Biophysics I (BPHS 3090)

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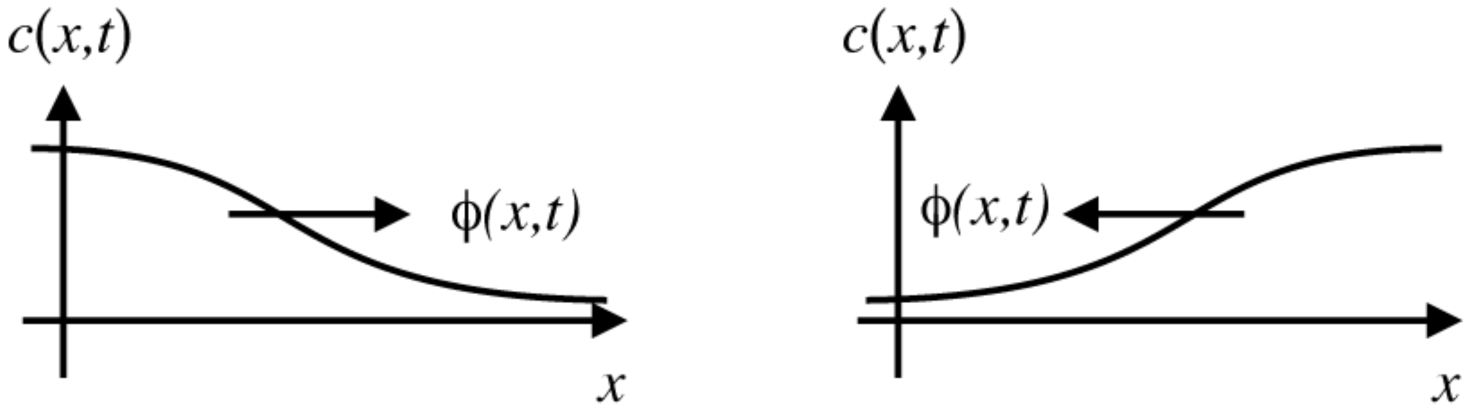
Website: http://www.yorku.ca/cberge/3090W2015.html

York University
Winter 2015
Lecture 2

Reference/Acknowledgement:
- TF Weiss (Cellular Biophysics)
- D Freeman

Diffusion (1-D)

From Graham's observations (~1830):



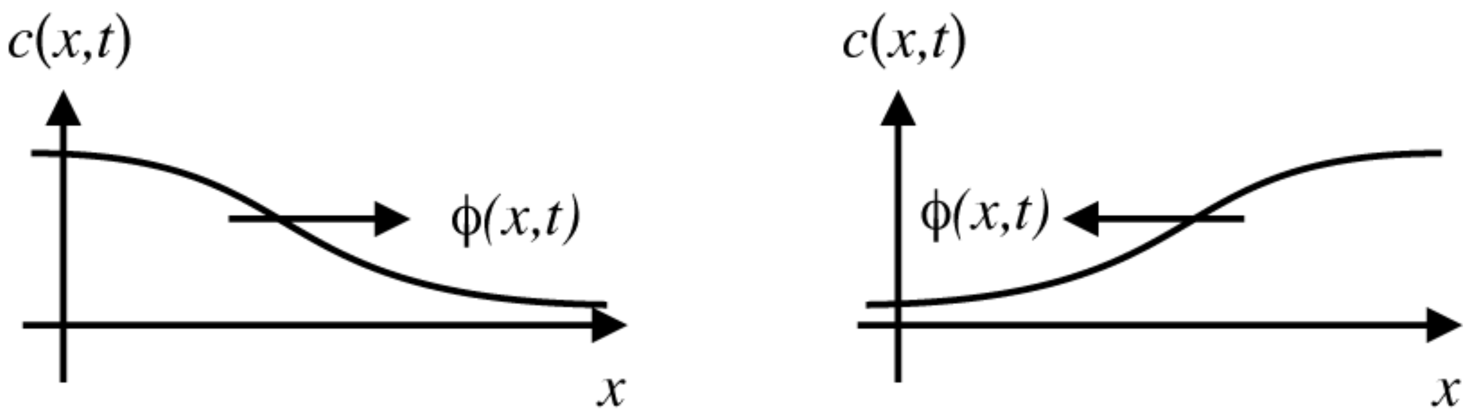
Freeman

" A few years ago, Graham published an extensive investigation on the diffusion of salts in water, in which he more especially compared the diffusibility of different salts. It appears to me a matter of regret, however, that in such an exceedingly valuable and extensive investigation, the development of a fundamental law, for the operation of diffusion in a single element of space, was neglected, and I have therefore endeavoured to supply this omission."

