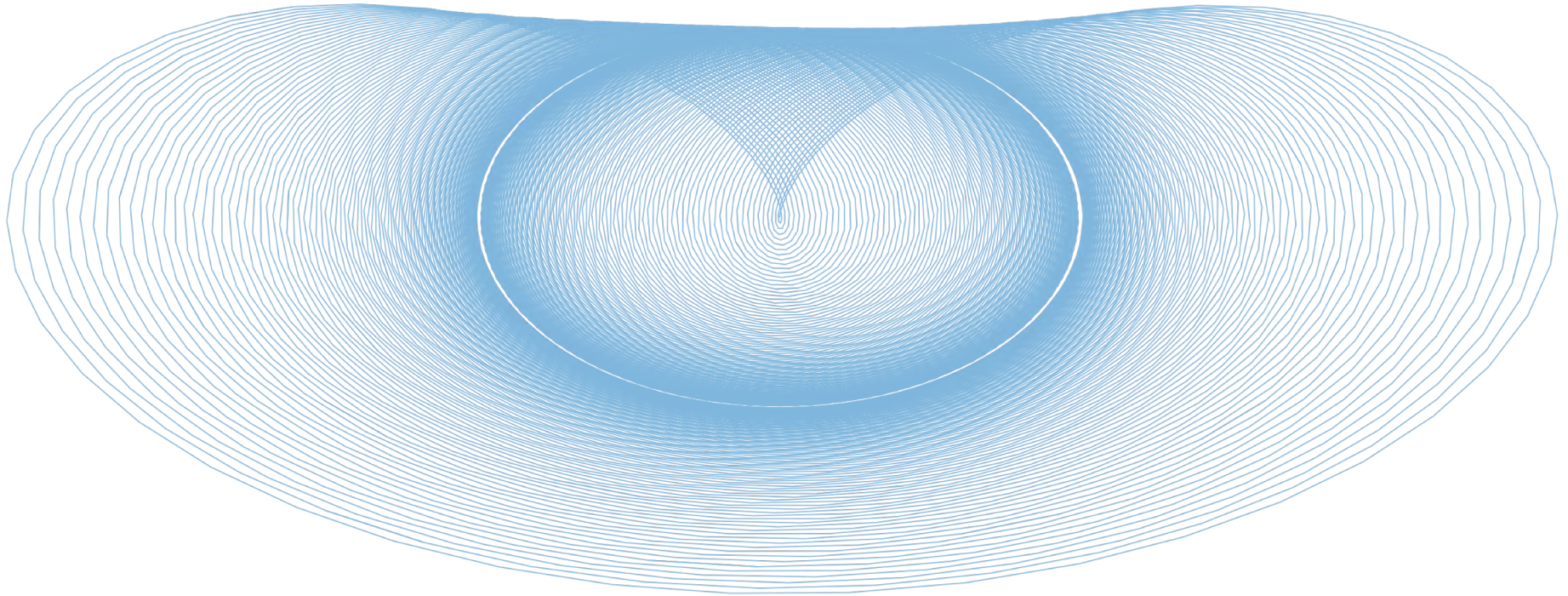PHYS 1420 (F19)
Physics with Applications to Life Sciences

2019.11.13
Relevant reading:
Kesten & Tauck ch. N/A

Christopher Bergevin
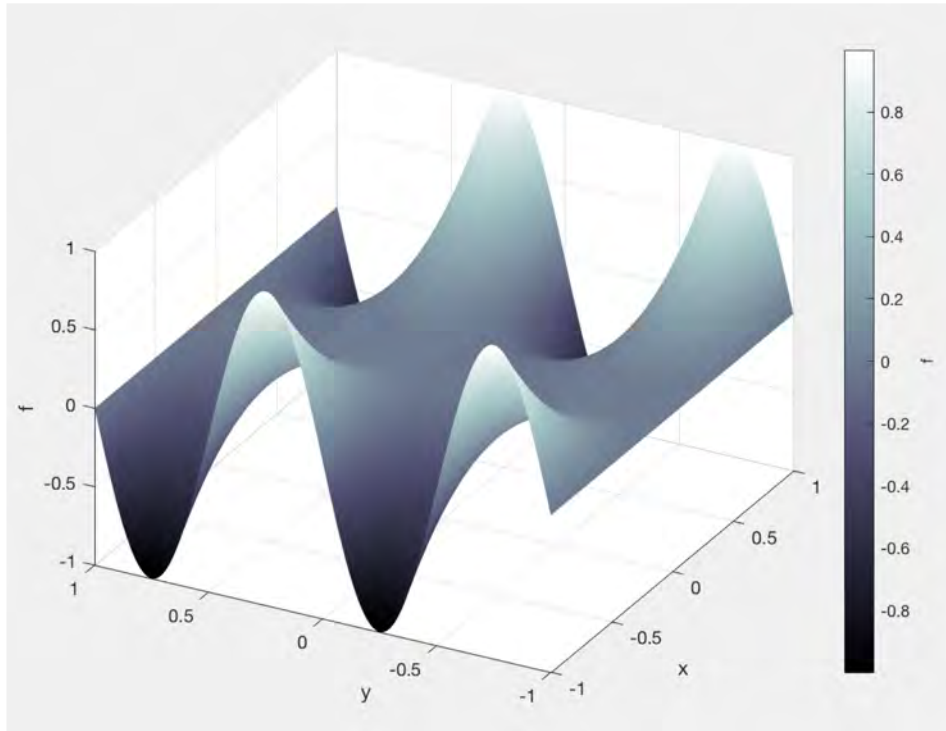York University, Dept. of Physics & Astronomy
Office: Petrie 240   Lab: Farq 103
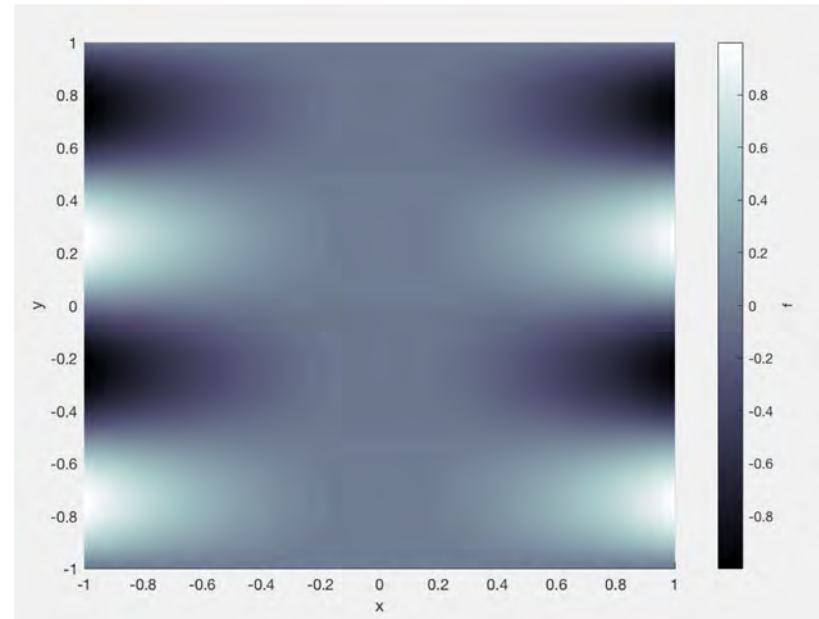cberge@yorku.ca

Ref. (re images):
Wolfson (2007), Knight (2017),
Kesten & Tauck (2012)

Top-down view

→ What is $f(x,y)$?

→ Written HW #2: Posted and due Friday 11/15 in class

→ Final exam: Saturday, Dec. 14 (start preparing!)

Some relevant underlying concepts of the day...

➢ Fick's Law & Diffusion equation

➢ "Swarming" & flocking

➢ Aside re *entropy*

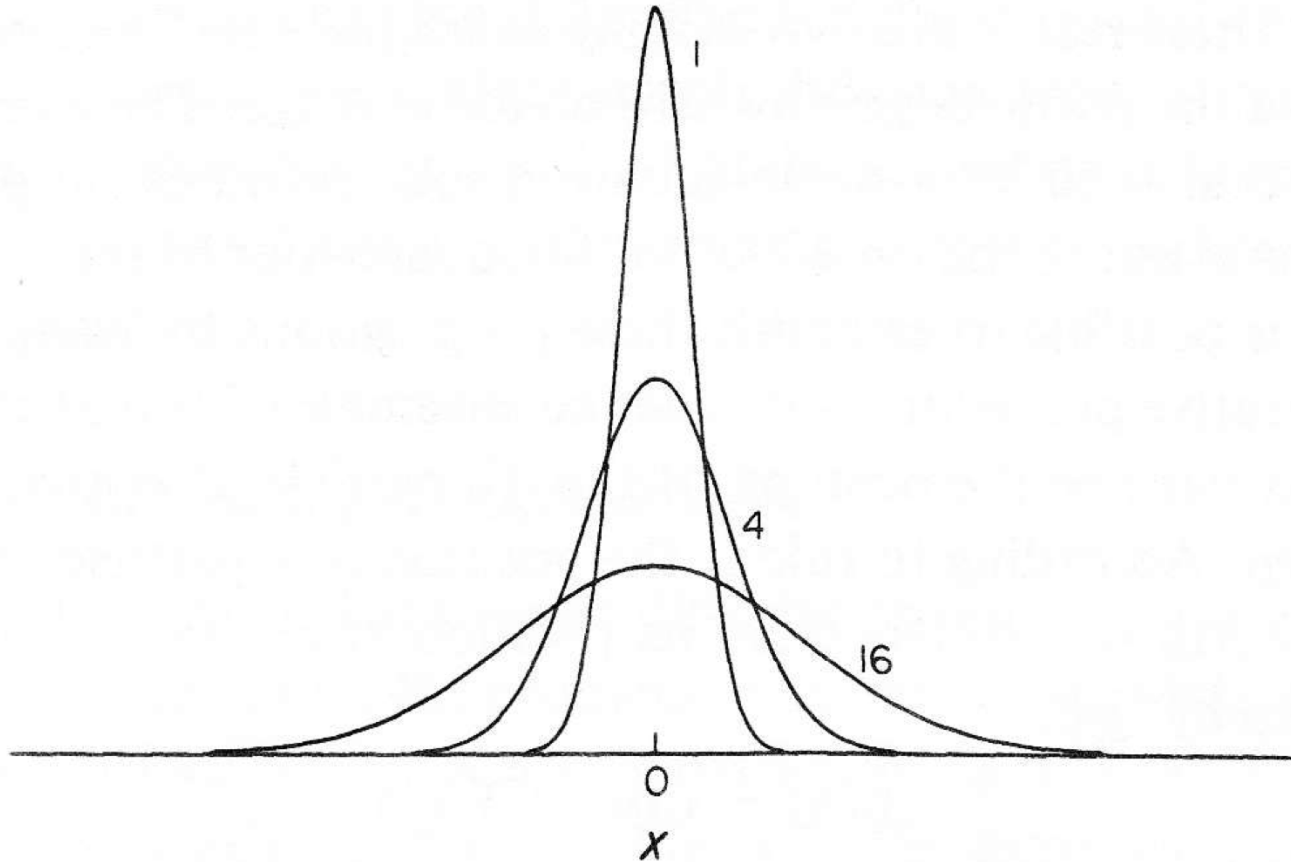➢ Motility
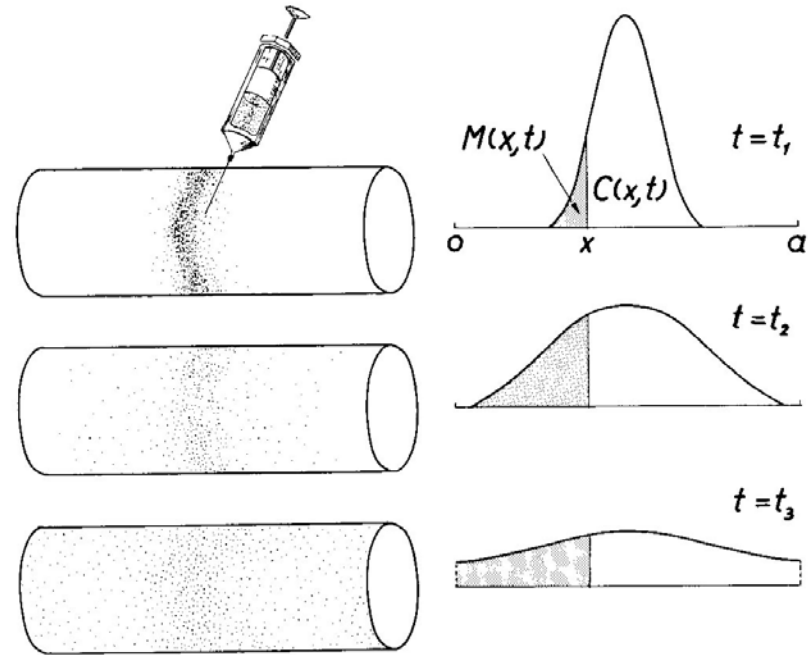
Diffusion: Microscopic → Macroscopic

