

# Rutgers 642:613 - Fall 2003

Instructor: Eduardo D. Sontag

Conservation Laws and Diffusion

<http://www.math.rutgers.edu/~sontag/613.html>

## Reaction-Diffusion Equations

let  $c(x, t)$  be the density of a chemical around a point  $x = (x_1, x_2, x_3)$  in space, at time  $t$

consider a region  $S$  and let  $C_S(t)$  be the total amount of chemical inside  $S$  at time  $t$ , i.e.:  $C_S(t) = \int_S c(x, t) dx$

let  $J(x, t)$  be the *flux* of  $c$ , a (possibly time-dependent) vector field which indicates the direction of flow, and the average amount of the chemical crossing, per unit time, a unit area perpendicular to  $J$

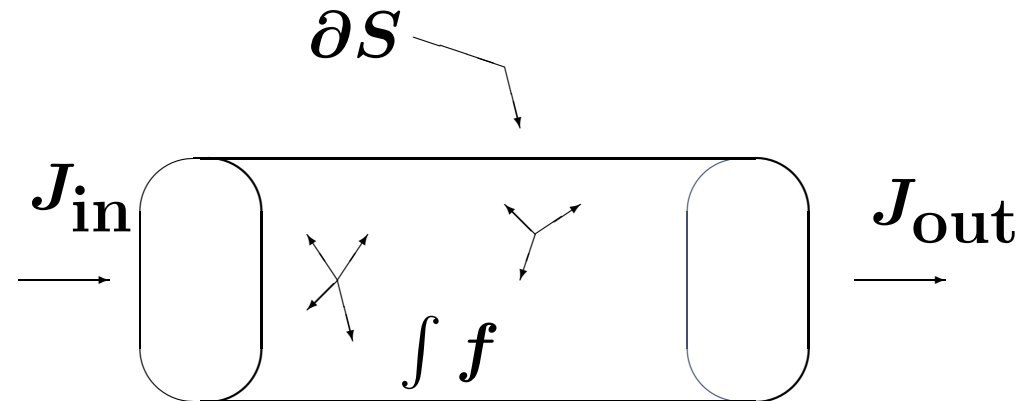
then, on the interval of time  $[t, t + h]$ , the net amount of chemical *exiting* through the boundary of  $S$  is

$$\int_t^{t+h} \int_{\partial S} J \cdot n dA$$

where  $n$  is the outward unit normal to the boundary

let  $f(x, t)$  be the amount of the chemical being *created* (or destroyed, if  $< 0$ ) at a point  $x$  in space, at time  $t$ ;

*total change in S = total created + net inflow*



$$\int_S [c(x, t+h) - c(x, t)] dx = \int_t^{t+h} \int_S f(x, t) dx - \int_t^{t+h} \int_{\partial S} J \cdot n dA$$

so dividing by  $h$  and taking limits as  $h \rightarrow 0$  we get:

$$\int_S \frac{\partial c}{\partial t} dx = \int_S f(x, t) dx - \int_{\partial S} J \cdot n dA$$

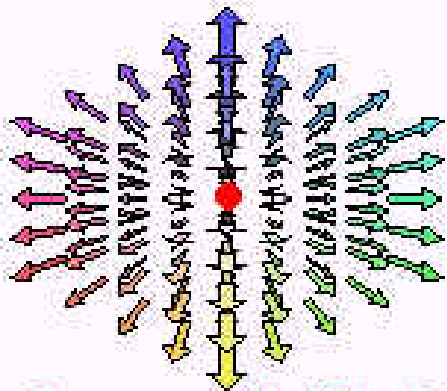
but (divergence, or Gauss') theorem says that

$$\int_S \nabla J dx = \int_{\partial S} J \cdot n dA$$

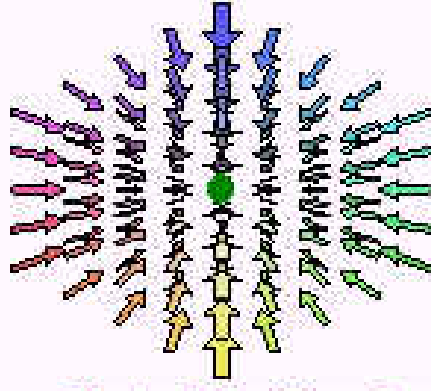
where *divergence* of  $J = (J_1, J_2, J_3)$ ,  $x = (x_1, x_2, x_3)$ :

$$\text{div } J = \text{“}\nabla \cdot J\text{”} = \frac{\partial J_1}{\partial x_1} + \frac{\partial J_2}{\partial x_2} + \frac{\partial J_3}{\partial x_3}$$