- A. Fick (1855)

Diffusion (1-D)

From Graham's observations (~1830):



$c(x,t)$ Concentration - of solute in solution [*mol/m*³]

$\phi(x,t)$ Flux - net # of moles crossing per unit time t through a unit area perpendicular to the x-axis [*mol/m*²·*s*]

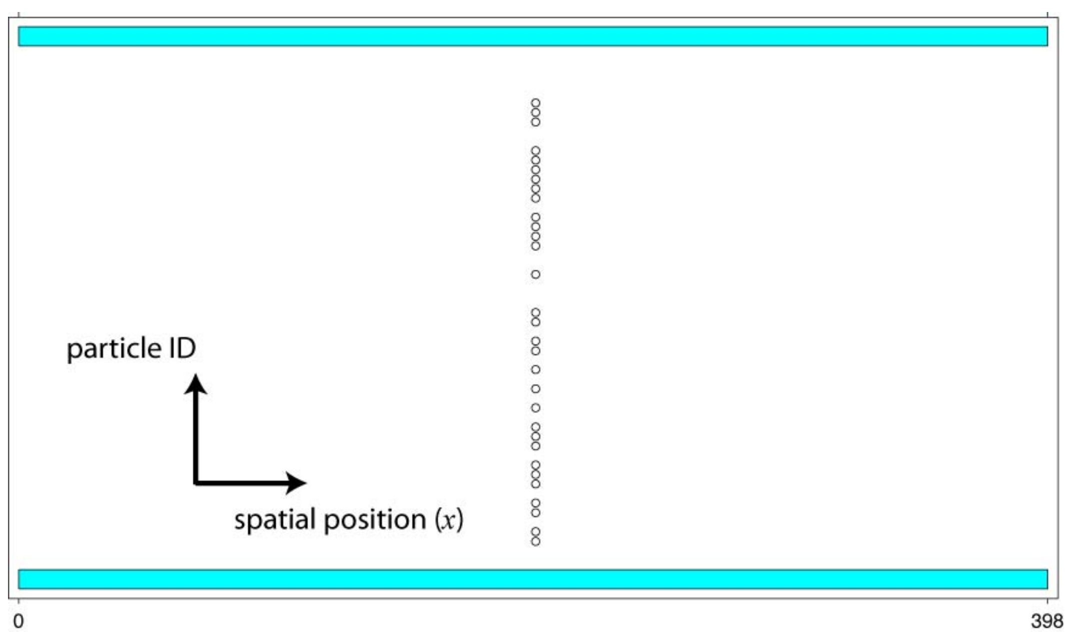
Note: flux is a vector!

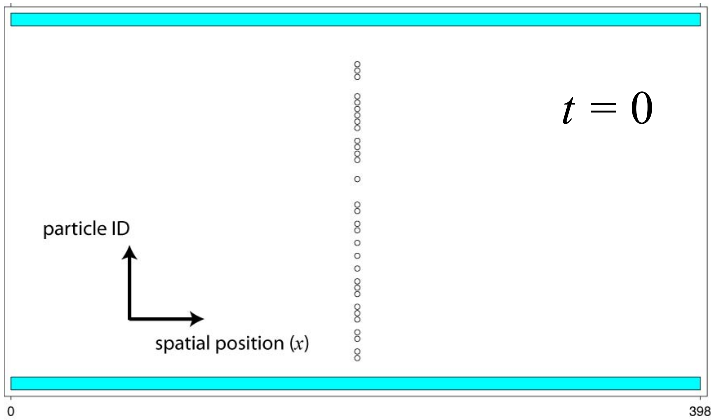
x, t Position [*m*], Time [*s*]

