# Diffusion PDE

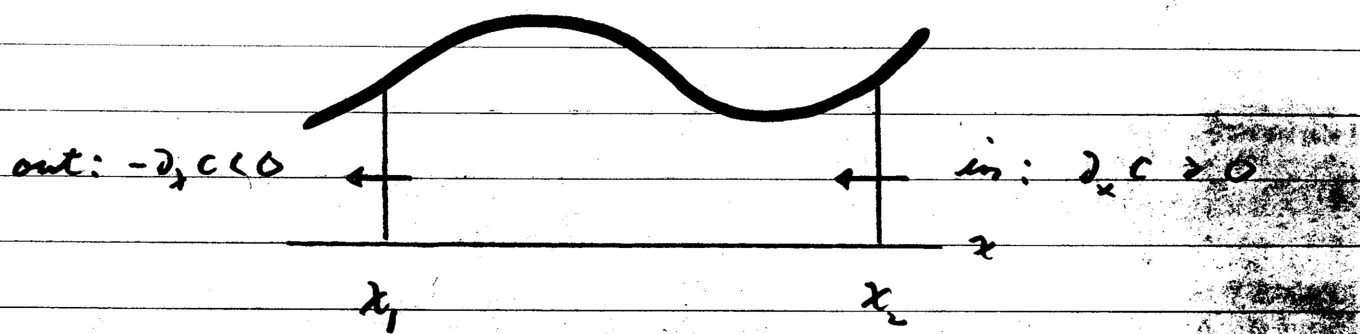
$c(x,t)$ = concentration of 'stuff'.

$\int_{x_1}^{x_2} c(x,t)\,dx$ = total amount of 'stuff' in $x_1 < x < x_2$

**Fick's' law**

$$\frac{d}{dt}\int_{x_1}^{x_2} c(x,t)\,dx = \underbrace{D(\partial_x c)(x_2,t)}_{\text{entering}} - \underbrace{D(\partial_x c)(x_1,t)}_{\text{leaving } x_1<x<x_2} \quad (1$$

rate of stuff entering leaving $x_1 < x < x_2$




$$(1) \iff \int_{x_1}^{x_2} \{ (\partial_t c)(x,t) - D(\partial_{xx} c)(x,t) \}\,dx = 0,$$

all $x_1, x_2 \Rightarrow$ $\boxed{\partial_t c = D\,\partial_{xx} c}$ Diffusion PDE (2

Units of <u>diffusion coef</u> $D$ $\quad \frac{1}{T} = [D]\frac{1}{L^2} \Rightarrow$

$[D] = \frac{L^2}{T}$. $\qquad [\;] \iff$ "units of" ie Diffusion of $Na^+$ ions in salt water

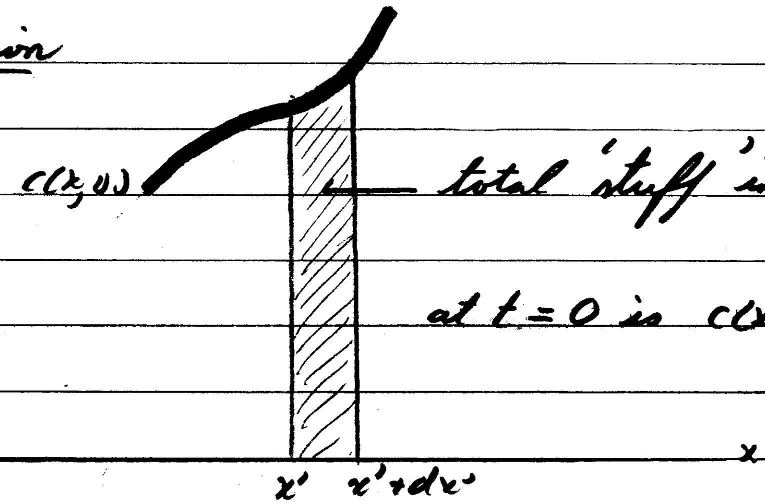
$D \simeq 10^{-5}\ cm^2/s$.

<u>Initial value problem</u> $c(x, 0)$ given for all $x$

Soltn of diffusion PDE for all $x$, all $t > 0$ is

$$c(x,t) = \frac{1}{2\sqrt{\pi D t}} \int_{-\infty}^{\infty} c(x', 0)\, e^{-\frac{(x-x')^2}{4Dt}}\, dx' \qquad (3)$$

<u>Interpretation</u>

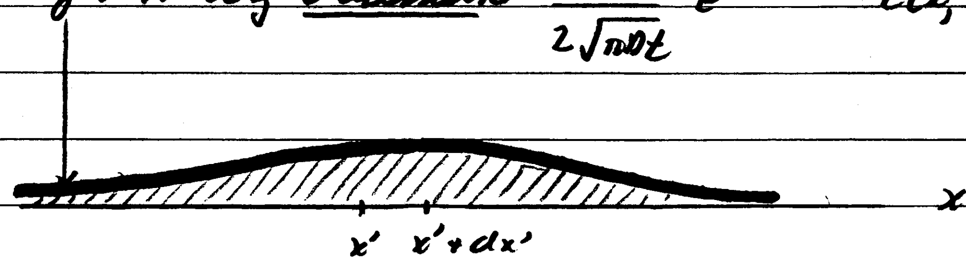



total 'stuff' in $x' < x < x'+dx'$

at $t = 0$ is $c(x', 0)\, dx'$.

