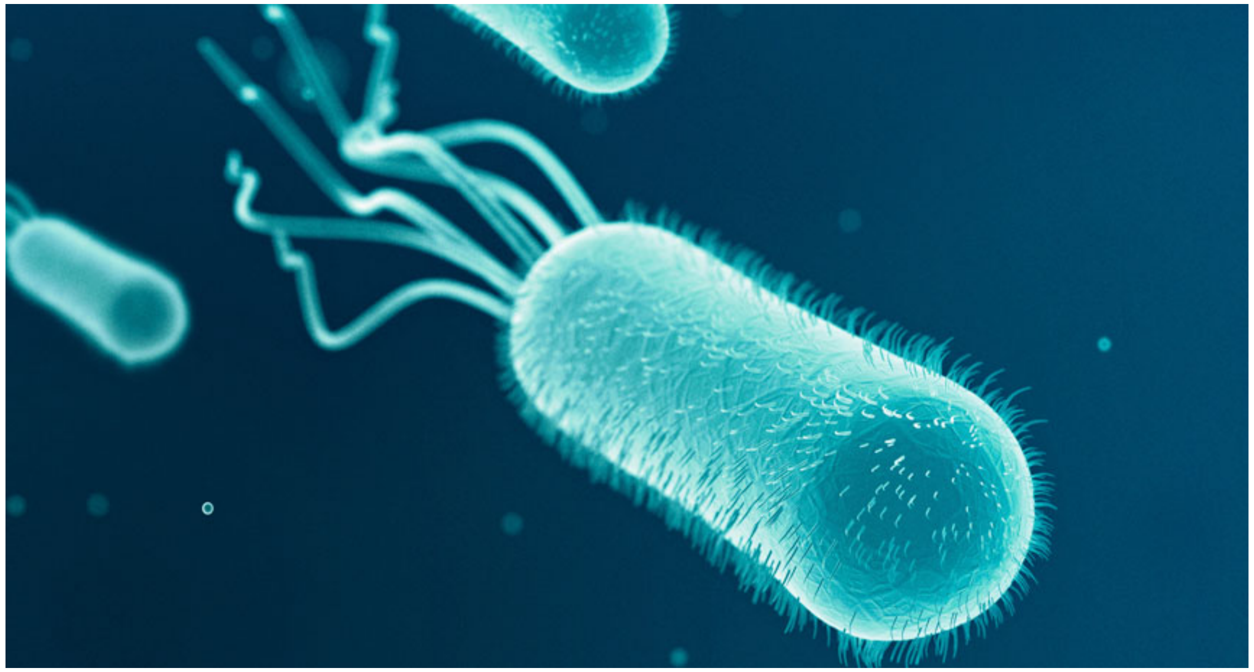
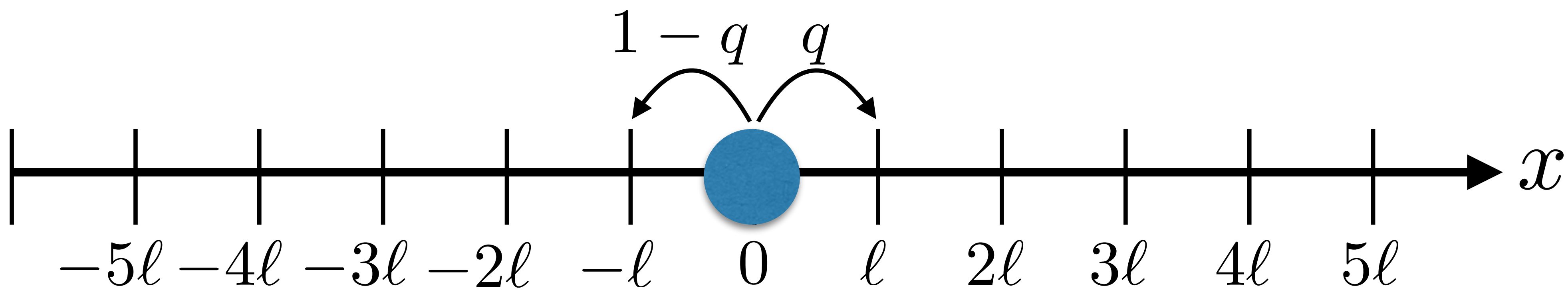
MAE 545: Lecture 18 (4/12)

Random walks

Chemotaxis of E. Coli

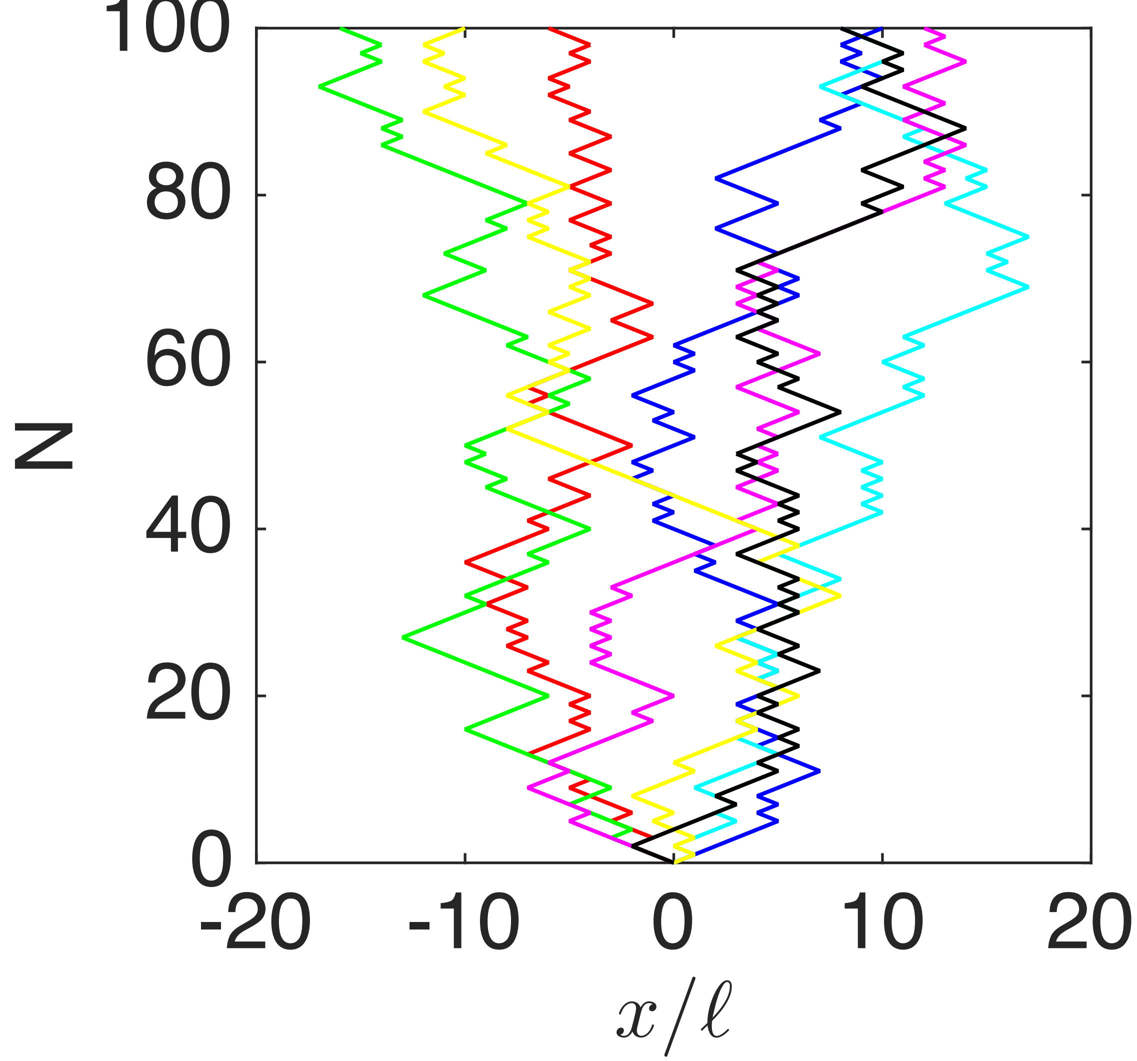


Random walk on a 1D lattice

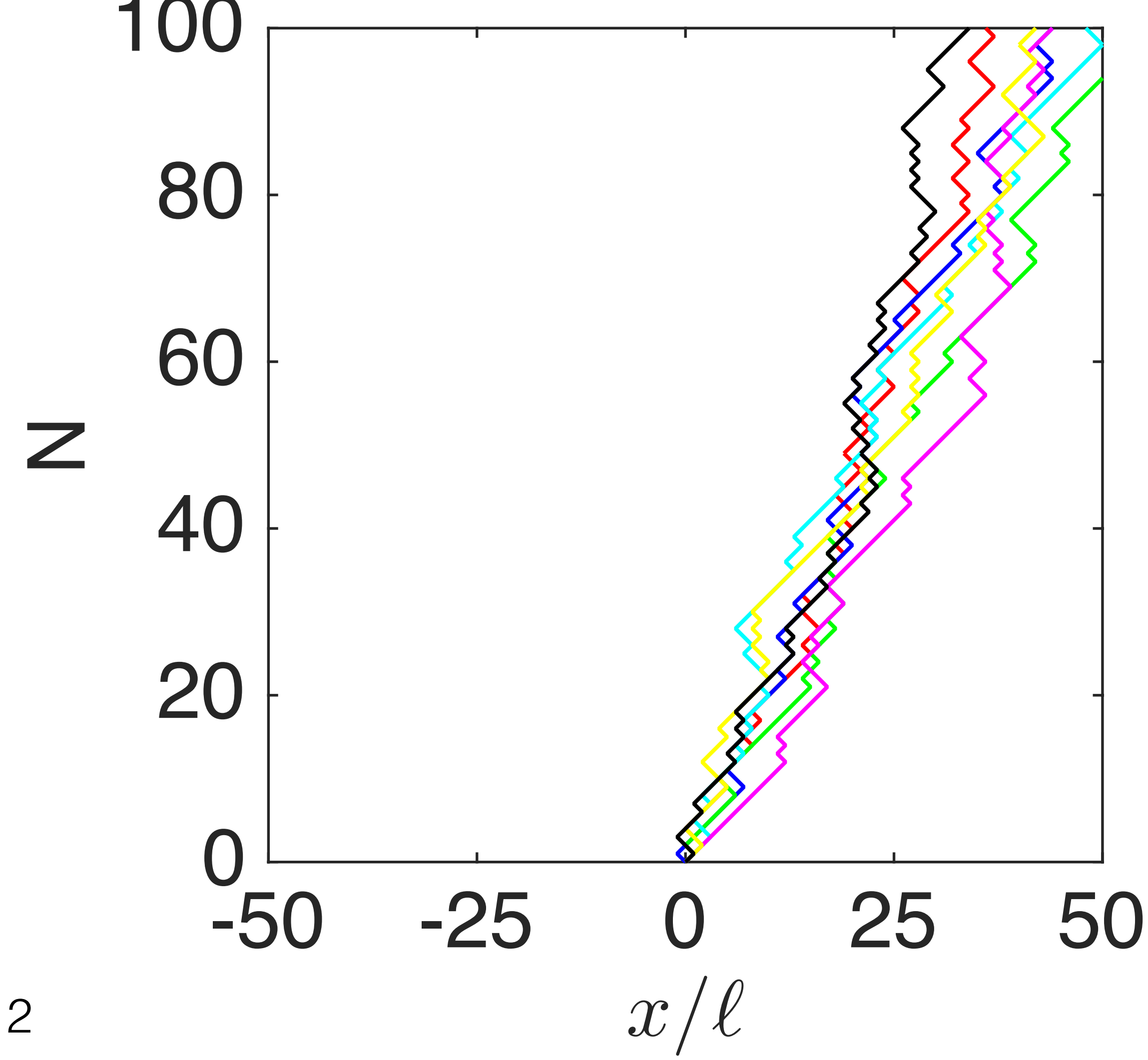


At each step particle jumps to the right with probability q and to the left with probability 1-q.