Short Excursion: Microscopic Basis for Diffusion

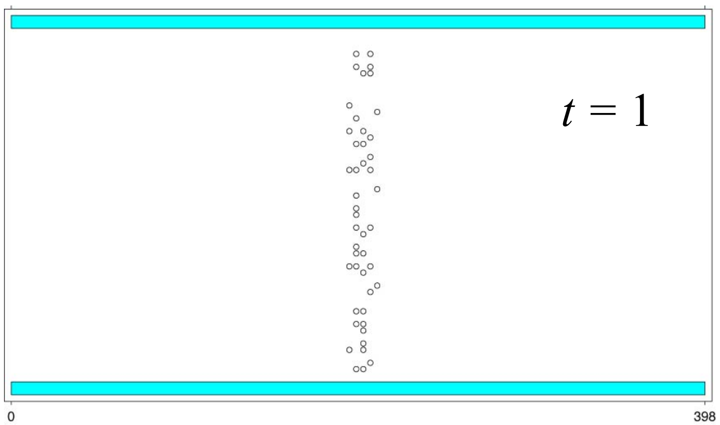
Brownian motion ⇒ ‘Random Walker’ (1-D)

Ensemble of Random Walkers

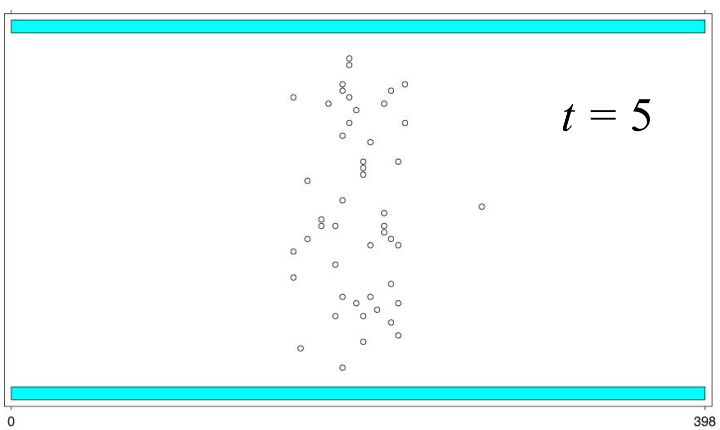




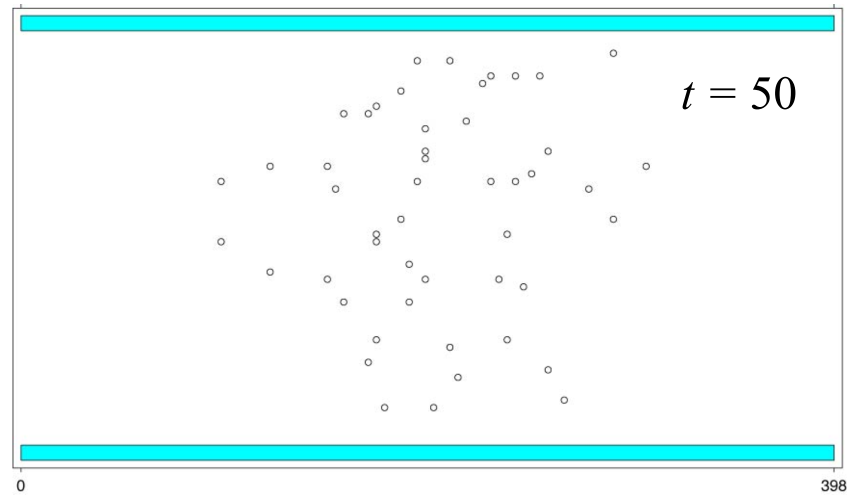
t = 0
particle ID
spatial position (x)
0
398



