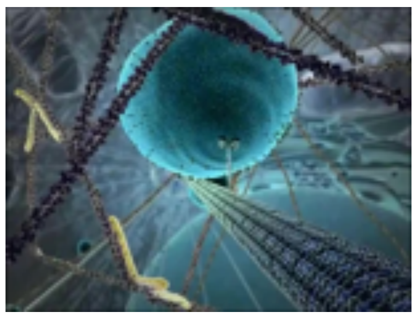
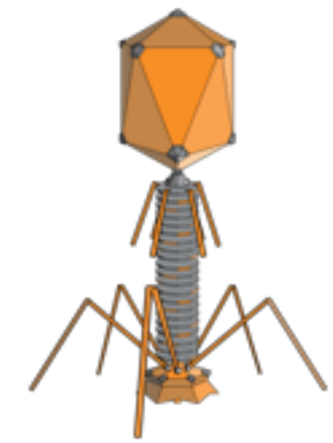
MAE 545

Special Topics - Lessons from Biology for Engineering Tiny Devices





Lectures:

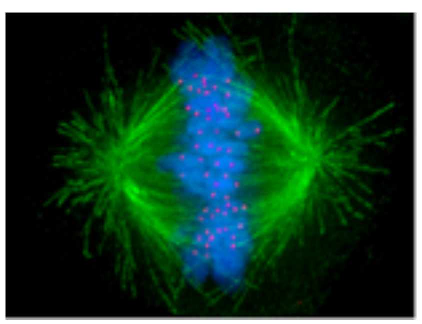
T, Th 1:30-2:50 PM,

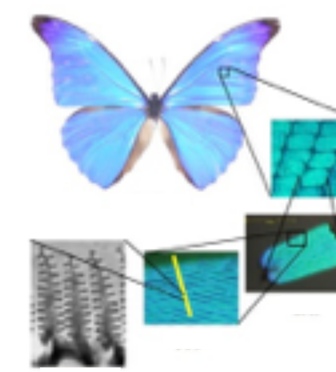
Friend Center 003

Office hours:

W 1:30-3:00 PM,

EQUAD D414





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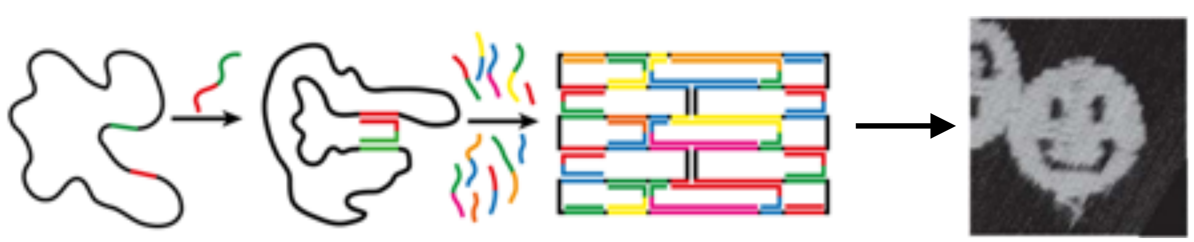


Lecture Notes

- **text books: none**
- **lecture slides will be posted on Blackboard**

http://blackboard.princeton.edu

course: MAE545_F2015

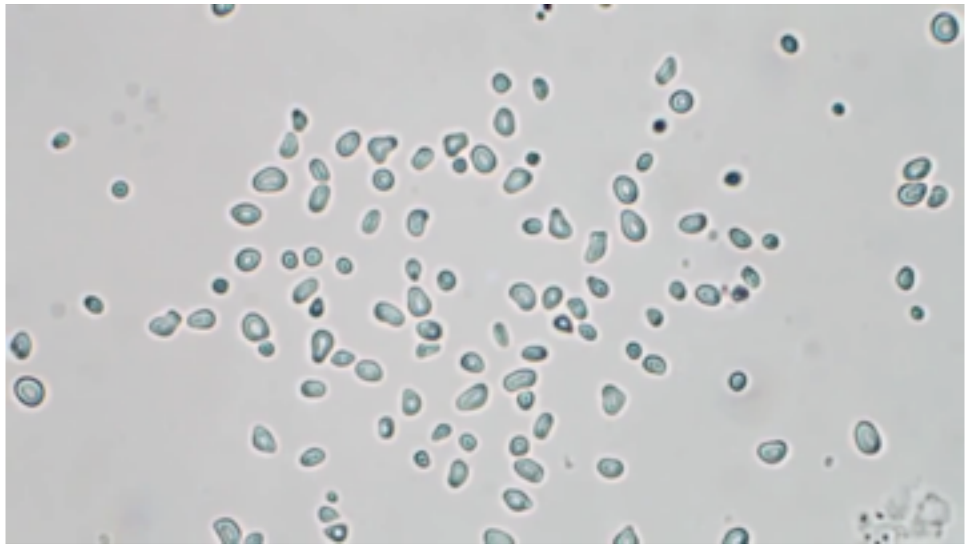
Assignments

- **presentation of research paper in class**
- **final paper (final project)**

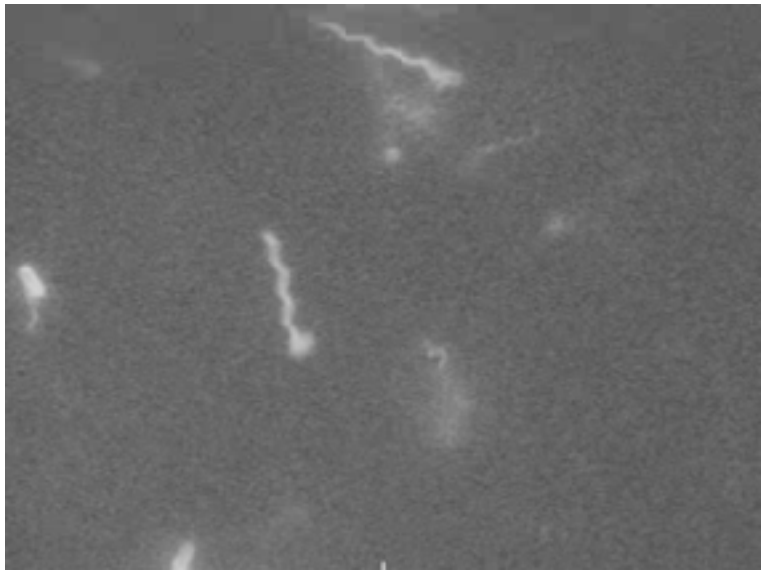
Syllabus

Random walks

Brownian motion

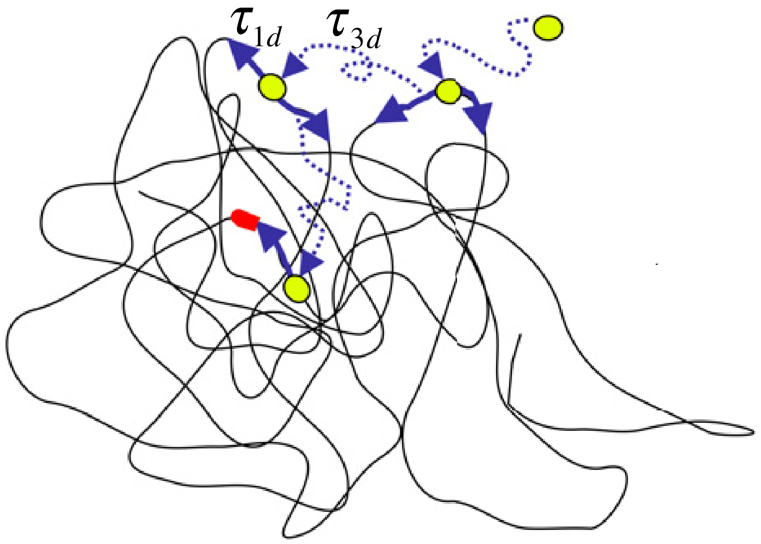


Swimming of E. coli



Polymer random coils

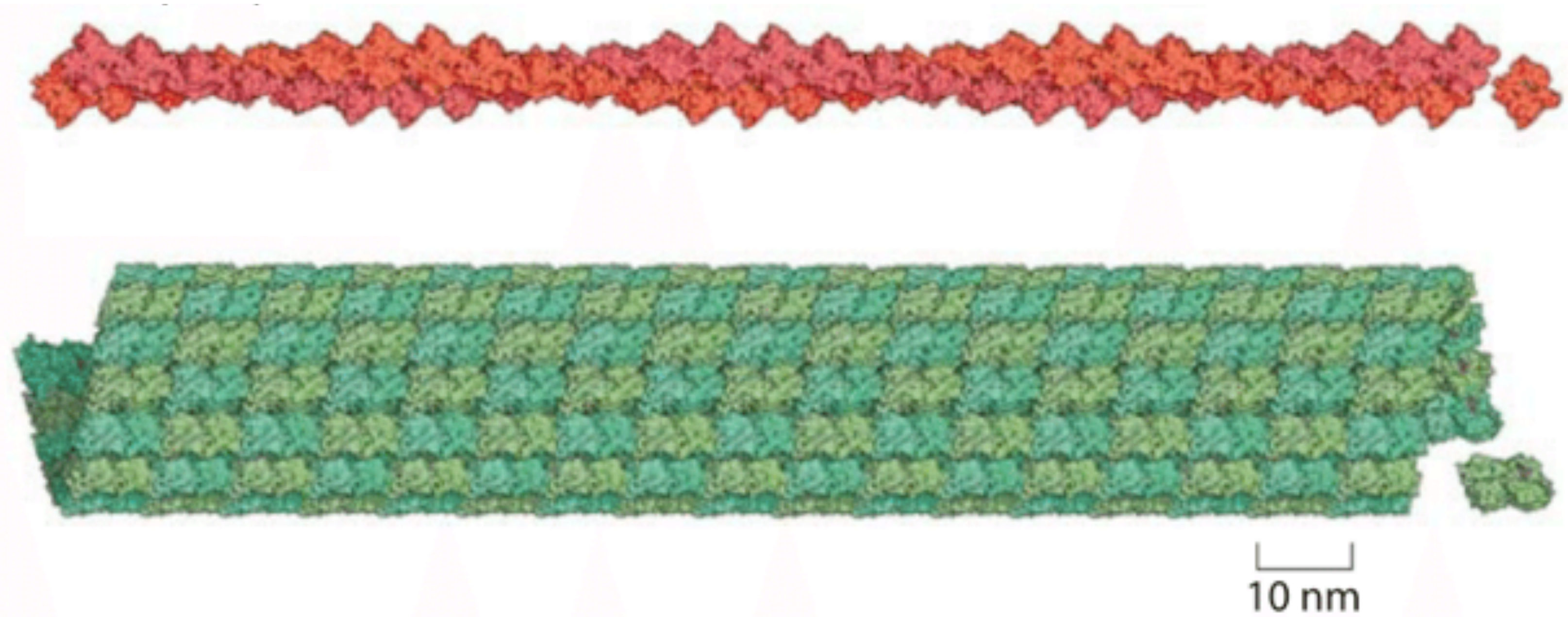
Protein search for a binding site on DNA