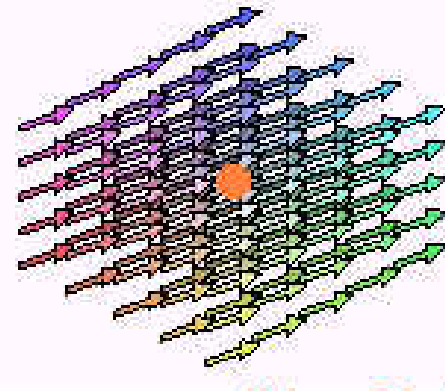
( $\forall$  smooth vector field  $J$ , net flow through the boundary of a region [bounded open subset of  $\mathbb{R}^n$  with smooth or piecewise smooth boundary] = total divergence in the region)



Source:  $\text{Div}(F) > 0$



Sink:  $\text{Div}(F) < 0$



Incompressible:  $\text{Div}(F) = 0$

so we conclude:

$$\int_S \frac{\partial c}{\partial t} dx = \int_S f(x, t) dx - \int_S \nabla J dx$$

and since this happens for all  $S$ , no matter how small (“function with zero integral on all regions must be zero”)

$\rightsquigarrow$

$$\frac{\partial c}{\partial t} = f - \nabla J$$

this applies in general; next: flux due to *diffusion*

## What is Diffusion?

one of the fundamental processes by which “particles” (atoms, molecules, even bigger objects) move

*Fick's Law, 1855*, based upon experimental observation: movement [higher  $\rightarrow$  lower] concentration regions  
 $\rightsquigarrow$  “flux  $J(x, t) \propto -\nabla c(x, t)$ ”

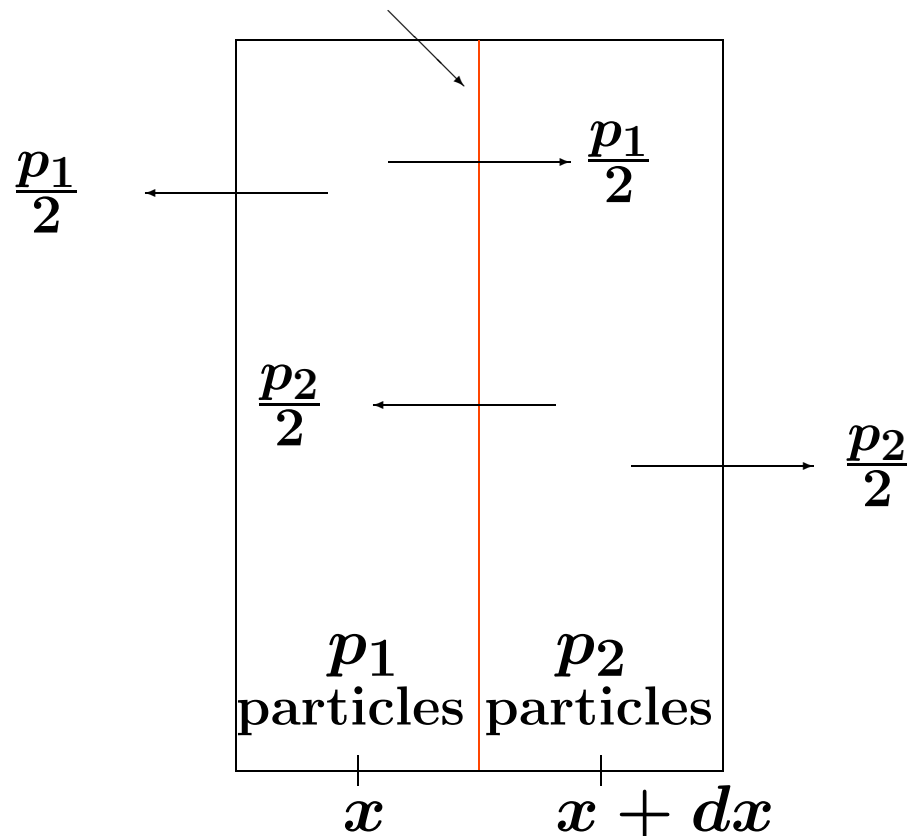
applies to movement of particles in a solution; proportionality constant depends on sizes of molecules (solvent, solute) and temperature and, when across membranes, permeability & thickness

main physical explanation is probabilistic, based on thermal motion of individual particles due to environment (e.g. molecules of solvent) constantly “kicking” the particles

(Brown 1828: pollen grains suspended in water move in a rapid but very irregular fashion; relation to Fick's Law explained mathematically in Einstein's Ph.D. thesis, 1905)

why  $J(x, t) \propto -\nabla c(x, t)$  ?

