Let $c(x,t)$ = concentration of a chemical in a region $(x, x+dx)$ at time t.
In 3 dimensions: $[c(x,t)] = ML^{-3}$.
In 1 dimension: $[c(x,t)] = ML^{-1}$.
Key: $c(x,t)$ is measurable

$$\int_a^b c(x,t)dx = \text{ total concentration of chemical in } (a,b) \text{ at time } t$$

Check the units

$$\left[\int_a^b c(x,t)dx\right] = ML^{-1} \times L = M$$

How does a chemical move? flux $J(x,t)$ – amount of substance that passes through x in the positive direction per unit time.
The rate of change of the amount is

$$\frac{d}{dt}\int_a^b c(x,t)dx = J(a,t) - J(b,t)$$

or

$$\int_a^b \left(\frac{\partial c}{\partial t} + \frac{\partial J}{\partial x}\right) dx = 0$$

This is the **Conservation of Mass!**

$$\frac{\partial c}{\partial t} + \frac{\partial J}{\partial x} = 0$$

What is the flux J?
How is it related to $c(x,t)$?

Chemical Diffusion

Fick's Law – chemical moves from regions of higher concentration to lower concentration.

$$J \propto -\frac{\partial c}{\partial x}$$

or

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

where D is the diffusion constant.
Substitute $J = -D\frac{\partial c}{\partial d}$ in

$$\frac{\partial c}{\partial t} + \frac{\partial J}{\partial x} = 0$$

$$\frac{\partial c}{\partial t} - D\frac{\partial^2 c}{\partial x^2} = 0 \tag{1}$$

Diffusion equation is a partial differential equation (PDE)
We need auxiliary equation conditions

- What was the concentration initially (at the start, $t = 0$)
- What happens at the endpoints a and b.

0.1.1 Aside

Diffusion equations arise in many other settings

Heat transfer

Heat energy is measured by temperature $[\theta]$
Let $u(x,t)$ = temperature in the bat at x and time t.
Same derivation as before:

$$\frac{\partial u}{\partial t} = -\frac{\partial J}{\partial x}$$

Now: $J(x,t)$ = heat flux
Fourier Law of Heat Conduction:

$$\begin{aligned} J &= -D\frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial t} &= D\frac{\partial^2 u}{\partial x^2} \end{aligned} \tag{2}$$

Probability

Let

Biomedical Application

Drug patch concentration = u_0 (fixed)
$u(x,t)$ = concentration at position x (depth) and time t

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \quad 0 < x < \infty, \quad t > 0$$

Initial condition: $u(x,0) = 0$.
Boundary condition: $u(0,t) = u_0$, $u \to 0, x \to \infty$

Dimensional Analysis

What is $[D]$?

$$\begin{aligned} \left[\frac{\partial u}{\partial t}\right] &= \left[D\frac{\partial^2 u}{\partial x^2}\right] \\ \left[\frac{\partial u}{\partial t}\right] &= [D]\left[\frac{\partial^2 u}{\partial x^2}\right] \\ ML^{-1}T^{-1} &= [D]ML^{-3} \\ L^2T^{-1} &= [D] \end{aligned}$$

0.2.1 Alternate Approach

1. Dimensional reduction to understand the form of the solution
2. Get non-dimensional problem
3. Use dimensionless variables to convert PDE $\rightarrow$ ODE

$$\begin{aligned}
u &= f(x,t,D,u_0)\\
[u] &= [x]^a[t]^b[D]^c[u_0]^d\\
ML^{-1} &= L^aT^b\left(L^2T^{-1}\right)^c\left(ML^{-1}\right)^d\\
M^1L^{-1}T^0 &= L^aT^bL^{2c}T^{-c}M^dL^{-d}\\
M^1L^{-1}T^0 &= L^{a+2c-d}T^{b-c}M^d
\end{aligned}$$

$$\begin{bmatrix} 1 & 0 & 2 & -1\\ 0 & 1 & -1 & 0\\ 0 & 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} a\\ b\\ c\\ d \end{bmatrix} = \begin{bmatrix} -1\\ 0\\ 1 \end{bmatrix}$$

$$\begin{aligned}
a+2c-d=-1 \qquad & b-c=0 \qquad & d=1\\
a=-2c \qquad & b=c \qquad & d=1
\end{aligned}$$

$$\begin{aligned}
\begin{bmatrix} a\\ b\\ c\\ d \end{bmatrix} &= \begin{bmatrix} -2c\\ c\\ c\\ 1 \end{bmatrix}\\
&= \begin{bmatrix} 0\\ 0\\ 0\\ 1 \end{bmatrix} + c\begin{bmatrix} -2\\ 1\\ 1\\ 0 \end{bmatrix}\\
&= u_0^1 + \left(t^1D^1x^{-2}\right)^c\\
&= u_0 + \left(\frac{tD}{x^2}\right)^c\\
u(x,t) &= u_0F\left(\frac{tD}{x^2}\right)
\end{aligned}$$

Boundary condition makes us multiple the vector within the nullspace by $-\frac{1}{2}$.

$$-\frac{1}{2}\begin{bmatrix} -2\\ 1\\ 1\\ 0 \end{bmatrix} = \begin{bmatrix} 1\\ -\frac{1}{2}\\ -\frac{1}{2}\\ 0 \end{bmatrix}$$

$$
\begin{aligned}
\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} &= \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} + c \begin{bmatrix} 1 \\ -\frac{1}{2} \\ -\frac{1}{2} \\ 0 \end{bmatrix} \\
&= u_0^1 + \left(t^{-\frac{1}{2}} D^{-\frac{1}{2}} x^1 \right)^c \\
&= u_0 + \left(\frac{x}{\sqrt{tD}} \right)^c \\
u(x,t) &= u_0 F \left(\frac{x}{\sqrt{tD}} \right) \\
\frac{u(x,t)}{u_0} &= F \left(\frac{x}{\sqrt{tD}} \right)
\end{aligned}
$$

We can make the similarity variable $\eta = \frac{x}{\sqrt{tD}}$. $[\eta] = 1$

$$u(x,t) = v(\eta)$$

$$N(x) = \text{ cumulative normal distribution } = \int \tag{3}$$