Physical Principles in Biology
Biology 3550
Spring 2024

# Lecture 17:

# Diffusion from a Sharp Boundary

# and

# Kinetic Energy

Friday, 16 February 2024


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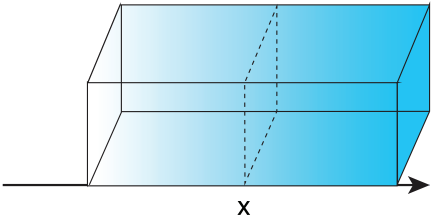
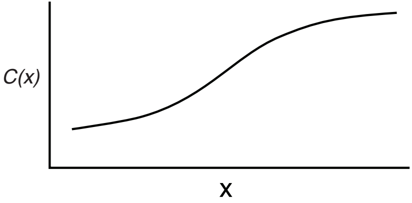
# Announcements

- Problem Set 3:
  - Due 11:59 PM, Monday, 26 February.
  - Download problems from Canvas.
  - Upload work to Gradescope.
  - Show your work!
  - Please don’t scrunch things up!
- Quiz 3:
  - Friday, 23 February
  - 25 min, second half of class.
- Review Session
  - 5:15 PM, Thursday, 22 February
  - HEB 2002
  - Come with questions!

# Fick's First and Second Laws of Diffusion




- First law:

$$J = -D\frac{dC}{dx}$$

- Flux, $J$, at position $x$ is proportional to the concentration gradient at that position.

- Second law:

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2}$$

- Rate of change in concentration at position $x$ is proportional to the derivative of the concentration gradient.

# Fick's Second Law of Diffusion

$$\frac{dC}{dt} = D\frac{d^2C}{dx^2}$$

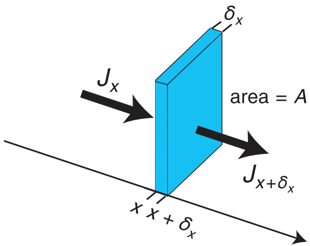
- A "second-order differential equation".
- The solution to the equation is a function:

$$C = f(x, t)$$

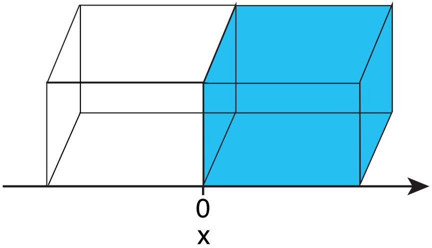
that satisfies the equation:

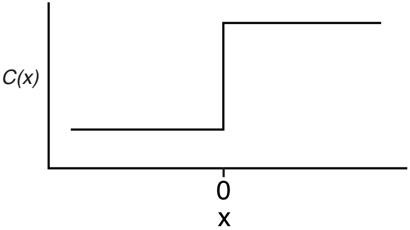
$$\frac{df(x, t)}{dt} = D\frac{d^2 f(x, t)}{dx^2}$$

- The trick is to find $C = f(x, t)$.
- The solution depends on the shape of the volume and the initial concentrations, the *boundary conditions*.



# Diffusion from a Sharp Boundary

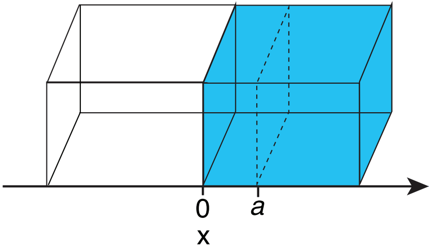


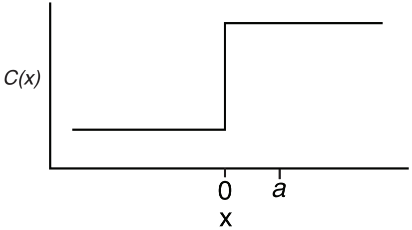




At $t = 0$

- For $x < 0$: $C(x) = 0$, $\dfrac{dC}{dx} = 0$, $\dfrac{d^2C}{dx^2} = 0$
- At $x = 0$: $\dfrac{dC}{dx} \to \infty$
- For $x > 0$: $C(x) = 1$, $\dfrac{dC}{dx} = 0$, $\dfrac{d^2C}{dx^2} = 0$