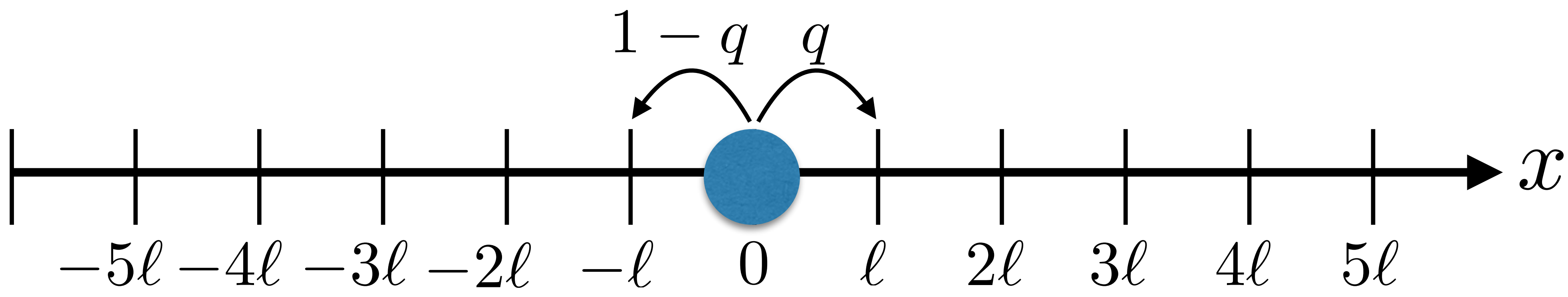
sample trajectories for q=1/2 (unbiased random walk)



sample trajectories for q=2/3 (biased random walk)



Gaussian approximation for p(x,N)



Position *x* after *N* jumps can be expressed as the sum of individual jumps $x_i \in \{-\ell, \ell\}$.

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

Mean value averaged over all possible random walks

$$\langle x \rangle = \sum_{i=1}^{N} \langle x_i \rangle = N \langle x_1 \rangle = N\left(q\ell - (1-q)\ell\right)$$

$$\boxed{\langle x \rangle = N\ell\,(2q-1)}$$

Variance averaged over all possible random walks

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = N\sigma_1^2 = N\left(\langle x_1^2 \rangle - \langle x_1 \rangle^2\right)$$

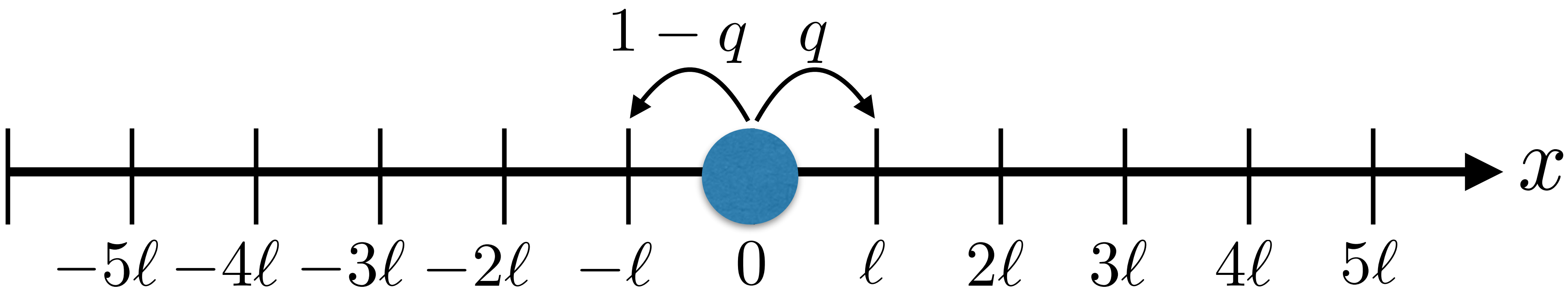
$$\sigma^2 = N\left(q\ell^2 + (1-q)\ell^2 - \langle x_1 \rangle^2\right)$$

$$\boxed{\sigma^2 = 4N\ell^2 q(1-q)}$$

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

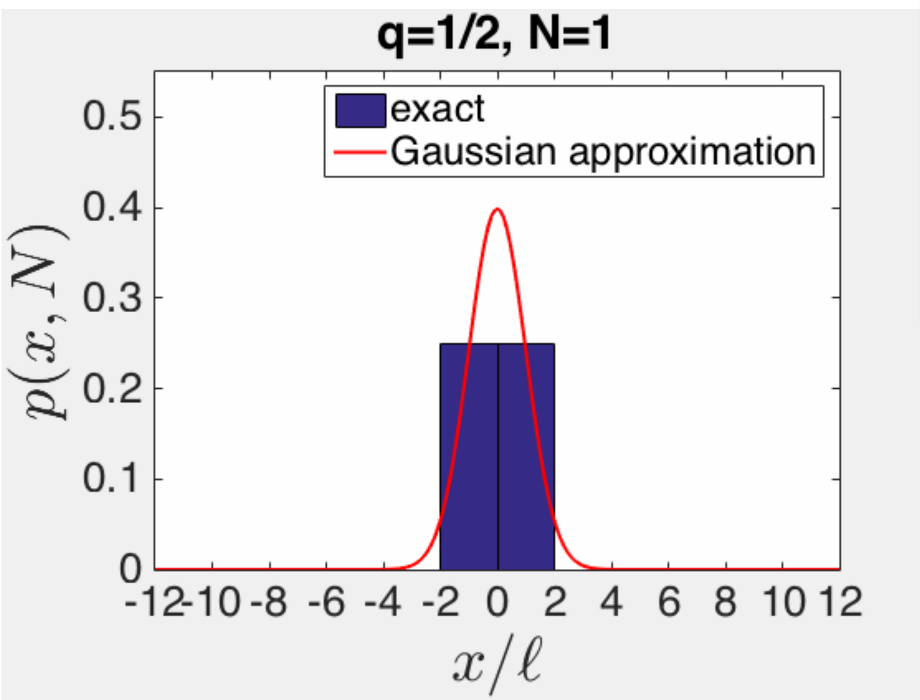
$$\boxed{p(x,N) \approx \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\langle x \rangle)^2/(2\sigma^2)}}$$

Random walk on a 1D lattice



unbiased random walk

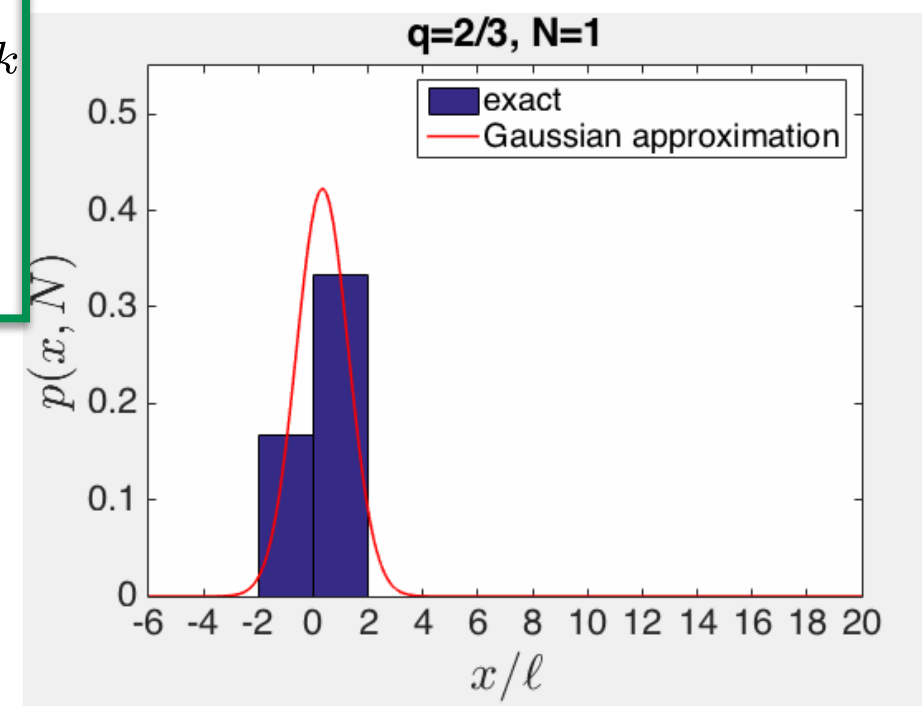
biased random walk

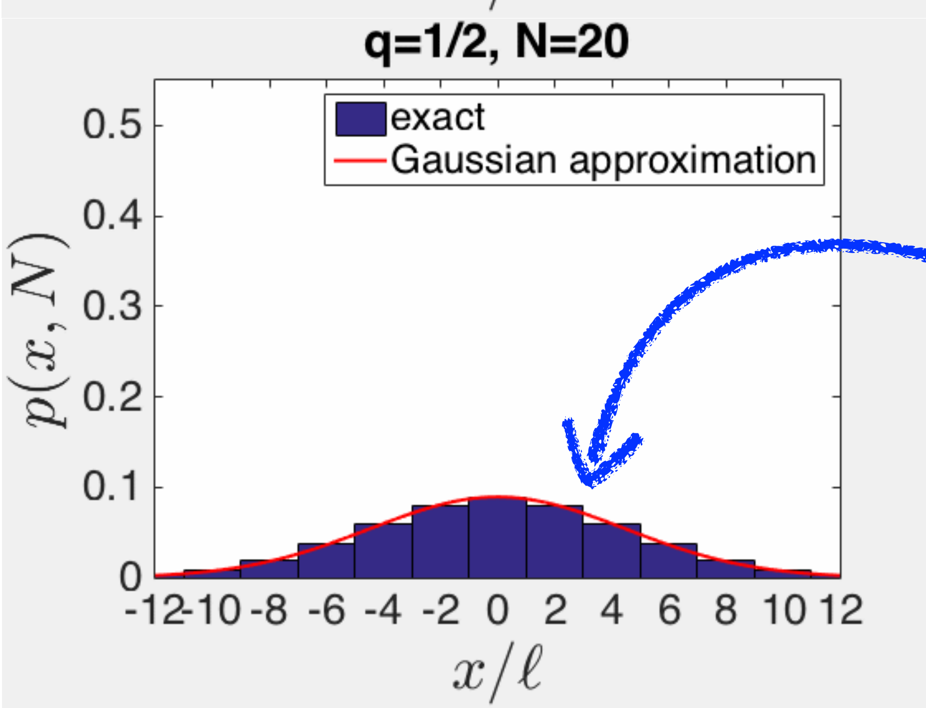


$$p(k,N) = \binom{N}{k} q^k (1-q)^{N-k}$$

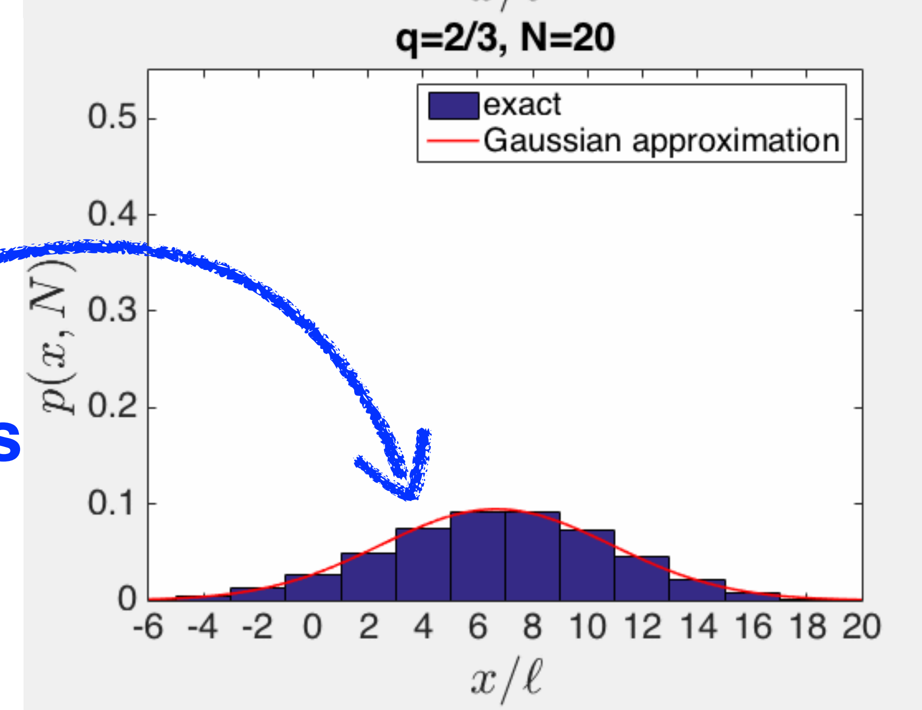
$$k = \frac{1}{2}\left(N + \frac{x}{\ell}\right)$$