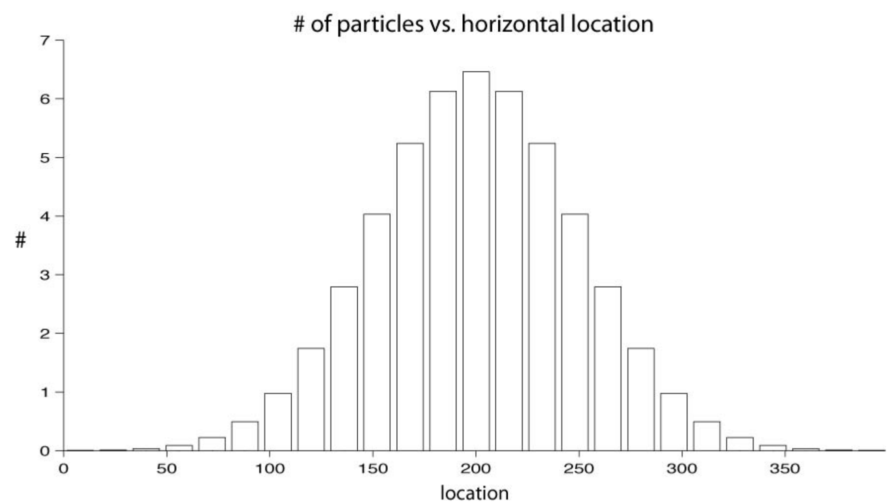
t = 1
0
398



t = 5
0
398



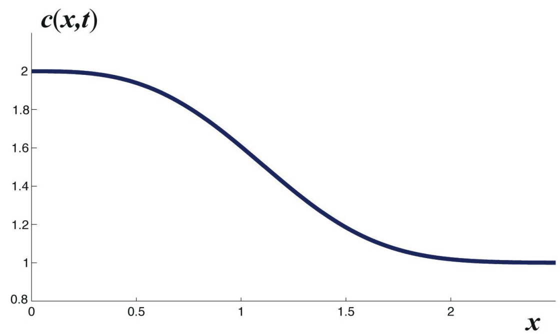
t = 50
0
398

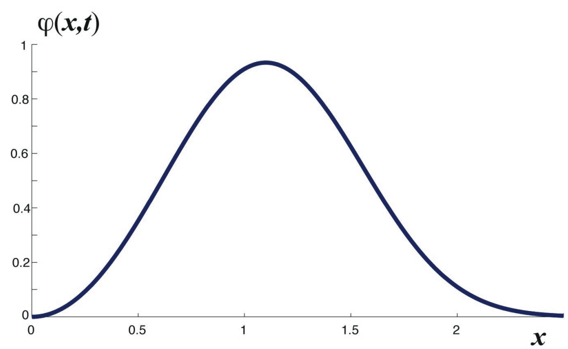


# of particles vs. horizontal location
#
location
0
1
2
3
4
5
6
7
0
50
100
150
200
250
300
350

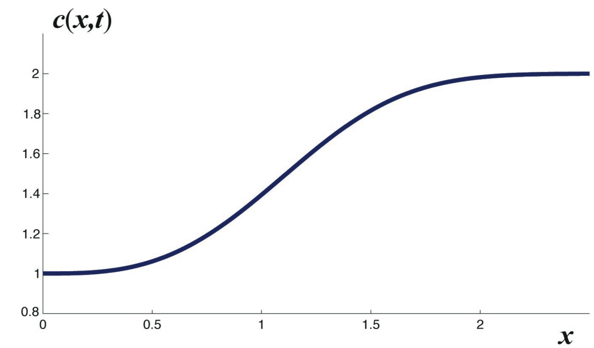
Fick's First Law (1-D)