“virtual wall” of unit area



probabilistic intuition  
(in one space dimension)

suppose particles move right or left with equal probability, so half of the  $p_1$  particles in the first box move right, and the other half move left; similarly for second box

**flux** (rightward) through virtual wall proportional to  $\frac{p_1}{2} - \frac{p_2}{2}$ , which is proportional to  $c(x, t) - c(x + dx, t)$ ,

which is proportional to  $-\frac{\partial c}{\partial x}$  (analogously in  $\mathbb{R}^3$ :  $-\nabla c(x, t)$ )

## Diffusion Equation

so  $J(x, t) = -D \nabla c(x, t)$  ( $D = \text{diffusion coefficient}$ )  
and, in general,  $\frac{\partial c}{\partial t} = f - \text{div } J$  (div = “ $\nabla \cdot$ ”)

⇨

$$\frac{\partial c}{\partial t} = D \nabla^2 c + f$$

where  $\nabla^2$  is the “Laplacian” (often “ $\Delta$ ”) operator:

$$\nabla^2 c = D \left( \frac{\partial^2 c}{\partial x_1^2} + \frac{\partial^2 c}{\partial x_2^2} + \frac{\partial^2 c}{\partial x_3^2} \right)$$

and in particular in dimension one:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + f$$

(note:  $\frac{1}{D} \propto \sqrt[3]{\text{volume}}$ , or equivalently to  $\sqrt[3]{\text{mass}}$ )

with no  $f$  nor additional constraints, eventually  $\rightarrow$  homogeneous concentration over space; but usually there are additional boundary conditions, creation and absorption rates, etc, superimposed on pure diffusion, so there’s a “trade-off” between the “smoothing out” effects of diffusion and other influences

## Remark: Speed of Diffusion (dim 1)

(ignore reaction term “ $f$ ” for now; will add back later)

Suppose  $c$  satisfies diffusion equation  $\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$ .

Assume also that the following hold:

$$C = \int_{-\infty}^{+\infty} c(x, t) dx$$

is independent of  $t$  (constant population), and

$$\lim_{x \rightarrow \pm\infty} x^2 \frac{\partial c}{\partial x}(x, t) = 0, \quad \lim_{x \rightarrow \pm\infty} xc(x, t) = 0.$$

( $c$  is small at infinity)  $\forall t$ . Define, for each  $t$ :

$$\sigma^2(t) = \frac{1}{C} \int_{-\infty}^{+\infty} x^2 c(x, t) dx \quad (\text{second moment finite})$$

which measures how the density “spreads out”

Then:

$$\sigma^2(t) = 2Dt + \sigma^2(0) \quad \forall t > 0$$

in particular, if the initial ( $t = 0$ ) population is concentrated near  $x = 0$  (“ $\delta$  function”), then  $\sigma^2(t) \approx 2Dt$

## Proof

use PDE and integrate by parts:

$$\begin{aligned}\frac{C d\sigma^2}{D dt} &= \frac{1}{D} \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} x^2 c dx = \frac{1}{D} \int_{-\infty}^{+\infty} x^2 \frac{\partial c}{\partial t} dx \\ &= \int_{-\infty}^{+\infty} x^2 \frac{\partial^2 c}{\partial x^2} dx = \left[ x^2 \frac{\partial c}{\partial x} \right]_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} 2x \frac{\partial c}{\partial x} dx \\ &= - [2xc]_{-\infty}^{+\infty} + \int_{-\infty}^{+\infty} 2c dx = 2 \int_{-\infty}^{+\infty} c(x, t) dx = 2C\end{aligned}$$

Cancelling  $C$ , we obtain

$$\frac{d\sigma^2}{dt}(t) = 2D$$

and hence, integrating over  $t$  we have, as wanted:

$$\sigma^2(t) = 2Dt + \sigma^2(0).$$

if  $c(x, 0) = 0$  for all  $|x| > \varepsilon$  then (with  $c = c(x, 0)$ ):

$$\int_{-\infty}^{+\infty} x^2 c dx = \int_{-\varepsilon}^{+\varepsilon} x^2 c dx \leq \varepsilon^2 \int_{-\varepsilon}^{+\varepsilon} c dx = \varepsilon^2 C(0)$$

so  $\sigma^2(0) \leq \varepsilon \approx 0$

## Suggested Problem

Show that, under analogous conditions to those in the theorem shown for dim 1, in dimension  $d$  (e.g.:  $d = 2, 3$ ) one has the formula:

$$\sigma^2(t) = 2dDt + \sigma^2(0)$$

(for  $d = 1$ , this is the same as previously)

the proof will be completely analogous, except that the first step in integration by parts

