Lecture notes for 12.086/12.586, Modeling Environmental Complexity

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September 10, 2014

Contents

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.

We now provide two examples in which such a connection can be shown explicity:

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

The interest in these models derives in part from their *statistical dynamics*.

1.1 Random walks

References: [1–3]

1.1.1 One-dimension, discrete time and space

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

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

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

- 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 ith walker after n steps. Then

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

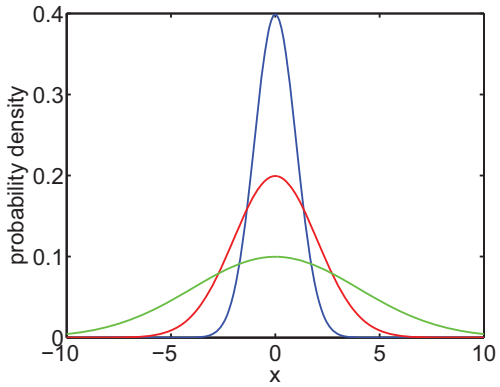
The mean position of a large ensemble of walkers after n steps is

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

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:



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

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

Because the mean of a sum of random variables is the sum of the means, the mean-square displacement in the ensemble is

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

In the second relation, we have replaced the average of a product with the product of averages because s is uncorrelated to x. (This also may be deduced from the observation that the walk contains no memory of past steps.)

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

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

Since $t = n\tau$, we have

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

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:

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

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

Indeed, in the plot above,

$$\left\langle x^2 \right\rangle^{1/2} = 1,\ 2,\ \text{and}\ 4$$

corresponding to times t such that

$$2Dt = 1,\ 4,\ \text{and}\ 16.$$

For a small molecule in water, $D \simeq 10^{-5}$ cm^2/s. So imagine you're a bacterium (size $\sim 10^{-4}$ cm), and you want to know how how long some molecular nutrient will take to diffuse a distance ℓ away from you. Identifying ℓ with $\left\langle x^2 \right\rangle^{1/2}$, the diffusion time τ_d is

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

Consider two particular cases:

ℓ (cm)	τ_d (s)
10^{-4}	5×10^{-4}
1	5×10^4

In other words, the molecule would stay within a length commensurate with 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 of the quadratic scaling $\tau_d \propto \ell^2$, a hallmark of diffusive processes.

In contrast, for a simple advective flow times scale linearly with distance.

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,

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

Since the mean-square distance from the origin is

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

we have

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

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 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

$$\begin{aligned} P(s = \delta) &= p \\ P(s = -\delta) &= q = 1 - p, \end{aligned}$$

i.e., the random walk takes positive steps of size δ 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

$$\left(\begin{array}{c} n \\ k \end{array} \right) \equiv \frac{n!}{k!(n-k)!}.$$

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

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

where $P(k)\mathrm{d}k$ is the probability that k is between k and $k + \mathrm{d}k$, and

$$\begin{aligned} \mu &= \langle k \rangle = np, \\ \sigma^2 &= \left\langle k^2 \right\rangle - \langle k \rangle^2 = npq. \end{aligned}$$

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 $p = q = 1/2$.

Note that in the symmetric case we can also substitute

$$\mathrm{d}x = 2\delta \mathrm{d}k, \qquad t = n\tau, \qquad D = \delta^2/2\tau$$

to obtain

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

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

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

$$\begin{aligned} \phi(k) &= \int_{-\infty}^{\infty} e^{ikx} P(x) \mathrm{d}x \\ P(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} \phi(k) \mathrm{d}k. \end{aligned}$$

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

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

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

$$\begin{aligned} \left. \frac{\mathrm{d}^j \phi(k)}{\mathrm{d}k^j} \right|_{k=0} &= i^j \int_{-\infty}^{\infty} x^j P(x) \mathrm{d}x \\ &= i^j \left\langle x^j \right\rangle , \end{aligned}$$

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

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

$$\begin{aligned} \phi(k) &= \phi(0) + k \left. \frac{\mathrm{d}\phi}{\mathrm{d}k} \right|_{k=0} + \frac{k^2}{2} \left. \frac{\mathrm{d}^2 \phi}{\mathrm{d}k^2} \right|_{k=0} + \mathcal{O}(k^3) \\ &= 1 + ik\langle x \rangle - \frac{k^2}{2} \left\langle x^2 \right\rangle + \mathcal{O}(k^3). \end{aligned}$$