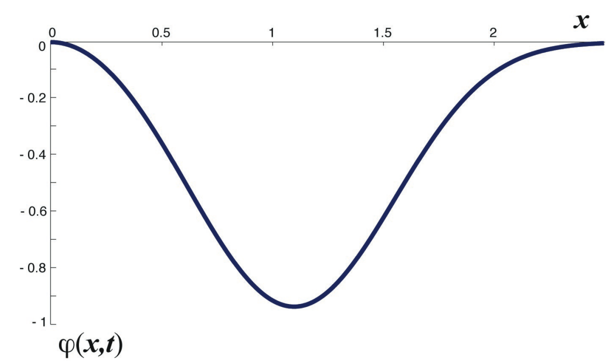
Profile 1





Profile 2





$$\phi(x,t) \propto -\frac{\partial c(x,t)}{\partial x}$$

<u>Diffusion Constant D</u>

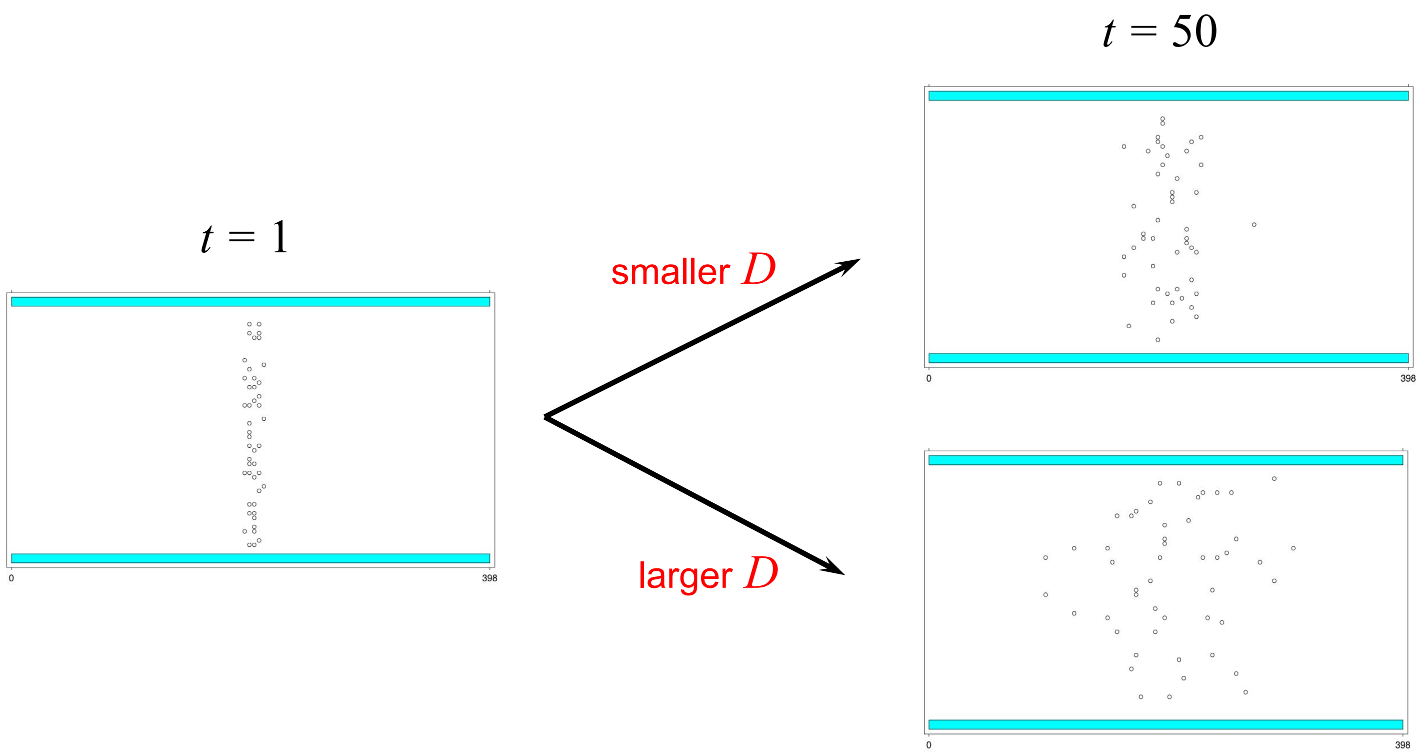
$$\phi(x,t) \propto -\frac{\partial c(x,t)}{\partial x}$$

constant of proportionality?

$$\boxed{\phi(x,t) = -D\frac{\partial c(x,t)}{\partial x}}$$

- diffusion constant is always positive (i.e., $D > 0$)
- determines time it takes solute to diffuse a given distance in a medium
- depends upon both solute and medium (solution)
- *Stokes-Einstein relation* predicts that D is inversely proportional to solute molecular radius

Diffusion Constant D



Generalizations

Higher Dimensions:

$$\phi(x,t) = -D\frac{\partial c(x,t)}{\partial x} \quad \longleftrightarrow \quad \vec{\phi} = -D\nabla c$$

$$\text{where} \quad \nabla c = \hat{x}\frac{\partial c}{\partial x} + \hat{y}\frac{\partial c}{\partial y} + \hat{z}\frac{\partial c}{\partial z} = \text{grad}(c)$$

Analogous Flux Laws:

Heat Flow (Fourier): $$\phi_h = -\sigma_h\frac{\partial T}{\partial x}$$ *heat flow, thermal conductivity, and temperature*