# Diffusion from a Sharp Boundary



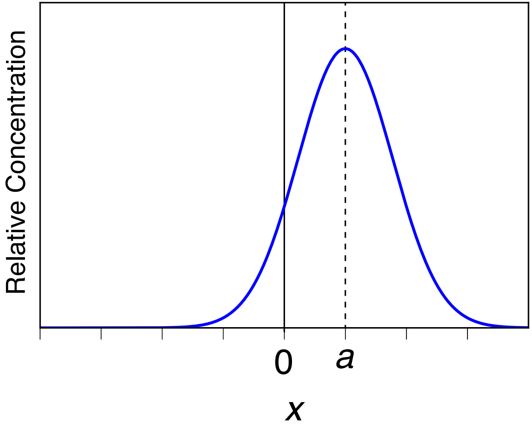




Consider molecules at a position $x = a > 0$:

- Molecules will begin to diffuse via a random walk.
- How will the molecules initially at position $a$ be distributed after a time, $t$?

# Diffusion from a Sharp Boundary

Distribution of molecules originally at position $x = a$



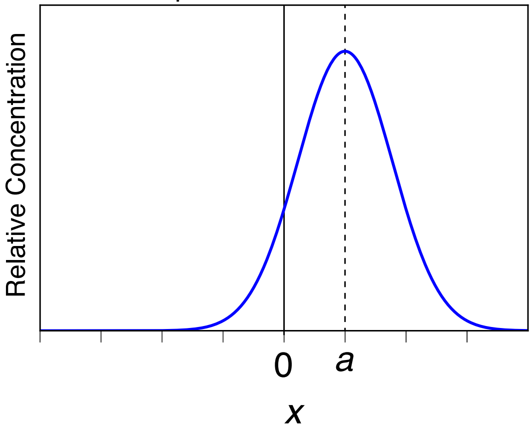

$$p(x) = \frac{1}{\sqrt{2\pi n\langle\delta_x^2\rangle}} e^{-(x-a)^2/(2n\langle\delta_x^2\rangle)}$$

$n$ = number of steps in random walk

$\langle\delta_x^2\rangle$ = mean-square step distance along $x$-axis

# Diffusion from a Sharp Boundary

Distribution of molecules originally at position $x = a$




$$p(x) = \frac{1}{\sqrt{2\pi n\langle\delta_x^2\rangle}} e^{-(x-a)^2/(2n\langle\delta_x^2\rangle)}$$

- Diffusion coefficient, $D = \frac{\delta_x^2}{2\tau}$

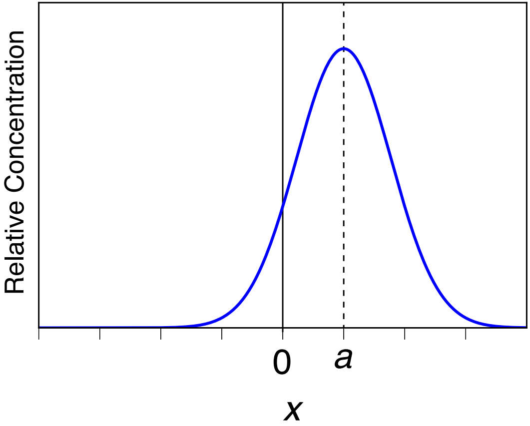
  $\tau$ = average time of each RW step

  After time, $t$, $n = t/\tau$

$$n\langle\delta_x^2\rangle = \frac{t\langle\delta_x^2\rangle}{\tau} = 2Dt$$

# Diffusion from a Sharp Boundary

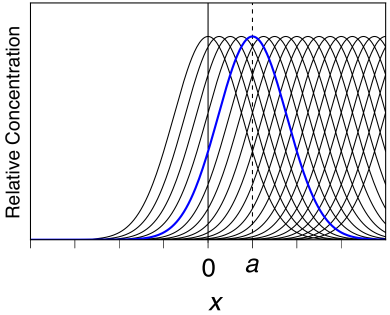
Distribution of molecules originally at position $x = a$




$$p(x) = \frac{1}{\sqrt{4\pi D t}} e^{-(x-a)^2/(4Dt)}$$

# Diffusion from a Sharp Boundary

- Distribution of molecules from all starting points, $a \geq 0$.




