12.086 / 12.586 Modeling Environmental Complexity Fall 2008

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Lecture notes for 12.086/12.586, Modeling Environmental Complexity

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# 1 From microdynamics to macrodynamics

Throughout the course we will suggest that simple idealized microdynamics, suitably averaged in space and/or time, suffices as a representation of complex macroscopic continuum behavior.

In this lecture we provide two examples in which such a connection can be shown explicity:

- Random walks  $\rightarrow$  diffusion.
- Lattice gas  $\rightarrow$  fluid flow (as in the previous lecture).

Applications of these ideas will be given in later lectures. For now, we just consider these problems as "toy models" of instrinsic interest themselves.

As we shall see, their intrinsic interest derives from their *statistical dynamics*.

## 1.1 Random walks

#### 1.1.1 One-dimension, discrete time and space

Consider a (drunkard's) random walk along a line (figure):

- Start at time t = 0 and position x = 0.
- Every  $\tau$  seconds, take a random step s to the left or right.
- Assume equiprobable steps of equal size  $\delta$ :

$$P(s = \delta) = P(s = -\delta) = 1/2.$$

• No memory (statistically independent jumps).

We think of this as a caricature of real diffusion (e.g., Brownian motion).

Now consider an ensemble of N independent random walks (i.e., many such drunkards, each acting with no awareness of the others).

Let  $x_i(n)$  be the position of the *i*th walker after *n* steps. Then

$$x_i(n) = x_i(n-1) + s.$$

The mean position of a large ensemble of walkers after n steps is

$$\langle x(n) \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{i=1}^{N} (x_i(n-1) + s)$$
  
=  $\langle x(n-1) \rangle + \langle s \rangle$   
=  $\langle x(n-1) \rangle.$ 

Here we have used the angle brackets  $\langle \cdot \rangle$  to denote the ensemble average. The result shows that the mean position is independent of n, thus retaining permanent memory of the initial condition:

$$\langle x(n) \rangle = 0.$$

Intuitively we understand that there should nevertheless be a wide spread in the probability P(x) that increases with time (figure).

We characterize this spread by the *root-mean-square displacement*  $\langle x^2(n) \rangle^{1/2}$ . To calculate it, first write

$$\begin{aligned} x_i^2(n) &= \left( x_i(n-1) + s \right)^2 \\ &= x_i^2(n-1) + 2sx_i(n-1) + s^2. \end{aligned}$$

The ensemble mean is

$$\begin{aligned} \langle x^2(n) \rangle &= \langle x^2(n-1) \rangle + 2\langle s \rangle \langle x(n-1) \rangle + \langle s^2 \rangle \\ &= \langle x^2(n-1) \rangle + \delta^2 \end{aligned}$$

where we have replaced the average of a product with the product of averages because of our assumption of no memory (ie, s is uncorrelated to x).

Note that our result is in the form of a recursion, which is readily put in the simpler form

$$\langle x^2(n)\rangle = n\delta^2$$

Since  $t = n\tau$ , we have

$$\langle x^2 \rangle = \delta^2 t / \tau = 2Dt,$$

where we have defined the *diffusion coefficient* 

$$D = \frac{\delta^2}{2\tau}.$$

Thus the mean-squared displacement increases linearly with time, like 2Dt. Consequently the root-mean-square displacement increases like the square-root of time:

$$\langle x^2 \rangle^{1/2} = (2Dt)^{1/2}.$$

Intuitively we understand that the width of some bell-shaped distribution P(x,t) increases like  $\sqrt{2Dt}$ . (figure)

For a small molecule in water,  $D \simeq 10^{-5} \text{ cm}^2/\text{s}$ . So imagine you're a bacterium (size ~  $10^{-4} \text{ cm}$ ), and you want to know how how long some molecular nutrient will take to diffuse a distance  $\ell$  away from you. Identifying  $\ell$  with  $\langle x^2 \rangle$ , the diffusion time  $\tau_d$  is

$$\tau_d \sim \ell^2 / 2D.$$

Then

$$\frac{\ell \text{ (cm)}}{10^{-4}} \frac{\tau_d \text{ (s)}}{5 \times 10^{-4} \text{ s}} \\
1 5 \times 10^4 \text{ s}$$

In other words, the molecule would stay within a length commensurate to a bug's size for only about a millisecond. But it would stay within 1 cm for about 14 hours!