density of <u>that</u> stuff at time $t > 0$

given by <u>Gaussian</u> $\frac{1}{2\sqrt{\pi D t}}\, e^{-\frac{(x-x')^2}{4Dt}}\, c(x', 0)\, dx'$




(3) comes from adding up Gaussians from all the $dx'$'s

Complex 'wave' solutions $c(x,t) = e^{\sigma t + i \underset{\substack{\uparrow \\ \text{real}}}{k} x}$ (4)

Get <u>real</u> wave solutions from LC of real and imaginary parts. Subst (4) into diffusion PDE (2):

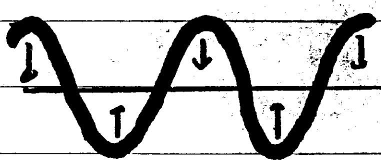
$$c_t = \sigma e^{\sigma t + ikx} = \sigma c$$

$$c_{xx} = (ik)^2 e^{\sigma t + ikx} = -k^2 c$$

$$0 = c_t - D c_{xx} = (\sigma + Dk^2)c = 0 \Rightarrow$$

$\boxed{\sigma = -Dk^2}$ 'Dispersion relation' (5)

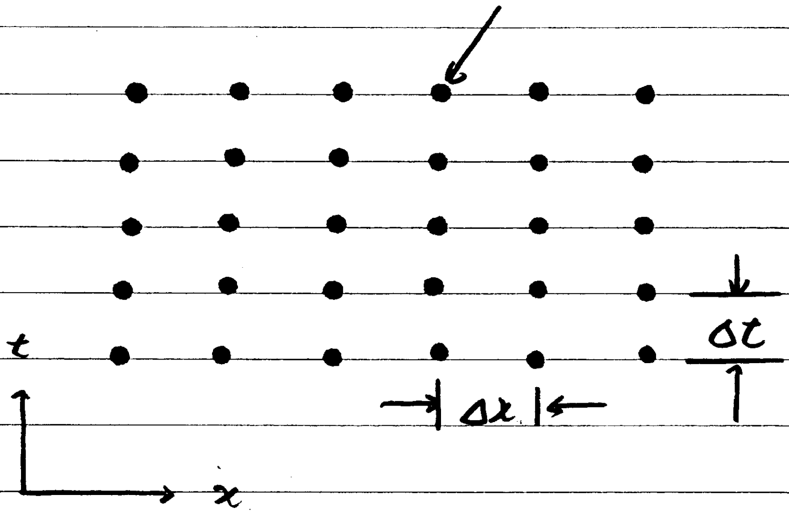
Hence, $c(x,t) = e^{-Dk^2 t + ikx}$ and a real solution $c(x,t) = e^{-Dk^2 t}\cos kx$



exponential decay in time. Shorter the wave, faster the decay.

## Numerical approximations

'Forward Euler' $\qquad (x,t) = (m\Delta x, n\Delta t)$




spacetime mesh

$\gamma_{m,n} \equiv$ numerical approximation to

$c(x,t)$ at $(x,t) = (m\Delta x, n\Delta t)$.

Recall:

$$(\partial_{xx}c)(x,t) = \frac{c(x+\Delta x,t) - 2c(x,t) + c(x-\Delta x,t)}{(\Delta x)^2} + O((\Delta x)^2) =$$

$$\frac{\gamma_{m+1,n} - 2\gamma_{m,n} + \gamma_{m-1,n}}{(\Delta x)^2} + O((\Delta x)^2)$$

$$(\partial_t c)(x,t) = \frac{c(x,t+\Delta t) - c(x,t)}{\Delta t} + O(\Delta t) =$$

$$\frac{\gamma_{m,n+1} - \gamma_{m,n}}{\Delta t} + O(\Delta t)$$

Hence <u>mesh approximation</u> 'of diffusion PDE

$$\boxed{\gamma_{m,n+1} - \gamma_{m,n} = \frac{D\Delta t}{(\Delta x)^2}\left(\gamma_{m+1,n} - 2\gamma_{m,n} + \gamma_{m-1,n}\right)} \qquad (6)$$

<u>'Wave solutions'</u> of mesh equations

$$\gamma_{m,n} = e^{\sigma(m\Delta t) + jk(n\Delta x)}$$

LHS of (6) =

$$\gamma_{m+1,n} - \gamma_{m,n} = \left(e^{\sigma\Delta t} - 1\right) e^{\sigma\Delta t + jk(n\Delta x)} =$$

$$\left(e^{\sigma\Delta t} - 1\right)\gamma_{m,n}.$$

RHS of (6) =

$$\frac{D\Delta t}{(\Delta x)^2}\left(e^{jk\Delta x} - 2 + e^{-jk\Delta x}\right)\gamma_{m,n} =$$