Fig. 1.3. The probability of finding particles at different points x at times $t = 1, 4,$ and 16. The particles start out at position $x = 0$ at time $t = 0$. The standard deviations (root-mean-square widths) of the distributions increase with the square-root of the time. Their peak heights decrease with the square-root of the time. See Eq. 1.22.

Note: Concentration of a solute in a solution (c) depends upon both spatial location (x) and time (t)

Multivariable function

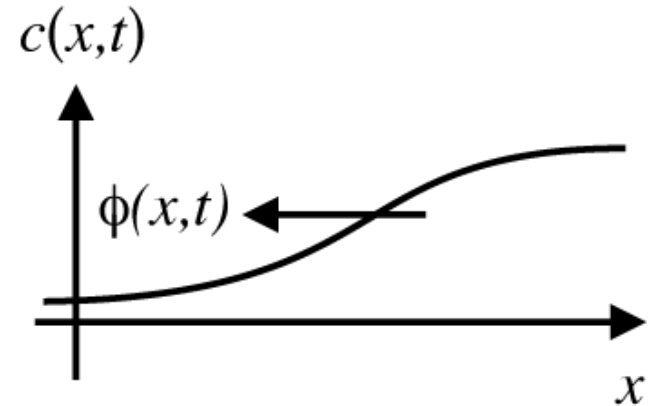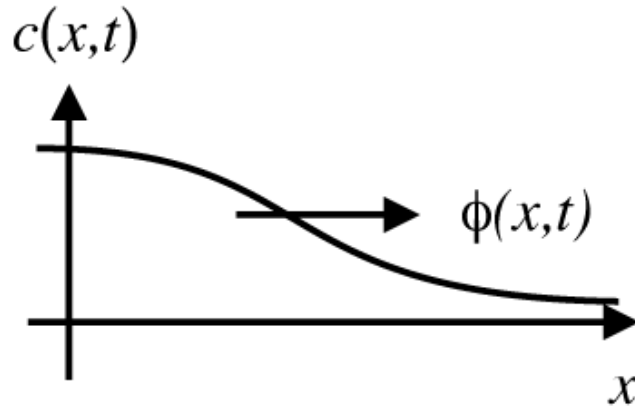$$f = f(x, y)$$

f - dependent variable

x, y - independent variables

➢ Multivariate functions are important in many various contexts throughout science

Diffusion: Macroscopic

Note: This is a multi-variable function(!!)

From Graham's observations (~1830):

$c(x,t)$ $\phi(x,t)$ x

$c(x,t)$ $\phi(x,t)$ x

" A few years ago, Graham published an extensive investigation on the diffusion of salts in water, in which he more especially compared the diffusibility of different salts. It appears to me a matter of regret, however, that in such an exceedingly valuable and extensive investigation, the development of a fundamental law, for the operation of diffusion in a single element of space, was neglected, and I have therefore endeavoured to supply this omission."

- A. Fick (1855)

Diffusion (1-D)

$$c(x,t)$$

Concentration - of solute in solution [*mol/m³*]

$$\phi(x,t)$$

Flux - net # of moles crossing per unit time t through a unit area perpendicular to the x-axis [*mol/m²·s*]

Note: flux is a vector!

$$x, t$$

Position [*m*], Time [*s*]

Fick's 1st Law (1-D)
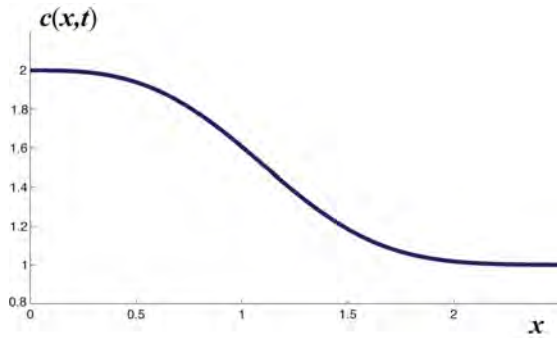
Profile 1

Profile 2
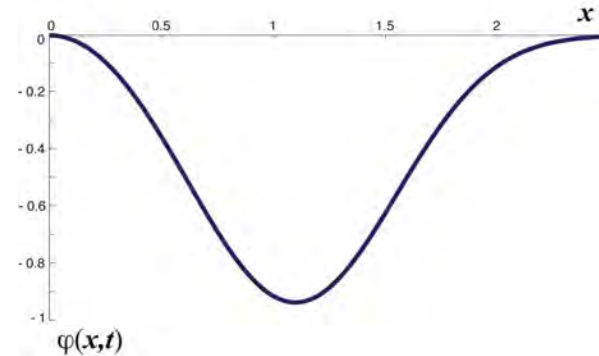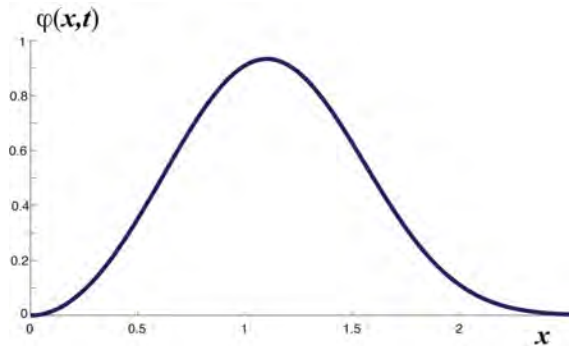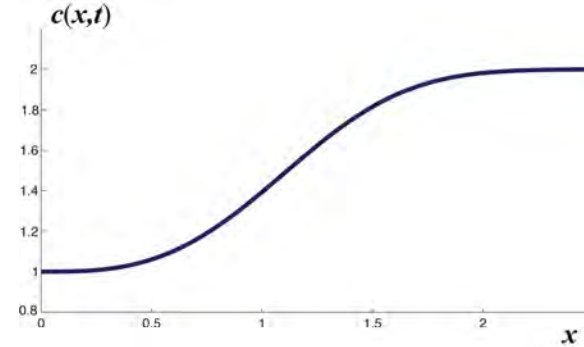
$$\phi(x,t) \propto -\frac{\partial c(x,t)}{\partial x}$$

In short, there is a net movement down a concentration gradient

Diffusion Constant (D)

$$\phi(x,t) \propto -\frac{\partial c(x,t)}{\partial x}$$

constant of proportionality?

$$\phi(x,t) = -D\frac{\partial c(x,t)}{\partial x}$$

- diffusion constant is always positive (i.e., $D > 0$)
- D determines time it takes solute to diffuse a given distance in a medium
- D depends upon both solute and medium (solution)
- *Stokes-Einstein relation* predicts that D is inversely proportional to solute molecular radius

Diffusion

$$\phi(x, t) = -D\frac{\partial c(x, t)}{\partial x}$$

(Fick's Law)

- diffusion constant is always positive (i.e., $D > 0$)
- D determines time it takes solute to diffuse a given distance in a medium
- D depends upon both solute and medium (solution)
- *Stokes-Einstein relation* predicts that D is inversely proportional to solute molecular radius

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

Diffusion equation
(combo of Fick's Law and continuity equation;
we do not derive this here)

Note: This is a PDE(!!)   → PDEs are beyond the scope of 1420

Diffusion processes

Impulse Response: Point-source of particles (n_o mol/cm²) at $t = 0$ and $x = 0$
[**Dirac delta function** $\delta(x)$]

given the inital/boundary conditions:

$$c(x,t) = n_o \delta(x) \quad \text{at} \quad t = 0 \quad \text{where} \quad \int_{-\infty}^{\infty} \delta(x)\,dx = 1$$

need to solve:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$
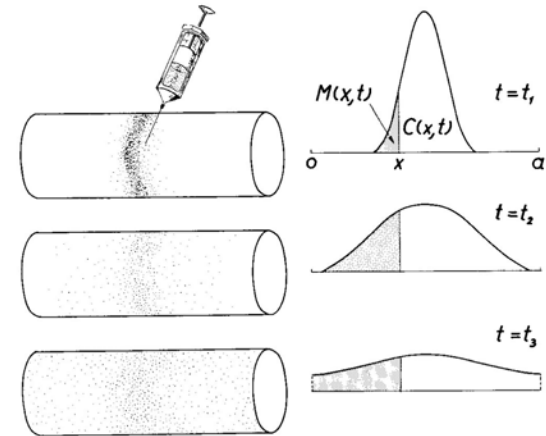
Batschelet Fig.12.5

[Aside: solution can be found by a # of different methods, one being by separation of variables and using a Fourier transform]

Solution
(for $t > 0$)

$$c(x,t) = \frac{n_o}{\sqrt{4\pi Dt}} e^{-x^2/4Dt}$$

Note: Historically, this ties in directly w/ the development of "Fourier analysis"

<u>Diffusion</u>: Microscopic → Macroscopic

Solution to "diffusion equation"