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

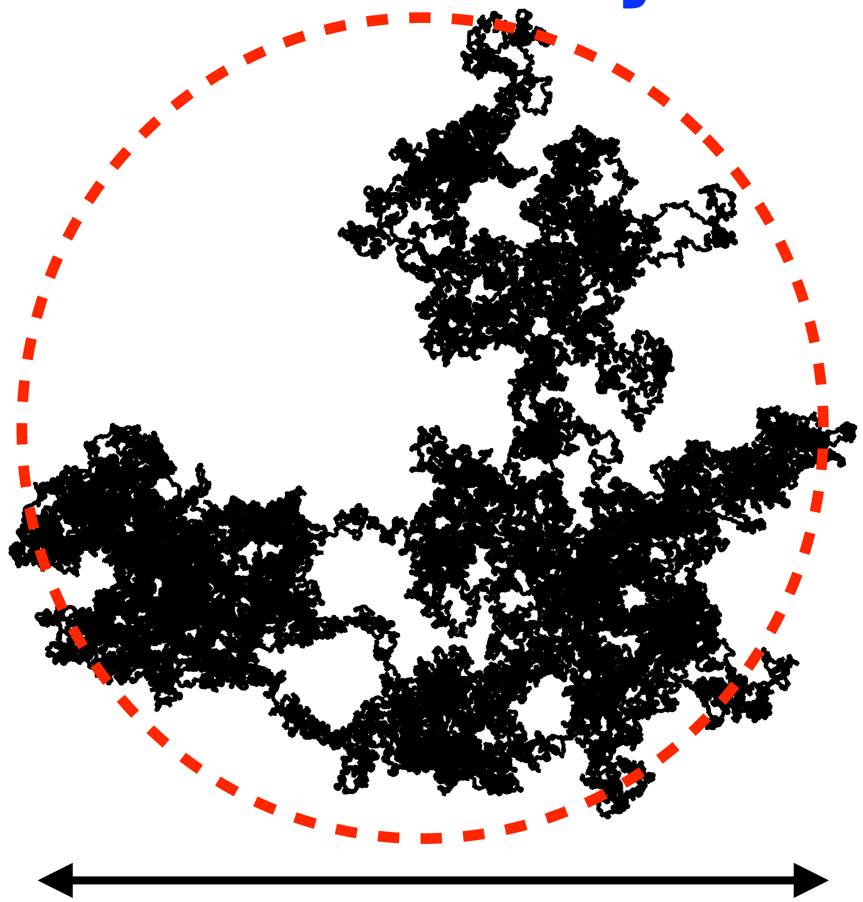




after several steps the probability distribution spreads out and becomes approximately Gaussian



Number of distinct sites visited by unbiased random walks



$$2r \propto \sqrt{N}$$

Total number of sites inside explored region after *N* steps

1D $N_{\text{tot}} \propto \sqrt{N}$

2D $N_{\text{tot}} \propto N$

3D $N_{\text{tot}} \propto N\sqrt{N}$

In 1D and 2D every site gets visited after a long time

In 3D some sites are never visited even after a very long time!

Shizuo Kakutani: "A drunk man will find his way home, but a drunk bird may get lost forever."

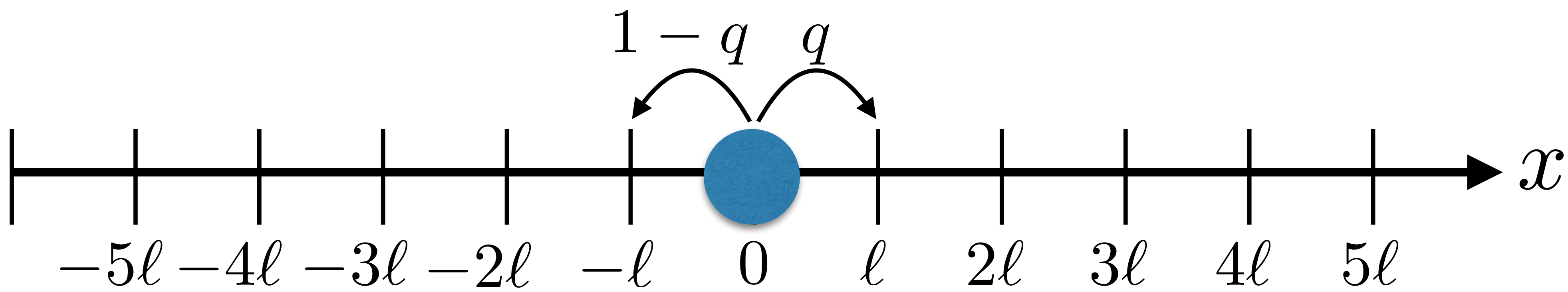
Number of distinct visited sites after *N* steps

1D $N_{\text{vis}} \approx \sqrt{8N/\pi}$

2D $N_{\text{vis}} \approx \pi N/\ln(8N)$

3D $N_{\text{vis}} \approx 0.66N$

Master 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*.

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

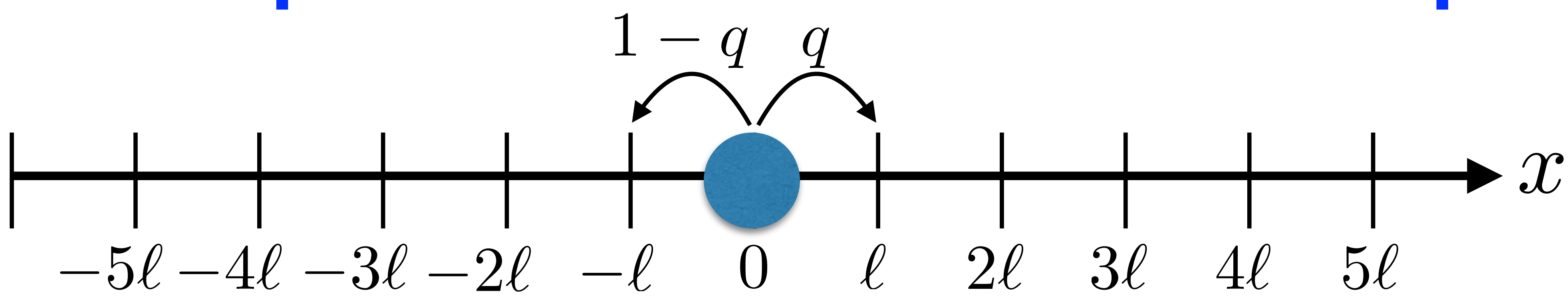
For our example the master equation reads:

$$p(x, N+1) = q\, p(x-\ell, N) + (1-q)\, p(x+\ell, N)$$

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

Probability distribution *p*(*x*,*N*) can be easily obtained numerically by iteratively advancing the master equation.

Master equation and Fokker-Planck equation



Assume that jumps occur in regular small time intervals: Δt

Master equation:

$$p(x, t + \Delta t) = q\, p(x - \ell, t) + (1 - q)\, p(x + \ell, t)$$

In the limit of small jumps and small time intervals, we can Taylor expand the master equation to derive an approximate drift-diffusion equation:

$$p + \Delta t \frac{\partial p}{\partial t} = q \left(p - \ell \frac{\partial p}{\partial x} + \frac{1}{2} \ell^2 \frac{\partial^2 p}{\partial x^2} \right) + (1 - q) \left(p + \ell \frac{\partial p}{\partial x} + \frac{1}{2} \ell^2 \frac{\partial^2 p}{\partial x^2} \right)$$

Fokker-Planck equation:

$$\frac{\partial p}{\partial t} = -v \frac{\partial p}{\partial x} + D \frac{\partial^2 p}{\partial x^2}$$

drift velocity $v = (2q - 1) \dfrac{\ell}{\Delta t}$

diffusion coefficient $D = \dfrac{\ell^2}{2 \Delta t}$

Diffusion equation

$$\frac{\partial p}{\partial t} = -v\frac{\partial p}{\partial x} + D\frac{\partial^2 p}{\partial x^2}$$

Solution of diffusion equation for a particle initially located at $x = x_0$:

$$p(x, t = 0) = \delta(x - x_0)$$

$$p(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-(x - x_0 - vt)^2/4Dt}$$

Mean and variance of probability distribution:

$$\langle x \rangle = \int dx\, x\, p(x,t) = x_0 + vt$$

$$\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle = \int dx\, (x - \langle x \rangle)^2\, p(x,t) = 2Dt$$

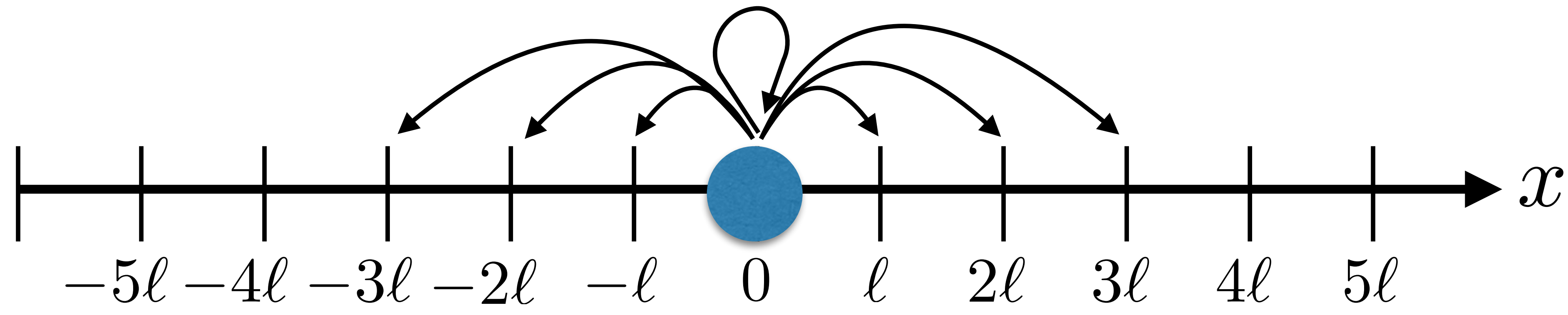
Generalization to *d* dimensions:

$$\frac{\partial p}{\partial t} = -\vec{v} \cdot \nabla p + D\nabla^2 p$$

$$p(\vec{r}, t) = \frac{1}{(4\pi D t)^{d/2}} e^{-(\vec{r} - \vec{r}_0 - \vec{v}t)^2/4Dt}$$

$$\langle \vec{r} \rangle = \vec{r}_0 + \vec{v}t \qquad \sigma^2 = 2dDt$$

Fokker-Planck equation



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

Generalized master equation:

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

Again Taylor expand the 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)

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

Lévy flights

Probability of jump lengths in *D* dimensions

$$\Pi(\vec{s}) = \begin{cases} C|\vec{s}|^{-\alpha}, & |\vec{s}| > s_0 \\ 0, & |\vec{s}| < s_0 \end{cases}$$

Normalization condition

$$\int d^D\vec{s}\,\Pi(\vec{s}) = 1 \longrightarrow \alpha > D$$

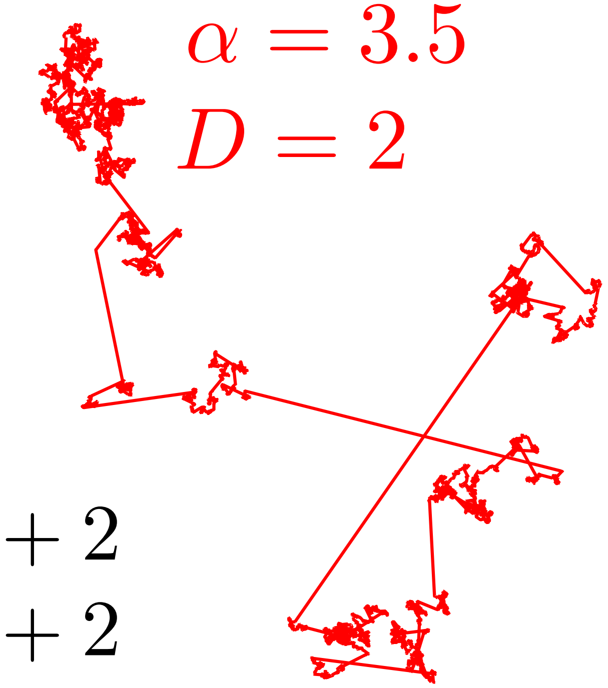
Moments of distribution

$$\langle \vec{s} \rangle = 0 \qquad \langle \vec{s}^{\,2} \rangle = \begin{cases} A_D s_0^2, & \alpha > D+2 \\ \infty, & \alpha < D+2 \end{cases}$$

Lévy flight trajectory

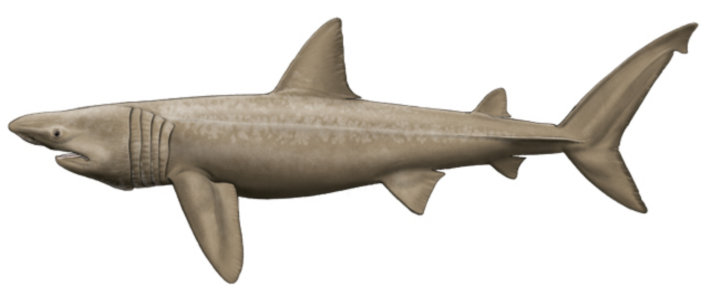
$\alpha = 3.5$

$D = 2$



2D random walk trajectory

Lévy flights are better strategy than random walk for finding prey that is scarce



D. W. Sims *et al.*
Nature **451**, 1098-1102 (2008)

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)

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

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 of *x***

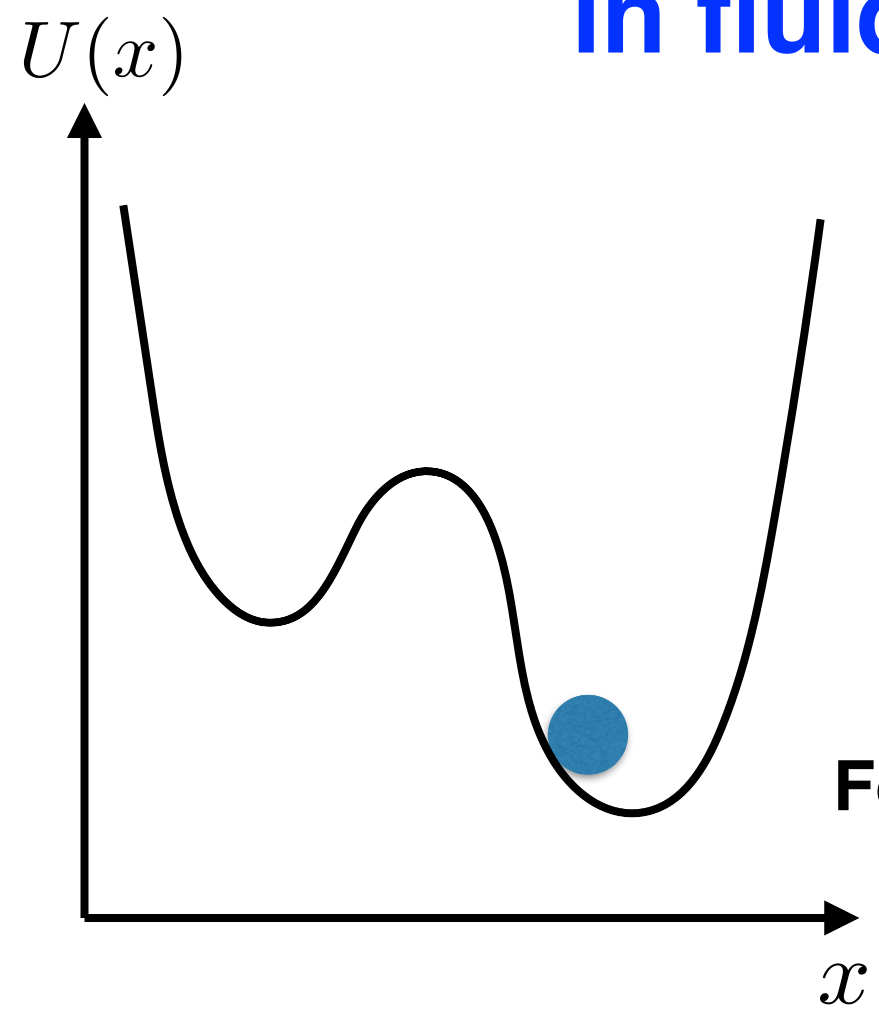
$$J^* \equiv v(x)p^*(x) - \frac{\partial}{\partial x}\left[D(x)p^*(x)\right] = \text{const}$$

Equilibrium probability distribution:

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: $\frac{\partial^2 x}{\partial t^2} \approx 0$

Drift velocity averaged over time $\langle v(x) \rangle = -\frac{1}{\lambda}\frac{\partial U(x)}{\partial x}$

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

Equilibrium probability distribution

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

(see previous slide) **(equilibrium physics)**

Einstein - Stokes equation

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

Diffusion at different temperatures

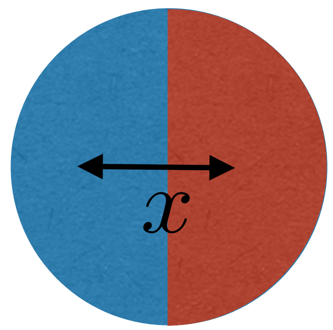
$$D = \frac{k_B T}{6\pi\eta R}$$

purple dye in hot water   blue dye in cold water

https://www.youtube.com/watch?v=A-5S2e1ubT8

Translational and rotational diffusion for particles suspended in liquid

Translational diffusion



$$\langle x^2 \rangle = 2D_T t$$

Stokes viscous drag: $\lambda_T = 6\pi\eta R$

Einstein - Stokes relation

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

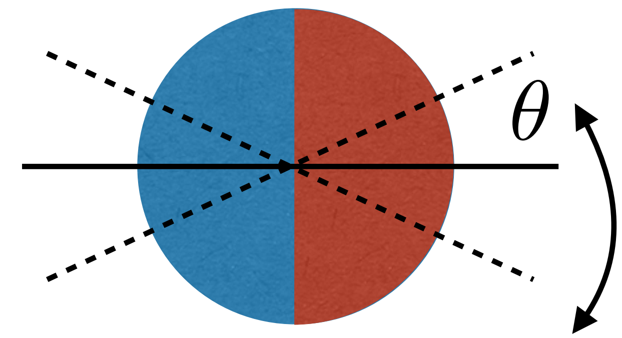
Time to move one body length in water at room temperature

$$\langle x^2 \rangle \sim R^2 \longrightarrow t \sim \frac{3\pi\eta R^3}{k_B T}$$

$$R \sim 1\mu\text{m} \longrightarrow t \sim 1\text{s}$$

$$R \sim 1\text{mm} \longrightarrow t \sim 100\,\text{years}$$

Rotational diffusion



$$\langle \theta^2 \rangle = 2D_R t$$

Stokes viscous drag: $\lambda_R = 8\pi\eta R^3$

Einstein - Stokes relation

$$D_R = \frac{k_B T}{8\pi\eta R^3}$$

Time to rotate by 90⁰ in water at room temperature

$$\langle \theta^2 \rangle \sim 1 \longrightarrow t \sim \frac{4\pi\eta R^3}{k_B T}$$

Boltzmann constant $k_B = 1.38 \times 10^{-23}\text{J/K}$

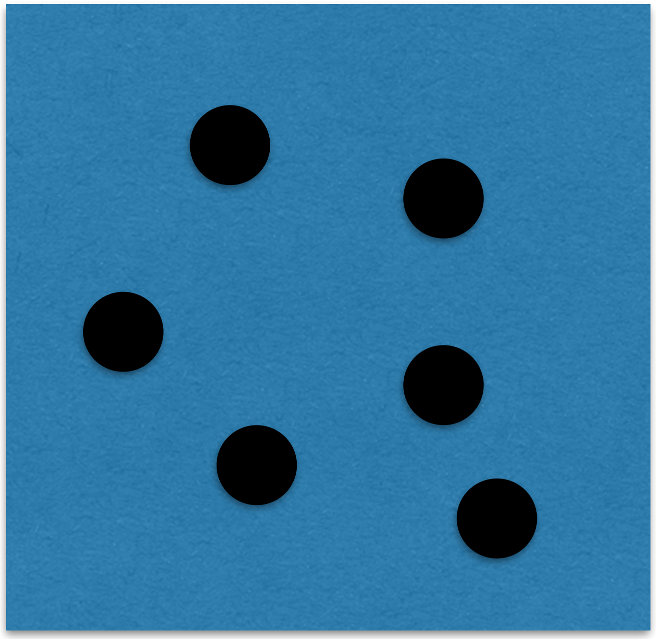
water viscosity $\eta \approx 10^{-3}\text{kg}\,\text{m}^{-1}\text{s}^{-1}$