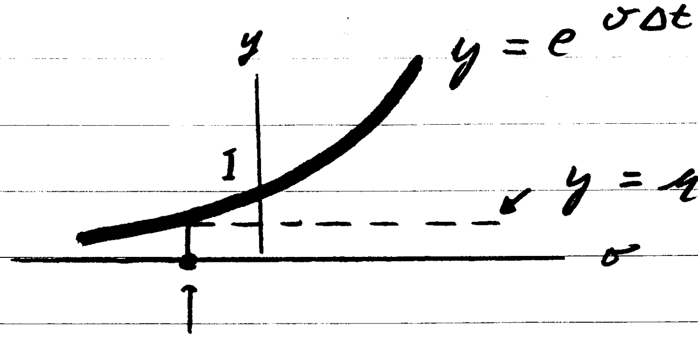
$$2\frac{D\Delta t}{(\Delta x)^2}\left(\cos k\Delta x - 1\right)\gamma_{m,n} = -4\frac{D\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right)\gamma_{m,n}$$

Hence, $\boxed{e^{\sigma\Delta t} - 1 = -\frac{4D\Delta t}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right)}$ <u>'Discrete'</u> dispersion relation

<u>Formal</u> limit $\Delta t, \Delta x \to 0$, <u>$k$ fixed</u>

$$LHS = \sigma\Delta t + O((\Delta t)^2)$$

Suppose $0 < \dfrac{D\Delta t}{(\Delta x)^2} < \dfrac{1}{4} \iff 0 < \mu < 1$




negative real $\sigma$. Mesh oscillation

<u>decays</u>.

<u>But</u> $\dfrac{D\Delta t}{(\Delta x)^2} > \dfrac{1}{4} \Rightarrow \mu < 0$. No real

solution of $e^{\sigma \Delta t} = \mu$ for $\sigma$. <u>Complex $\sigma$?</u>

$s \equiv \sigma \Delta t = S + iW$. Then (7) reads (for $\mu < 0$)

$$e^{S+iW} = e^{S}(\cos W + i \sin W) = -|\mu| \iff$$

$$\underbrace{e^{S}\cos W = -|\mu|}, \quad \underbrace{e^{S}\sin W = 0}$$

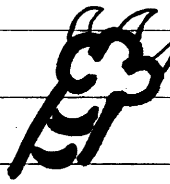
$$\Rightarrow W = N\pi \Rightarrow$$

$$e^{S}(-1)^N = -|\mu| \longleftarrow \cos W = (-1)^N.$$

$$RHS = -\frac{4D\Delta t}{(\Delta x)^2}\left\{\left(\frac{k\Delta x}{2}\right)^2 + O((\Delta x)^4)\right\} =$$

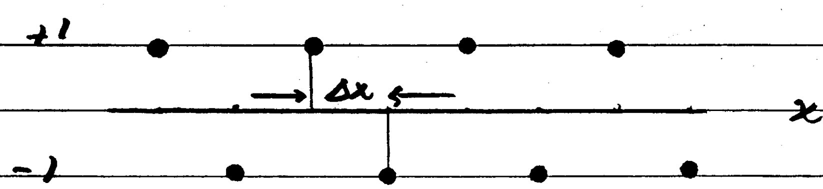
$$-Dk^2\Delta t + O(\Delta x(\Delta x)^2)$$

so get limit $\sigma = -Dk^2$, same as 'exact' dispersion relation (3). How nice.



But numerical roundoff errors, or 'noise' in IC can produce 'waves' with large $k$.

For instance take $k = \frac{\pi}{\Delta x}$ and $e^{jkx} = e^{j\left(\frac{\pi}{\Delta x}\right)(n\Delta x)} =$ $e^{j\pi n} = (-1)^n$. The 'wave' is much oscillations




For $k = \frac{\pi}{\Delta x}$, discrete dispersion relation gives

$$\boxed{e^{\sigma\Delta t} = q = 1 - 4\frac{D\Delta t}{(\Delta x)^2}} \qquad (7)$$

Take $\nu = 1 \Rightarrow e^{\delta} = 1 + q$. Solve to get a real $\delta$, and hence $\sigma = \frac{\delta}{\Delta t}$. Our 'wave' looks like

$$\gamma_{mn} = e^{m(\sigma \Delta t) + ik(n\Delta x)} =$$

$$e^{m(\delta + \underbrace{i\pi}_{W = \pi}) + i\left(\frac{\pi}{\Delta x}\right)(n\Delta x)} =$$

$$e^{m\delta + i\pi(m+n)} = e^{m\delta}\underbrace{(-1)^{m+n}}.$$

oscillates in time (m) as well as space

What about $e^{m\delta}$?

$-1 < q < 0 \Rightarrow \delta < 0$ <u>decay</u>

$q < -2 \Longleftrightarrow \frac{D\Delta t}{(\Delta x)^2} > \frac{1}{2}$ <u>growth</u>

So if $\frac{D\Delta t}{(\Delta x)^2} > \frac{1}{2}$, spatial mesh oscillation grows exponentially in time, contrary to <u>any</u> exact wave solution of diffusion PDE.