→ Time-dependent Gaussian!!
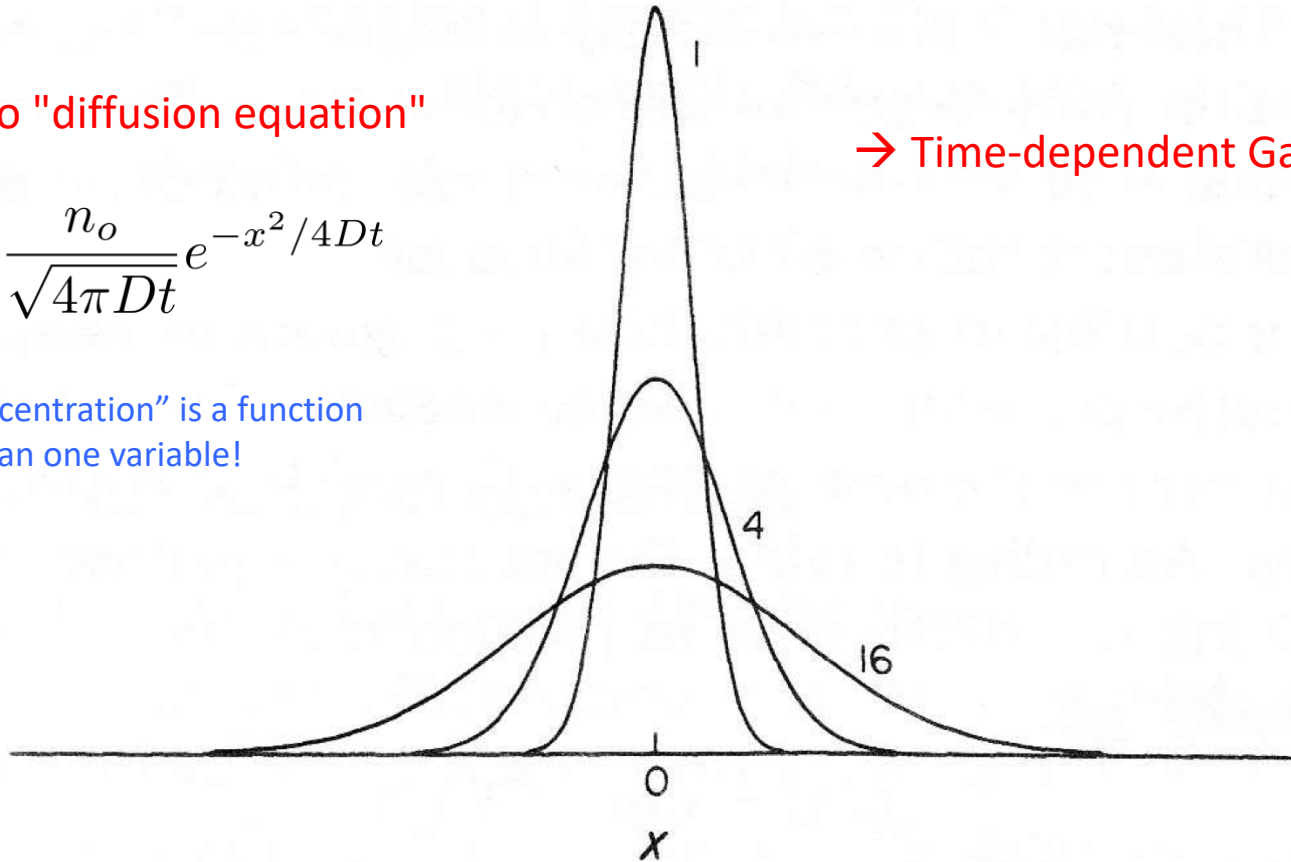
$$c(x, t) = \frac{n_o}{\sqrt{4\pi D t}} e^{-x^2/4Dt}$$

<u>Note</u>: "concentration" is a function of more than one variable!

Fig. 1.3. The probability of finding particles at different points x at times $t = 1, 4,$ and 16. The particles start out at position $x = 0$ at time $t = 0$. The standard deviations (root-mean-square widths) of the distributions increase with the square-root of the time. Their peak heights decrease with the square-root of the time. See Eq. 1.22.

"Diffusion math" → Multivariable functions

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$
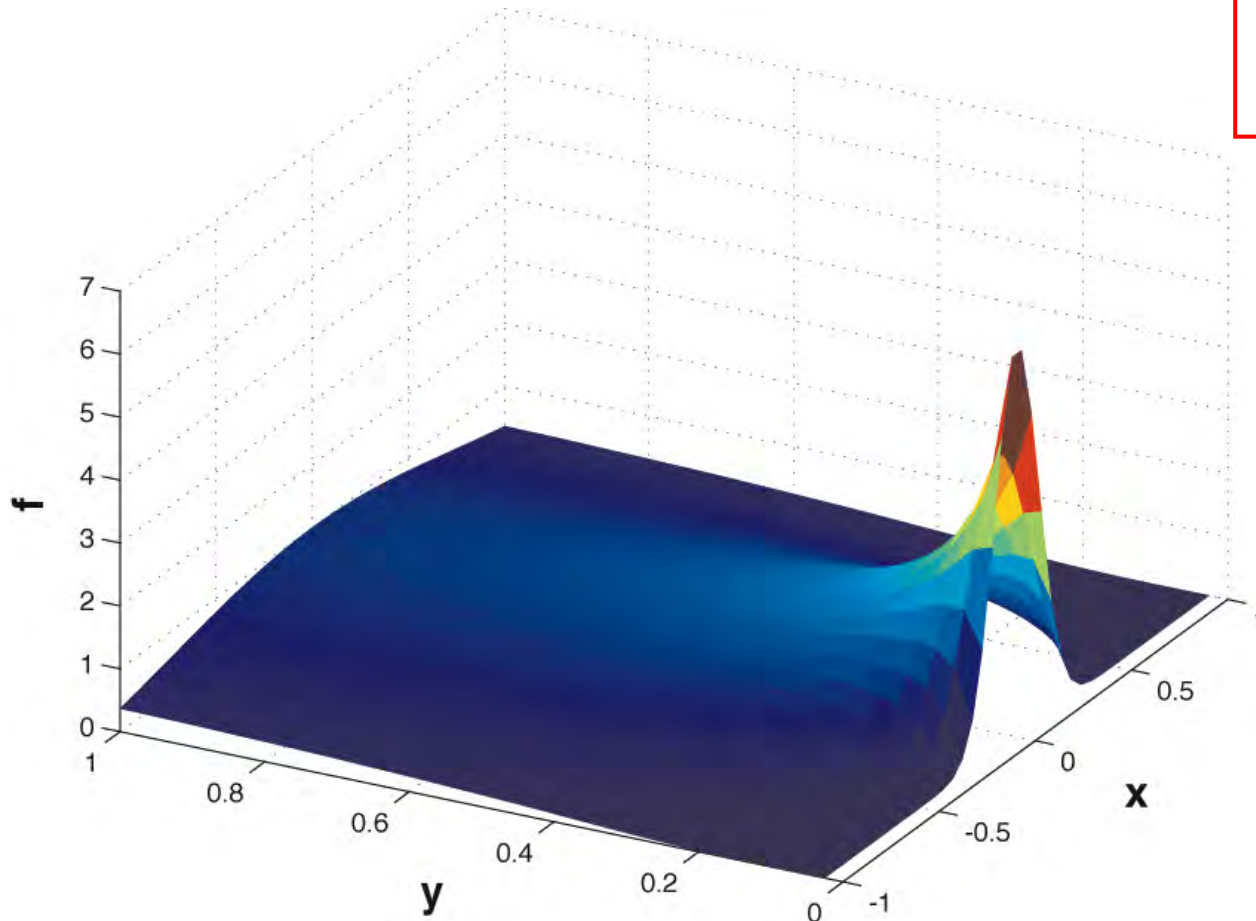
$$f(x, y) = \frac{1}{\sqrt{y}} e^{-x^2/y}$$

Solution to diffusion equation

Diffusion

Weiss Fig.3.14 (modified)
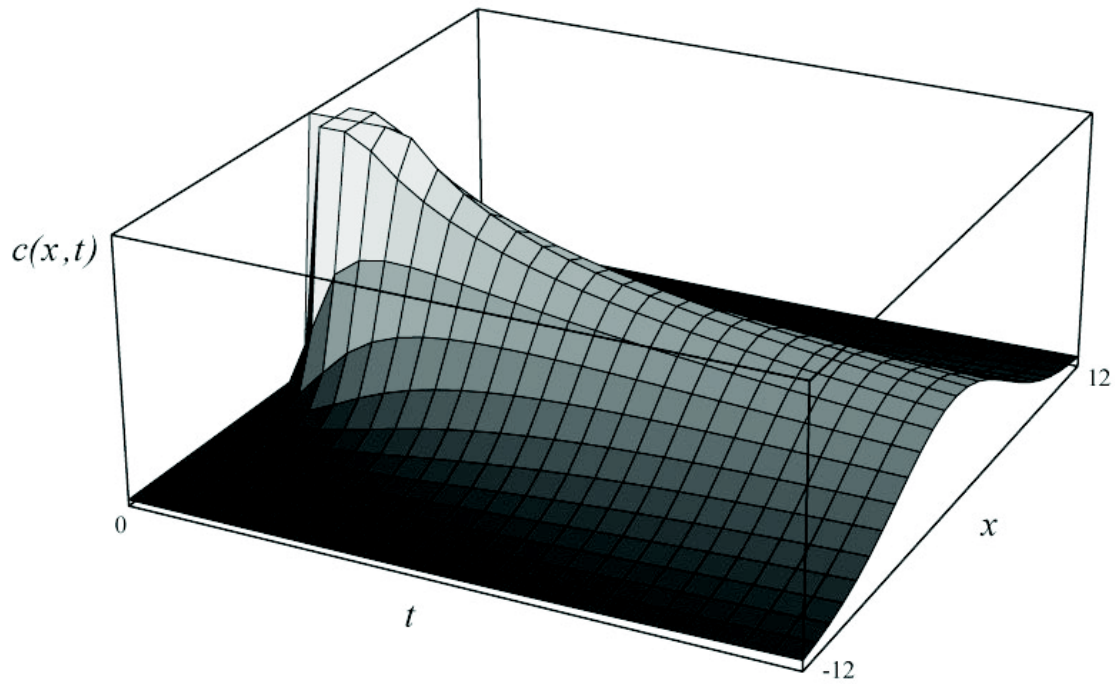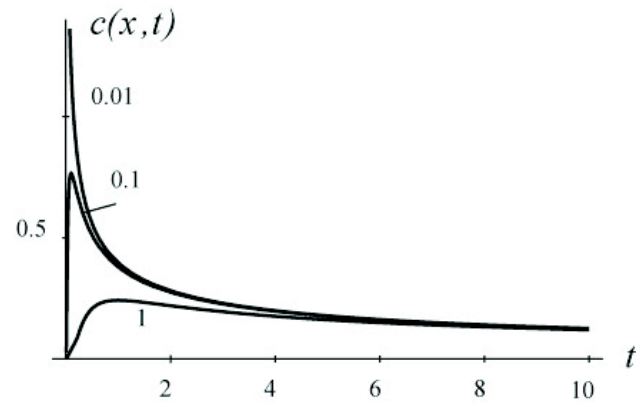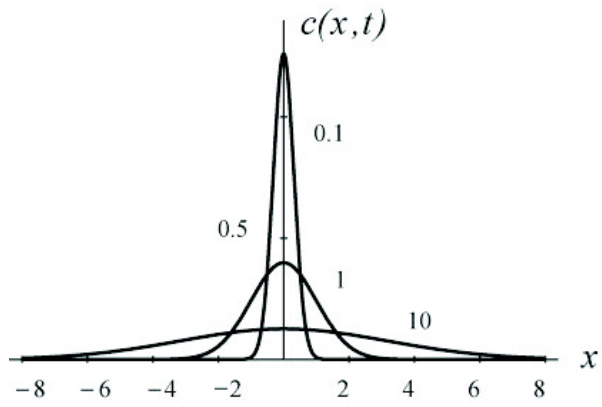
Importance of scale