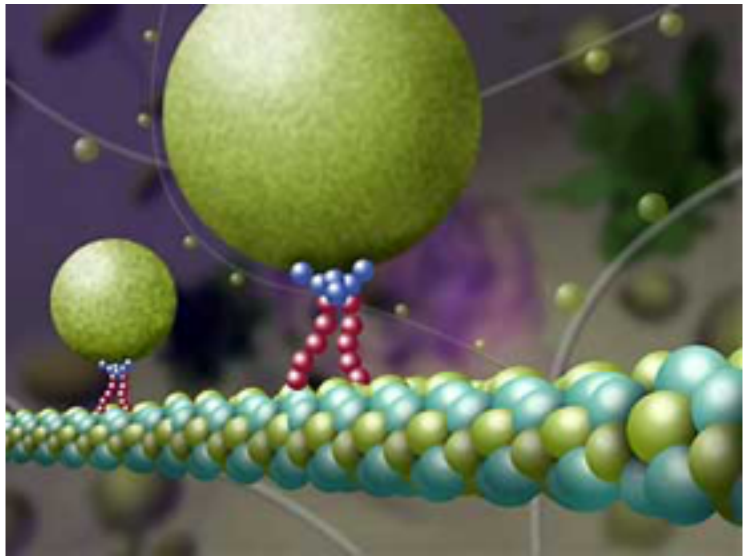
Protein filaments

Actin filament

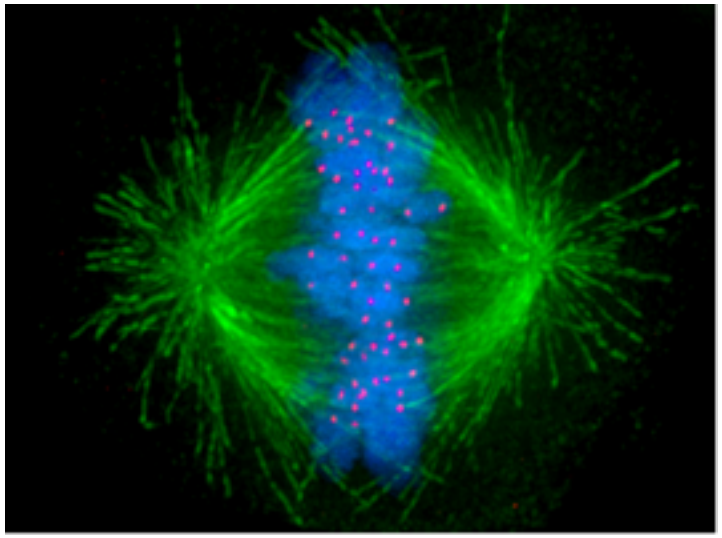
Microtubule



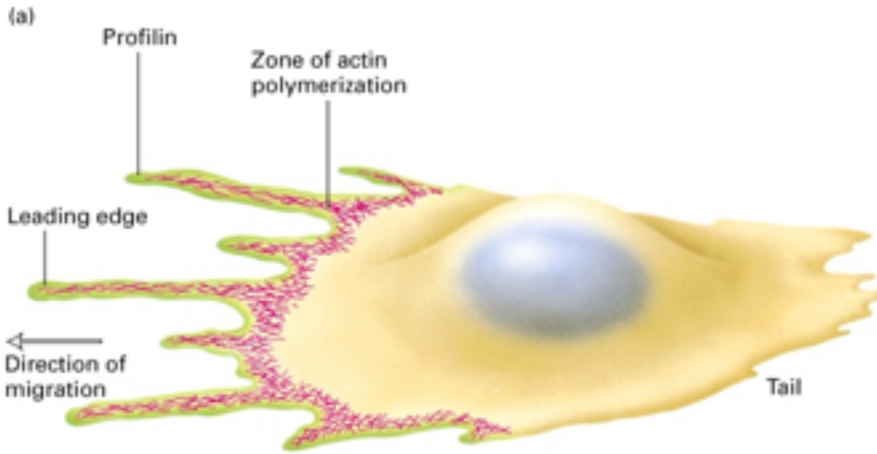
Cargo transport



Segregation of chromosomes during cell division



Crawling of cells

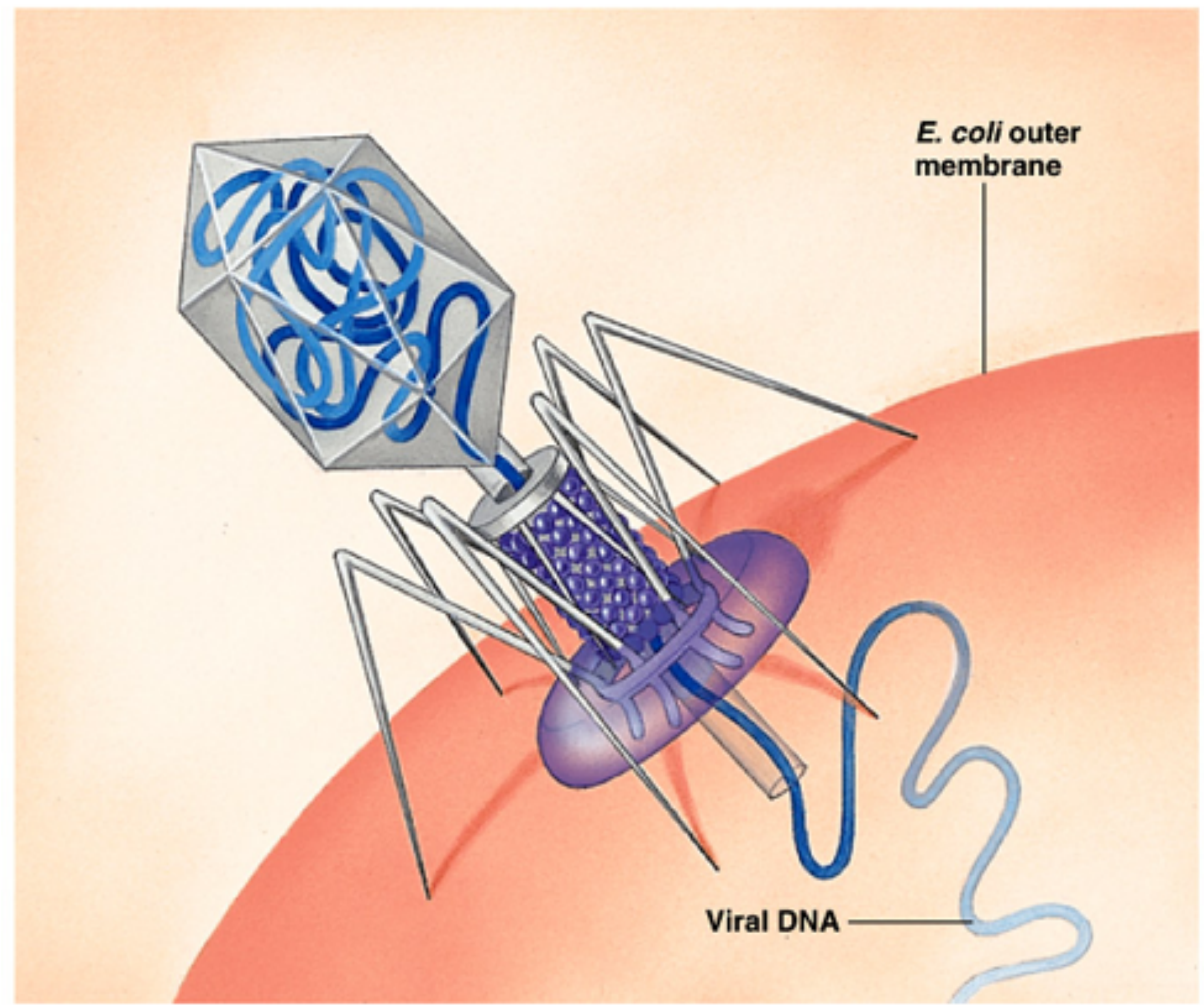


Viruses

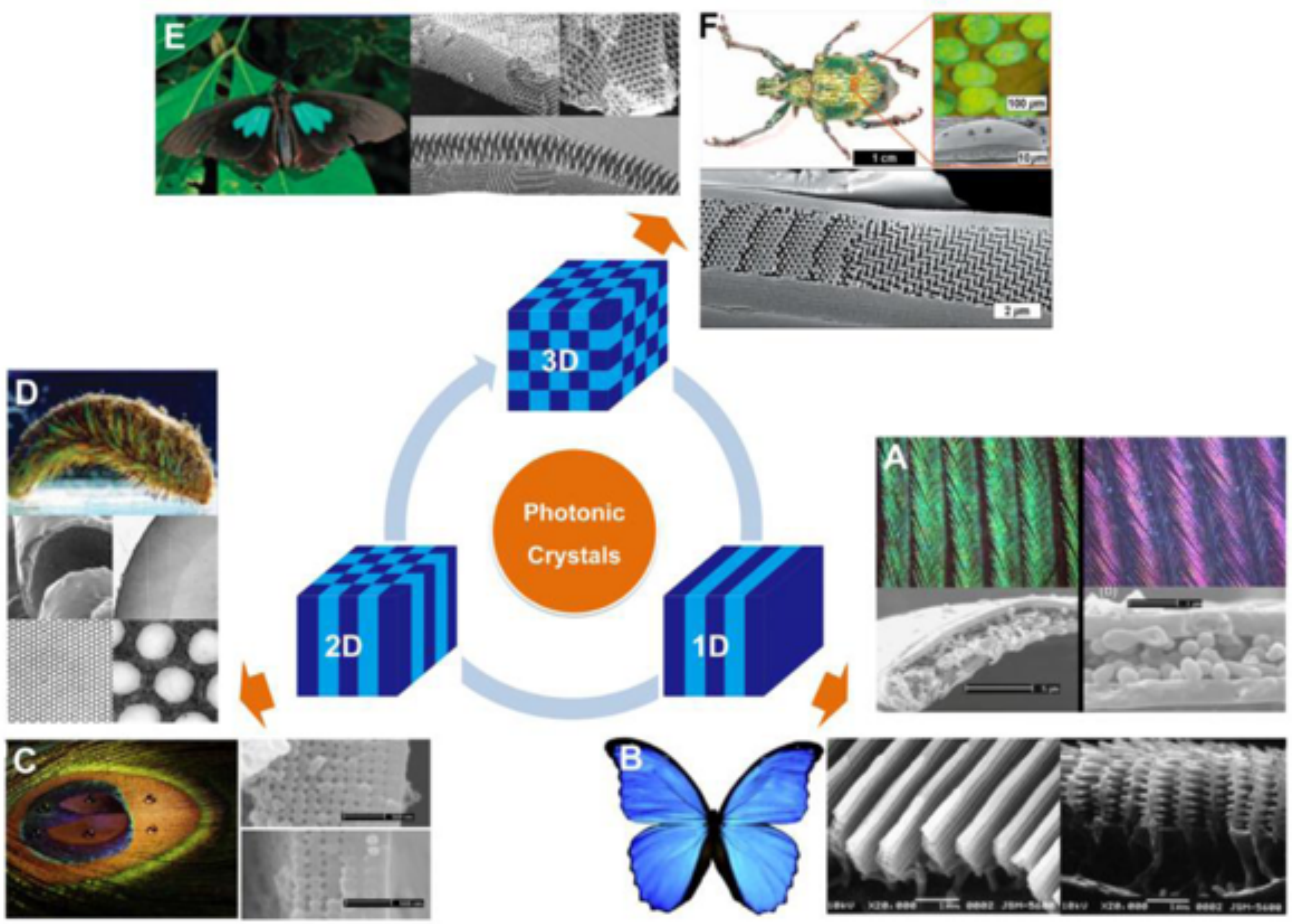
assembly of
viral capsids

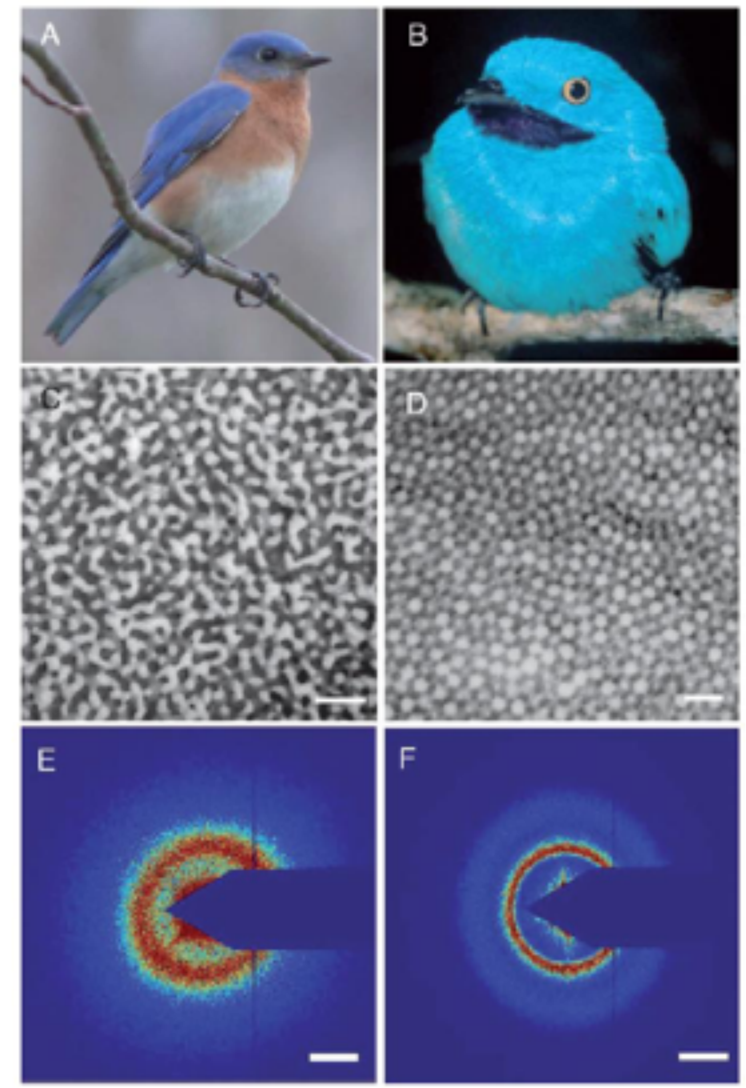
packing of viral DNA
inside the capsid

infection of cells



Structural colors





H. Wang and K-Q. Zhang, Sensors (2013)

H. Cao, Yale