This huge change is a consequence  $\tau \propto \ell^2$ , a hallmark of diffusive processes. (Contrast with flow, or advection, in which  $\tau \propto \ell$ .)

#### 1.1.2 Higher dimensions

Before moving on, we first argue that our little toy problem is equally valid in higher dimensions.

In, say, two dimensions, the random walker is on a plane. In our discrete approximation, this corresponds to a lattice with a "Manhattan metric," with the drunkard originating at his corner bar and moving  $\pm \delta$  in each dimension at each time step.

Because the drunk's motion in x is independent of his motion in y,

$$\langle x^2 \rangle = \langle y^2 \rangle = 2Dt$$

Since the mean-square distance from the origin is

$$r^2 = x^2 + y^2,$$

we have

$$\langle r^2 \rangle = 4Dt.$$

The generalization to higher dimensions is obvious. The point is that we retain the diffusive scaling  $\ell^2 \propto t$ .

#### 1.1.3 The binomial distribution and the large n (Gaussian) limit

We return now to one dimension, and seek the probability P(x, n) that a random walker is at position x after n steps.

In doing so, we generalize the toy problem so that

$$P(s = \delta) = p$$
  
$$P(s = -\delta) = q = 1 - p,$$

i.e., the random walk takes positive steps of size  $\delta$  with probability p and negative steps with probability q = 1 - p.

The displacement after k positive steps is

$$\begin{aligned} x(n) &= [k - (n - k)]\delta \\ &= (2k - n)\delta \end{aligned}$$

The probability of arriving at this point by a specific sequence of k positive steps and n - k negative steps is

$$p^k q^{n-k}$$
.

Since there are two choices per step, there are  $2^n$  possible sequences of steps. The number of possible sequences in which k of the n steps are positive is

$$\binom{n}{k} \equiv \frac{n!}{k!(n-k)!}.$$

The probability of having exactly k positive steps in n attempts is the *binomial distribution* 

$$P(k,n) = \frac{n!}{k!(n-k)!} p^k q^{n-k}.$$

For large n (long times) the binomial distribution approaches the Gaussian distribution

$$P(k,n)dk = \frac{1}{(2\pi\sigma^2)^{1/2}}e^{(k-\mu)^2/2\sigma^2}dk$$

where P(k)dk is the probability that k is between k and k + dk, and

$$\mu = \langle k \rangle = np,$$
  

$$\sigma^2 = \langle k^2 \rangle - \langle k \rangle^2 = npq.$$

We can write this in a simpler form by substituting  $x = (2k - n)\delta$ . The resulting distribution then corresponds to an unbiased random walk about x = 0 with p = q = 1/2.

Substituting also

$$dx = 2\delta dk, \qquad t = n\tau, \qquad D = \delta^2/2\tau,$$

we obtain

$$P(x,t)dx = \frac{1}{(4\pi Dt)^{1/2}}e^{-x^2/4Dt}dx,$$

i.e., a Gaussian with mean  $\langle x \rangle = 0$  and variance  $\langle x^2 \rangle = 2Dt$ .

#### 1.1.4 Central-limit theorem

The previous result is in fact more general. No matter what distribution P(s) the step size is drawn from, the long-time limit of P(x) is still Gaussian.

To show this, we shall use the Fourier-transform pair

$$\phi(k) = \int_{-\infty}^{\infty} e^{ikx} P(x) dx$$
$$P(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} \phi(k) dk.$$

The first relation also defines the average (or *characteristic function*)

$$\phi(k) = \langle e^{ikx} \rangle.$$

Note that the jth derivative evaluated at zero has the simple form

$$\left. \frac{\mathrm{d}^{j}\phi(k)}{\mathrm{d}k^{j}} \right|_{k=0} = i^{j} \langle x^{j} \rangle,$$

where  $\langle x^j \rangle$  is the *j*th moment of P(x).

We express  $\phi(k)$  as a Taylor series of the moments:

$$\phi(k) = 1 + ik\langle x \rangle - \frac{k^2}{2}\langle x^2 \rangle + \mathcal{O}(k^3)$$

Now return to our random walk. The distribution P(x) derives from the sum of random steps  $s_i$ , i = 1, ..., n.

