,dB(t). \tag{1.25}$$

Although the derivative $\xi(t) = dB/dt$ is not well-defined mathematically, Eq. (1.25) is in the physics literature often written in the form

$$\dot{X}(t) = u + \sqrt{2D}\,\xi(t). \tag{1.26}$$

The random driving function $\xi(t)$ is then referred to as Gaussian white noise, characterized by

$$\langle \xi(t) \rangle = 0\,, \qquad \langle \xi(t)\xi(s) \rangle = \delta(t-s), \tag{1.27}$$

with $\langle \cdot \rangle$ denoting an average with respect to the Wiener measure.

$$\delta(x) = \begin{cases} +\infty, & x = 0 \\ 0, & \text{otherwise} \end{cases} \qquad f(y) = \int_{-\infty}^{+\infty} dx\; \delta(x-y)\, f(x)$$

Dirac's Delta-function

Mean displacement

$$\dot{X}(t) = \sqrt{2D}\,\xi(s)$$

Direct integration with $X(0) = 0$

$$X(t) = \sqrt{2D}\int_0^t ds\,\xi(s)$$

Averaging

$$\langle X(t)\rangle = \left\langle \sqrt{2D}\int_0^t ds\,\xi(s)\right\rangle = \sqrt{2D}\int_0^t ds\,\langle\xi(s)\rangle = 0$$

↑

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

Mean square displacement

$$X(t) = \sqrt{2D} \int_0^t ds\, \xi(s)$$

$$\begin{aligned}
\langle X(t)^2 \rangle &= \left\langle \left[\sqrt{2D} \int_0^t ds\, \xi(s) \right] \cdot \left[\sqrt{2D} \int_0^t du\, \xi(u) \right] \right\rangle \\
&= \left\langle 2D \int_0^t ds \int_0^t du\, \xi(s) \cdot \xi(u) \right\rangle \\
&= 2D \int_0^t ds \int_0^t du\, \langle \xi(s) \cdot \xi(u) \rangle \\
&= 2D \int_0^t ds \int_0^t du\, \delta(s-u) \\
&= 2D \int_0^t ds \\
&= 2Dt
\end{aligned}$$