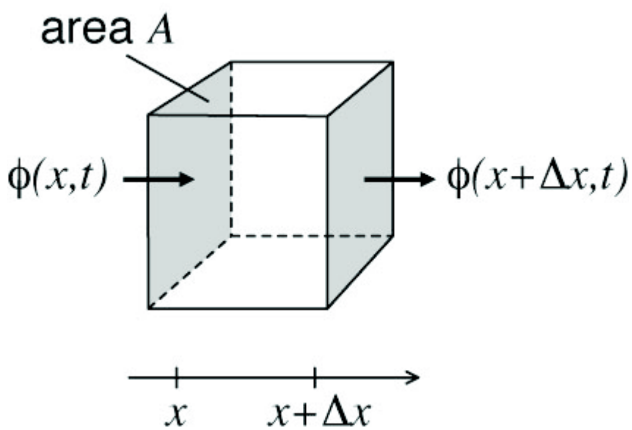
Electric Conduction (Ohm): $$J = -\sigma_e\frac{\partial \psi}{\partial x}$$ *current density, electrical conductivity, and electric potential*

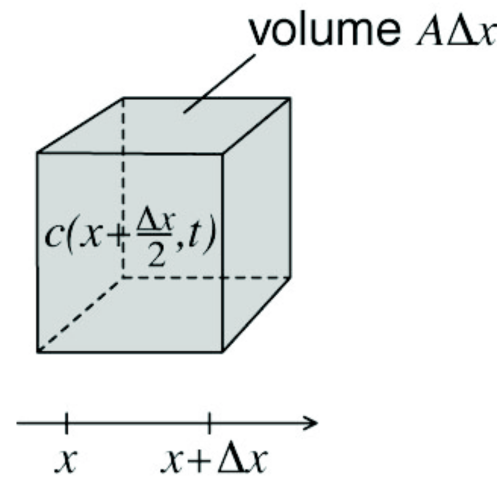
Convection (Darcy): $$\Phi_v = -\kappa\frac{\partial p}{\partial x}$$ *fluid flow, hydraulic permeability, and pressure*

Diffusion (Fick): $$\phi = -D\frac{\partial c}{\partial x}$$

Continuity Equation

$\Rightarrow$ imagine a cube (with face area A and length Δx) and a time interval Δt

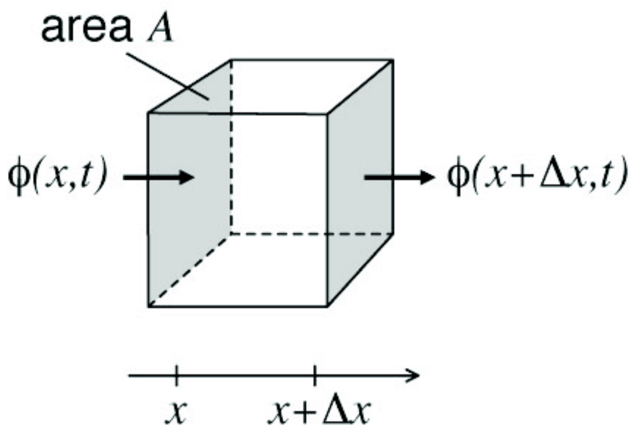


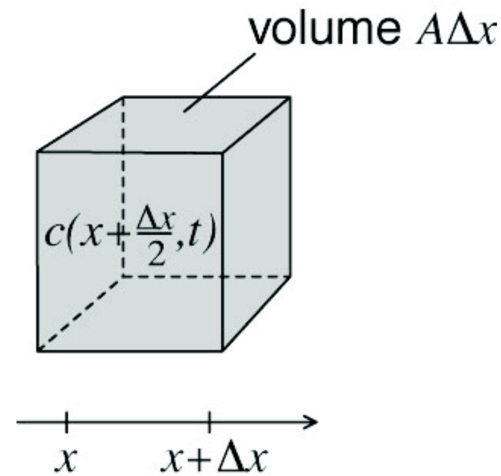


solute entering from *<u>left</u>* - solute exiting from *<u>right</u>* (during time interval [t, $t+\Delta t$]) = change in amount of solute *<u>inside</u>* cube (during time interval [t, $t+\Delta t$])