We allow  $s_i$  to derive from *any* probability distribution with finite mean and finite variance. For convenience we assume that all  $s_i$  are drawn from the same distribution with zero mean (but it doesn't matter).

Assuming the walk starts at the origin, the location of the walk after n steps is given by the sum

$$x(n) = \sum_{i=1}^{n} s_i.$$

The mean-square distance is

$$\langle x^2 \rangle = \sum_{i,j=1}^n \langle s_i s_j \rangle = n \langle s^2 \rangle = n \sigma^2,$$

where  $\sigma^2 \equiv \langle s^2 \rangle$  is the variance of s.

Since  $\langle x^2 \rangle$  grows with n, we consider the reduced sum

$$w(n) = x(n)/n^{1/2},$$

whose variance  $\langle w^2 \rangle$  is constant.

We seek the probability density P(w). To do so, we write its characteristic function

$$\phi_w(k) = \langle e^{ikw(n)} \rangle$$

$$= \left\langle \exp\left(\frac{ik}{n^{1/2}}\sum_{j=1}^n s_j\right) \right\rangle$$

$$= \left\langle \prod_{j=1}^n e^{iks_j/n^{1/2}} \right\rangle$$

$$= \prod_{j=1}^n \langle e^{iks_j/n^{1/2}} \rangle$$

$$= \langle e^{iks/n^{1/2}} \rangle^n$$

$$= \left[ \phi_s(k/\sqrt{n}) \right]^n$$

Expanding  $\phi_s(k/\sqrt{n})$  in powers of the moments, we have

$$\phi_s(k/\sqrt{n}) = 1 - \frac{k^2 \sigma^2}{2n} + \mathcal{O}\left(\frac{k^3}{n^{3/2}}\right),$$

where the first-order term vanished from the assumption that  $\langle s \rangle = 0$ .

For large n, the third-order term is small. Substitution of the remaining expansion into the expression for  $\phi_w(k)$  then yields

$$\phi_w(k) = \lim_{n \to \infty} \left( 1 - \frac{k^2 \sigma^2}{2n} \right)^n$$
$$= e^{-k^2 \sigma^2/2}$$

The final step is the inverse Fourier transform to obtain P(w):

$$P(w) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikw} \phi_w(k) dk.$$
$$= \frac{1}{\sqrt{2\pi\sigma^2}} e^{-w^2/2\sigma^2},$$

i.e., a Gaussian distribution with mean zero and variance  $\sigma^2$ .

This is the *central limit theorem*: for large n, the sum of random numbers drawn from *any* distribution with finite variance asymptotically approaches the Gaussian distribution.

Our rescaling by  $1/\sqrt{n}$  hides the growing variance but does not change the result: the distribution P(x) of the random walk is Gaussian, no matter how the steps are made.

This is an elementary statement of *universality*: in the long-time limit, the details of the "microdynamics"—i.e., the step-size distribution—do not matter. The long-time limit of the Gaussian requires only that the probability of extremely large events be extremely small.

This result underlies the ubiquity of the Gaussian distribution: any process that results from "sums" of random variables is likely to yield Gaussian fluctuations.

### 1.1.5 Macrodynamics: the diffusion equation

We now proceed to derive the diffusion equation from our random walk.

Suppose we have a long tube of cross-section A in which particles undergo random walks. We are interested in N(x), the number of particles at x (i.e., between  $x - \delta/2$  and  $x + \delta/2$ ), along with the particle flux  $J_x$ .

How many particles move through across a unit area in unit time, from x to  $x + \delta$ ? And in the other direction?

In other words, what is the net flux  $J_x$ ?

We imagine an imaginary boundary between x and  $x + \delta$ . During one time step  $\tau$ , half the particles at x cross over to the right, and half the particles at  $x + \delta$  cross over to left.

The net flux (number particles per unit area per unit time) is

$$J_x = \left(\frac{N(x)}{2} - \frac{N(x+\delta)}{2}\right)\frac{1}{A\tau}$$

where the factor of 1/2 comes from the fact that half the particles at each location move away from the boundary rather than towards it.