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

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

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

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

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

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

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

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

$$\begin{aligned} \phi_w(k) &= \left\langle e^{ikw(n)} \right\rangle \\ &= \left\langle \exp\left(\frac{ik}{n^{1/2}} \sum_{j=1}^{n} s_j \right) \right\rangle \end{aligned}$$

where we have merely used the definitions of ϕ, w, and x. Since the exponential of a sum is a product of exponentials,

$$\begin{aligned} \phi_w(k) &= \left\langle \prod_{j=1}^{n} e^{iks_j/n^{1/2}} \right\rangle \\ &= \prod_{j=1}^{n} \left\langle e^{iks_j/n^{1/2}} \right\rangle \end{aligned}$$

where in the latter relation we have used the independence of each random step s_j. Since each term in the product above is equal,

$$\begin{aligned} \phi_w(k) &= \left\langle e^{iks/n^{1/2}} \right\rangle^n \\ &\equiv \left[\phi_s\left(k/\sqrt{n}\right) \right]^n. \end{aligned}$$

where we have implicitly defined the characteristic function ϕ_s.

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

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

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

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

$$\begin{aligned}
\lim_{n\to\infty} \phi_w(k) &= \lim_{n\to\infty} \left(1 - \frac{k^2\sigma^2}{2n}\right)^n \\
&= \lim_{n\to\infty} \exp\left[n \log\left(1 - \frac{k^2\sigma^2}{2n}\right)\right] \\
&= \lim_{n\to\infty} \exp\left[n\left(\frac{-k^2\sigma^2}{2n} + \frac{1}{2}\left(\frac{k^2\sigma^2}{2n}\right)^2 + \ldots\right)\right] \\
&= e^{-k^2\sigma^2/2}.
\end{aligned}$$

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

$$\begin{aligned}
P(w) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ikw}\phi_w(k)\mathrm{d}k. \\
&= \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-w^2/2\sigma^2},
\end{aligned}$$

i.e., a Gaussian distribution with zero mean and variance σ^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

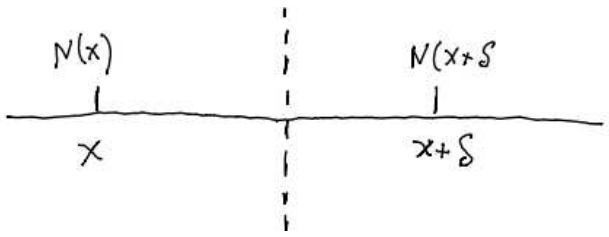
We now proceed to derive the diffusion equation from our random walk.

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 pass through 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 a boundary between x and $x + \delta$. During one time step τ, 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 δ^2/δ^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

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

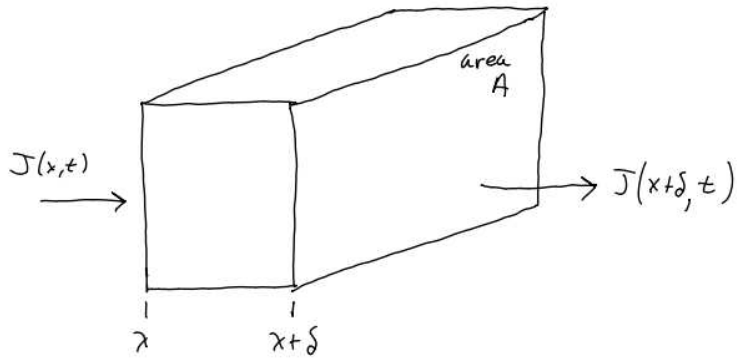
Letting $\delta \to 0$, we obtain

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

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 and Hooke's law. 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 independently of one another.

Now consider particles flowing into and out of a box with cross-sectional area A perpendicular to and width δ parallel to the x-axis.



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

In τ units of time the concentration changes as

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

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 the *diffusion equation*:

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

These developments can be derived succinctly by an alternative approach. Let

$$P_n(i) = \text{probability that a random walker is at site } i \text{ after } n \text{ steps.}$$

Since steps to the left and right occur with equal probability, we have

$$P_n(i) = \frac{1}{2}P_{n-1}(i+1) + \frac{1}{2}P_{n-1}(i-1)$$

Now set

$$t = n\tau \quad \text{and} \quad x = i\delta$$

and consider the probability to be spread over an interval of size δ so that

$$P_n(i) = \delta \cdot p(x,t).$$

Then

$$p(x,t) = \frac{1}{2}p(x+\delta, t-\tau) + \frac{1}{2}p(x-\delta, t-\tau).$$

Multiplying both sides by $1/\tau$ and rearranging, we have

$$\frac{1}{\tau}\left[p(x,t) - p(x,t-\tau)\right] = \frac{\delta^2}{2\tau}\cdot\frac{1}{\delta^2}\left[p(x+\delta,t-\tau) - 2p(x,t-\tau) + p(x-\delta,t-\tau)\right]$$

We recognize the LHS as a finite difference in time and the RHS as a finite difference of finite differences in space.