- At position $x$, concentration is the sum of molecules that have diffused from $a \geq 0$

$$C(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_0^{\infty} e^{-(x-a)^2/(4Dt)} da$$

# Does the "Solution" Satisfy Fick's Second Law?

- Putative solution:

$$C(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_0^{\infty} e^{-(x-a)^2/(4Dt)} da$$

- Fick's second law:

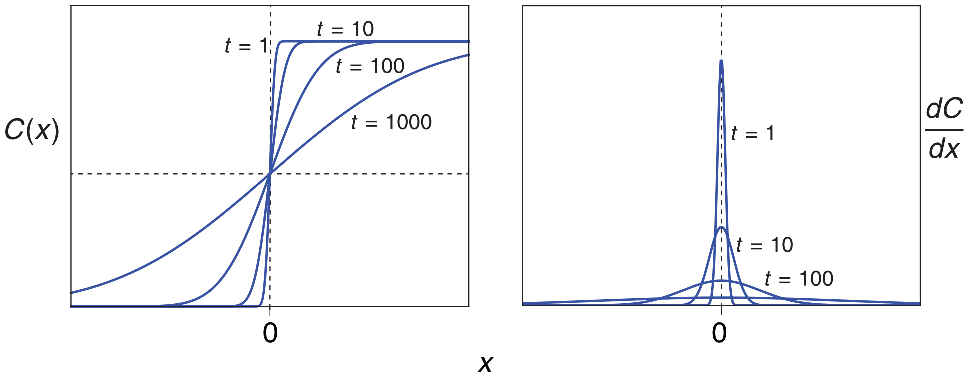
$$\frac{dC}{dt} = D\frac{d^2C}{dx^2}$$

- Need to evaluate $\frac{dC}{dt}$ and $\frac{d^2C}{dx^2}$ and see if they satisfy the equation.

  They do!

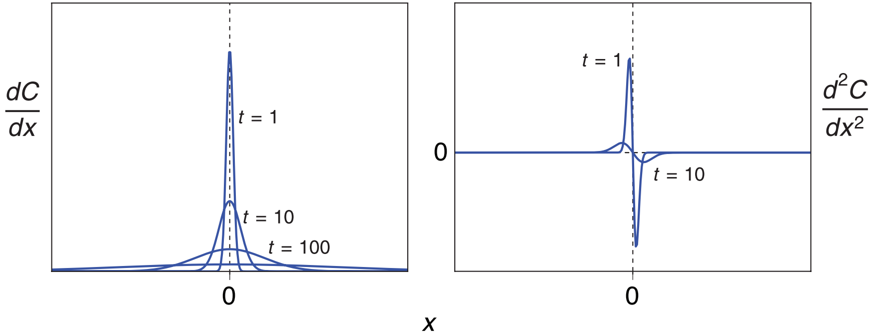
- $C(x,t)$ can't be evaluated analytically, but it can be numerically.

# Diffusion from a Sharp Boundary




- $C(x, t)$ is the integral of a Gaussian function with respect to $x$.
- The derivative of $C(x, t)$ with respect to $x$ is a Gaussian function!

# Diffusion from a Sharp Boundary




- Concentration increases most rapidly where the second derivative is most postitive.
- Concentration decreases most rapidly where the second derivative is most negative.
- Concentration does not change at $x = 0$, where the flux, $J$, is greatest!