$$A\,\Delta t\,\phi(x,t) \qquad\qquad A\,\Delta x\,c(x,t)$$

Weiss





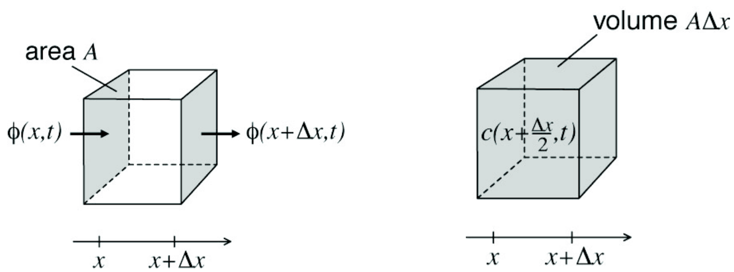
solute entering from left - solute exiting from right = change in amount of solute inside cube
(during time interval $[t, t+\Delta t]$) (during time interval $[t, t+\Delta t]$)

$$\underbrace{A\,\Delta t\,\phi(x, t+\Delta t/2)}_{\text{amount of solute entering on left side of cube}} - \underbrace{A\,\Delta t\,\phi(x+\Delta x, t+\Delta t/2)}_{\text{amount of solute leaving on right side of cube}} = \underbrace{A\,\Delta x\,c(x+\Delta x/2, t+\Delta t)}_{\text{amount of solute in cube at the end of the interval}} - \underbrace{A\,\Delta x\,c(x+\Delta x/2, t)}_{\text{amount of solute in cube at the start of the interval}}$$

$$-\frac{\phi(x+\Delta x, t+\Delta t/2) - \phi(x, t+\Delta t/2)}{\Delta x} = \frac{c(x+\Delta x/2, t+\Delta t) - c(x+\Delta x/2, t)}{\Delta t}$$

$$-\frac{\phi(x+\Delta x, t+\Delta t/2) - \phi(x, t+\Delta t/2)}{\Delta x} = \frac{c(x+\Delta x/2, t+\Delta t) - c(x+\Delta x/2, t)}{\Delta t}$$

$$\lim_{\Delta t, \Delta x \to 0} \implies \boxed{\frac{\partial \phi}{\partial x} = -\frac{\partial c}{\partial t}}$$



$\Rightarrow$ conservation of mass within the context of our imaginary cube yielded the *continuity equation*

Diffusion Equation

1. Fick's First Law:

$$\phi = -D\frac{\partial c}{\partial x}$$

+

2. Continuity Equation:

$$\frac{\partial \phi}{\partial x} = -\frac{\partial c}{\partial t}$$

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

(Fick's Second Law)

Diffusion Processes

1. Equilibrium: Zero flux and concentration is independent of time

D ≠ 0 ⇒ concentration is independent of space and time

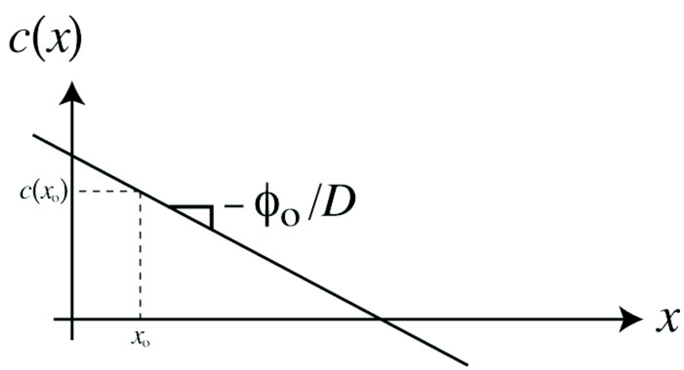
D = 0 ⇒ non-diffusible solute is automatically at equilibrium

2. Steady-state: Flux can be non-zero, but flux and concentration are independent of time

$$\frac{\partial \phi}{\partial x} = 0 \quad \Rightarrow \quad \int \phi_o \, dx = \int -D \, dc \quad \Rightarrow \quad c(x) = c(x_o) - \frac{\phi_o}{D}(x - x_o)$$

[integrate Fick's 1st Law]

[x_o is a reference location where the concentration is known]