( $uv' = (uv)' - u'v$ , the Leibnitz rule for derivatives)

must be generalized to vectors ( $\nabla \cdot$  acts like a derivative)

and the second step (the Fundamental Theo of Calc) should be replaced by an application of Gauss' divergence theorem

so, in a rough sense, diffusion has “speed”  $\propto \sqrt{t}$

(a different, probabilistic, interpretation is given later)

*travelling distance  $L$  requires time  $L^2$*

diffusion is simple and energetically “cheap”:

no need for building machinery for locomotion; no loss due to conversion to mechanical energy (e.g. cellular motors)

at the right scales, very efficient: fast method for nutrients and signals that must be carried along for *short* distances,

...but not for long distances... example:

if can travel  $10^{-6}\text{m}$  ( $= 1\mu\text{m}$ ) in  $10^{-3}$  seconds

(typical order of magnitude in cell),

then how much time needed to travel 1 meter?

since  $x^2 = 2Dt$ , solve  $(10^{-6})^2 = 2D10^{-3} \rightsquigarrow D = 10^{-9}/2$

so,  $1 = 10^{-9}t \Rightarrow t = 10^9$  seconds, i.e. about 27 years (!)

not a feasible way to move things along a large organism,

...or even a big cell (e.g., long neuron)

$\Rightarrow$  circulatory systems, cell motors, microtubules, etc

the “fundamental solution”

for  $n = 1$ , this is *one* solution of the diffusion equation:

$$c_0(x, t) = \frac{C}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

(where  $C$  is any constant – verify by plugging-in)

for  $t = 0$  solution is not well-defined; it tends to “ $\delta$ ”

think as “spread from a point source”

moreover, for arbitrary continuous  $g$

$$c(x, t) = \int_{-\infty}^{+\infty} \frac{C}{\sqrt{4\pi Dt}} e^{-\frac{(x-\xi)^2}{4Dt}} g(\xi) d\xi$$

solves diff eq and has initial condition  $c(x, 0) = g(x)$

(continuous function, satisfies PDE for  $t > 0$ )

*convolution*  $c_0 * g$  with “Green’s function” for PDE

more generally ( $r^2 = x_1^2 + \dots + x_d^2$ ), this is a solution:

$$c_0(x, t) = \frac{C}{(4\pi Dt)^{d/2}} e^{-\frac{r^2}{4Dt}}$$

with radial ( $d = 2$ ) or spherical ( $d = 3$ ) symmetry

## probabilistic interpretation: random walks

above looks  $\approx$  Gaussian (normal) distribution. . . coincidence?  
intuition (dimension 1, but similar for arbitrary  $d$ ):

*each individual particle* is undergoing Brownian motion  
if particles move independently (small, no collisions)  
then, concentration in a region  $R$  is proportional to  
the probability of any given particle being in  $R$

so, soln of diffusion equation  $c(x, t)$  should be proportional  
to the *probability density* of the random variable that  
gives the position of a random-walk at time  $t$

if starting at  $x = 0$ , one obtains Gaussian distribution  $c_0$   
intuition from discrete steps:

suppose we can move left or right with a unit displacement  
and equal probability (each step independent of the rest)

what is the position after  $t$  steps?

do a histogram, let us say for 4 steps:

ending	possible sequences	count	
-4	-1-1-1-1	1	x
-2	-1-1-1+1,-1-1+1-1,...	4	xxxx
0	-1-1+1+1,-1+1+1-1,...	6	xxxxxx
2	1+1+1-1,1+1-1+1,...	4	xxxx
4	1+1+1+1	1	x

tends to normal (Central Limit Theorem), and has variance:

$$\sigma^2(t) = E(X_1 + \dots + X_t)^2 = \sum_{i=1}^t \sum_{j=1}^t EX_i X_j = \sum_{i=1}^t EX_i^2 = \sigma^2 t$$

since independent (so  $EX_i X_j = 0$  for  $i \neq j$ )

again this leads to the formula “ $\sigma(t)$  proportional to  $\sqrt{t}$ ”

*exercise:* prove that the average displacement of a Gaussian r.v. is proportional to  $\sqrt{t}$  (hint: substitute  $u = x/\sigma$ ):

$$E(|X|) = \frac{2}{\sigma\sqrt{2\pi}} \int_0^\infty x e^{-x^2/(2\sigma^2)} dx = \frac{\sigma}{\sqrt{\pi}}$$

similarly,  $E(\sqrt{x_1^2 + \dots + x_d^2})$