Rearranging and multiplying by  $\delta^2/\delta^2$ ,

$$J_x = -\frac{\delta^2}{2\tau} \frac{1}{\delta} \left( \frac{N(x+\delta)}{A\delta} - \frac{N(x)}{A\delta} \right)$$

Defining the number density or concentration  $C = N/A\delta$  and recalling  $D = \delta^2/2\tau$ , we have

$$J_x = -D\frac{C(x+\delta) - C(x)}{\delta}.$$

Letting  $\delta \to 0$ , we obtain

$$J_x = -D\frac{\partial C}{\partial x}.$$

This is Fick's (first) law: the concentration flux goes down the concentration gradient, at a rate given by the diffusivity D.

Fick's law is an example of a "linear-response relation." Others include Ohm's law, Hooke's law, Darcy's law, etc. The linearity is essentially an assumption, which follows in our case from assuming that the two sides of the boundary through which particles flow act independent of one another.

Now consider particles flowing into and out of a box with cross-sectional area A and width  $\delta$  perpendicular to to the x-axis. (figure)

The concentration C(t) inside the box changes with the net flux into it.

In  $\tau$  units of time the concentration changes as

$$C(t+\tau) - C(t) = \left(J_x(x) - J_x(x+\delta)\right) \frac{A\tau}{A\delta}$$

The factor of  $A\tau$  converts the concentration flux to the number of particles flowing through the face, and the factor of  $1/A\delta$  converts that number to a concentration. Simplifying, we obtain

$$\frac{1}{\tau} \big( C(t+\tau) - C(t) \big) = -\frac{1}{\delta} \big( J_x(x+\delta) - J_x(x) \big).$$

Letting  $\tau \to 0$  and  $\delta \to 0$ , we obtain

$$\frac{\partial C}{\partial t} = -\frac{\partial J_x}{\partial x}$$

Substituting Fick's first law for  $J_x$  then yields

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

commonly called the *diffusion equation* (and sometimes Fick's second law).

Note that in higher dimensions, Fick's first law is

$$\vec{J} = -D\nabla C$$

and mass conservation yields

$$\frac{\partial C}{\partial t} = -\nabla \cdot \vec{J}.$$

Combining the two, we have

$$\frac{\partial C}{\partial t} = D\nabla^2 C.$$

*Conclusion:* The simplest possible random walks are solutions to the diffusion equation. Consequently:

- We can think about diffusive processes as random walks.
- We can equally think about random walks as diffusive.
- Should we wish to numerically *solve* the diffusion equation, we can simulate random walks instead.

### 1.2 The lattice gas

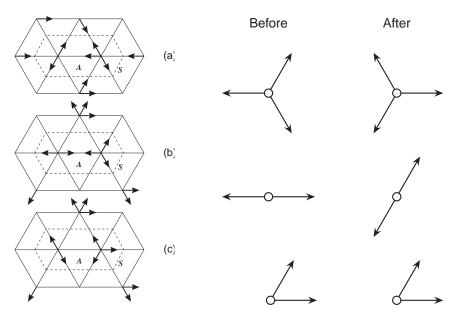
We now return to the lattice gas of Lecture 1 and sketch its relation to the equations of fluid dynamics.

In some sense, the continuum limit of the lattice gas follows similar arguments to that for the diffusion equation.

However there two additional issues: symmetry and scale separation. We comment briefly on the first and in some detail on the second.

### 1.2.1 Microdynamical equations

Recall the model's evolution:



The particle dynamics evolve as

 $n_i(\mathbf{x} + \mathbf{c}_i, t+1) = n_i(\mathbf{x}, t) + \Delta_i[\mathbf{n}(\mathbf{x}, t)].$ 

The quantities  $\mathbf{n} = (n_1, n_2, \dots, n_6)$  are *Boolean* variables that indicate the presence  $(n_i = 1)$  or absence  $(n_i = 0)$  of particles.

Particles move from sites  $\mathbf{x}$  to neighboring sites at  $\mathbf{x} + \mathbf{c}_i$ .

Particles move with unit speed in the directions given by

$$\mathbf{c}_i = (\cos \pi i/3, \sin \pi i/3), \qquad i = 1, 2, \dots, 6.$$

 $\Delta_i \in \{-1, 0, 1\}$  is the *collision operator*. Example: the three-body collision:

$$\Delta_i^{(3)} = n_{i+1}n_{i+3}n_{i+5}\bar{n}_i\bar{n}_{i+2}\bar{n}_{i+4} - n_in_{i+2}n_{i+4}\bar{n}_{i+1}\bar{n}_{i+3}\bar{n}_{i+5},$$

where  $\bar{n}_i = 1 - n_i$  and a subscript x is taken to imply "x mod 6".