Thus in the limit as $\tau \to 0$ and $\delta \to 0$, we have

$$\frac{\partial p}{\partial t} = D\frac{\partial^2 p}{\partial x^2}, \qquad D = \frac{\delta^2}{2\tau}$$

expressing the diffusion of probability.

Reverting back to the concentration C, 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 the *diffusion equation*

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

which may be straightforwardly obtained by generalization of our random walk to higher dimensions.

By deriving the diffusion equation via a random walk, we have exposed the connection of diffusion to random motion.

The universality of the Gaussian distribution tells us that only the diffusivity D changes as the distribution of step sizes (or waiting times) changes, not the diffusion equation itself, provided that the step size and waiting time distributions are not too wide.

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

References: [4, 5]

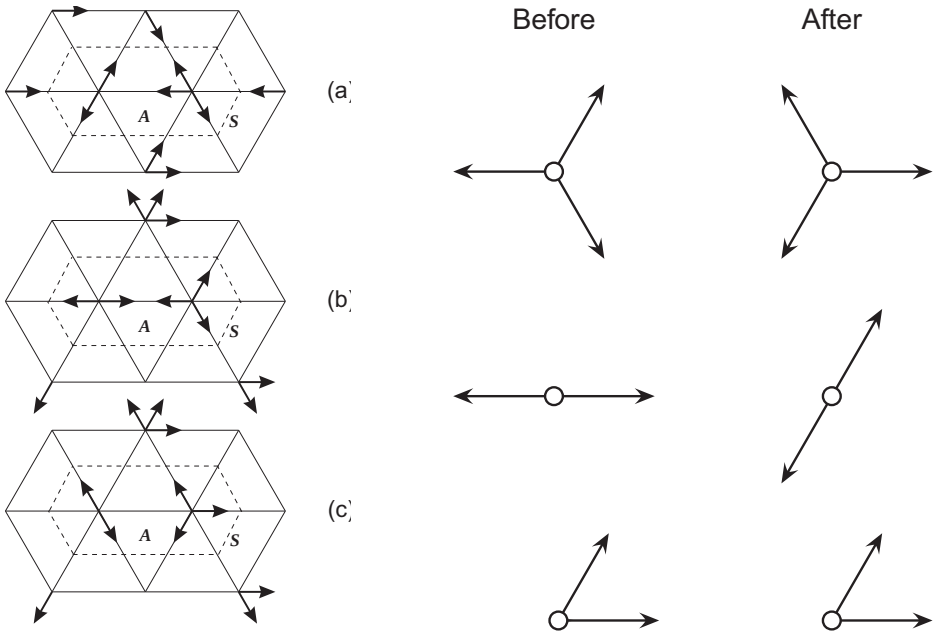
We now return to the lattice gas of Lecture 1 and sketch its relation to the equations of fluid dynamics.

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

However there are 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 $\mathbf{n} = (n_1, n_2, \ldots, n_6)$ 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

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

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

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

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 [4].

Note that Δ_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_{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 the left-hand side above as the 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 α-component of the ith 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 α-component of momentum.
- $\sum_i \langle n_i \rangle c_{i\alpha} c_{i\beta}$: slowly varying α-momentum carried by $\langle n_i \rangle$ in the β-direction.

Thus the LHS averages to the time derivative of α-momentum and the RHS is the divergence of the flux of α-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

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

is the 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 hexagonally symmetric (rather than isotropic).

In the real world, the inviscid momentum flux density tensor takes the form

$$\Pi^{(0)^\star}_{\alpha\beta} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta$$

where p is the pressure and

$$\delta_{\alpha\beta} = \begin{cases} 1 & \alpha = \beta \\ 0 & \text{else} \end{cases}.$$

Through symmetry arguments one may obtain the general form of the lattice analog when the average velocity u is small. Expanding to second order, one obtains

$$\Pi^{(0)}_{\alpha\beta} = p_0(\rho)\delta_{\alpha\beta} + \lambda_{\alpha\beta\gamma\delta}(\rho) u_\alpha u_\beta + \mathcal{O}(u^4).$$

In real fluids, $\lambda_{\alpha\beta\gamma\delta}$ is *isotropic*, meaning that it is invariant under rotation. The isotropy of the lattice gas turns out to depend on the symmetry properties of fourth-order tensors made from

$$\sum_i c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta}.$$

Surprisingly, it turns out that six velocities suffice for isotropy! (This result is indeed familiar in elasticity theory, where it is often shown that the stress-strain relation in a hexagonally symmetric system is isotropic.)

