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

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

This is the **Conservation of Mass!**

$$\frac{\partial c}{\partial t} + \frac{\partial J}{\partial x} = 0 \tag{1}$$

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 $J = -D\frac{\partial c}{\partial d}$ into (1)

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

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

$$\left.\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}, \qquad \begin{matrix} a < x < b \\ t > 0 \end{matrix}\right\}$$

- 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 bar at x and time t.
Same derivation as before:

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

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

$$\begin{aligned} J &= -D\frac{\partial u}{\partial x} \\ \frac{\partial u}{\partial t} &= D\frac{\partial^2 u}{\partial x^2} \end{aligned} \tag{3}$$

where D = thermal diffusion constant

Probability

Let $p(x,t)$ = probability density function of a stochastic process $X(t)$

$$Pr\left[a \le X(t) < b\right] = \int_a^b p(x,t)dx \tag{4}$$

Example: Random wale (discrete) $\rightarrow$ Brownian motion (continuous)
Brownian motion's pdf:

$$\frac{\partial p}{\partial t} = \frac{1}{2}\frac{\partial^2 p}{\partial x^2}, \quad -\infty < x < \infty, t > 0 \tag{5}$$

where the initial condition $(X(0) = 0) \Rightarrow p(x,0) = \delta$ (The dirac delta function)

$$\delta(x) = \begin{cases} 0 & x \neq 0 \\ \infty & x = 0 \end{cases}$$

such that

$$\int_{-\infty}^{\infty} \delta(x)dx = 1$$

Biomedical Application

Drug patch concentration $= u_0$ (fixed)
$u(x,t)$ = concentration at position x (depth) and time t ($x = 0$ is the surface of the skin)

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

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

Dimensional Analysis

What is $[D]$?

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

Exact solution of u is hard!
Try Laplace transforms

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

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

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

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

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

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

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

is a huge reduction.
Introduce a non-dimensional variable into u.

$$v(x,t) = \frac{u(x,t)}{u_0},$$

$[v] = 1, 0 \leq v < 1$
We can make the similarity variable $\eta = \frac{x}{\sqrt{tD}}$. $[\eta] = 1$

$$u(x,t) = v(\eta)$$
$$u_t = Du_{xx} \Rightarrow v_t = Dv_{xx}$$

The chain rule from Multivariate calculus says that $v(x,t) = v(\eta(x,t))$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial t} = -\frac{1}{2}\frac{x}{\sqrt{D}}\frac{1}{t^{3/2}}\frac{\partial}{\partial \eta}$$
$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \eta}\frac{\partial \eta}{\partial x} = \frac{1}{\sqrt{tD}}\frac{\partial}{\partial n}$$
$$\frac{\partial^2}{\partial x^2} = \frac{1}{Dt}\frac{\partial^2}{\partial \eta^2} \leftarrow \text{ be able to derive!!}$$

Plug into $u_t = Du_{xx}$

$$-\frac{1}{2}\frac{x}{\sqrt{D}}\frac{1}{t^{3/2}}v' = D\frac{1}{Dt}v''$$
$$-\frac{1}{2}\frac{x}{\sqrt{D}}\frac{1}{t^{3/2}}v' = \frac{1}{t}v''$$
$$-\frac{1}{2}\frac{x}{\sqrt{D}}\frac{1}{t^{1/2}}v' = v''$$
$$-\frac{1}{2}\frac{x}{\sqrt{D}t^{1/2}}v' = v''$$
$$-\frac{1}{2}\frac{x}{\sqrt{Dt}}v' = v''$$
$$-\frac{1}{2}\eta v' = v''$$
$$v'' + \frac{1}{2}\eta v' = 0$$

Initial conditional(s) and boundary conditions must be consistent Boundary conditions:

$$\frac{u(0,t)}{u_0} = \frac{u_0}{u_0} \Rightarrow v(0) = 1$$

$$x = 0 \Rightarrow \eta = \frac{x}{Dt} = 0$$
$$u \to 0 \text{ as } x \to \infty \Rightarrow v \to 0 \text{ if } \eta \to \infty$$

Initial condition:

$$u(x,0) = 0$$
$$t = 0 \Rightarrow \eta \to \infty \Rightarrow v(\infty) = 0$$

Boundary Value ODE Problem

$$v'' + \frac{1}{2}\eta v' = 0, \quad 0 < \eta < \infty$$
$$v(0) = 1, \quad v(\infty) = 0$$

2nd order, linear, not constant coefficient homogeneous.

Let $g = v'$

$$\begin{aligned}
g' + \frac{1}{2}\eta g &= 0 \\
I &= e^{\int \frac{1}{2}\eta d\eta} \\
&= e^{\frac{\eta^2}{4}} \\
e^{\frac{\eta^2}{4}} g' + \frac{1}{2}\eta e^{\frac{\eta^2}{4}} g &= 0 \\
\left(e^{\frac{\eta^2}{4}} g\right)' &= 0 \\
e^{\frac{\eta^2}{4}} g &= C \\
g &= Ce^{-\frac{\eta^2}{4}} \\
&= c_2 e^{-\frac{\eta^2}{4}}
\end{aligned}$$

$$\begin{aligned}
v &= \int g d\eta \\
&= c_1 + c_2 \int_0^\eta e^{-\frac{\zeta^2}{2}} d\zeta \\
v(0) = 1 &\Rightarrow c_1 = 1 \\
v &= 1 + c_2 \int_0^\eta e^{-\frac{\zeta^2}{2}} d\zeta \\
v(\infty) &= 0 \\
0 &= 1 + c_2 \int_0^\infty e^{-\frac{\zeta^4}{2}} d\zeta \\
0 &= 1 + c_2[\sqrt{\pi}] \\
-1 &= c_2\sqrt{\pi} \\
-\frac{1}{\sqrt{\pi}} &= c_2 \\
v(\eta) &= 1 - \frac{1}{\sqrt{\pi}} \int_0^\eta e^{\frac{-s^2}{4}} ds
\end{aligned}$$

Change this back to the original variable: $\eta = \frac{x}{\sqrt{DT}}, v = \frac{u}{u_0}$

$$\begin{aligned}
\frac{u(\eta)}{u_0} &= 1 - \frac{1}{\sqrt{\pi}} \int_0^\eta e^{\frac{-s^2}{4}} ds \\
\frac{u(x,t)}{u_0} &= 1 - \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{Dt}} e^{\frac{-s^2}{4}} ds \\
u(x,t) &= u_0 \left[1 - \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{Dt}} e^{\frac{-s^2}{4}} ds\right] \\
&= u_0 \left[1 - \operatorname{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right]
\end{aligned}$$

where erf is the error function

$$\mathrm{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-s^2} ds \tag{6}$$

$$\begin{aligned} \mathrm{erfc} &= 1 - \mathrm{erf} \\ u(x,t) &= u_0 \left[1 - \mathrm{erf}\left(\frac{x}{2\sqrt{Dt}}\right)\right] \\ &= u_0 \mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right) \end{aligned}$$

Method of Similarity Variables

0.2.2 Aside 2 (Amother way of writing erfc)

$$N(x) = \text{ cumulative normal distribution } = \int_{-\infty}^{x} \frac{e^{-\frac{s^2}{2}} ds}{\sqrt{2\pi}} \tag{7}$$

$N(-\infty) = 0, N(\infty) = 1$

$$N(x) = \frac{1 + \mathrm{erf}\left(\frac{x}{\sqrt{2}}\right)}{2}$$