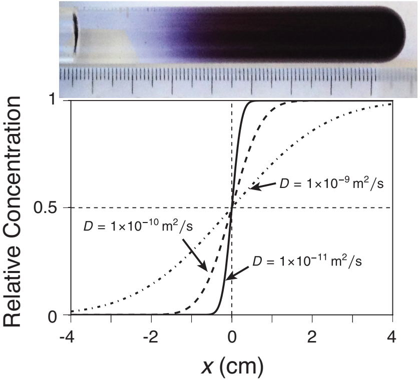
# Estimating $D$ from Diffusion from a Sharp Boundary

$$C(x,t) = \int_0^\infty \frac{1}{\sqrt{4\pi D t}} e^{-(x-a)^2/(4Dt)} da$$

$$t = 48\,\text{hr} = 1.7 \times 10^5\,\text{s}$$

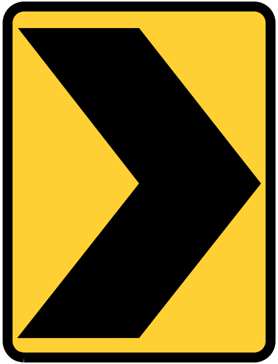
$$D \approx 2 \times 10^{-10}\,\text{m}^2/\text{s}$$

$$D = \frac{\delta_x^2}{2\tau}$$




- What are the average length ($\delta_x$) and duration ($\tau$) of the random walk steps?
- We could answer these questions if we knew the velocity of the molecules, $\delta_x/\tau$.

# Warning!



# Direction Change

Molecular Motion and Kinetic Energy

# Molecular Motion and Kinetic Energy

- What is energy?

  Capacity to do work.

- What is work?

  Mechanical work: The application of force over distance:

$$w = \int_a^b F\,dx$$

- The units of work and energy.
  - Force: Units defined by Newton's second law: $F = \text{mass} \times \text{acceleration}$

    SI unit of mass: Kg

    Acceleration: change in velocity (m/s) with time. SI units: $\text{m}/\text{s}^2$

    SI units of Force: $\text{Kg} \cdot \text{m}/\text{s}^2$ $\qquad 1\,\text{N} = 1\,\text{Kg} \cdot \text{m}/\text{s}^2$
  - Work or energy: $\text{Kg} \cdot \text{m}^2/\text{s}^2$ $\qquad 1\,\text{J} = 1\,\text{N} \cdot \text{m} = 1\,\text{Kg} \cdot \text{m}^2/\text{s}^2$

# Kinetic Energy

- A object of mass, $m$, moving with velocity, $v$, in the $x$-direction has kinetic energy in that direction of:

$$E_{k,x} = mv_x^2/2$$

Check the units: $\mathrm{Kg} \times (\mathrm{m/s})^2 = \mathrm{Kg} \cdot \mathrm{m}^2/\mathrm{s}^2$ It's OK!

- What does this mean?
  - The energy required to accelerate the mass, $m$, from rest to velocity, $v_x$.
  - Also the energy released during the deceleration of the mass from velocity, $v_x$, to rest.
  - Kinetic energy does not depend on the rate of acceleration or deceleration, only the final velocity.
  - But, amount of <u>wasted</u> energy likely does depend on rate of acceleration!
  - $E_{k,x}$ is proportional to $v_x^2$. What are the implications?

# Clicker Question #1

What is the kinetic energy of a baseball ($m = 145\,\mathrm{g}$) with a velocity of 40 m/s ($\approx 90\,\mathrm{miles/h}$)?

**A)** $3\,\mathrm{J}$

**B)** $50\,\mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s}^2$

**C)** $100\,\mathrm{Nm}$

**D)** $200\,\mathrm{J}$

**E)** $200\,\mathrm{N}$

$$E_\mathrm{k} = \frac{1}{2}mv^2 = \frac{1}{2}0.145\,\mathrm{Kg}(40\,\mathrm{m/s})^2 = 120\,\mathrm{Kg}\cdot\mathrm{m}^2\mathrm{s}^{-2} = 120\,\mathrm{Nm} = 120\,\mathrm{J}$$