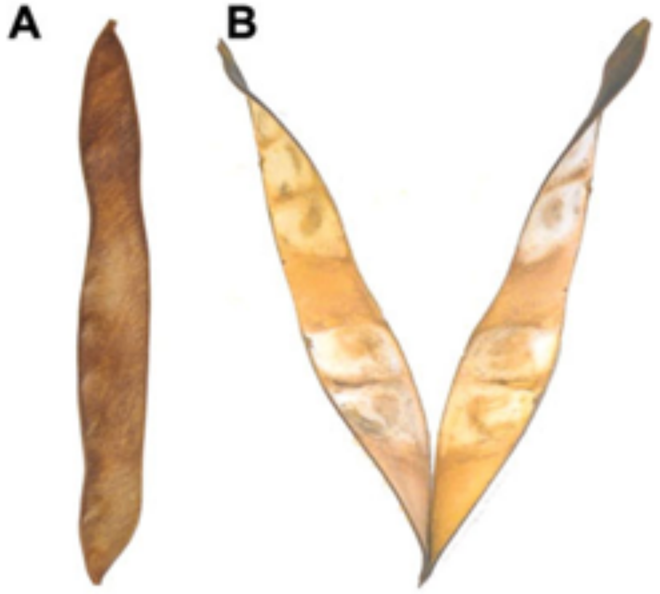
Structure and form of organs and plants

Brain

Gut

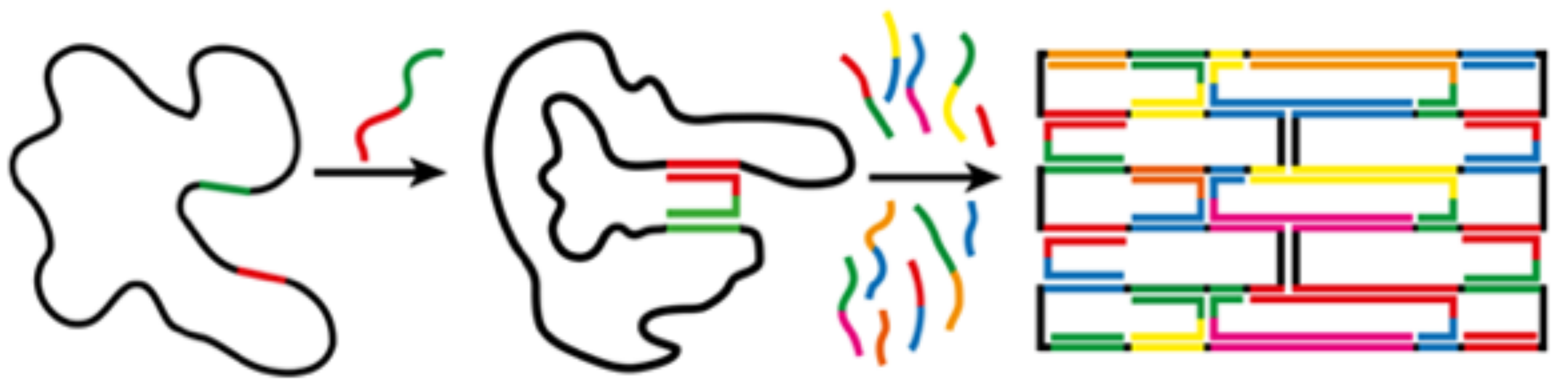
Plantain Lily leaf

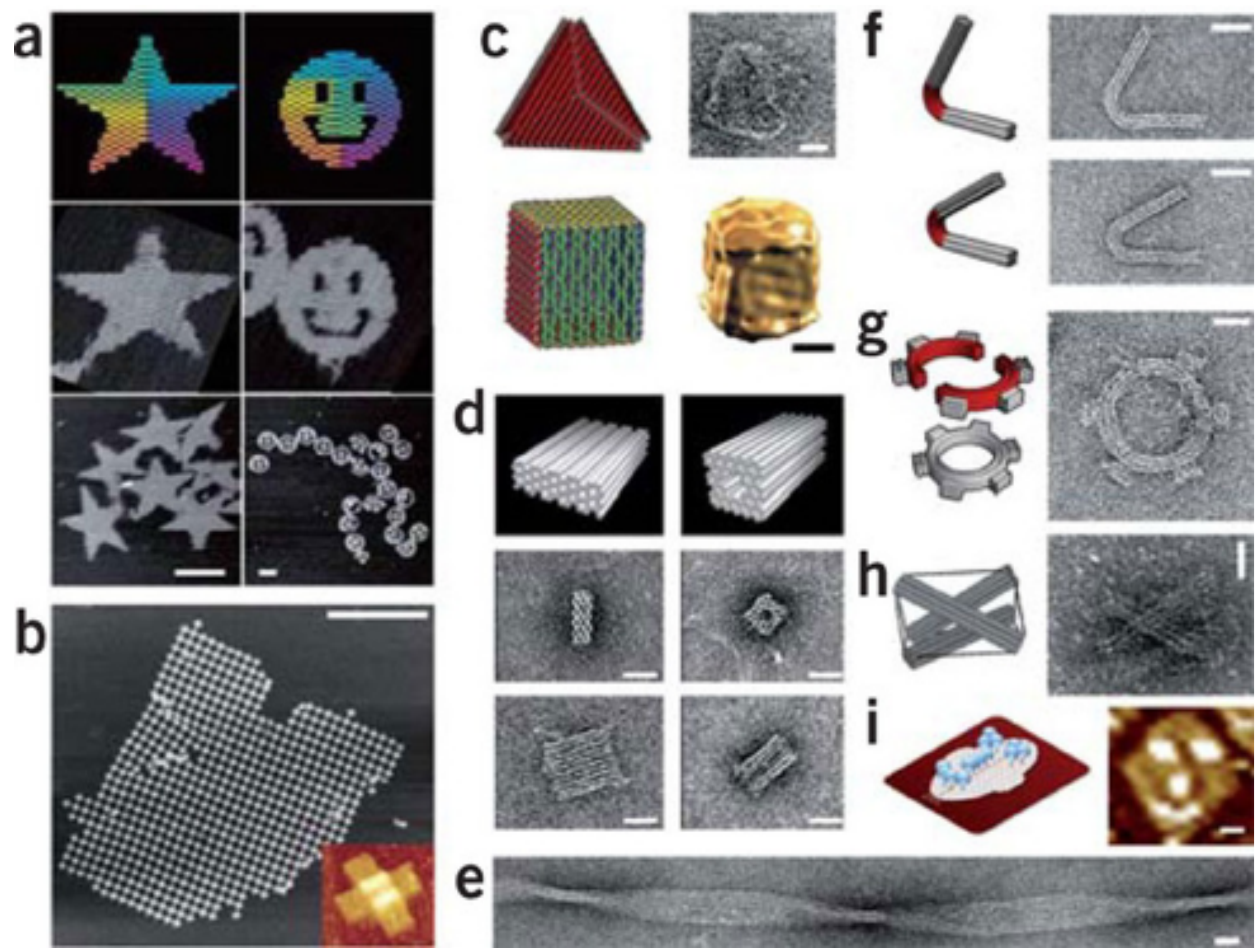
Bauhinia seed pods



(A and B) Closed and open Bauhinia pods

DNA Origami

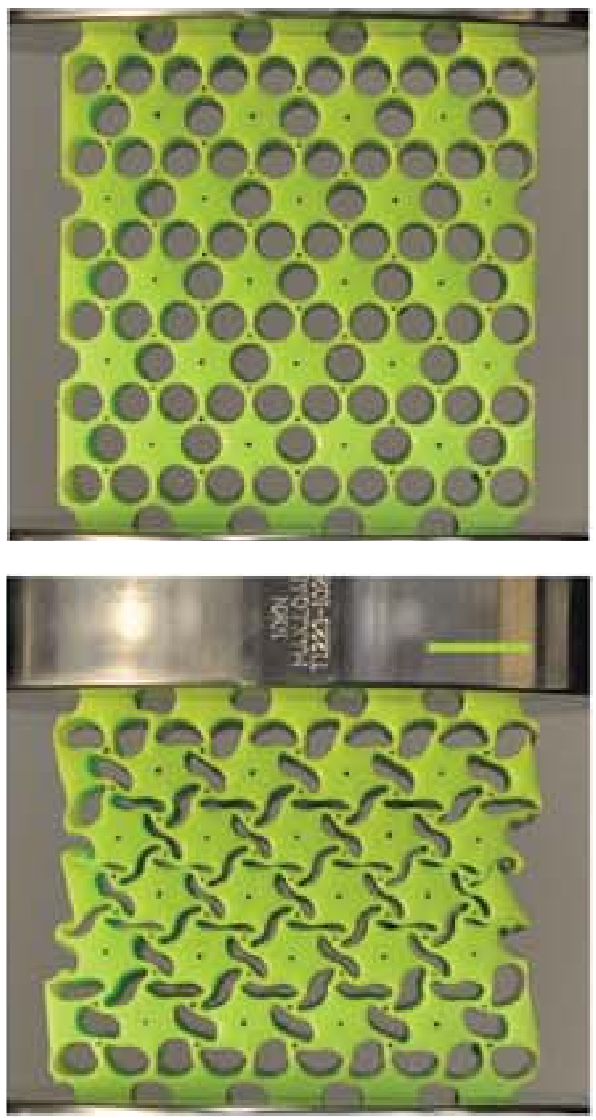




C. E. Castro et al., Nature methods (2011)

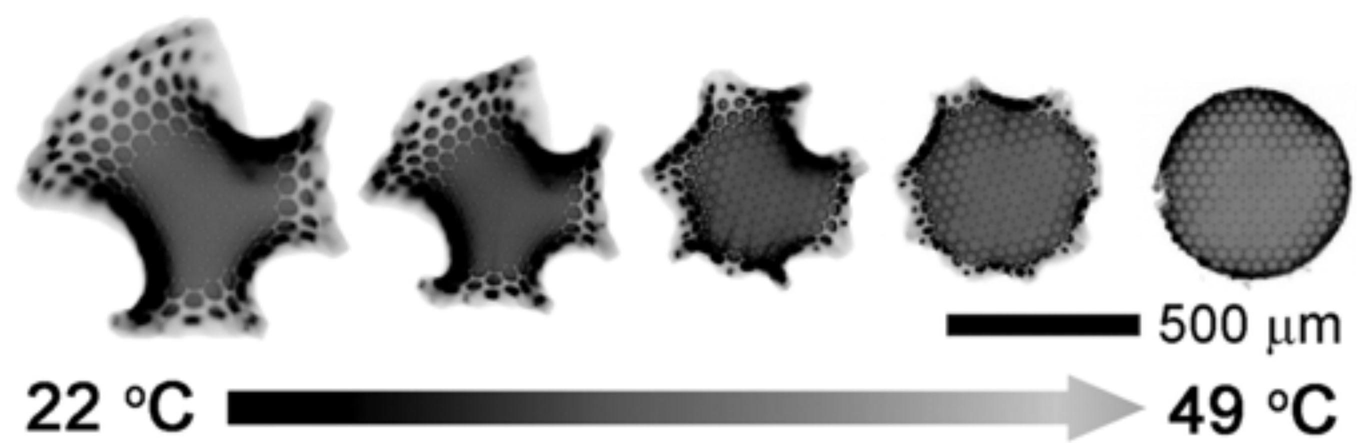
Elastic metamaterials

phononic crystals



buckliball

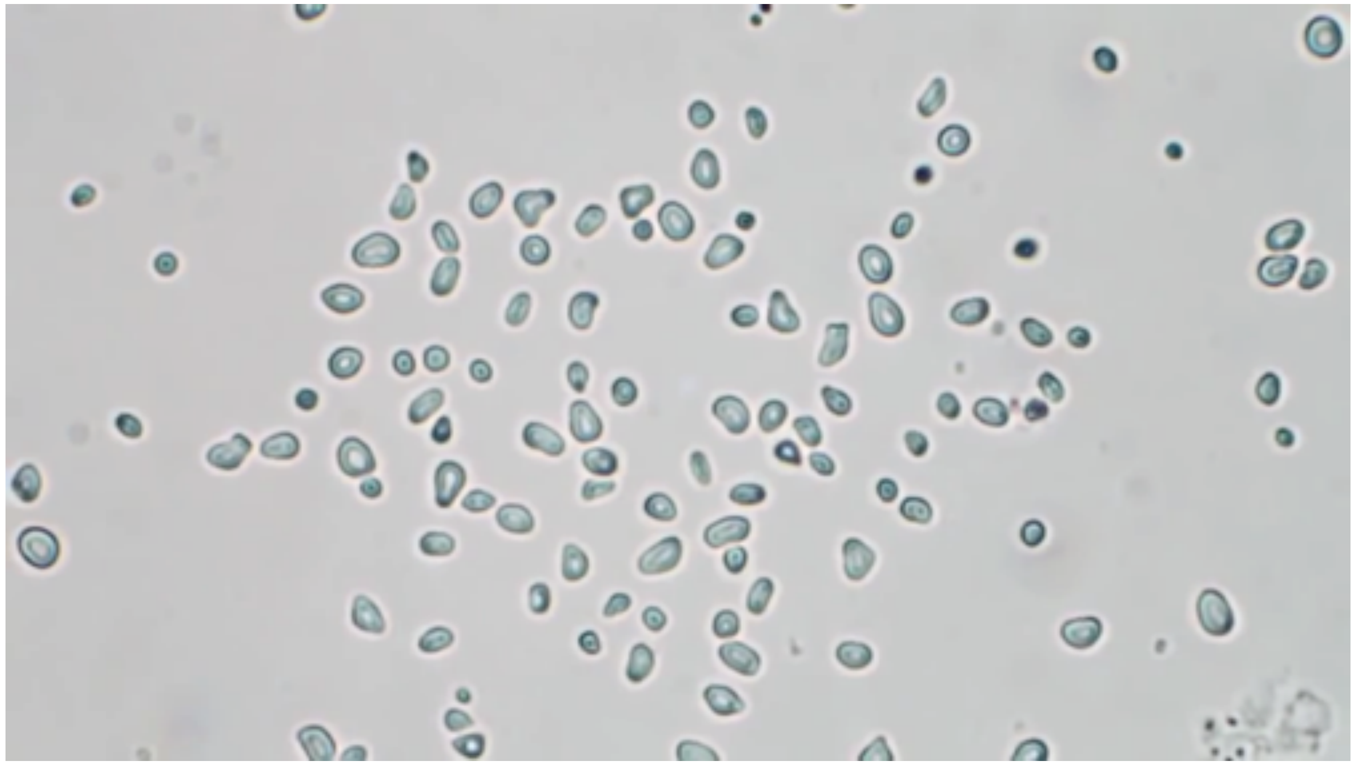
swelling of patterned gels



Lecture 1 (9/17)
Brownian motion of small particles