room temperature $T = 300\text{K}$

Fick's laws

Adolf Fick 1855

N noninteracting Brownian particles



Local concentration of particles

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

Fick's laws are equivalent to Fokker-Plank equation

First Fick's law

Flux of particles

$$J = vc - D\frac{\partial c}{\partial x}$$

Second Fick's law

Diffusion of particles

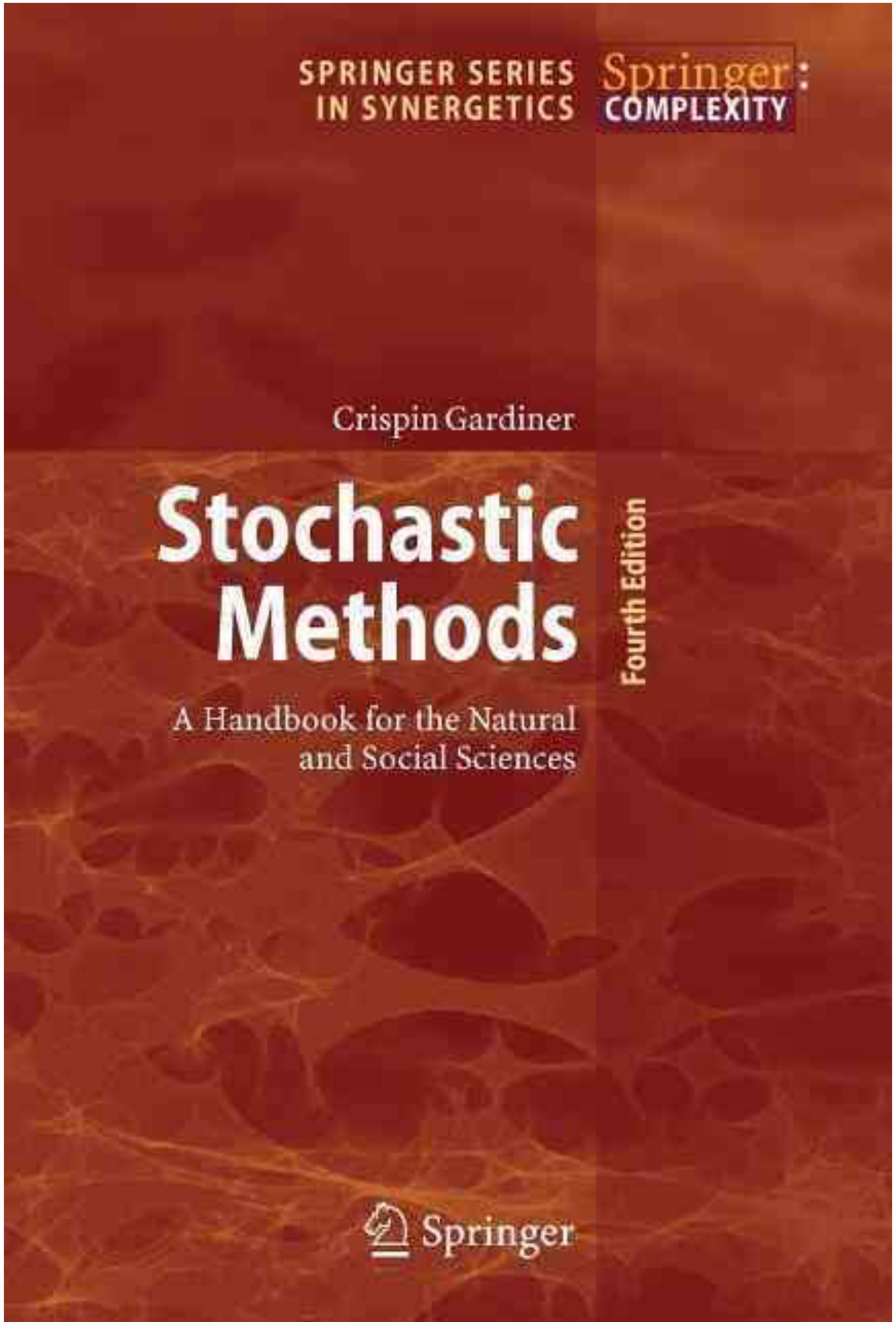
$$\frac{\partial c}{\partial t} = -\frac{\partial J}{\partial x} = -\frac{\partial}{\partial x}\Big[vc\Big] + \frac{\partial}{\partial x}\Big[D\frac{\partial c}{\partial x}\Big]$$

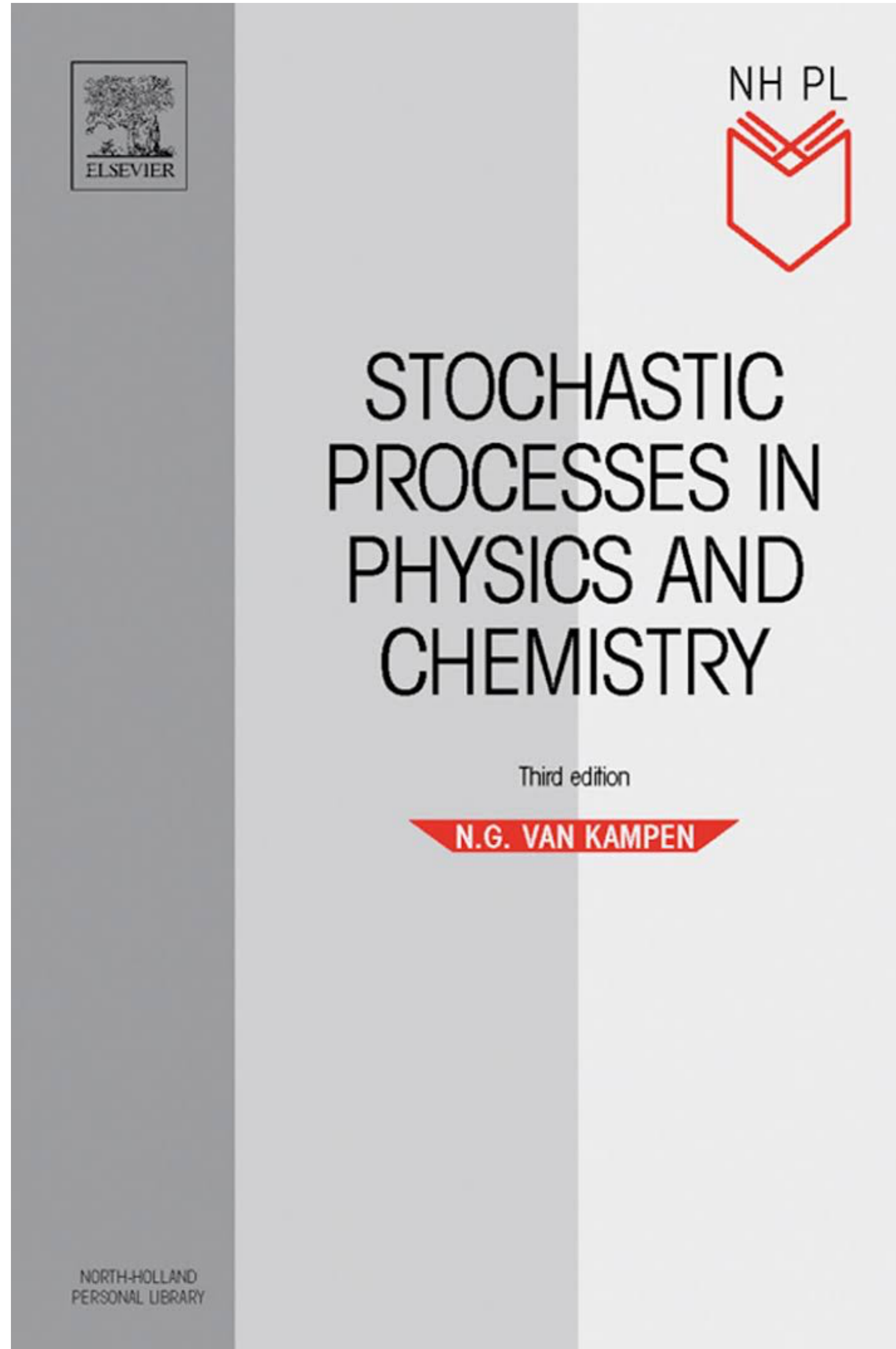
Generalization to higher dimensions

$$\vec{J} = c\vec{v} - D\vec{\nabla}c$$

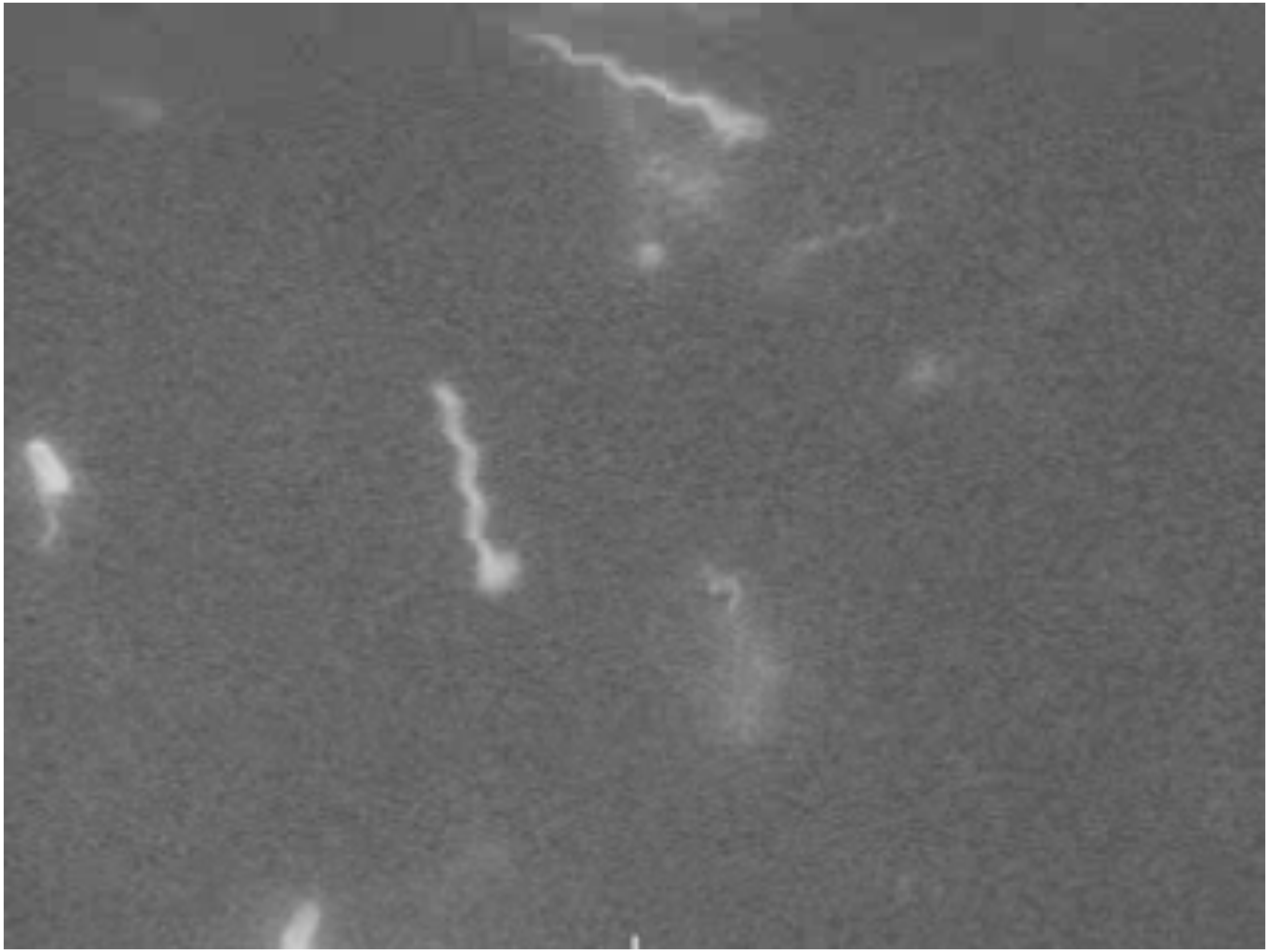
$$\frac{\partial c}{\partial t} = -\vec{\nabla}J = -\vec{\nabla}\cdot(c\vec{v}) + \vec{\nabla}\cdot(D\vec{\nabla}c)$$