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

In this case, in the continuum limit we no longer relate second-rank tensors (e.g., stress and strain) via a fourth-rank tensor, but instead we relate vectorial quantities (mass flux and concentration gradient) via a second-rank tensor.

One may then show that symmetry rests only on the isotropy of second-rank tensors formed from

$$\sum_i c_{i\alpha} c_{i\beta},$$

for which 4-fold symmetry (i.e., a square lattice) suffices for isotropy.

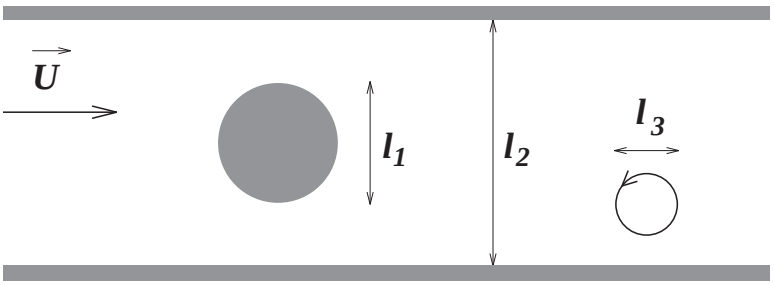
Further information can be found in Ref. [5].

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.

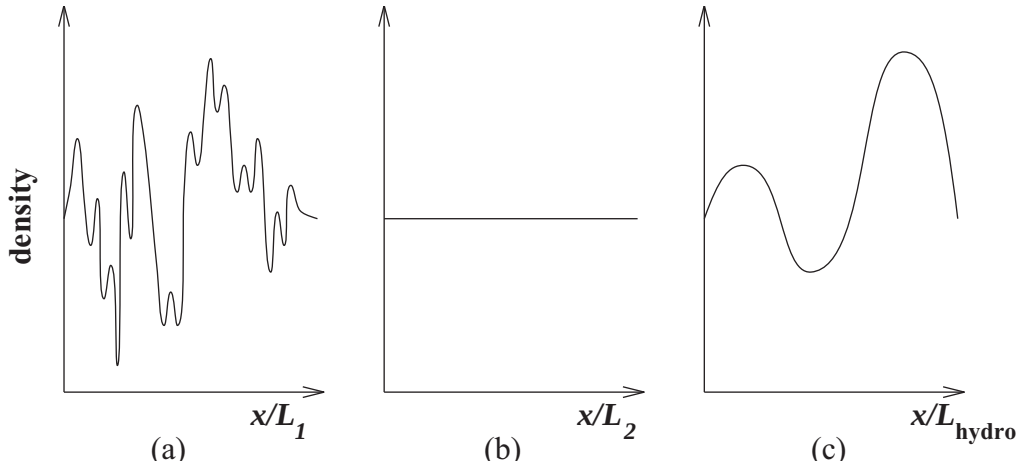
Fluids may be regarded as *continuous fields* if

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

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 ℓ using some particularly sensitive device. We then move the device in the x-direction over a distance of roughly 10ℓ.

Suppose $\ell \sim L_1 \sim \ell_{\rm mfp}$. 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 ℓ 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 ℓ.)

On the other hand, if $\ell \sim L_{\rm hydro}$ (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.

References

[1] Berg, H. C. *Random Walks in Biology* (Princeton University Press, Princeton, 1993).

[2] Tennekes, H. & Lumley, J. L. *A First Course in Turbulence* (MIT Press, Cambridge, MA, 1972).

[3] Ma, S.-K. *Statistical Mechanics* (World Scientific, Singapore, 1985).

[4] Frisch, U., Hasslacher, B. & Pomeau, Y. Lattice-gas automata for the Navier-Stokes equations. *Phys. Rev. Lett.* **56**, 1505–1508 (1986).

[5] Rothman, D. H. & Zaleski, S. *Lattice-gas Cellular Automata: Simple Models of Complex Hydrodynamics* (Cambridge University Press, Cambridge, 1997).

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Fall 2014