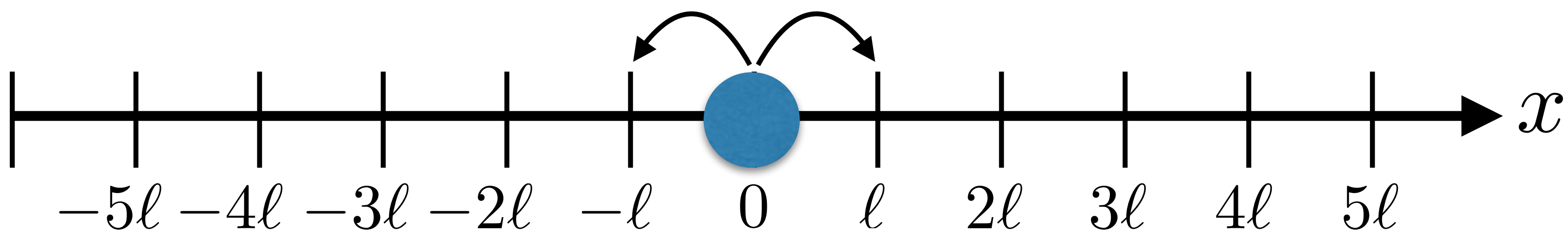
History

1827 Robert Brown: observed irregular motion of small pollen grains suspended in water



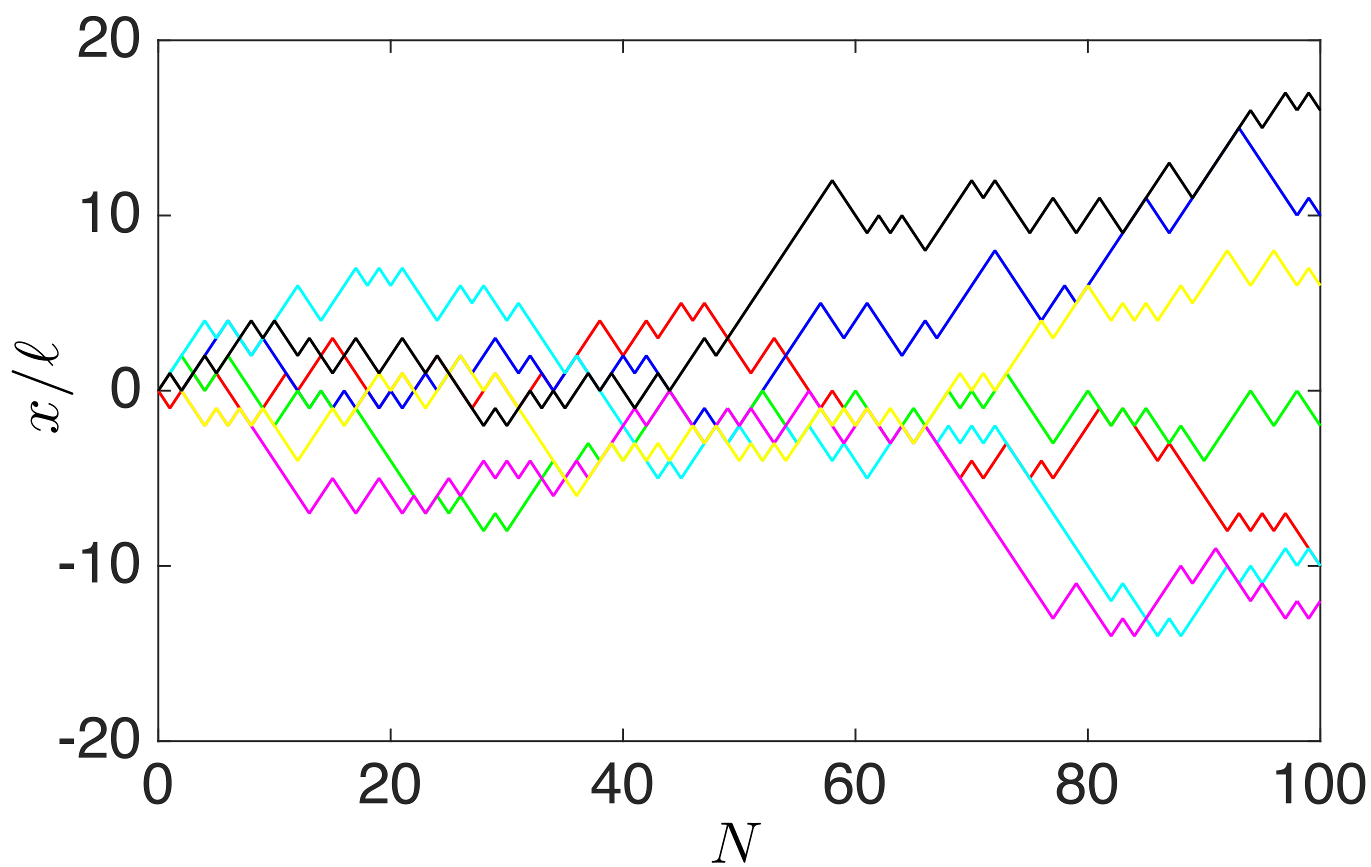
1905-06 Albert Einstein, Marian Smoluchowski: microscopic description of Brownian motion and relation to diffusion equation

Random walk on a 1D lattice



At each step particle jumps left or right with probability 1/2.

What is the probability *p(x,N)* that we find particle at position *x* after *N* jumps?



Probability that particle makes *k* jumps to the right and *N-k* jumps to the left obeys the binomial distribution