Freeman

Diffusion Processes

3. Impulse Response: Point-source of particles (n_o mol/cm^2) at t = 0 and x = 0

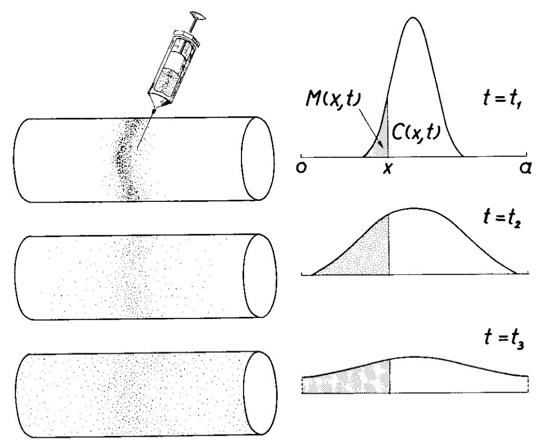
[Dirac delta function $\delta(x)$]

given the inital/boundary conditions:

$$c(x,t) = n_o \delta(x) \qquad \text{at} \quad t = 0 \qquad \text{where} \quad \int_{-\infty}^{\infty} \delta(x)\, dx = 1$$

need to solve:

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

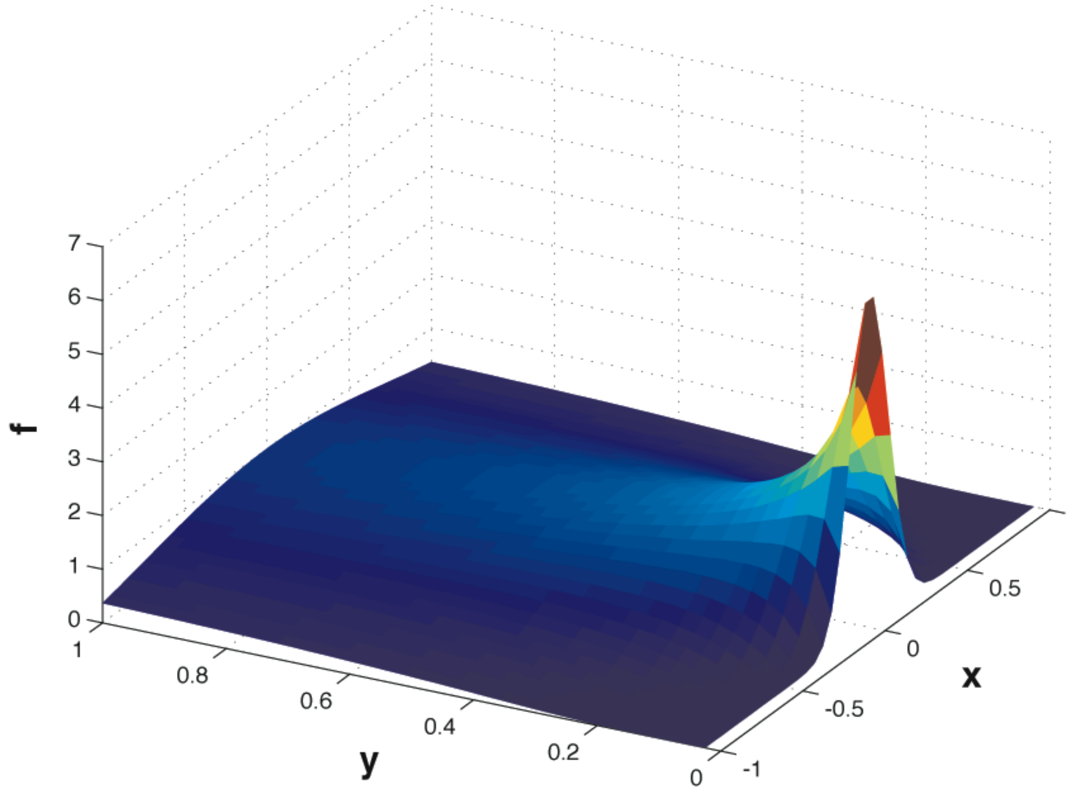


Batschelet Fig.12.5

[Aside: solution can be found by a # of different methods, one being by separation of variables and using a Fourier transform]

Solution
(for t > 0)

$$\boxed{c(x,t) = \frac{n_o}{\sqrt{4\pi D t}} e^{-x^2/4Dt}}$$



$$f(x,y) = \frac{1}{\sqrt{y}} e^{-x^2/y}$$

solution to
diffusion equation!