$$c(x,t) = \frac{n_o}{\sqrt{4\pi D t}} e^{-x^2/4Dt}$$

Gaussian function with zero mean and standard deviation:
$$\sigma = \sqrt{2Dt}$$
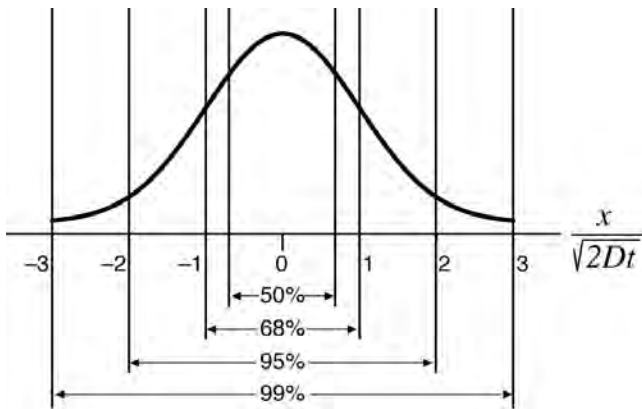
Question: How long does it take ($t_{1/2}$) for ~1/2 the solute to move at least the distance $x_{1/2}$?

$$\frac{x_{1/2}}{\sqrt{2Dt_{1/2}}} \approx \frac{2}{3} \implies t_{1/2} \approx \frac{x_{1/2}^2}{D}$$

For small solutes (e.g. K$^+$ at body temperature) $D \approx 10^{-5} \ \frac{\text{cm}^2}{\text{s}}$

	$x_{1/2}$	$t_{1/2}$
membrane sized	10 nm	$\frac{1}{10}$ μsec
cell sized	10 μm	$\frac{1}{10}$ sec
dime sized	10 mm	10^5 sec $\approx$ 1 day

➢ Cells are typically 1-100 um or so in size. Why?

What determines cell size?

Wallace F Marshall[*1], Kevin D Young[2], Matthew Swaffer[3], Elizabeth Wood[3], Paul Nurse[3,4,5], Akatsuki Kimura[6], Joseph Frankel[7], John Wallingford[8], Virginia Walbot[9], Xian Qu[10] and Adrienne HK Roeder[11]

➢ Non-trivial question and likely a # of factors (e.g., optimizing volume to surface area), but….

➢ … limits stemming from diffusion are likely central

	$x_{1/2}$	$t_{1/2}$
membrane sized	10 nm	$\frac{1}{10}$ μsec
cell sized	10 μm	$\frac{1}{10}$ sec
dime sized	10 mm	10^5 sec ≈ 1 day

Summary (re Diffusion)

Note: Lots of "objects in direct contact" here!

Heat-transfer mechanisms

When two objects are in direct contact, such as the soldering iron and the circuit board, heat is transferred by *conduction*.
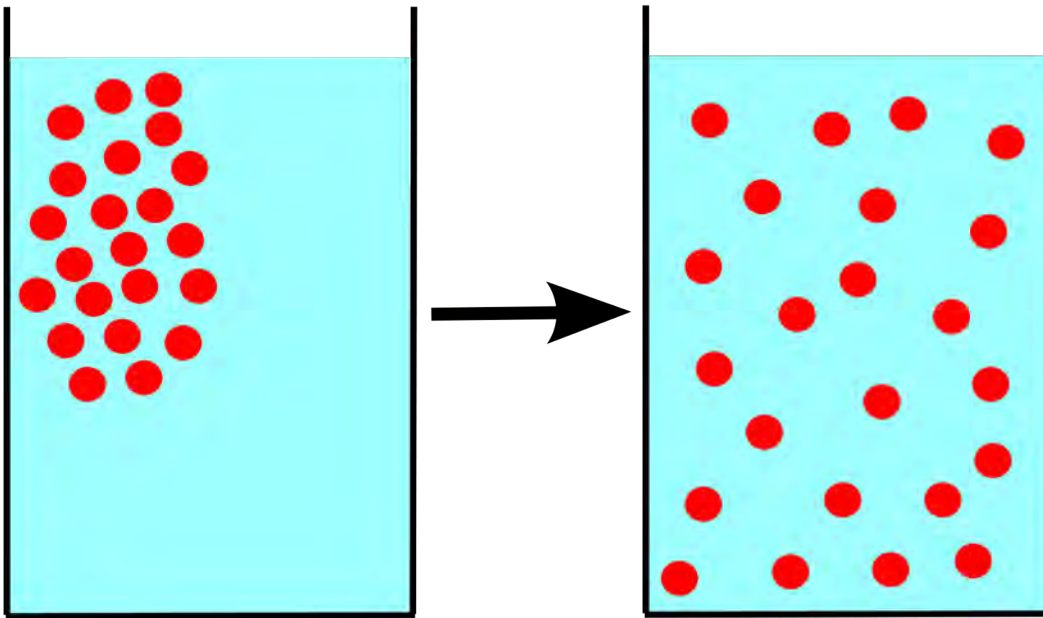
→ Diffusion is a macroscopic movement of stuff stemming from lots of random walks at the microscopic level
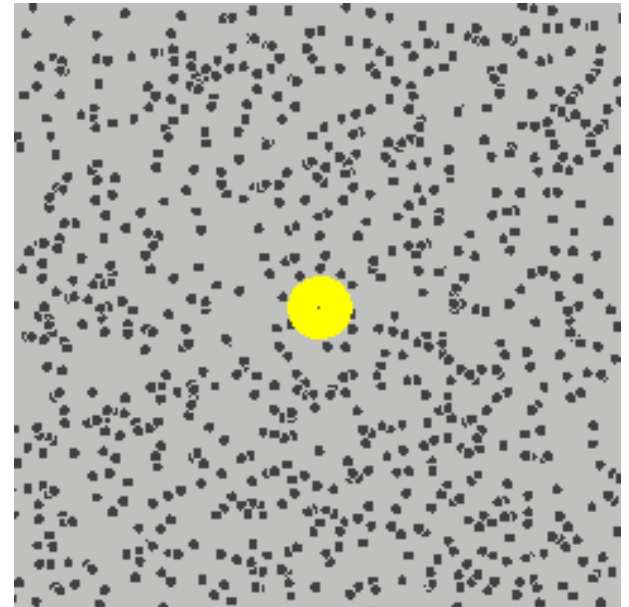
Summary (re Diffusion)

Heat-transfer mechanisms

When two objects are in direct contact, such as the soldering iron and the circuit board, heat is transferred by *conduction*.
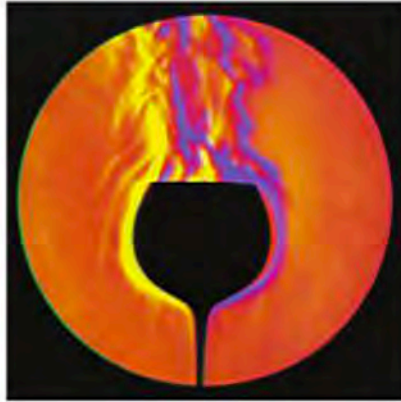
Air currents near a warm glass of water rise, taking thermal energy with them in a process known as *convection*.

The lamp at the top shines on the lambs huddled below, warming them. The energy is transferred by *radiation*.

Blowing on a hot cup of tea or coffee cools it by *evaporation*.

Goal now is to build up a theme focusing on one of these in particular....

... and that is a key principle underlying *conduction*

→ We have delved into a physical means by which conduction occurs

3.14 The time course of one-dimensional diffusion of a solute from a point source in space and time has the form

$$c_n(x, t) = \frac{n_o}{\sqrt{4\pi Dt}} e^{-x^2/4Dt},$$

where n_o is the number of moles of solute per unit area placed at $x = 0$ at $t = 0$. As shown in Figure 3.50, $c_n(x, t)$ is computed for locations x_a and x_b. Is $x_a > x_b$, or is $x_a < x_b$? Explain.
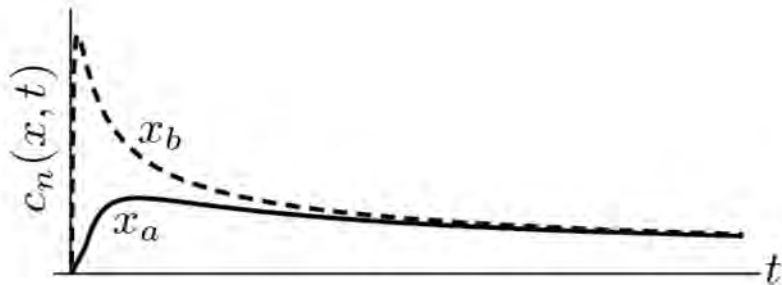
Figure 3.50 Concentration of solute n as a function of time for two locations, x_a and x_b (Exercise 3.14).

Recall: Biophysical notion of *Passive vs Active*

➢ Passive: movement is subject to the medium you are in moving you around

➢ Active: you move yourself around (e.g., swim)

MOTILE BEHAVIOR OF BACTERIA

JANUARY 2000   PHYSICS TODAY

E. coli, a self-replicating object only a thousandth of a millimeter in size, can swim 35 diameters a second, taste simple chemicals in its environment, and decide whether life is getting better or worse.

Howard C. Berg

→ What happens when you have a LOT of (random?) *swimmers* together?

