MATE664 L08

Jan - 28 - 2026

Recap: discussion about solving diffusion eqn

	I. C.		Solution
①	Step function	$\longrightarrow$	error function
	Dirac δ-function	$\longrightarrow$	Gaussian

super impose
reflection $\Big\}$ $\longrightarrow$ general solutions

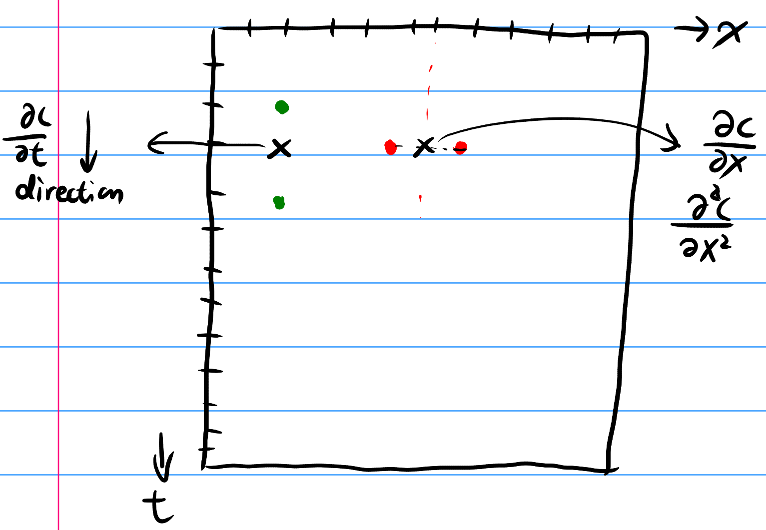
② separation of variables $\Rightarrow$ solution $C(x,t) = X(x)\,T(t)$

$\begin{cases} \text{Fourier series in space} \\ \text{Exp decay in time} \end{cases}$

Numerical solutions to diffusion equation

What do we need in the equation?

$$\begin{cases} \dfrac{\partial c}{\partial t} \\[2ex] \dfrac{\partial c}{\partial x} \\[2ex] \dfrac{\partial^2 c}{\partial x^2} \end{cases} \quad \xrightarrow{\text{Discretize on grid } \Delta t,\ \Delta x} \quad \begin{matrix} \dfrac{C(x, t_{i+1}) - C(x, t_{i-1})}{2\Delta t} \\[2ex] \dfrac{C(x_{i+1}, t) - C(x_{i-1}, t)}{2\Delta x} \\[2ex] \dfrac{C(x_{i+1}, t) + C(x_{i-1}, t) - 2C(x_i, t)}{(\Delta x)^2} \end{matrix}$$



How to choose Δx & Δt?

Generally

$$\Delta t < \frac{(\Delta x)^2}{2D}$$

D: diffusivity

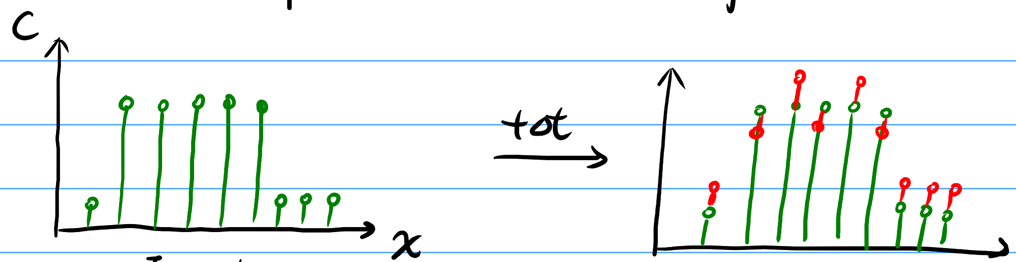
Math packages usually "know" the stability limit

How do we use FD to solve the PDE of diffusion?

Think in "method of lines" (MOL)

1) At each x_i, the series $\{C(x_i, t_0), C(x_i, t_1) \cdots C(x_i, t_j)\}$ is easy to be computed using ODE integration

2) The diffusion problem is now a series of ODE on x-domain



Initial Condition
(t=0)

: change of x_i from previous t

Applications: of finite difference method

1) Initial value problem (IVP)
2) non-isotropic D
3) spatially verying D
4) time-dependent D
5) 2D, 3D geometries (Finite element, Finite volume)

How do you know solution is correct?

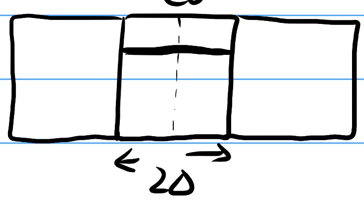
1) Convergence of solution over Δx (Δt usually implicitly imposed by solver)

2) Stability (do the numbers' floating precision satisfy?
example: Poisson-Boltzmann type diffusion
$\exp(\varphi_i c_i z_i)$ can explode!

Examples 1.