Further reading



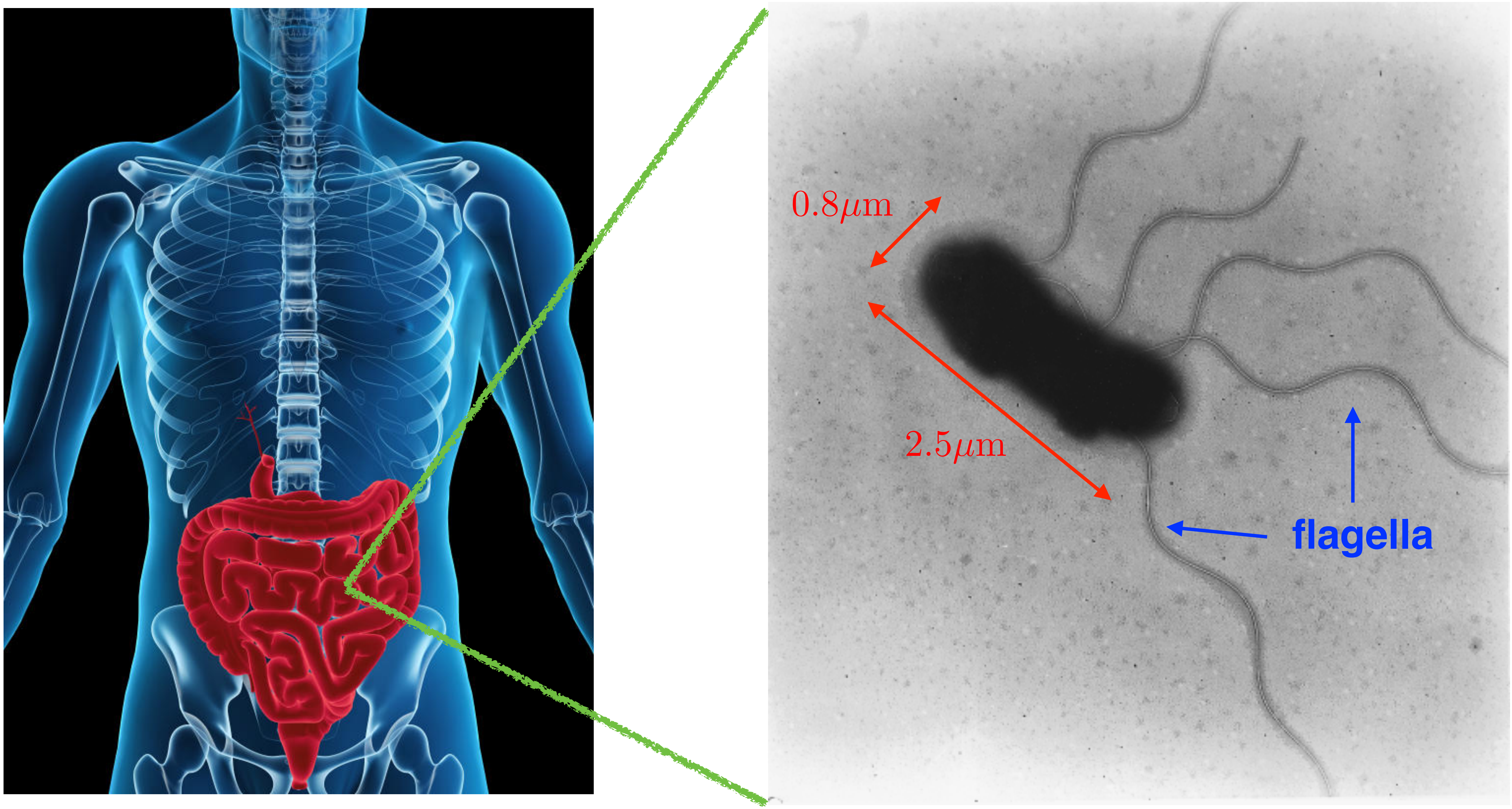


E. coli chemotaxis



L. Turner, W.S. Ryu, H.C. Berg**,** J. Bacteriol. **182,** 2793-2801 (2000)

Escherichia coli



E. coli is a part of gut flora that helps us digest food.

In normal conditions E. coli divide and produce 2 daughter cells every ~20min.

Concentration of E. coli $\sim 10^9 \mathrm{cm}^{-3}$

Total concentration of bacteria $\sim 10^{11} \mathrm{cm}^{-3}$

In one day one E. coli could produce ~7x10^{10} new cells!

Flagella filaments and rotary motors

Flagellum filament

left handed helix

helix diameter

$d \approx 0.4\mu\mathrm{m}$

filament diameter

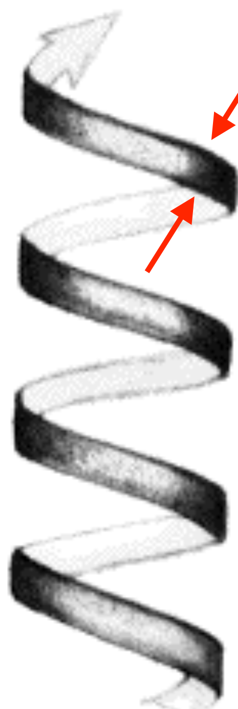
$\approx 20\mathrm{nm}$

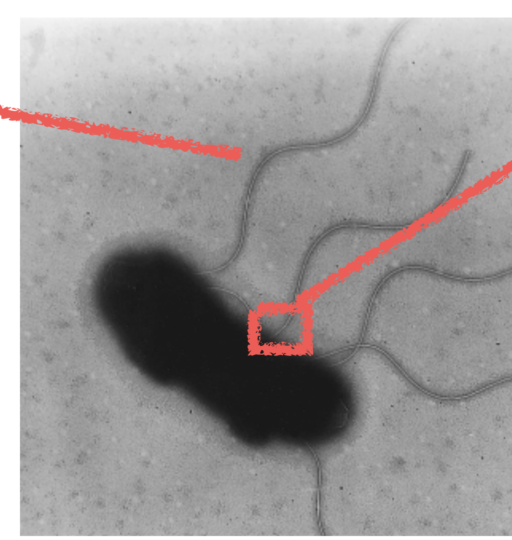
length

$L \lesssim 10\mu\mathrm{m}$

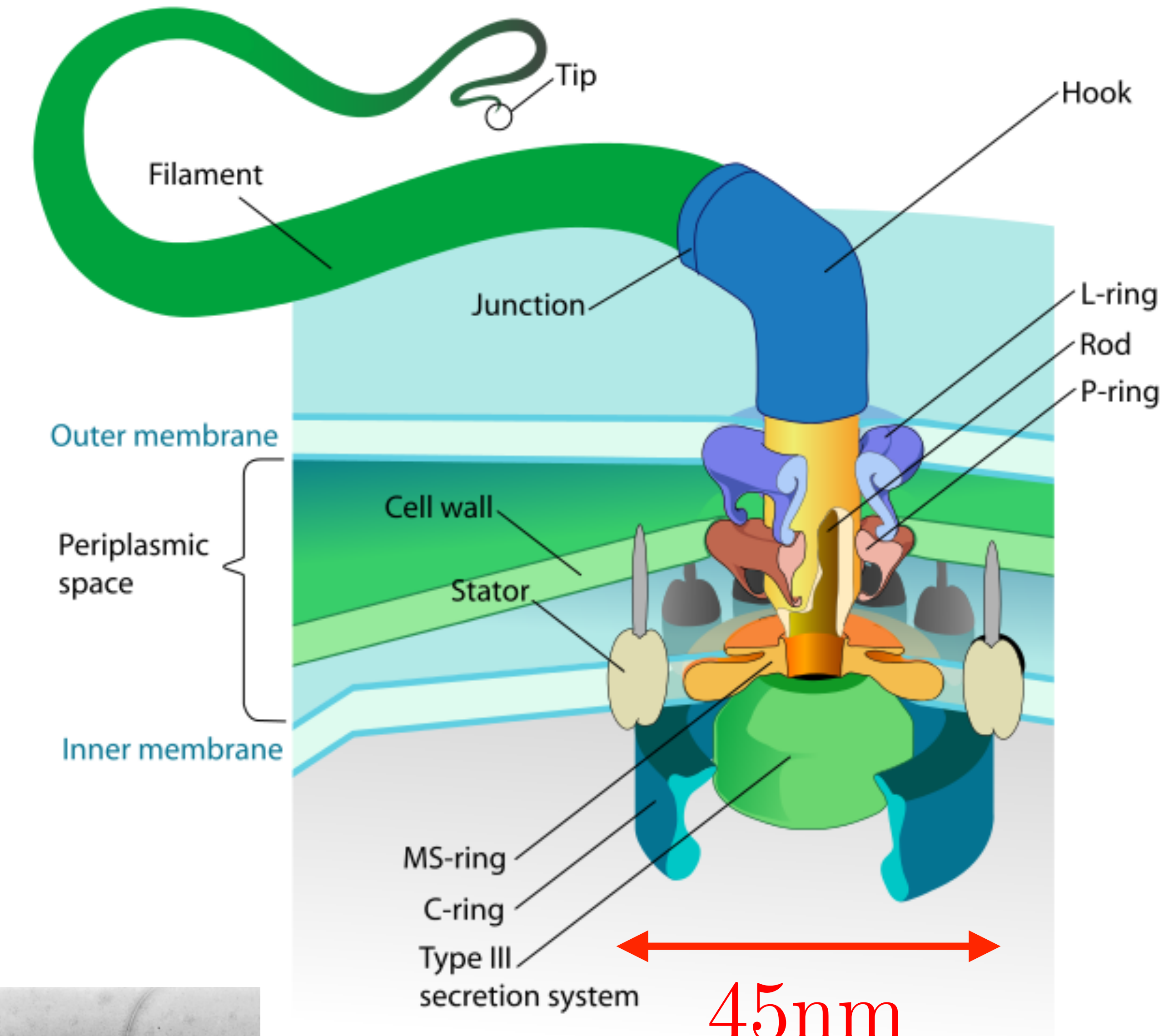
pitch

$p \approx 2.3\mu\mathrm{m}$



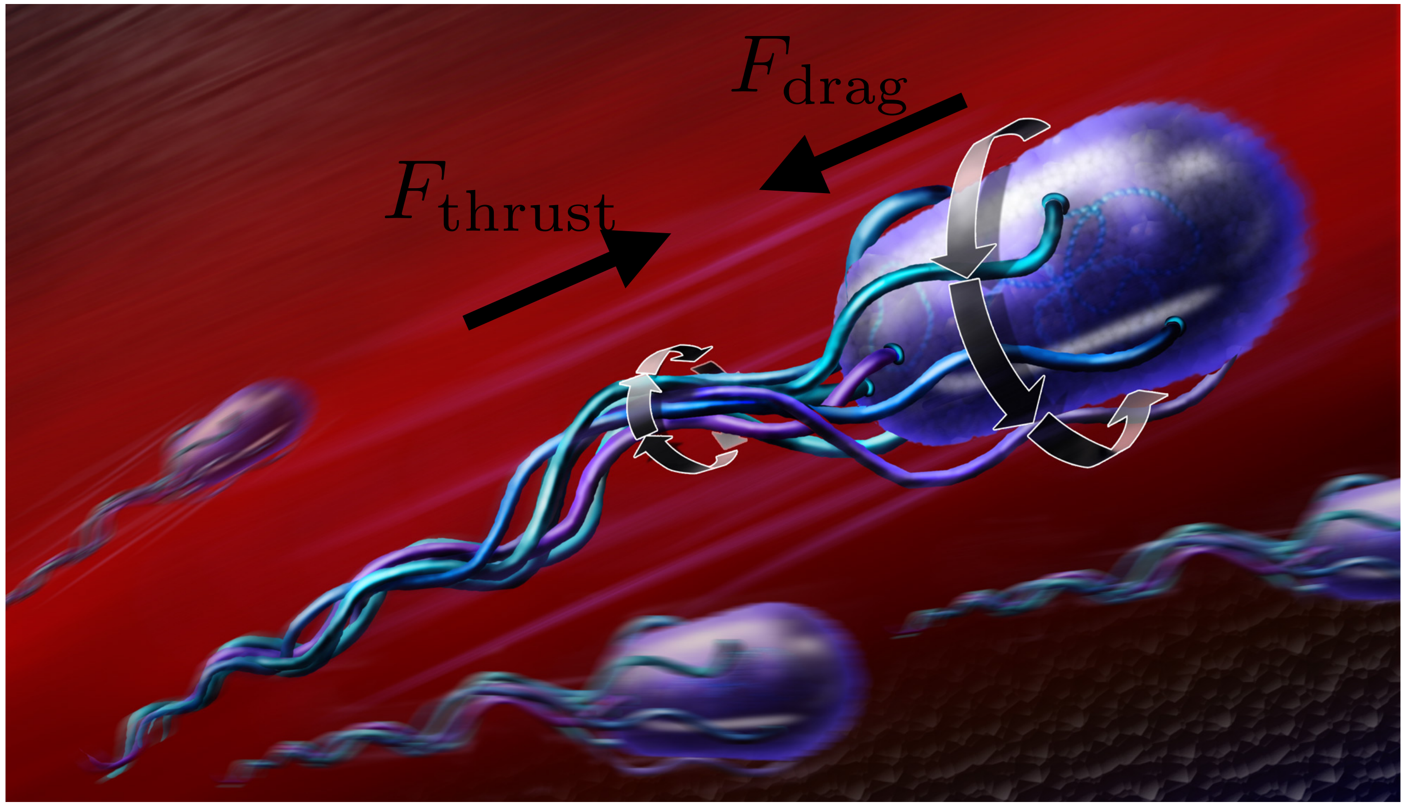


Rotary motor



$45\mathrm{nm}$

Swimming of E. coli



swimming speed	$v_s \sim 20\mu\text{m/s}$
body spinning frequency	$f_b \sim 10\text{Hz}$
spinning frequency of flagellar bundle	$f_r \sim 100\text{Hz}$