$$\binom{N}{k} 2^{-N}$$

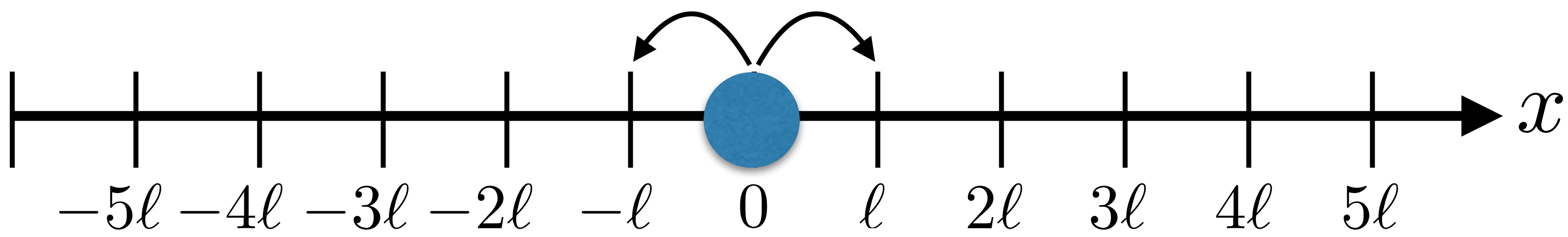
This corresponds to particle position

$$x = k\ell - (N-k)\ell = (2k - N)\ell$$

Therefore

$$p\Big(x = (2k-N)\ell, N\Big) = \binom{N}{k} 2^{-N}$$

Random walk on a 1D lattice



Gaussian approximation for *p(x,N)*

Position *x* after *N* jumps can be expressed as the sum of individual jumps x_i

$$x = \sum_{i=1}^{N} x_i$$

Mean value averaged over all possible random walks

$$\langle x \rangle = N \langle x_1 \rangle = N \left(\frac{1}{2}\ell - \frac{1}{2}\ell \right) = 0$$