Case study: Swarming
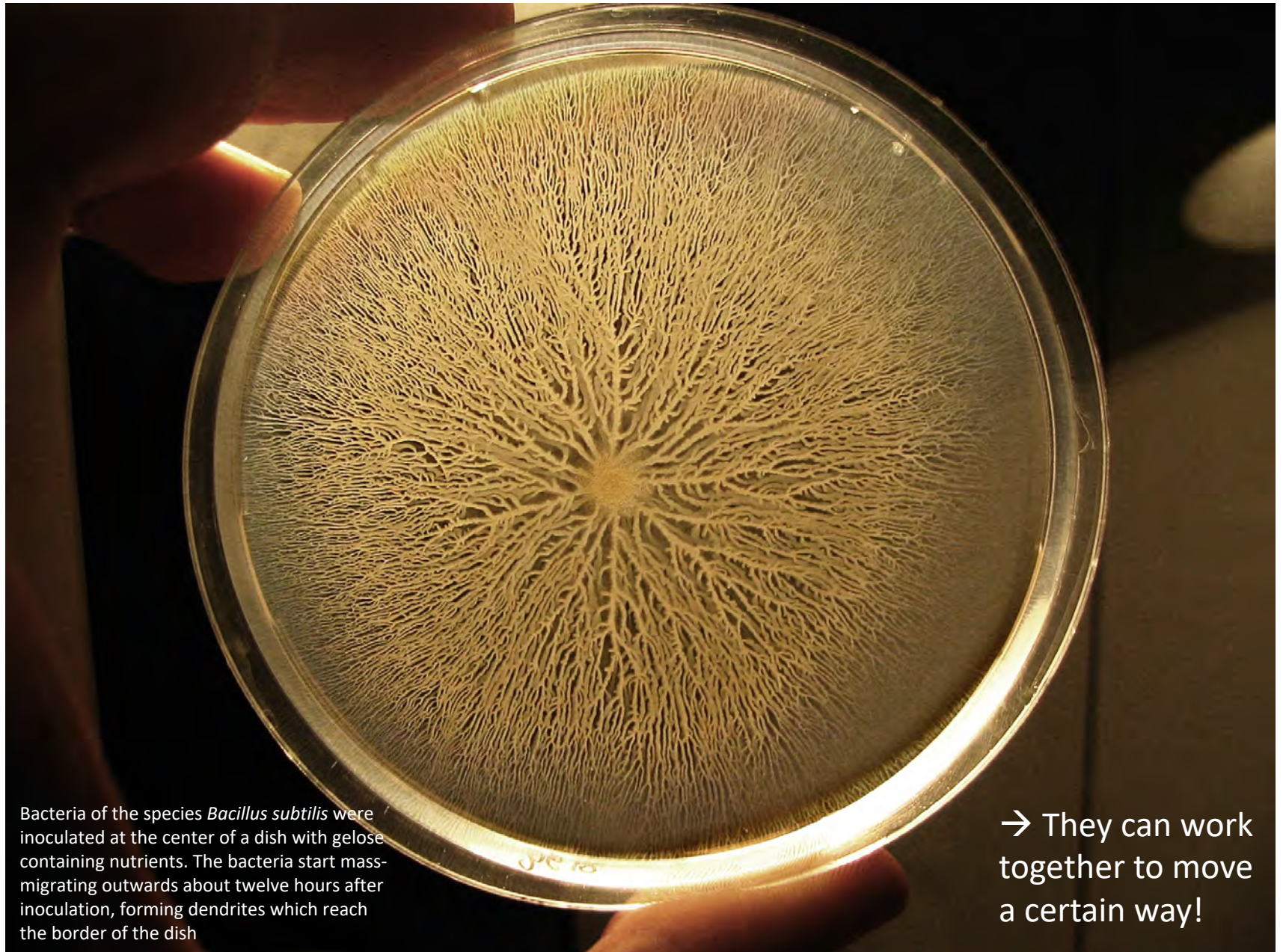
Bacteria of the species *Bacillus subtilis* were inoculated at the center of a dish with gelose containing nutrients. The bacteria start mass-migrating outwards about twelve hours after inoculation, forming dendrites which reach the border of the dish

→ They can work together to move a certain way!

Case study: Swarming

➢ Key idea here is that the swimmers can interact

➢ Notion of collective dynamics

→ The "whole" is more/different from the sum of the parts
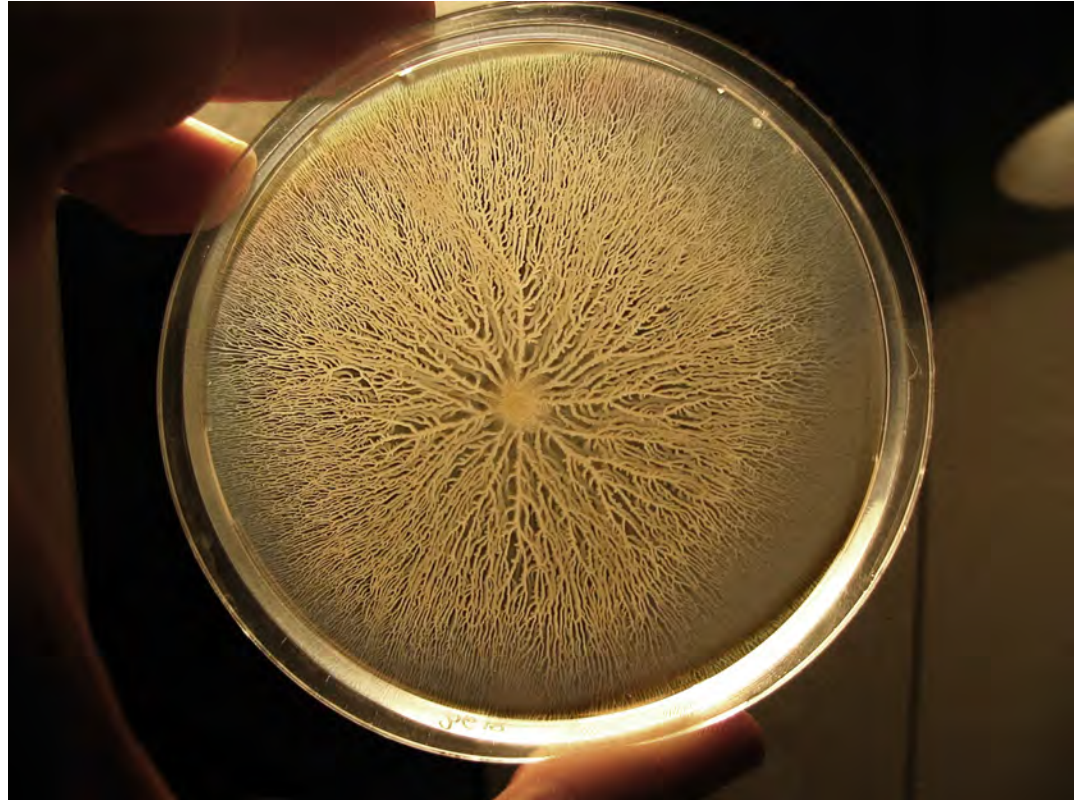
Flocking is a typical example of emergent collective behavior, where interactions between individuals produce collective patterns on the large scale. Here we show how a quantitative microscopic theory for directional ordering in a flock can be derived directly from field data. We construct the minimally structured (maximum entropy) model consistent with experimental correlations in large flocks of starlings. The maximum entropy model shows that local, pairwise interactions between birds are sufficient to correctly predict the propagation of order throughout entire flocks of starlings, with no free parameters. We also find that the number of interacting neighbors is independent of flock density, confirming that interactions are ruled by topological rather than metric distance. Finally, by comparing flocks of different sizes, the model correctly accounts for the observed scale invariance of long-range correlations among the fluctuations in flight direction.

animal groups | statistical inference

Case study: Flocking

A swarm-like flock of starlings

Case study: Flocking

Fig. 1. The raw data. (*A*) One snapshot from flocking event 28 – 10, $N = 1,246$ birds (see *SI Appendix*, Table S1). (*B*) Instantaneous vector velocities of all the individuals in this snapshot, normalized as $\vec{s}_i = \vec{v}_i/|\vec{v}_i|$.

The maximum entropy distribution consistent with the directional correlations C_{ij} is

$$P(\{\vec{s}_i\}) = \frac{1}{Z(\{J_{ij}\})} \exp\left[\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} \vec{s}_i \cdot \vec{s}_j\right],$$

Note: Plenty of mathematical concepts here we've dealt w/ in 1420!
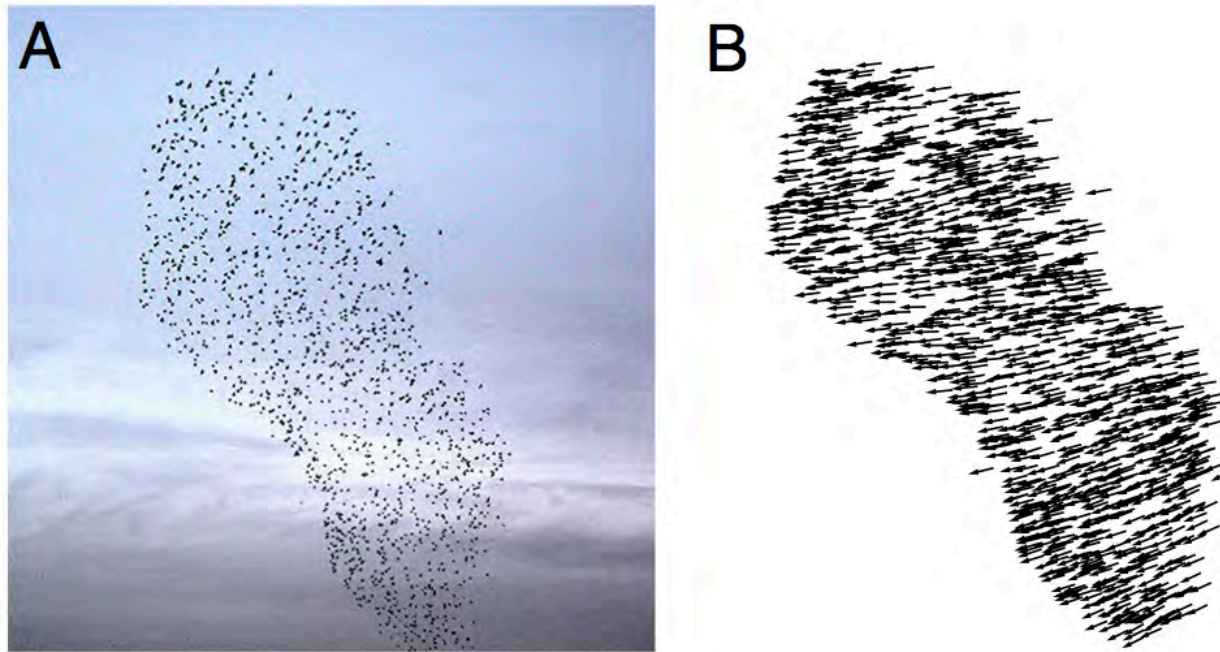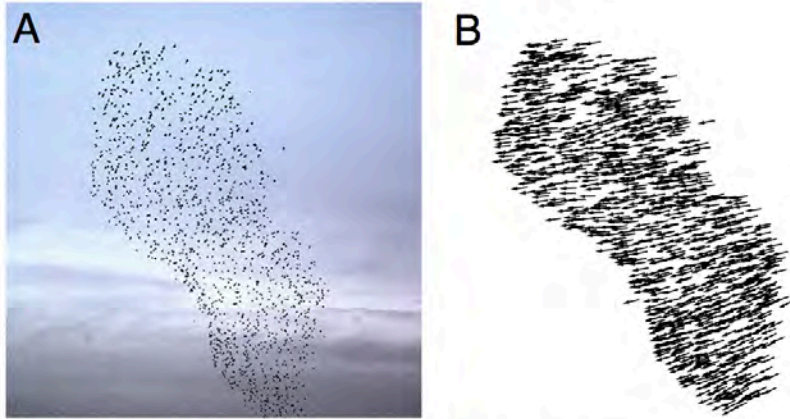
Interdisciplinary Connection: Entropy

Fig. 1. The raw data. (*A*) One snapshot from flocking event 28 − 10, $N = 1{,}246$ birds (see *SI Appendix*, Table S1). (*B*) Instantaneous vector velocities of all the individuals in this snapshot, normalized as $\vec{s}_i = \vec{v}_i / |\vec{v}_i|$.

