Introduction to the mathematical modeling of multi-scale phenomena

Diffusion

MCB/MATH 303

Brownian motion

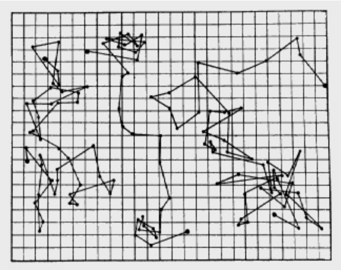
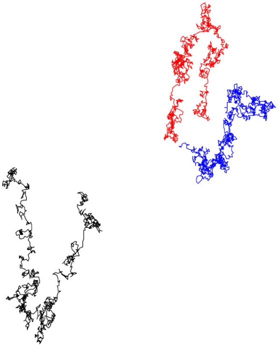


Image (public domain) from J. B. Perrin, *Mouvement Brownien et réalité moléculaire*, Ann. de Chimie et de Physique **18**, 5-114 (1909).

- Brownian motion (named after botanist Robert Brown) refers to the random motion of particles suspended in a fluid as they are "pushed around" by the smaller fluid molecules.
- This phenomenon may be modeled in terms of a random walk.
- The diffusion MATLAB GUI illustrates that, on average, a particle performing a random walk on the plane is, after time t, at a distance proportional to $\sqrt{t}$ from the origin.

Random walk



Trajectories of three particles performing a 1000-step random walk on the plane.

- This immediately allows us to introduce a dimensionless quantity DT/L^2, where T is a characteristic time, L a characteristic length, and D a diffusion coefficient.
- We recognize the same dimensionless combination that appears in the heat equation,

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

One can in fact show that a random walk at the microscopic level can be described at the macroscopic level by a diffusion equation.

Reaction-diffusion equations

- The dynamics of macroscopic dynamics of quantities that both diffuse and interact, such as chemicals in a reaction, is typically described in terms of a reaction-diffusion equation of the form
$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2} + F(u),$$
where F is a reaction term.

- Reaction-diffusion systems often lead to the formation of Turing patterns, such as hexagons or stripes.

- Such patterns, which have been reproduced in chemical reaction experiments, are also thought to be observed on animal coats and fish skins.

Microscopic versus macroscopic aspects of diffusion

- The macroscopic description of a microscopic phenomenon is typically obtained by taking averages. As a consequence, individual aspects are lost and replaced by quantities such as densities, which can be measured at the macroscopic level.
- Since a random walk at the microscopic level can be described at the macroscopic level by a diffusion equation, the same reasoning may be applied to describe any motion that involves a random walk, regardless of the scale at which it happens.
- In particular, flagellated bacteria such *Bacillus subtilis* swim in a series of runs and tumbles, which can be modeled by a random walk.

Motion of *B. subtilis* on agar

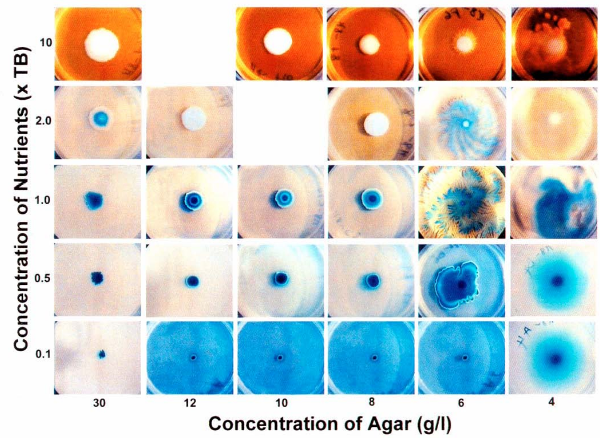
Bacillus subtilis is a flagellated rod-like bacterium

Movie (made in 2001 by then undergraduate student Cathy Ott in N. Mendelson's lab) showing *Bacillus subtilis* bacteria swimming on agar.

▸ Larger Movie

- Length: 2 to 3 μm.
- Diameter: ~ 0.7 μm.
- Swimming speed: about 10 times its length per second.
- It moves by a succession of runs and tumbles.

Colony forms for *B. subtilis*



N.H. Mendelson, and B. Salhi, *Patterns of reporter gene expression in the phase diagram of Bacillus subtilis colony forms*, J. Bacteriol. **178**, 1980-1989 (1996).

(Diameter of petri dishes: 6 cm)

Reaction-diffusion models

It is therefore not surprising that branched bacterial colony shapes may be captured by means of reaction-diffusion models.

$$\frac{\partial S}{\partial t} = D^S \nabla^2 S - \eta N S$$

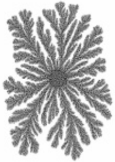
S : density of nutrients
N : density of bacteria

- These models often involve nonlinear diffusion,

$$\frac{\partial N}{\partial t} = \nabla \left(D^N N^k \nabla N \right) + NS - \mu N$$

S. Kitsunezaki, J. Phys. Soc. Jpn. **66**, 1544-1550 (1997)

- Possibly with a stochastic diffusion coefficient:



$$\frac{\partial N}{\partial t} = \nabla \left(D^N (1 + \sigma) NS \nabla N \right) + NS$$

K. Kawasaki et al., J. Theor. Biol. **188**, 177-185 (1997)

Images from I. Golding et al., Physica **A 260**, 510-554 (1998).

Foraging behaviors

- It is natural to push the analogy even further, to describe the dynamics of "objects" of even bigger size, such as animals foraging for food.
- But of course, the scaling law $L^2 \propto T$ is only valid if the directions allowed for each step in the random walk are equally likely, and if steps are taken at regular intervals.
- In particular, if the random walker stops and stays put for a while, the average distance L after time T will grow more slowly than $\sqrt{T}$. This is called subdiffusion.
- Similarly, if the walker takes unusually large steps, L^2 will grow faster than T and superdiffusion will be observed.
- The above ideas have been applied in ecology to describe the foraging behaviors of animals.

Summary

- We started with multi-scale aspects of various physical or biological systems.
- We introduced the concept of scales and discussed examples of scale-free systems, such as fractals and self-similar systems found in nature.
- We then turned to a discussion of how ideas of scales appear in models that involve differential equations. This led us to dimensional analysis and self-similar solutions of partial differential equations.
- We studied random walks and used scalings to associate them with diffusion at the macroscopic level. This took us back to patterns via reaction-diffusion equations.
- Finally, we extended the concept of a random walk to phenomena occurring at the scales of a few microns (bacteria) and at our own scale (foraging animals).

Motion of B. subtilis on agar

Movie by Cathy Ott

Back