Variance averaged over all possible random walks

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = N \langle x_1^2 \rangle = N \ell^2$$

$$\sigma^2 \equiv 2DN$$

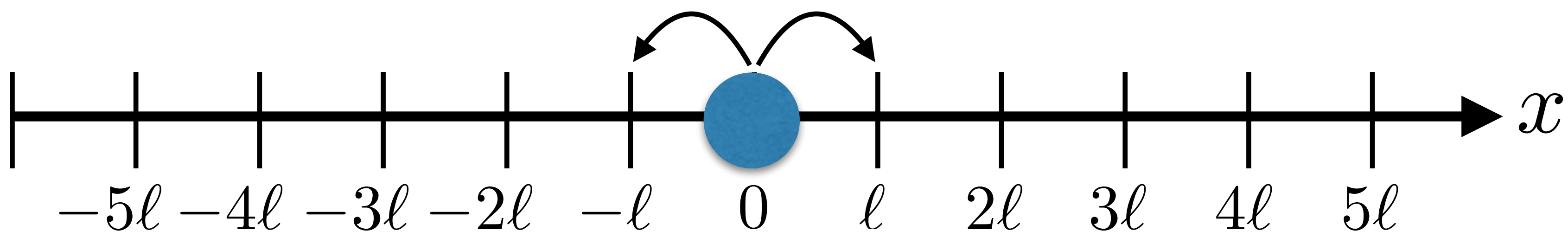
effective diffusion constant

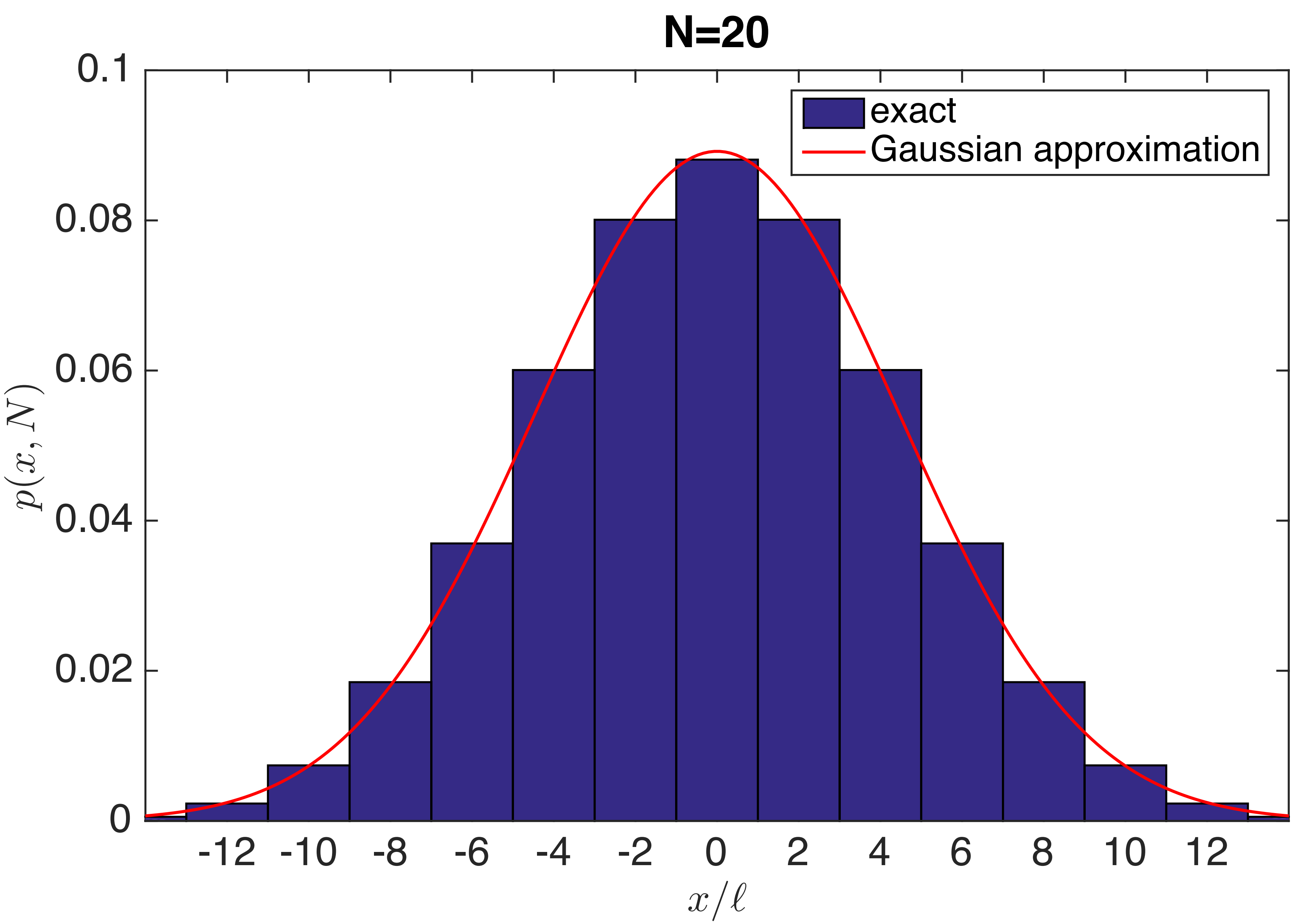
$$D = \ell^2 / 2$$

According to the central limit theorem *p(x,N)* approaches gaussian distribution for large *N*

$$p(x, N) \approx \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}$$

Random walk on a 1D lattice





Exact distribution

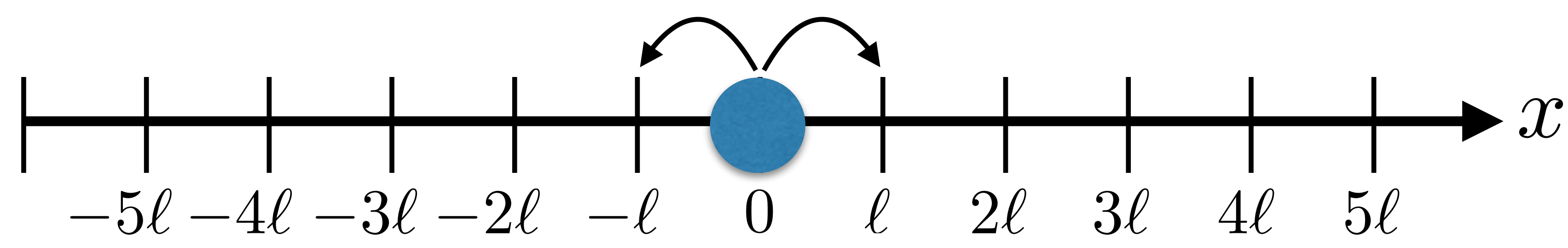
$$p\left(x = (2k - N)\ell, N\right) = \binom{N}{k} 2^{-N}$$

Gaussian approximation

$$p(x, N) \approx \frac{1}{\sqrt{2\pi N \ell^2}} e^{-x^2/2N\ell^2}$$

Note: exact discrete distribution has been made continuous by replacing discrete peaks with boxes whose area corresponds to the same probability.

Master equation and diffusion equation



Master equation provides recursive relation for the evolution of probability distribution, where $\Pi(x,y)$ describes probability for a jump from *y* to *x*.

$$p(x, N+1) = \sum_y \Pi(x,y)p(y,N)$$

For our example master equation reads

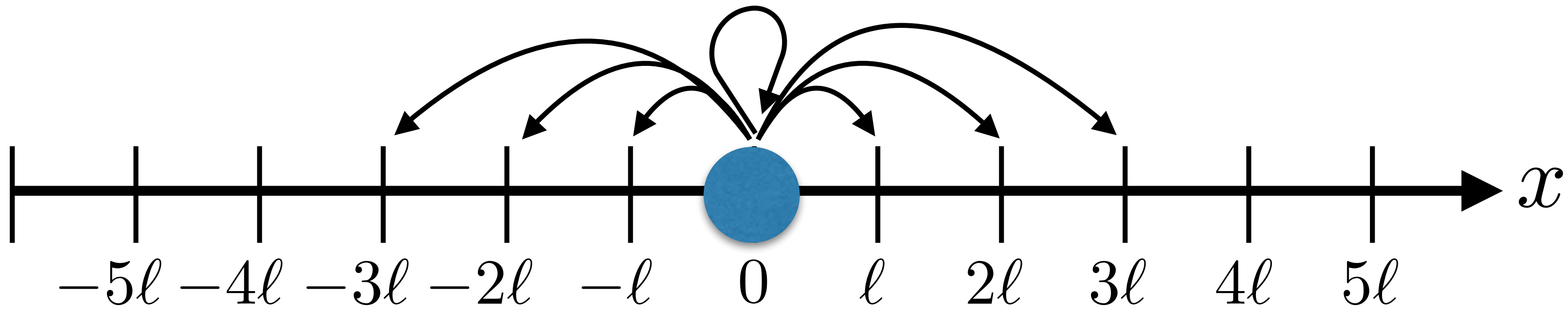
$$p(x, N+1) = \frac{1}{2}p(x-\ell, N) + \frac{1}{2}p(x+\ell, N)$$

Initial condition $p(x, N=0) = \delta(x)$

In the limit of large number of jumps *N* and small step size ℓ, we can Taylor expand master equation to derive an approximate diffusion equation

$$\frac{\partial p(x,N)}{\partial N} = D\frac{\partial^2 p(x,N)}{\partial x^2} \qquad D = \ell^2/2$$

Fokker-Planck equation



In general the probability distribution Π of jump lengths *s* can depend on the particle position *x*. $\Pi(s|x)$

Assume that jumps occur in regular small time intervals Δt

Generalized master equation $p(x, t + \Delta t) = \sum_s \Pi(s|x - s) p(x - s, t)$

Again Taylor expand master equation above to derive the Fokker-Planck equation

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}\Big[v(x)p(x,t)\Big] + \frac{\partial^2}{\partial x^2}\Big[D(x)p(x,t)\Big]$$

drift velocity (external fluid flow, external potential)

$$v(x) = \sum_s \frac{s}{\Delta t}\Pi(s|x) = \frac{\langle s(x)\rangle}{\Delta t}$$

diffusion coefficient (e.g. position dependent temperature)

$$D(x) = \sum_s \frac{s^2}{2\Delta t}\Pi(s|x) = \frac{\langle s^2(x)\rangle}{2\Delta t}$$

Probability current

Fokker-Planck equation

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[v(x)p(x,t)\right] + \frac{\partial^2}{\partial x^2}\left[D(x)p(x,t)\right]$$