The maximum entropy distribution consistent with the directional correlations C_{ij} is

$$P(\{\vec{s}_i\}) = \frac{1}{Z(\{J_{ij}\})} \exp\left[\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} \vec{s}_i \cdot \vec{s}_j\right], \qquad [1]$$

→ Entropy is a key consideration in chemistry and thermodynamics

We consider flocks of European starlings, *Sturnus vulgaris*, as in Fig. 1*A*. At any given instant of time, following refs. 11–13, we can attach to each bird i a vector velocity $\vec{v}_i$ and define the normalized velocity $\vec{s}_i = \vec{v}_i / |\vec{v}_i|$ (Fig. 1*B*). On the hypothesis that flocks have statistically stationary states, we can think of all these normalized velocities as being drawn (jointly) from a probability distribution $P(\{\vec{s}_i\})$. It is not possible to infer this full distribution directly from experiments, because the space of states specified by $\{\vec{s}_i\}$ is too large. However, what we can measure from field data is the matrix of correlations between the normalized velocities, $C_{ij} = \langle \vec{s}_i \cdot \vec{s}_j \rangle$. There are infinitely many distributions $P(\{\vec{s}_i\})$ that are consistent with the measured correlations, but out of all these distributions, there is one that has minimal structure: It describes a system that is as random as it can be while still matching the experimental data. This distribution is the one with maximum entropy (10).

It should be emphasized that the maximum entropy principle is not a "modeling assumption;" rather it is the absence of assumptions. Any other model that accounts for the observed correlations will have more structure and hence (explicitly or implicitly) assumes something about the nature of the interactions in the flock beyond what is required to match the data. Of course the fact that the maximum entropy model is minimally structured does not make it correct. It could be, for example, that individual birds set their flight direction by computing a complicated nonlinear combination of the velocities from multiple neighbors, in which case correlations among pairs of birds would be insufficient to capture the essence of the ordering mechanism. We view the maximum entropy model as a powerful starting point, from which, as we will see, we can generate detailed and testable predictions.

Related: "Flying spaghetti monster,"

The Flying Spaghetti Monster Lives

The deeply weird creatures oil workers spot near deep-water rigs.

By Jim Festante

VIDEO — SLATE IN MOTION. — AUG. 14 2015 2:52 PM

Slate

11.3k   138   10

Dive Number: 794

> "Although a *siphonophore* appears to be a single organism, each specimen is actually a colony composed of many individual animals"

Aside: Entropy

entropy *noun*

1   *thermodynamics* : a measure of the unavailable energy in a closed thermodynamic system that is also usually considered to be a measure of the system's disorder, that is a property of the system's state, and that varies directly with any reversible change in heat in the system and inversely with the temperature of the system

   broadly : the degree of disorder or uncertainty in a system

2   a   : the degradation of the matter and energy in the universe to an ultimate state of inert uniformity

      // *Entropy* is the general trend of the universe toward death and disorder.
      — James R. Newman

   b   : a process of degradation or running down or a trend to disorder

      // The deterioration of copy editing and proof-reading, incidentally, is a token of the cultural *entropy* that has overtaken us in the postwar years.
      — John Simon

3   : CHAOS, DISORGANIZATION, RANDOMNESS

4   *statistical mechanics* : a factor or quantity that is a function of the physical state of a mechanical system and is equal to the logarithm of the probability for the occurrence of the particular molecular arrangement in that state

5   *communication theory* : a measure of the efficiency of a system (such as a code or a language) in transmitting information, being equal to the logarithm of the number of different messages that can be sent by selection from the same set of symbols and thus indicating the degree of initial uncertainty that can be resolved by any one message

Note also:

Merriam-Webster   SINCE 1828

$t = 0$

particle ID

spatial position (x)

$t = 50$
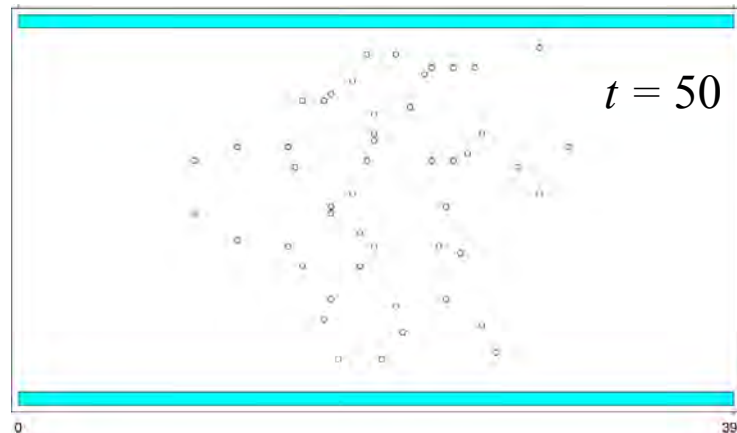
<u>Aside</u>: Entropy

In statistical mechanics, **entropy** is an extensive property of a thermodynamic system. It is closely related to the number Ω of microscopic configurations (known as microstates) that are consistent with the macroscopic quantities that characterize the system (such as its volume, pressure and temperature). Entropy expresses the number Ω of different configurations that a system defined by macroscopic variables could assume.[1] Under the assumption that each microstate is equally probable, the entropy S is the natural logarithm of the number of microstates, multiplied by the Boltzmann constant k_B. Formally (assuming equiprobable microstates),

$$S = k_B \ln \Omega.$$

```matlab
% ### EXcoffee.m ###    11.16.14    {C. Bergevin}
% [modified version of EXrandomWalk2D.m motivated by the problem shown in
% Giordano (1997) Fig.7.18ff]
% **NOTE**: There is a minor bug in this version such that it is possible for
% some 'cream' to leave the 'cup' (despite the specifed boundary conditions)
clear;
% -------------
N= 10;        % one plus sqrt of total # of (independent) walkers (each starts at unique x,y point about origin)
M= 300;         % Total # of steps for each walker
method= 2;    % see comments above
BND= 10;      % bounding limits for initial grid of walkers at t=0
axisLim= 100;   % size of coffee cup
diffC= 1;     % diffusion const. (i.e., scaling factor for step size)
framerate= 1/30;    % pause length [s] for animation
Sgrid= 8;            % grid spacing for entropy calculation
% -------------
% +++
space= (2*BND)/N;
[X,Y]= meshgrid(-BND:space:BND,-BND:space:BND);
E= size(X,1); % # of elements
SgridX= linspace(-axisLim,axisLim,Sgrid);    % set grid bounds for entropy calc.
SgridY= linspace(-axisLim,axisLim,Sgrid);

figure(1); clf; grid on; xlabel('x-postion'); ylabel('y-postion');
% visualize before onset?
if (1==1), plot(X,Y,'ko','MarkerSize',5); axis([-axisLim axisLim -axisLim axisLim]);    end
% +++
% To do
% - apply boundary condition (i.e., ensure no steps past walls)
% - fix entropy calc. (i.e., if prob.=0??)
for r= 1:M

    if method==1
        % random L/R and U/D step with equal probability
        tempX= rand(E,E);    tempY= rand(E,E);   % determine random vals.
        temp2X= tempX<0.5;   temp2Y= tempY<0.5;  % determine L vs R and U vs D
        X(temp2X)= X(temp2X)+1; X(~temp2X)= X(~temp2X)-1;
        Y(temp2Y)= Y(temp2Y)+1; Y(~temp2Y)= Y(~temp2Y)-1;
    else
        % sample step from normal distribution
        stepX= randn(E,E); stepY= randn(E,E);
        X= X+ diffC*stepX;  Y= Y+ diffC*stepY;
        % verify step is not past walls; if so, bounce back in opposite direction
        [aa,bb]= find(abs(X)>axisLim); [cc,dd]= find(abs(Y)>axisLim);

        % +++ --> correct for points that have moved past the walls
        % not quite right, but kinda works
        X(aa,bb)= X(aa,bb)-2*diffC*stepX(aa,bb); Y(cc,dd)= Y(cc,dd)-2*diffC*stepY(cc,dd);

        % more right (I think), but doesn't work
        %X(aa,bb)= sign(X(aa,bb))*2*axisLim-X(aa,bb); Y(cc,dd)= Y(cc,dd)-2*diffC*stepY(cc,dd);

        % uncomment to allow for flagging when 'cream' leaves the cup
        if(max(abs(X(:))>axisLim)), return;   end
    end
    % visualize
    figure(1)
    plot(X,Y,'ko','MarkerSize',5); axis([-axisLim axisLim -axisLim axisLim]); pause(framerate);
    % do binning to determine 'probability' distribution
    histS= hist2(X(:),Y(:),SgridX,SgridY)/E^2; % use external function hist2.m; and normalize to a probability
    histS= histS(:);     % convert to a single column vector
    zeroI= ~histS==0; % need to filter out states with zero elements so to avoid computational error (since 0*log(0)= NaN)
    S(r)= -sum(histS(zeroI).*log(histS(zeroI))); % calculate entropy (S)
end;

figure(2)
plot(S,'LineWidth',2); hold on; grid on;
xlabel('time step'); ylabel('entropy');
```
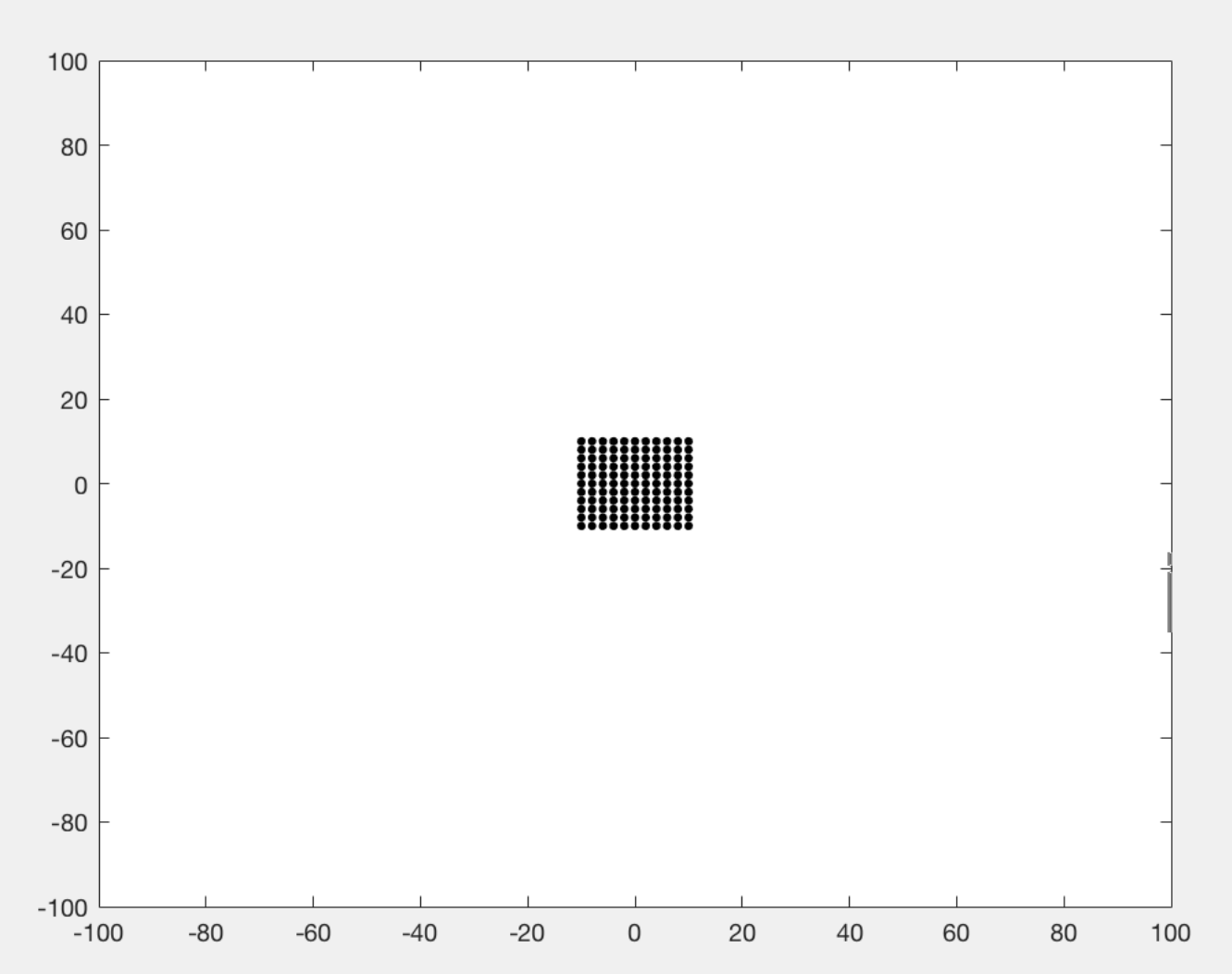
100 2-D non-interacting random walkers

