Introduction to the mathematical modeling of multi-scale phenomena

Diffusion

MCB/MATH 303
Brownian motion

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

This immediately allows us to introduce a dimensionless quantity $\frac{DT}{L^2}$, 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.
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.
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

- **Length**: 2 to 3 $\mu$m.
- **Diameter**: $\sim$ 0.7 $\mu$m.
- **Swimming speed**: about 10 times its length per second.
- It moves by a succession of runs and tumbles.

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


(Diameter of petri dishes: 6 cm)
It is therefore not surprising that branched bacterial colony shapes may be captured by means of reaction-diffusion models.

\[
\frac{\partial S}{\partial t} = D^S \nabla^2 S - \eta NS \\
S: \text{density of nutrients} \\
N: \text{density of bacteria}
\]

These models often involve nonlinear diffusion,

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


Possibly with a stochastic diffusion coefficient:

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


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