Conservation law of probability
(no particles created/removed)

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

By comparing equations above we can define probability current

$$J(x,t) = v(x)p(x,t) - \frac{\partial}{\partial x}\left[D(x)p(x,t)\right]$$

Note that for the steady state distribution, where $\partial p^*(x,t)/\partial t \equiv 0$

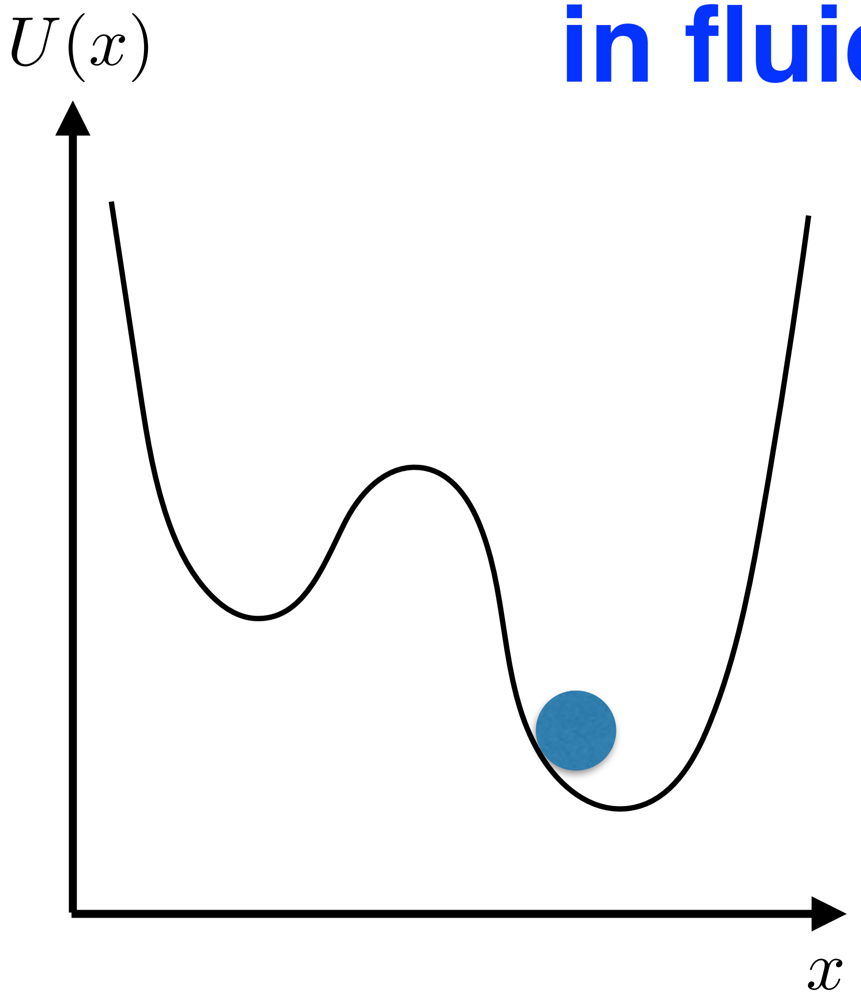
the steady state current is constant and independent on *x*

$$J^* \equiv v(x)p^*(x) - \frac{\partial}{\partial x}\left[D(x)p^*(x)\right] = \mathrm{const}$$

If we don't create/remove particles at boundaries then *J=0**

$$p^*(x) \propto \frac{1}{D(x)} \exp\left[\int_{-\infty}^{x} dy \frac{v(y)}{D(y)}\right]$$

Spherical particle suspended in fluid in external potential



Newton's law

$$m\frac{\partial^2 x}{\partial t^2} = -\lambda v(x) - \frac{\partial U(x)}{\partial x} + F_r$$

fluid drag — **external potential force** — **random Brownian force**

For simplicity assume overdamped regime and ignore inertial term on the left hand side. This produces average drift velocity

$$\langle v(x)\rangle = -\frac{1}{\lambda}\frac{\partial U(x)}{\partial x}$$

Equilibrium probability distribution

$$p^*(x) = Ce^{-U(x)/\lambda D} = Ce^{-U(x)/k_B T}$$

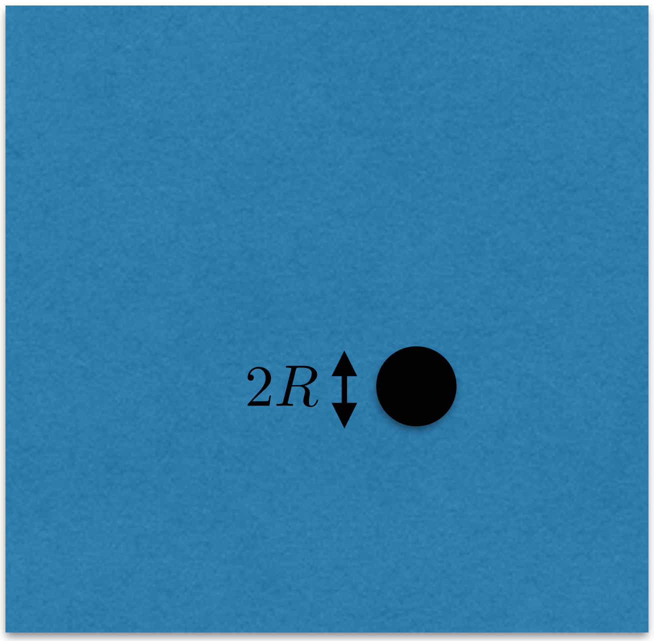
(see previous slide) (equilibrium physics)

R	**particle radius**
η	**fluid viscosity**
$\lambda = 6\pi\eta R$	**Stokes drag coefficient**
k_B	**Boltzmann constant**
T	**temperature**
D	**diffusion constant**

Einstein - Stokes equation

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

Example of Einstein-Stokes equation



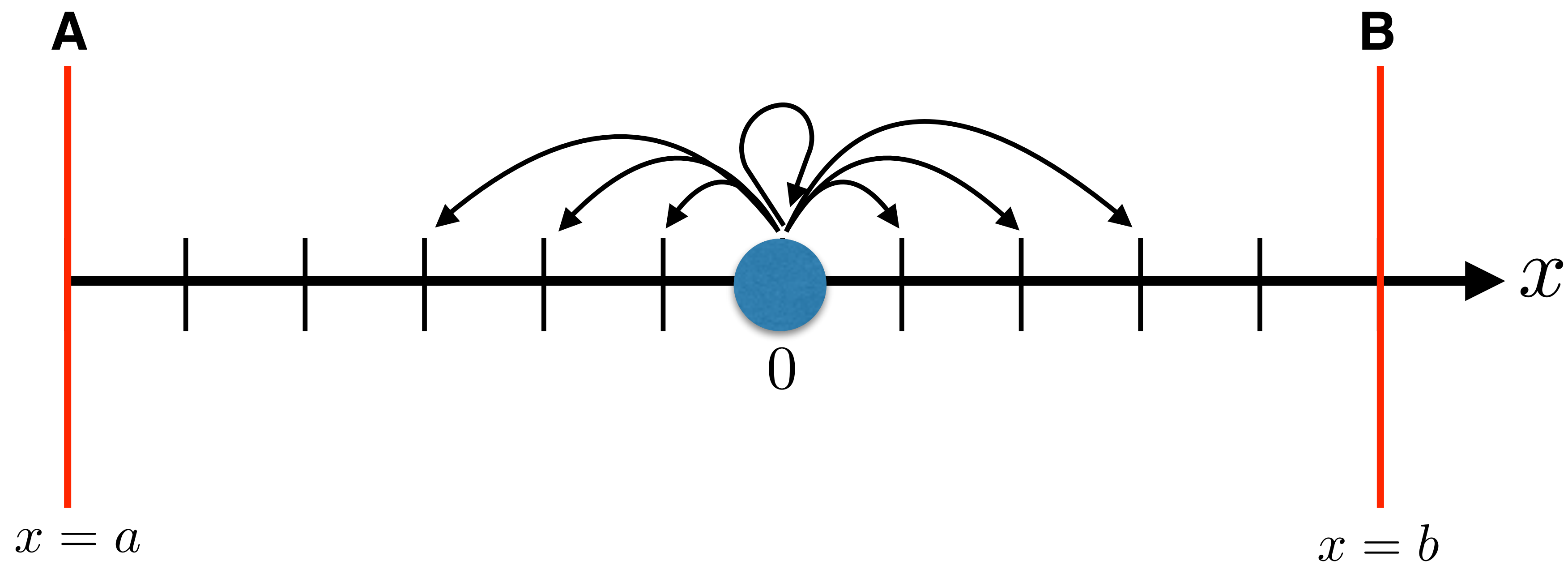
$$D = \frac{k_B T}{\lambda} = \frac{k_B T}{6\pi\eta R}$$

Spherical particle suspended in water at room temperature

water viscosity	$\eta \approx 10^{-3}\text{kg m/s}$
temperature	$T = 300\text{K}$
Boltzmann constant	$k_B = 1.38 \times 10^{-23}\text{J/K}$

particle radius	$R = 1\mu\text{m}$	$R = 1\text{mm}$
	↓	↓
diffusion constant	$D \approx 0.2\mu\text{m}^2/\text{s}$	$D \approx 2 \times 10^{-4}\mu\text{m}^2/\text{s}$
	diffusion important	**small diffusion**

Random walk with absorbing boundaries



What is the probability $P_B(x)$ that particle that starts at position *x* gets absorbed at site B?