There is a also a two-body collision  $\Delta_i^{(2)}$ . Then

$$\Delta_i = \Delta_i^{(2)} + \Delta_i^{(3)}.$$

This is the entire dynamics, due to Frisch, Hasslacher, and Pomeau (1986). Note that  $\Delta_i$  conserves mass,

$$\sum_{i} \Delta_i(\mathbf{n}) = 0,$$

and momentum,

$$\sum_{i} \mathbf{c}_i \Delta_i(\mathbf{n}) = 0.$$

Using mass conservation, we sum the microdynamical equation over each direction i to obtain

$$\sum_{i} n_i(\mathbf{x} + \mathbf{c}_i, t+1) = \sum_{i} n_i(\mathbf{x}, t).$$

Similarly

$$\sum_{i} \mathbf{c}_{i} n_{i}(\mathbf{x} + \mathbf{c}_{i}, t+1) = \sum_{i} \mathbf{c}_{i} n_{i}(\mathbf{x}, t).$$

These are the microscopic mass-balance and momentum-balance equations of the lattice gas.

#### 1.2.2 Macrodynamical equations of the lattice gas

Consider an area  $\mathcal{A}$  of lattice sites enclosed by a perimeter  $\mathcal{S}$ .

Mass conservation requires that

$$\sum_{\mathbf{x}\in\mathcal{A}}\sum_{i}[n_i(\mathbf{x},t+1)-n_i(\mathbf{x},t)] = -(\text{net mass flux out of }\mathcal{S}).$$

Now define the average particle occupancy  $\langle n_i \rangle$ . The averages  $\langle \cdot \rangle$  are constructed so that they vary slowly in space and time—more on this later, when we will refer to the macroscopic length scale as  $L_{\text{hydro}}$ .

In terms of the averaged quantities, we have

- $\sum_i \langle n_i \rangle$ : slowly varying mass.
- $\sum_i \langle n_i \rangle \mathbf{c}_i$ : slowly varying mass flux.

We identify left-hand side above be written as a time derivative of the mass and, the right-hand side as the divergence of the mass flux. Then

$$\partial_t \sum_i \langle n_i \rangle = -\partial_\alpha \sum_i \langle n_i \rangle c_{i\alpha},$$

where the  $\alpha$ -component of the *i*th velocity vector  $\mathbf{c}_i$  is given by  $c_{i\alpha}$ , and repeated Greek indices are summed (i.e.,  $X_{\alpha}Y_{\alpha} = \sum_{\alpha=1}^{d} X_{\alpha}Y_{\alpha}$ .)

We describe the momentum flux similarly, i.e.,

$$\sum_{\mathbf{x}\in\mathcal{A}}\sum_{i}[n_{i}(\mathbf{x},t+1)-n_{i}(\mathbf{x},t)]c_{i\alpha}=-(\text{net flux of }\alpha\text{-momentum out of }\mathcal{S}).$$

Averaging allows identification of

- $\sum_{i} \langle n_i \rangle c_{i\alpha}$ : slowly varying  $\alpha$ -component of momentum.
- $\sum_{i} \langle n_i \rangle c_{i\alpha} c_{i\beta}$ : slowly varying  $\alpha$ -momentum carried by  $\langle n_i \rangle$  in the  $\beta$ -direction.

The the LHS averages to the time derivative of  $\alpha$ -momentum and the RHS is the divergence of the flux of  $\alpha$ -momentum:

$$\partial_t \sum_i \langle n_i \rangle c_{i\alpha} = -\partial_\beta \sum_i \langle n_i \rangle c_{i\alpha} c_{i\beta}.$$

Now define the mass density

$$\rho = \sum_{i} \langle n_i \rangle,$$

and the momentum density

$$\rho u_{\alpha} = \sum_{i} \langle n_i \rangle c_{i\alpha}.$$

Substitution above then yields the continuity equation,

$$\partial_t \rho = -\partial_\alpha (\rho u_\alpha),$$

and the macroscopic momentum-balance equation,

$$\partial_t(\rho u_\alpha) = -\partial_\beta \Pi^{(0)}_{\alpha\beta},$$

where

$$\Pi^{(0)}_{\alpha\beta} = \sum_{i} \langle n_i \rangle c_{i\alpha} c_{i\beta}$$

inviscid momentum flux density tensor.