Roberts-Austen weight fraction Au in diffusivity estimation (1894)

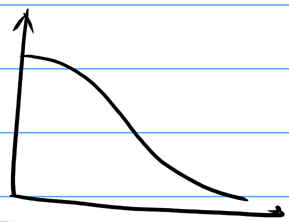
Au diffusion in molten Pb



$2\delta = 2.108$ cm $T = 492°C$

$t = 6.96d$

Analytical solution



$$C(x,t) = \frac{C_0}{2}\left[\mathrm{erf}\left(\frac{x+\delta}{\sqrt{4Dt}}\right) - \mathrm{erf}\left(\frac{x-\delta}{\sqrt{4Dt}}\right)\right]$$

Least square fitting

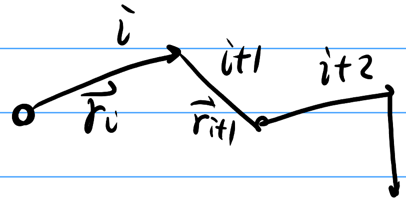
To do fitting (see online demo)

Guess D, Guess C_0 $\xrightarrow{\text{Solve Fick}}$ $\hat{C}(x, t=t_e)$, $C_{exp}(x, t=t_e)$ $\xRightarrow{\text{Loss func}}$ $\mathcal{L} = \sum\left[\hat{C}(x_i, t=t_e) - C_{exp}(x_i, t=t_e)\right]^2$

minimize

Roberts-Austen exp $\Rightarrow$ $\hat{D}_{Au-Pb} \approx 3.00\ cm^2/d = 3.47 \times 10^{-9}\ m^2/s$

Atomic model of diffusion



Jump vector $\vec{r}_i$

Frequency Γ (unit 1/s)

① How many jumps ?

$$N_\tau = \Gamma \cdot \tau$$

② Why change direction? Atomistic collision

③ Total displacement $\vec{R}(N_\tau)$

$$\vec{R} = \sum_{i=1}^{N_\tau} \vec{r}_i$$

Average of $\vec{R} \Rightarrow \langle \vec{R} \rangle = 0$ if same concentration

But not mean squared displacement

$$\langle R^2(N_\tau) \rangle = \langle \vec{R}(N_\tau) \cdot \vec{R}(N_\tau) \rangle$$

$$\vec{R} = \sum_i^{N_\tau} \vec{r}_i \Rightarrow R^2(N_\tau) = \sum_{i \neq j} \vec{r}_i \cdot \vec{r}_j + \sum_{i=} \vec{r}_i \vec{r}_i$$

$$= \sum_i \sum_j |r_i||r_j| \cos\theta_{ij} + \sum |r_i|^2$$

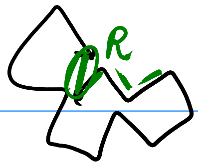
For R^2 jump, we have

① diagonal : $\langle r^2 \rangle = \frac{1}{N_\tau} \sum |r_i|^2 > 0$

mean jump dist

② angle / off-diag

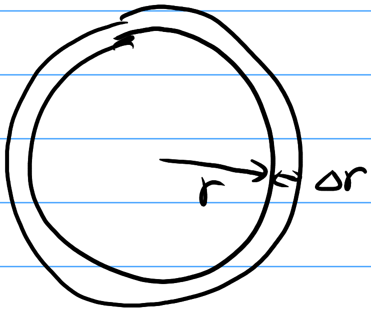
$$\langle R^2(N_\tau) \rangle = N_\tau \cdot \langle r^2 \rangle + \langle \sum_{i \neq j} |r_i||r_j| \cos\theta \rangle$$



$\langle (\text{Length each jump})^2 \rangle = \langle r^2 \rangle$

$\langle (\text{Final disp})^2 \rangle = \langle R^2(N_\tau) \rangle$

Einstein (1904) showed If a point source in 3D space freely diffuse into $\pm\infty$,



$\langle R^2(t) \rangle$ Can be measured

$$\langle R^2(t) \rangle = \frac{\text{int } r^2 \cdot N^{\#} \text{ particle}}{\text{int } N^{\#} \text{ particle on shell } r \text{ to } r}$$

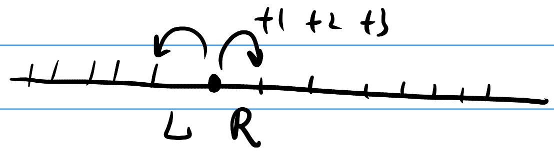
$$= \frac{\int_0^\infty r^2 \, C(r,t) \, 4\pi r^2 dr}{\int_0^\infty C(r,t) \, 4\pi r^2 dr}$$

What's the solution to $C(r,t)$? From last lecture it's

$$C(x,t) = \frac{N}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right) \quad 1D$$

$$C(r,t) = \frac{N}{(\sqrt{4\pi D t})^3} \cdot \exp\left(-\frac{r^2}{4Dt}\right) \quad r^2 = x^2 + y^2 + z^2$$

Random walk model



Total N_T steps $\quad N_L$ left steps

$\qquad\qquad\qquad\quad N_R$ right steps

Probability after N_T steps, at position n ?

$p(n, N_T)$ Constraints $\begin{cases} N_L + N_R = N_T \\ N_R - N_L = n \end{cases}$

Binomial ways

$$\mathcal{U}(n, N_t) = \frac{N_T!}{N_L!\, N_R!} = \frac{N_T!}{\left[\frac{(N_T+n)}{2}\right]!\, \left(\frac{N_T-n}{2}\right)!}$$

all possibilities $\left(\frac{1}{2}\right)^{N_T}$

$$p(n, N_T) \sim \exp\left(-\frac{n^2}{2N_T}\right)$$

$$\langle x^2 \rangle = \langle n^2 \rangle (\Delta x)^2 \sim \Gamma t\, (\Delta x)^2$$

$\langle x^2 \rangle \Downarrow \langle R^2 \rangle$ $\qquad \Gamma \downarrow \langle r \rangle$

Einstein eqn $\langle R^2 \rangle = 2Dt$

$\langle x^2 \rangle = \Gamma(\Delta x)^2 . t \Rightarrow D = \frac{\Gamma(\Delta x)^2}{2}$