Thrust force generated by spinning flagellar bundle

$$F_{\text{thrust}} = F_{\text{drag}} \approx 6\pi\eta R v_s$$

$$F_{\text{thrust}} \sim 0.4\text{pN} = 4 \times 10^{-13}\text{N}$$

Torque generated by spinning flagellar bundle

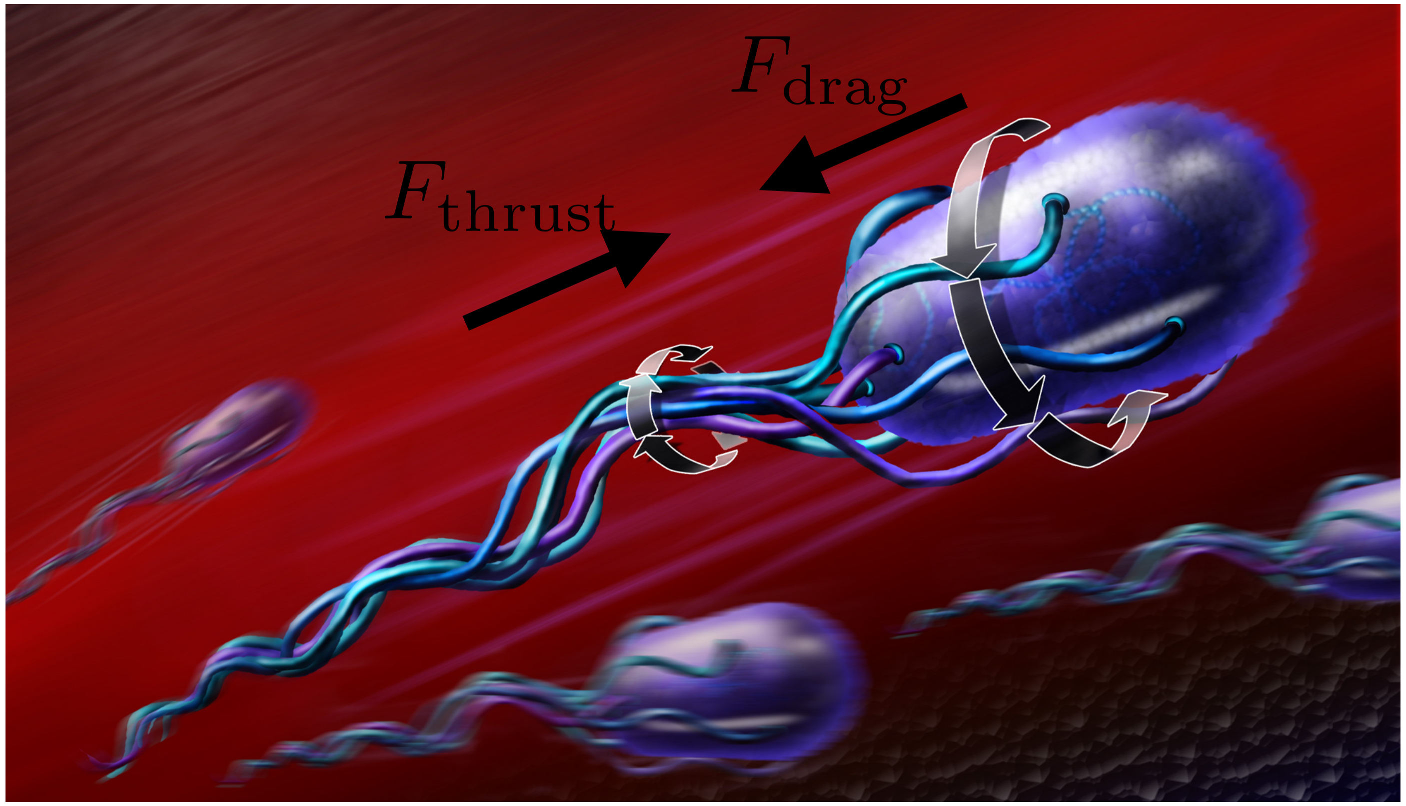
$$N = N_{\text{drag}} \approx 8\pi\eta R^3 \omega_b$$

$$N \sim 2\text{pN}\,\mu\text{m} = 2 \times 10^{-18}\text{Nm}$$

size of E. coli $R \approx 1\mu\text{m}$

water viscosity $\eta \approx 10^{-3}\text{kg}\,\text{m}^{-1}\text{s}^{-1}$

How quickly E. coli stops if motors shut off?



swimming speed	$v_s \sim 20\mu\text{m/s}$
size of E. coli	$R \approx 1\mu\text{m}$
water viscosity	$\eta \approx 10^{-3}\text{kg}\,\text{m}^{-1}\text{s}^{-1}$
mass of E. coli	$m \sim \frac{4\pi R^3 \rho}{3} \sim 4\text{pg}$

Newton's law

$$m\ddot{x} = -6\pi\eta R\dot{x}$$

$$x = x_0\left[1 - e^{-t/\tau}\right]$$

$$\tau \approx \frac{m}{6\pi\eta R} \approx \frac{2\rho R^2}{9\eta} \sim 0.2\mu\text{s}$$

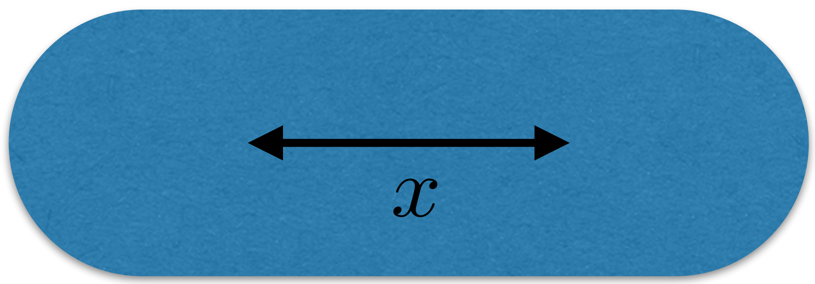
$$x_0 = v_s\tau \sim 0.1\text{Å}$$

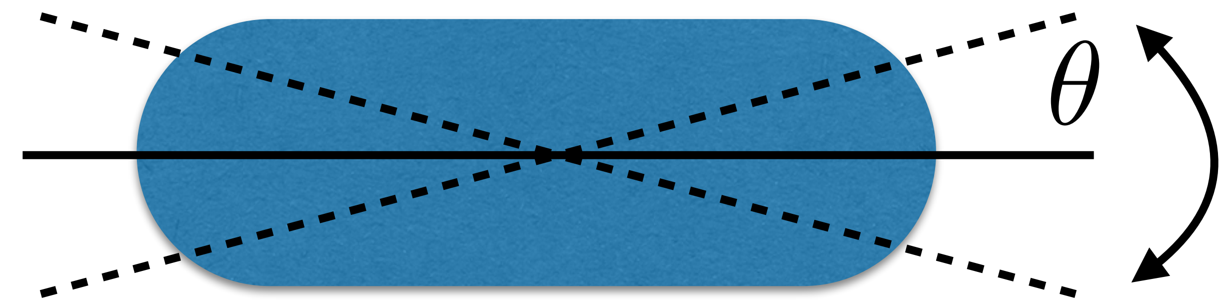
E. coli stops almost instantly!

signature of low Reynolds numbers

$$\text{Re} = \frac{R v_s \rho}{\eta} \sim 2 \times 10^{-5}$$

Translational and rotational diffusion of E. coli





$$\langle x^2 \rangle = 2 D_T t$$

$$\langle \theta^2 \rangle = 2 D_R t$$

Einstein - Stokes relation

$$D_T \approx \frac{k_B T}{6 \pi \eta R} \approx 0.2 \mu\mathrm{m}^2/s$$

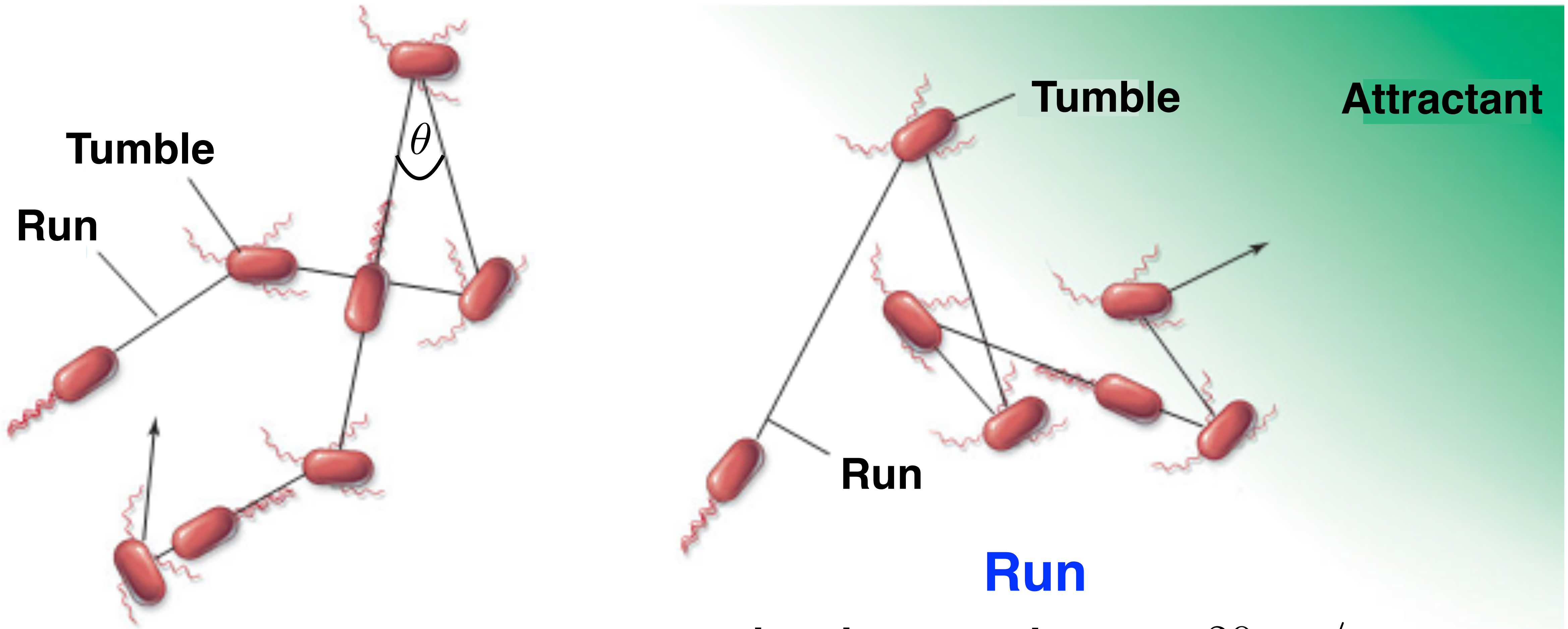
Einstein - Stokes relation

$$D_R \approx \frac{k_B T}{8 \pi \eta R^3} \sim 0.2\,\mathrm{rad}^2/\mathrm{s}$$

After ~10s the orientation of E. coli changes by 90^0 due to the Brownian motion!

size of E. coli	$R \approx 1 \mu\mathrm{m}$
water viscosity	$\eta \approx 10^{-3} \mathrm{kg}\,\mathrm{m}^{-1}\mathrm{s}^{-1}$
Boltzmann constant	$k_B = 1.38 \times 10^{-23} \mathrm{J/K}$
temperature	$T = 300\mathrm{K}$

E. coli chemotaxis



Run

swimming speed: $v_s \sim 20\mu\mathrm{m/s}$

typical duration: $t_r \sim 1\mathrm{s}$

all motors turning counter clockwise

Increase (Decrease) run durations, when swimming towards good (harmful) environment.