### 1.2.3 Symmetry

The arguments above provide the basic foundation of the continuum limit and its correspondence to real fluid dynamics.

However one should ask whether the appearance of terms like  $c_{i\alpha}c_{i\beta}$  in the momentum flux cause the fluid motion to be hexagonnally symmetric (rather than isotropic).

Surprisingly, it turns out the six velocities suffice for isotropy! (This result follows from the symmetry properties of fourth-order tensors made from  $\sum_{i} c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta}$ .)

Note that a similar question could be asked for our random walk: Is a random walk on a lattice isotropic?

It turns out that for diffusion, one needs only four-fold symmetry (i.e., a square lattice) for isotropy.

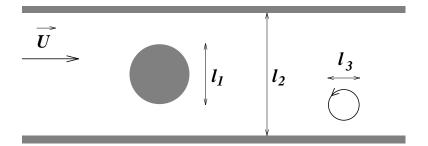
Further information can be found in Ref. [1].

#### 1.2.4 Separation of scales

A related question of more general importance concerns the separation of length scales between that of the lattice unit and that of the fluid continuum.

Because real fluids are made of atoms or molecules, our remarks below are in that context, but they easily translate to our lattice model.

Consider the following macroscopic length scales in a flow:



Of the length scales  $l_i$  we define

 $L_{\rm hydro}$ : the smallest characteristic length scale of macroscopic motions.

We are also interested in the mean free path

 $\ell_{\rm mfp}$ : the characteristic length scale between molecular collisions.

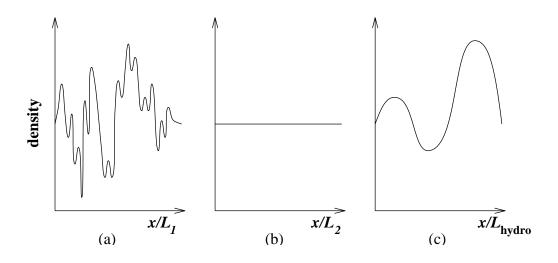
Fluids may be regarded as *continuous fields* if

 $L_{\rm hydro} \gg \ell_{\rm mpf}.$ 

When this condition holds, the evolution of the macroscopic field may be described by *continuum mechanics*, i.e., partial differential equations.

To make this idea clearer, consider a thought experiment in which we measure the density of a fluid over a length scale  $\ell$  using some particularly sensitive device. We then move the device in the x-direction over a distance of roughly  $10\ell$ .

Suppose  $\ell \sim L_1 \sim \ell_{mpf}$ . Then we expect the density to vary greatly in space as in Figure (a) below:



We expect that the fluctuations in (a) should decrease as  $\ell$  increases. (Statistics tells us that these fluctuations should decrease like  $1/N^{1/2}$ , where  $N \propto \ell^3$  is the average number of molecules in a box of size  $\ell$ .)

On the other hand, if  $\ell \sim L_{\text{hydro}}$  (see (c)), variations in density should reflect density changes due to macroscopic motions (e.g., a rising hot plume), not merely statistical fluctuations.

Our assumption of a continuum implies that there is an intermediate scale,  $\ell \sim L_2$ , over which fluctuations are small. Thus the continuum hypothesis implies a *separation of scales* between the molecular scale,  $L_1 \sim \ell_{\rm mfp}$ , and the hydrodynamic scale,  $L_{\rm hydro}$ .

Both the lattice gas and real fluids provide the happy situation in which there is a genuine "scale-gap" between phenomena like (a) and (c). Such situations give confidence to the notion of a continuum and the partial differential equation that models it.

However in many "complex" problems, especially non-physical (i.e., biological) problems, the existence of such a separation is not obvious. For example:

- Physical: flow through (fractal) fractures.
- Biological: ecological interactions between organisms.

In such cases it may be better to concentrate directly on connectivity and the way it varies with scale. We next address an elementary physical example of connectivity: river networks.

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