Note: Cream in reality likely mixes w/ coffee primarily more via convection and "conduction"
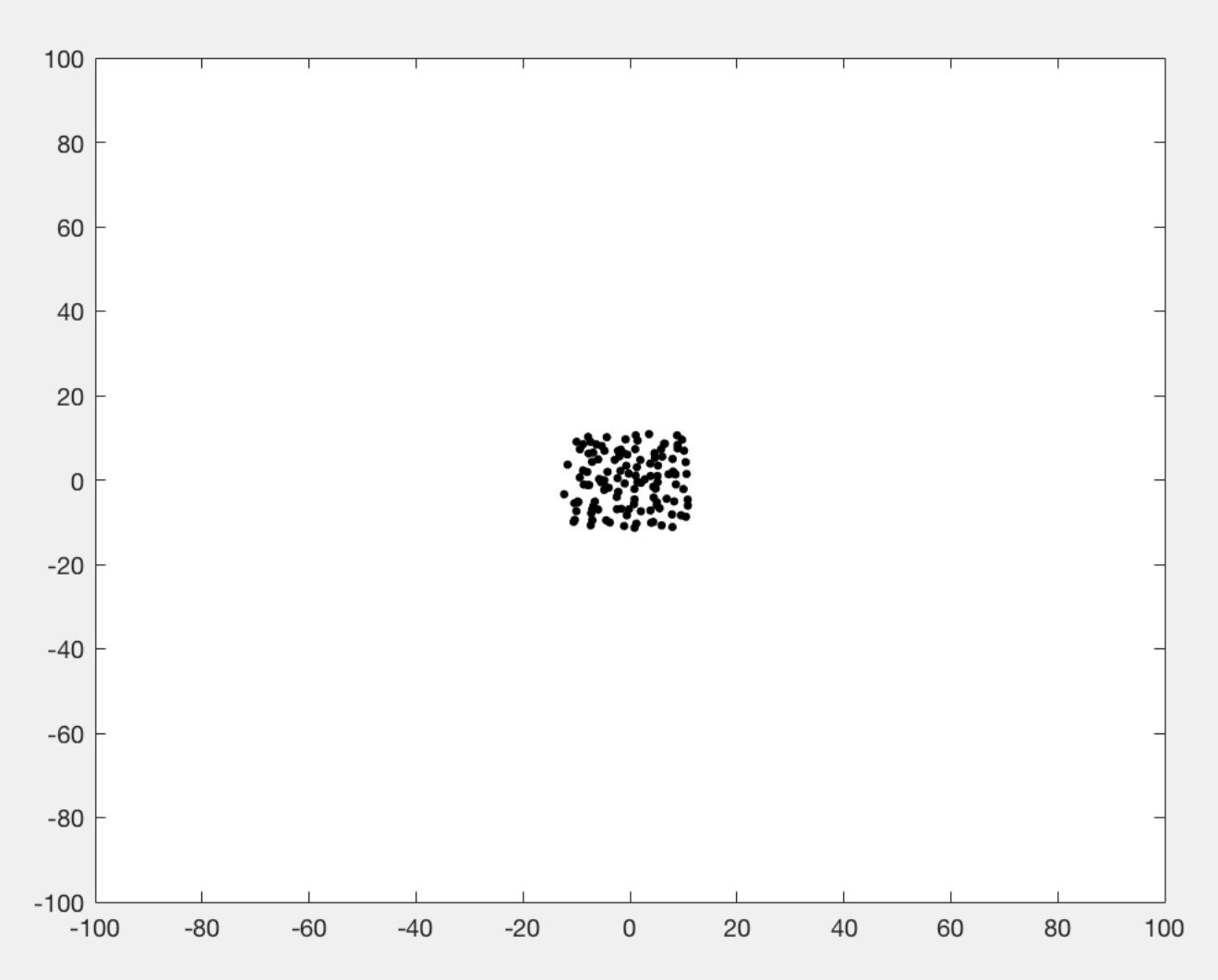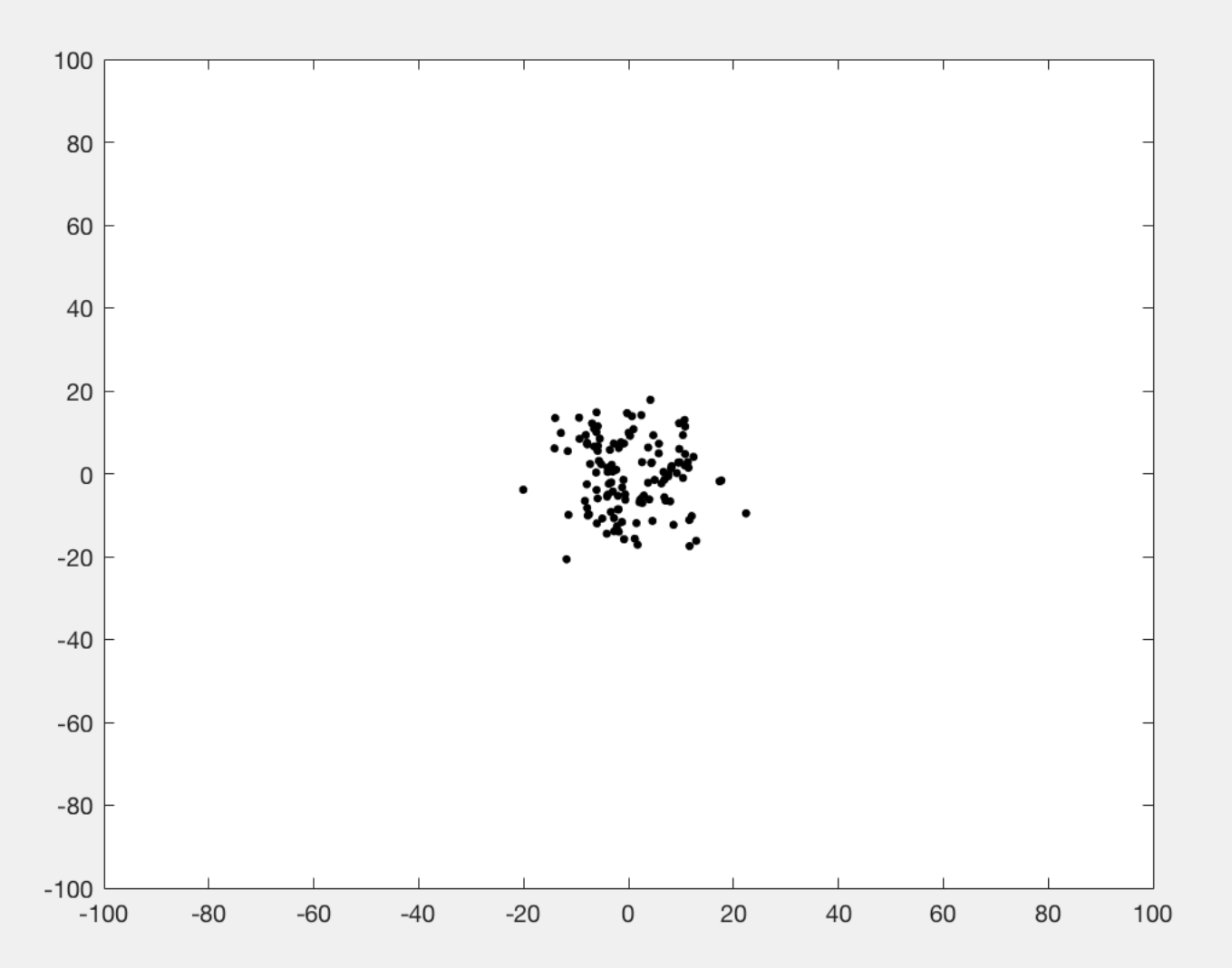
Aside: Entropy

