Diffusion of a density in a static fluid

$u(x, y, z, t)$, density (M/L^3) of a substance (dye). Diffusion: motion of particles from places where the density is higher to places where it is lower, due to random independent motion (http://en.wikipedia.org/wiki/Diffusion).

Ficks law (1870): flux vector

$$\underbrace{\mathbf{J}}_{M/(TL^2)} = -\underbrace{D}_{L^2/T}\ \underbrace{\nabla u}_{M/L^4},$$

where $\int_\Sigma \mathbf{J}\cdot\mathbf{n}\, d\mathcal{S}$ (M/T) is the net flux of mass per unit time crossing Σ in the direction of $\mathbf{n}$. D: diffusivity.

Balance of mass:

$$\frac{d}{dt}\int_{\Omega_0} u\, d\mathcal{V} = -\int_{\partial\Omega_0} \mathbf{J}\cdot\mathbf{n}\, d\mathcal{S} + \int_{\Omega_0} \underbrace{g}_{\text{reaction}}\ d\mathcal{V},$$

$$u_t = \nabla\cdot(D\nabla u) + g,\quad \textbf{diffusion equation}.$$

$$u_t = \nabla \cdot (D \nabla u) + g$$

- $D \equiv D_0$, Laplacian, linear diffusion.
- $D = D(u) = D_0 m u^{m-1}$, porous medium equation, $m > 1$.
- $D = D(\nabla u) = D_0 |\nabla u|^{p-1}$ p-laplacian, $p > 2$.
- $g = g(u)$ (kinetics), reaction-diffusion equation. The reaction part is the ODE

$$\frac{du}{dt} = g(u).$$

1-dimensional random walk (Bachelier, 1900, finance)

A particle moves in a net $\{x = x_i = ih; i \in \mathbb{Z}\} \subset \mathbb{R}$ jumping each Δt either left or right with probability $1/2$ ($h, \Delta t > 0$). Let $u(x,t)$ be the probability that the particle occupies the position x at time t.

$$u(x, t+\Delta t) = \frac{1}{2}[u(x+h,t) + u(x-h,t)]$$

$$\frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} = \frac{h^2}{2\Delta t}\,\frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2}$$

If $h \to 0$ and $\Delta t \to 0$ with $h^2/(2\Delta t) \to D_0$ (better with the *density* $u' = u/h$), then we get

$$u_t = D_0 u_{xx}.$$

Observe that if $h^2/(2\Delta t) \to D_0 > 0$ then the *speed* $h/\Delta t \to \infty$.
Observe $h \sim \sqrt{\Delta t}$.
This deduction gives an interpretation for the diffusivity D_0.

Observe that if $\int_{-\infty}^{\infty} u \, dx = 1$ initially, then the same will hold in the future.

The same deduction holds when $u(x, t)$ is the density of individuals between $x - h/2$ and $x + h/2$ (the number of individuals being then hu) at time t when half of them jump right and half of them jump left each Δt.

Then, the total population $\int_{-\infty}^{\infty} u \, dx$ is no longer restricted to be 1, but can be arbitrary (positive).

Problem 2.1: Suppose that a particle in $\mathbb{R}^n$ moves in the net $\{(i_1 h, i_2 h, \dots i_n h); i_j \in \mathbb{Z}\}$ and jumps every Δt from one point to one of its neighbours (along one of the axes) with a probability $1/(2n)$. Deduce $u_t = D_0 \nabla^2 u$ and state the hypotheses on how $h \to 0$ and $\Delta t \to 0$.

Problem 2.2 : (anisotropic diffusion) Consider the situation of the previous problem for $n = 2$ and supose that the probability of jumping left is $d/2$, right is $d/2$, up is $(1-d)/2$ and down is $(1-d)/2$, for some $0 < d \leq 1$. Write the limit equation in the form $u_t = \nabla \cdot M_0 \nabla u$, where now M_0 is a 2×2 matrix.

Problem 2.3: Suppose a particle moves in a 1-dimensional net $\{x = x_i = ih; i \in \mathbb{Z}\} \subset \mathbb{R}$, and each Δt either remains in its place with a probability $(1-d)$, or with a probability d jumps either left or right with probability $d/2$. We suppose $0 < d \leq 1$. Deduce $u_t = D_0 u_{xx}$, for some D_0 and state the hypotheses.