$$P_A(x) = 1 - P_B(x)$$

$$P_B(x) = \sum_s \Pi(s|x) P_B(x+s)$$

$$0 = v(x)\frac{dP_B(x)}{dx} + D(x)\frac{d^2 P_B(x)}{dx^2}$$

boundary conditions

$$P_B(x = b) = 1$$

$$P_B(x = a) = 0$$

Example

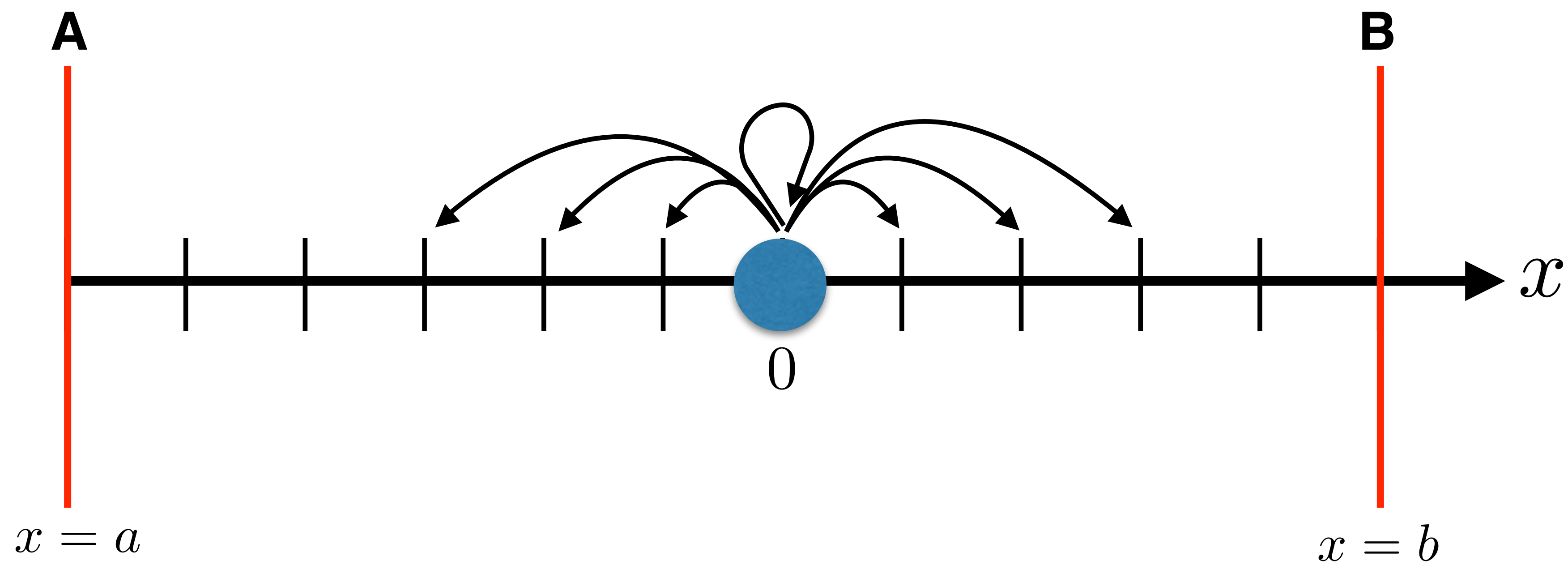
$v = 0, D = \mathrm{const}$

$$P_B(x) = \frac{(x-a)}{(b-a)}$$

$v, D = \mathrm{const}$

$$P_B(x) = \frac{(1 - e^{-v(x-a)/D})}{(1 - e^{-v(b-a)/D})}$$

Random walk with absorbing boundaries



What is the mean time $T(x)$ that particle that starts at position *x* gets absorbed at either site?

$$T(x) = \sum_s \Pi(s|x) T(x+s) + \Delta t$$

$$-1 = v(x)\frac{dT(x)}{dx} + D(x)\frac{d^2T(x)}{dx^2}$$

boundary conditions

$$T(x=a) = 0$$

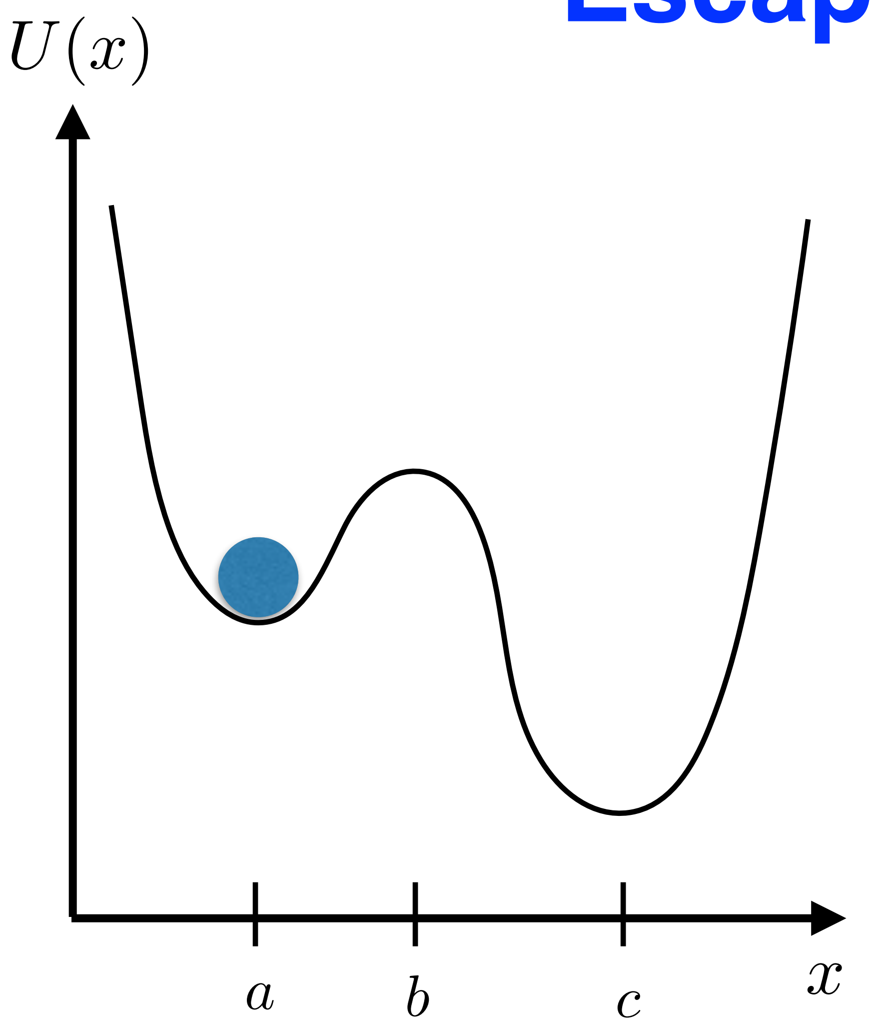
$$T(x=b) = 0$$

Example

$v = 0, D = \mathrm{const}$

$$T(x) = \frac{(x-a)(b-x)}{2D}$$

Escape over a potential barrier



$$\langle v(x)\rangle = -\frac{1}{\lambda}\frac{\partial U(x)}{\partial x}$$

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

What is the average time T_{esc} it takes for a particle to escape over a barrier?

Once particle crosses the peak it quickly descends into the global minimum. Therefore estimate the escape time, by placing reflecting boundary at *x*=*a* and absorbing boundary at *x*=*b*.

$$-1 = v(x)\frac{dT(x)}{dx} + D(x)\frac{d^2T(x)}{dx^2}$$

boundary conditions

$$\frac{dT}{dx}(x=a) = 0$$

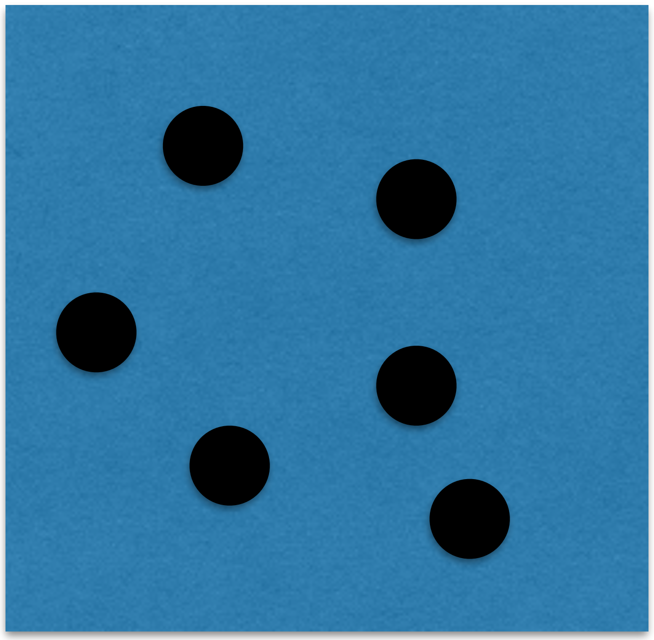
$$T(x=b) = 0$$

Arrhenious Law

$$T_{\text{esc}} = T(a) \approx \frac{\pi\lambda}{\sqrt{U''(a)U''(b)}} e^{[U(b)-U(a)]/k_B T}$$

Fick's laws

N noninteracting
Brownian particles



Local concentration $c(x,t) = Np(x,t)$

Fick's laws below directly follow
from Fokker-Plank equations

First Fick's law

Concentration flux

$$J = vc - \frac{\partial}{\partial x}\Big[Dc\Big]$$

Second Fick's law

Diffusion of concentration

$$\frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}\Big[vc\Big] + \frac{\partial^2}{\partial x^2}\Big[Dc\Big]$$

Generalization to higher dimensions

$$\vec{J} = \vec{v}c - \vec{\nabla}(Dc)$$

$$\frac{\partial c}{\partial t} = -\vec{\nabla}\cdot(\vec{v}c) + \vec{\nabla}^2(Dc)$$

Further reading