timestep 0
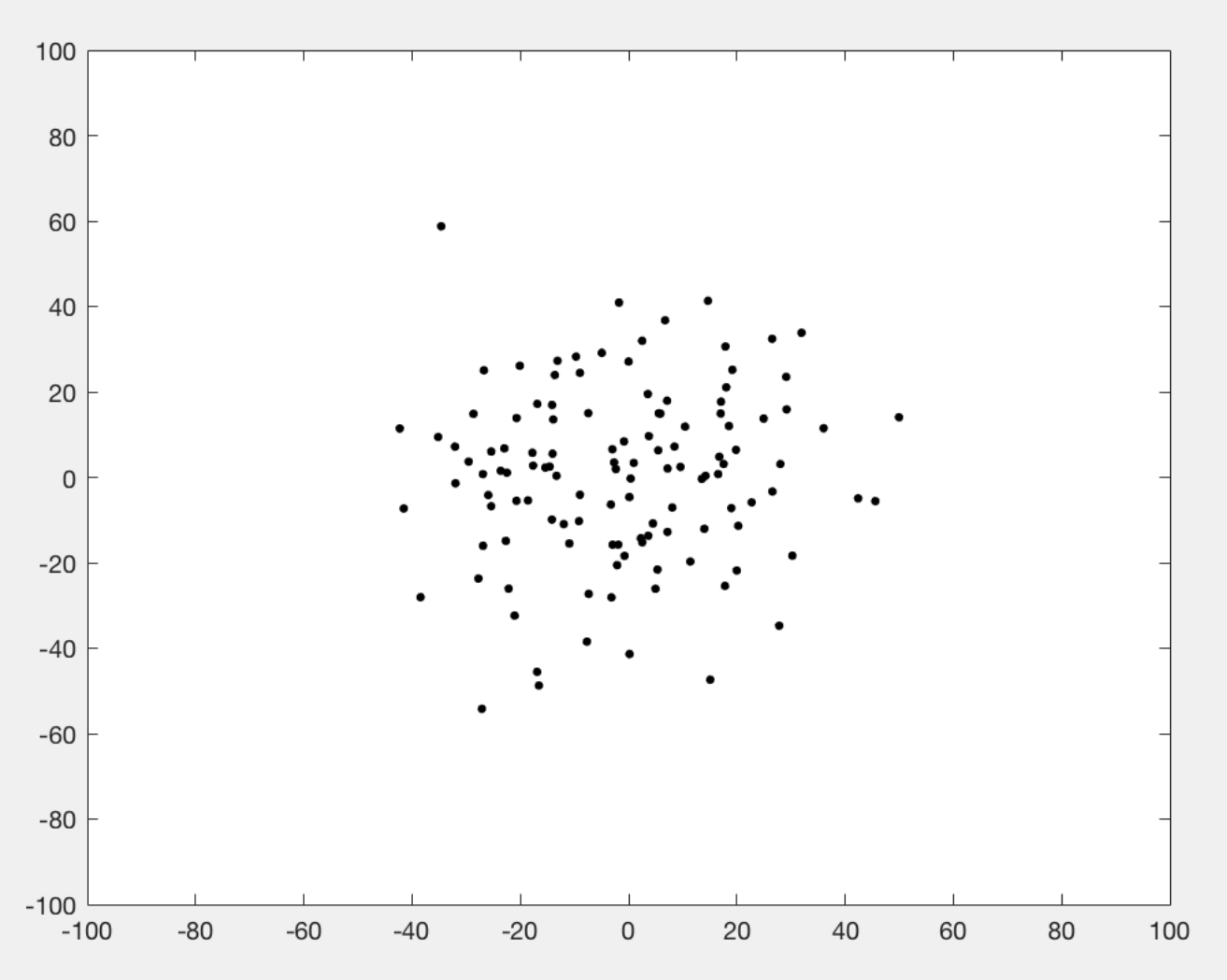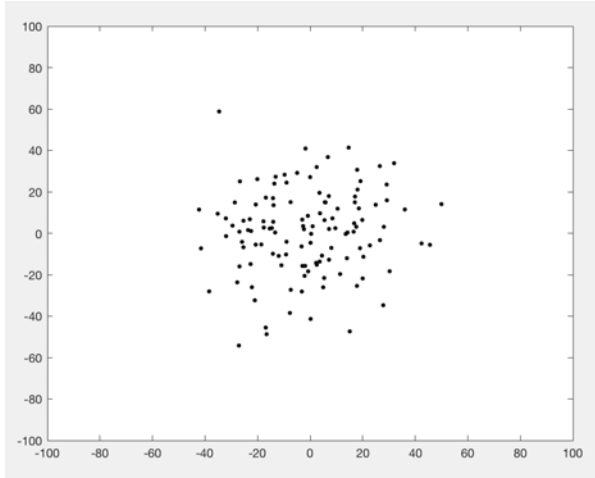
Aside: Entropy

Aside: Entropy

timestep 30

Aside: Entropy

timestep 300

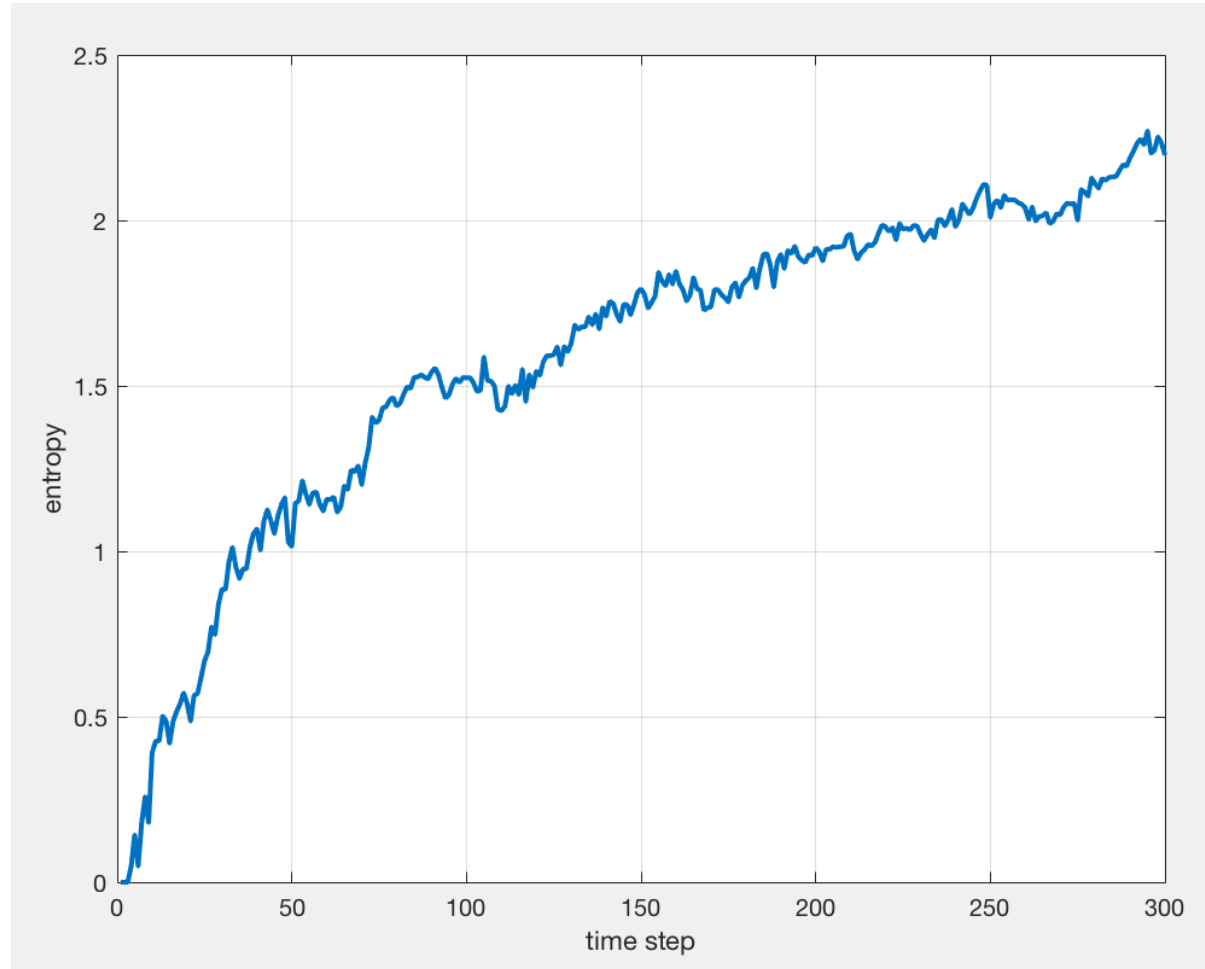## Aside: Entropy

→ Can determine the associated entropy as a function of time!

$$S = -\sum_i P_i \ln P_i$$

$$S = k_{\mathrm{B}} \ln \Omega.$$

Giordano (1997)

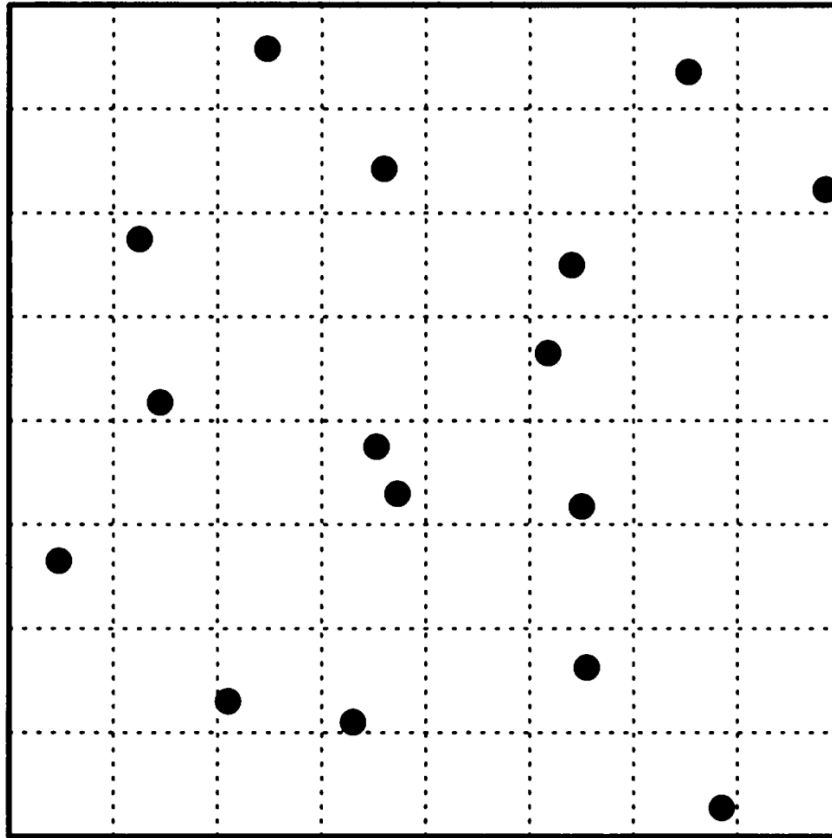$$S = -\sum_{i} P_i \ln P_i$$

Figure 7.20: Schematic division of our coffee cup into grid cells, with a few molecules distributed throughout the cup. P_i is the probability of finding a molecule in cell i.