Heat Conduction, Fourier's Law

Heat conduction in an equilibrium isotropic solid.

u, temperature (degrees); Q is the heat density (energy/volume); ρ, density (mass/volume); C heat capacity (specific heat) (energy/(temperature$\times$mass)).

$$Q = \rho C u.$$

The quantities u and Q, the *unknowns*, depend on space and time. In non-homogeneous solids also ρ and C can depend on $\mathbf{x}$, or, in more realistic but complicate situations, also on u. The total heat in Ω_0 is

$$Q_{\Omega_0} = \int_{\Omega_0} Q \, d\mathcal{V}.$$

One postulates the existence of a *flux vector* $\mathbf{q}$ (energy/(area $\times$ time)) whose integral gives us the net heat flux:

$$\frac{d}{dt}\int_{\Omega_0} Q\, d\mathcal{V} = -\underbrace{\int_{\partial\Omega_0} \mathbf{q}\cdot\mathbf{n}\, d\mathcal{S}}_{\text{conduction}} + \underbrace{\int_{\Omega_0} f\, d\mathcal{V}}_{\textit{generation}}.$$

Fourier's Law(1822): (isotropic case)

$$\mathbf{q} = -k\nabla u,$$

where k is the *thermal conductivity* (large in metals, low in isolating materials).

$$\rho C u_t = \nabla\cdot(k\nabla u) + f \quad \text{heat equation.}$$

If ρ, C, k are constants and $f = 0$ then $u_t = D\nabla^2 u$, where $D = k/(\rho C)$ is the *thermal diffusivity*.

A self-similar solution

A solution of $u_t = Du_{xx}$ of the form $u = \varphi(r(t)x)$, with φ bounded. We use the new variables $\xi = rx$ and t, and the special function $\mathrm{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\sigma^2}\, d\sigma$ and obtain (**Problem 2.4**: make this calculation)

$$u(x,t) = \frac{u_\infty + u_{-\infty}}{2} + \frac{u_\infty - u_{-\infty}}{2} \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right),$$

whose initial condition is

$$u(x,0) = \begin{cases} u_{-\infty} & \text{for } x < 0 \\ u_\infty & \text{for } x > 0 \end{cases} .$$

Take $u_{-\infty} = 0$, $u_\infty = 1$ and $D = 1$, then

$$U(x,t) = \frac{1}{2} + \frac{1}{2}\,\text{erf}\left(\frac{x}{2\sqrt{t}}\right).$$

We see that $U(x,0) \equiv 0$ for $x < 0$, but $U > 0$ for $t > 0$ (infinite speed of propagation). The same happens with $U(x-a,t) - U(x-b,t)$. We see also the irreversibility of the diffusion.

Observe that the Gaussian

$$G(x,t) = U_x = \frac{1}{\sqrt{4\pi t}} e^{-\frac{x^2}{4t}}$$

satisfies $\int_{-\infty}^{\infty} G(x,t)\,dx = 1$ and has as its initial condition Dirac's δ-function. From here, Poisson's formula

$$u(x,t) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} e^{-\frac{(x-x')^2}{4t}} u(x',0)\,dx'.$$

Also, in 2 dimensions, $U(x)U(y)$ is also a solution of $u_t = u_{xx} + u_{yy}$, and we get (in n dimensions)

$$u(\mathbf{x}, t) = \frac{1}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{||\mathbf{x}-\mathbf{x}'||^2}{4t}} u(\mathbf{x}', 0)\, d\mathcal{V}(\mathbf{x}').$$

Problem 2.5: Deduce this last formula from what we know about $G(x, t)$.

Problem 2.6: Are there more (bounded) solutions of $u_t = u_{xx}$ of the form $u = r(t)\varphi(r(t)x)$ apart from $G(x, t)$?

A. Einstein calculation on Brownian motion (1905)

Suppose $X(t)$ is a random variable depending on time (a random process) such that

$$X(t+\Delta t) = \begin{cases} X(t)+h & \text{with probability } d/2 \\ X(t) & \text{with probability } (1-d) \\ X(t)-h & \text{with probability } d/2 \end{cases}$$

for some $0 < d \leq 1$.

A. Einstein claim (1905): The (net) displacement is not proportional to the elapsed time, but to its square root (supposing $\Delta t, h \ll 1$).

Proof: Supposing Δt and h small and defining $D = dh^2/(2\Delta t)$, the position of the particle at time t has a pdf $u(x,t)$ such that

$$u_t = Du_{xx}$$

(one of the problems above), and since the initial pdf is a Dirac delta function then

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}.$$

So, the average square of the net displacement is

$$\overline{x^2} = \int_{-\infty}^{\infty} \frac{x^2}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}} = 2Dt,$$

Problem 2.7: Check the last equality. That was the expected value of x^2. Calculate the expected value of $|x|$. Check also that $X(t) - X(s) \sim \mathcal{N}(0, 2D(t-s))$ (normal distribution, $\mathcal{N}(\mu, \sigma^2)$).

Einstein calculation, in other words, says that the *variance* of $X(1)$ is $\sigma^2 = 2D$. This is the reason of the *probabilistic* tradition of writing the diffusion equation as $u_t = \frac{\sigma^2}{2} u_{xx}$.
Einstein's calculation was used (by him) to support *atomic theory* and to calculate Avogadro's number.

https://en.wikipedia.org/wiki/Brownian_motion
https://en.wikipedia.org/wiki/Louis_Bachelier

Diffusion and advection

By adding to Fick's law the flux due to advection by a velocity field $\mathbf{v}(x, t)$ one gets

$$J = -D\nabla u + u\mathbf{v}$$

and the *advection-diffusion* equation

$$u_t + \nabla \cdot (u\mathbf{v}) = D\nabla^2 u.$$