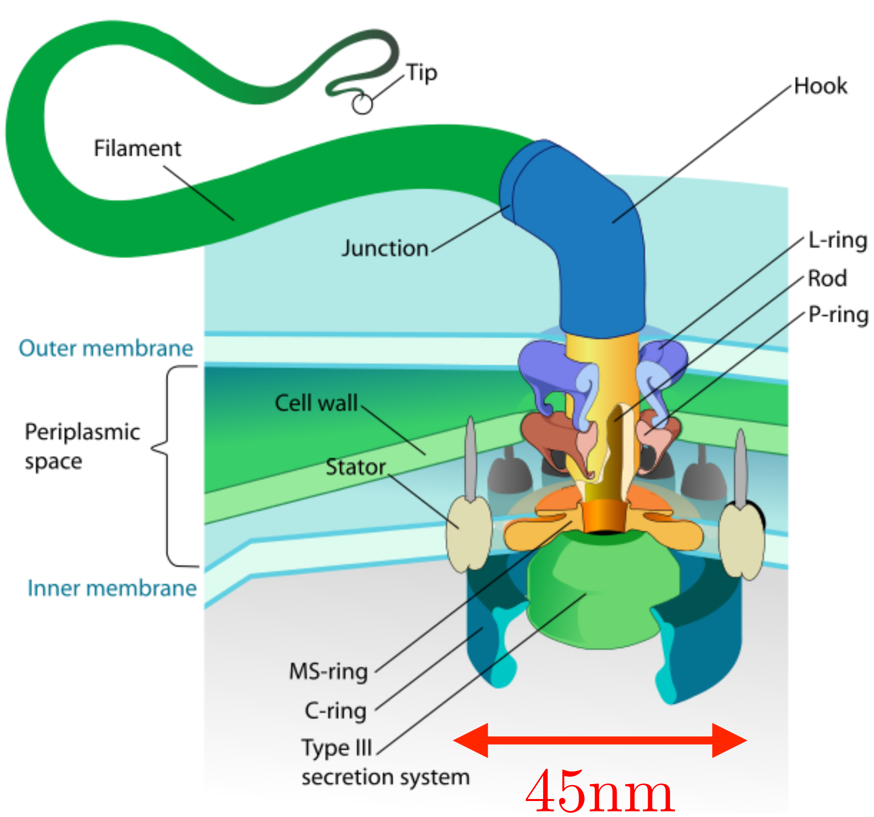
Tumble

random change in orientation $\langle\theta\rangle = 68^\circ$

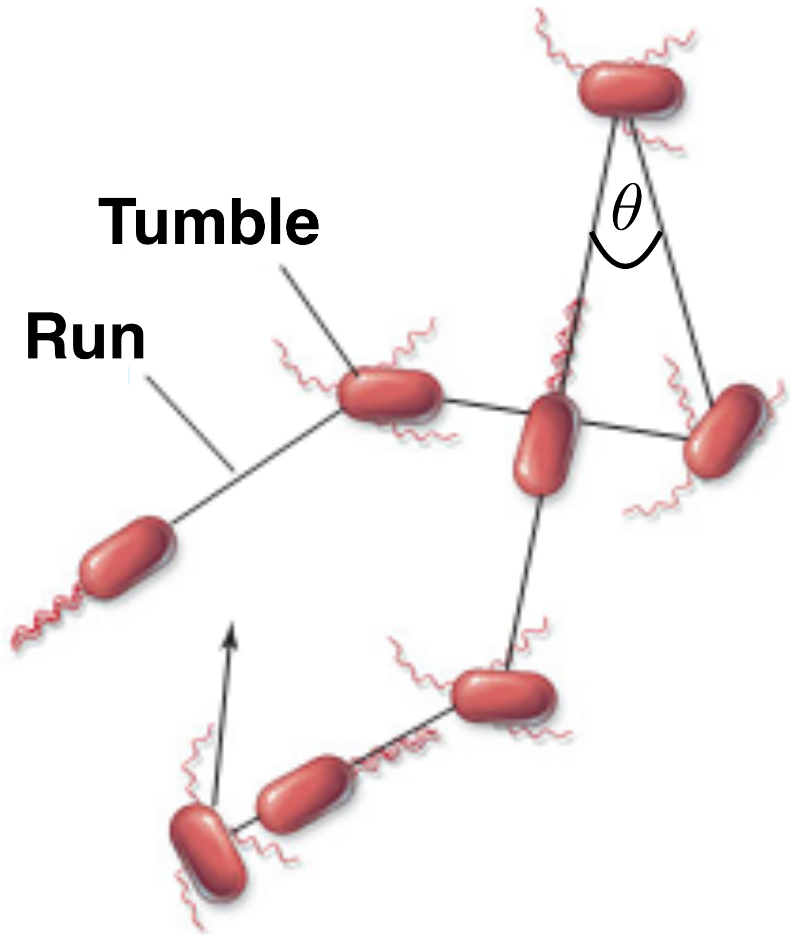
typical duration: $t_t \sim 0.1\mathrm{s}$

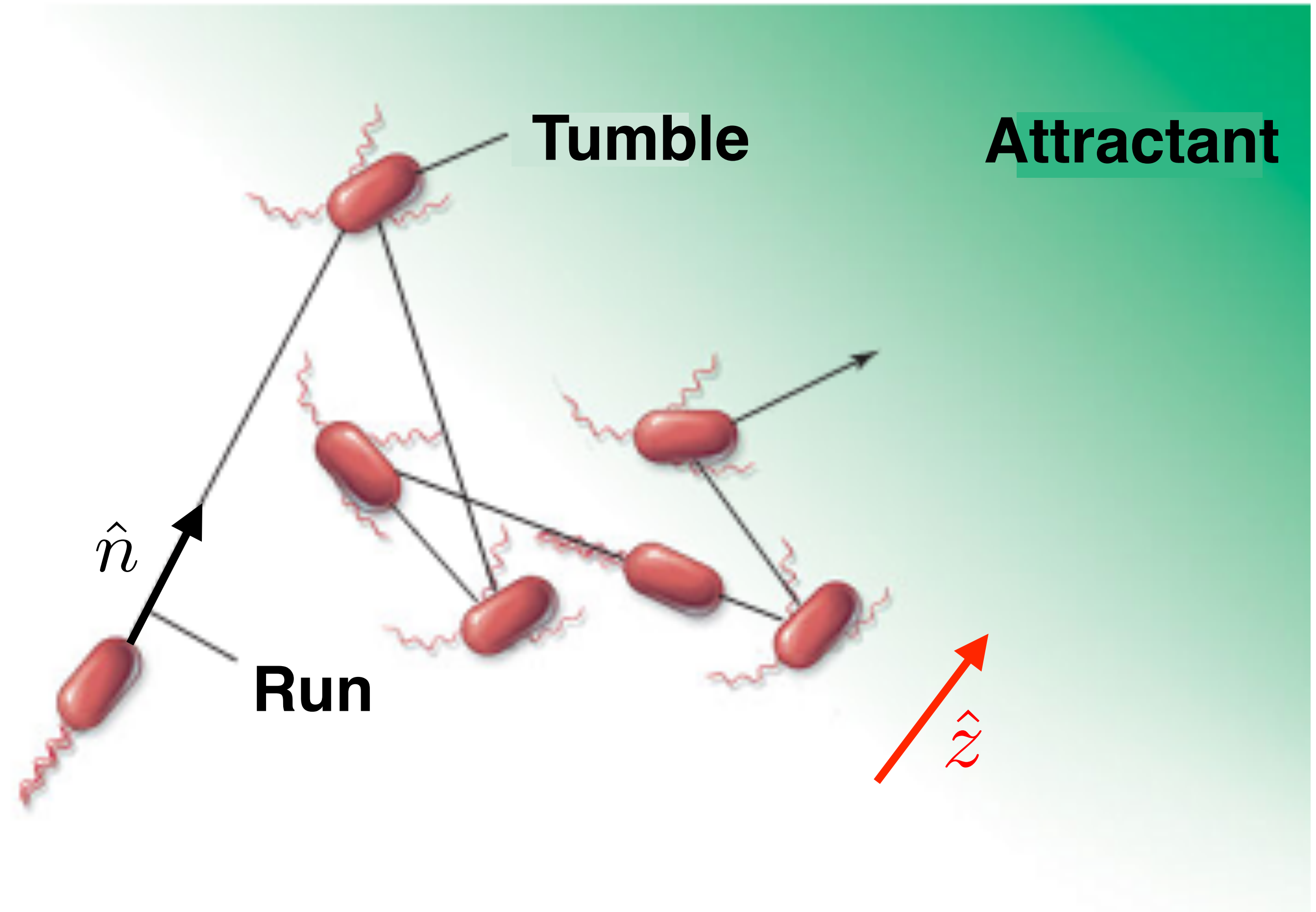
one or more motors turning clockwise

Rotary motor



E. coli chemotaxis





Homogeneous environment

run duration: $t_r \sim 1\mathrm{s}$

tumble duration: $t_t \sim 0.1\mathrm{s}$

swimming speed: $v_s \sim 20\mu\mathrm{m/s}$

drift velocity

$$v_d = 0$$

effective diffusion

$$D_{\mathrm{eff}} = \frac{\langle \Delta \ell^2 \rangle}{6 \langle \Delta t \rangle}$$

$$D_{\mathrm{eff}} \approx \frac{v_s^2 t_r^2}{6(t_r + t_t)} \sim 60\mu\mathrm{m}^2/\mathrm{s}$$

Gradient in “food” concentration

run duration increases (decreases) when swimming towards (away) from “food”

$$t_r(\hat{n}) = \bar{t}_r + \alpha(\hat{n}\cdot\hat{z})(\partial c/\partial z)$$

drift velocity

$$v_d = \frac{\langle \Delta z \rangle}{\langle \Delta t \rangle} \approx \frac{v_s \alpha (\partial c/\partial z)}{3(\bar{t}_r + t_t)}$$

$$\langle \Delta z \rangle = \langle v_z(\hat{n}) t_r(\hat{n}) \rangle = \langle v_s (\hat{n}\cdot\hat{z}) t_r(\hat{n}) \rangle$$