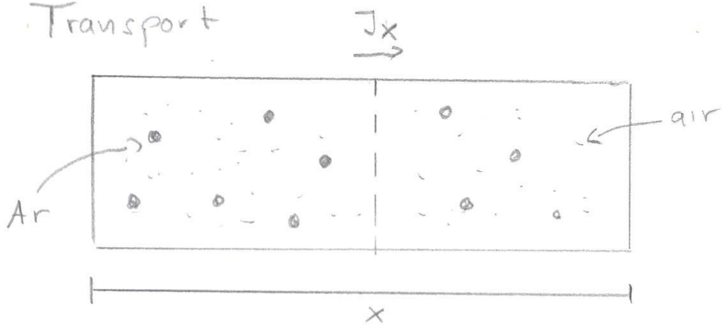
Transport



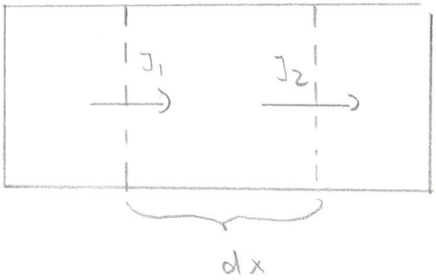
Diffusion of Argon in air

diffusion coefficient

flux $\quad J_x = -D \frac{\partial c}{\partial x}$ } concentration gradient $\quad$ Fick's first law

$\left[\frac{\#}{m^2 s}\right] \quad \left[\frac{m^2}{s}\right]$

concentration c is a function of time and location $c(x,t)$



$$\underline{\partial c(x,t)} = - \frac{\overbrace{(J_2 - J_1)}^{\text{flux divergence}} A \,\partial t}{\underbrace{A\,\partial x}_{\text{Volume}}}$$

$$\frac{\partial c(x,t)}{\partial t} = - \frac{\partial J}{\partial x} = \frac{\partial}{\partial x} D \frac{\partial c}{\partial t}$$

3D: $c(x,y,z,t)$

$$\frac{\partial c}{\partial t} - \frac{\partial}{\partial x} D \frac{\partial c}{\partial x} - \frac{\partial}{\partial y} D \frac{\partial c}{\partial y} - \frac{\partial}{\partial z} D \frac{\partial c}{\partial z} = 0$$

$$\frac{\partial c}{\partial t} - \nabla \cdot (D \nabla c) = 0$$

$$\frac{\partial c}{\partial t} - \nabla \cdot (D \nabla c) = S$$

internal sources or sinks

Advection: transport by flow

$$Dc(x,y,z,t) = \frac{\partial c}{\partial x}dx + \frac{\partial c}{\partial y}dy + \frac{\partial c}{\partial z}dz + \frac{\partial c}{\partial t}dt$$

↑

total derivative

$$\frac{Dc}{dt} = \frac{\partial c}{\partial x}\underbrace{\frac{dx}{dt}}_{u_x} + \frac{\partial c}{\partial y}\underbrace{\frac{dy}{dt}}_{u_y} + \frac{\partial c}{\partial z}\underbrace{\frac{dz}{dt}}_{u_z} + \frac{\partial c}{\partial t}$$

$\vec{u} = [u_x, u_y, u_z]$
flow vector

$$\underbrace{(\vec{u}\cdot\nabla)}_{\text{advection operator}} = [u_x, u_y, u_z]\cdot\left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right]$$

$$\frac{Dc}{dt} = \frac{\partial c}{\partial t} + (\vec{u}\cdot\nabla)c$$

more general

$$= \frac{\partial c}{\partial t} + \underbrace{\nabla\cdot(\vec{u}c)}$$

$\vec{u}\cdot(\nabla c) + (\nabla c)\cdot\vec{u}$ "product rule"

$(\vec{u}\cdot\nabla)c + (\nabla\cdot\vec{u})c$

$\nabla\cdot\vec{u} = 0$ for incompressible flow advection - diffusion equation

$$\underbrace{\frac{\partial c}{\partial t}}_{\text{local change}} - \underbrace{\nabla(D\nabla c)}_{\text{diffusion}} + \underbrace{\nabla\cdot(\vec{u}c)}_{\text{advection}} = \underbrace{S}_{\text{sources - sinks}}$$

Heat equation

$$\rho c_p \frac{\partial T}{\partial t} - \nabla(k\nabla T) + \nabla\cdot(\vec{u}T) = \underbrace{q}_{\text{heat added / subtracted to unit volume}}$$

$$\left[\frac{kg}{m^3}\right]\left[\frac{J}{kg\,K}\right]\left[\frac{K}{s}\right]$$

$$\frac{J}{s\,m^3} \qquad\qquad \frac{J}{s\,m^3}$$

Basic 1D heat equation

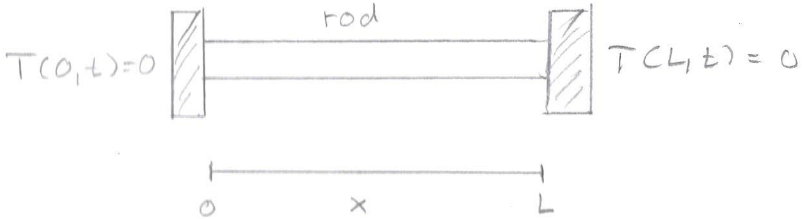
- no advection $(\nabla \cdot (\vec{u} T) = 0)$
- no sources / sinks $(q = 0)$
- 1 dimension $\left(\frac{\partial T}{\partial y} = 0 \quad \frac{\partial T}{\partial z} = 0 \right)$
- $k, \rho, c_p =$ constant

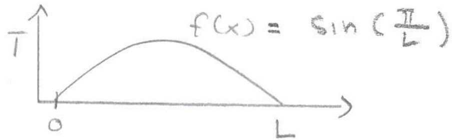
$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} k \frac{\partial T}{\partial x}$$

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \qquad \alpha = \frac{k}{\rho c_p} \quad \left[\frac{m^2}{s} \right]$$

"thermal diffusivity"

Solving PDEs: Separation of variables





$T(x,0) = f(x)$

PDE: $\dfrac{\partial T}{\partial t} = \alpha \dfrac{\partial^2 T}{\partial x^2}$

Problem: seek $T(x,t)$ that satisfies initial and boundary conditions

Approach: seperation of variables (functions)

- works for linear + homogeneous systems

- assume that solutions will be a product of two functions each function only with one variable

$$T(x,t) = A(x)\,B(t)$$

- apply proposed solution to PDE

$$\frac{\partial(A(x)B(t))}{\partial t} = \alpha\,\frac{\partial^2(A(x)B(t))}{\partial x^2}$$

$$A\,\frac{dB}{dt} = \alpha B\,\frac{d^2A}{dx^2}$$

- seperate functions

$$\underbrace{\frac{1}{\alpha B}\,\frac{dB}{dB}}_{\text{function of } t \text{ only}} = \underbrace{\frac{1}{A}\,\frac{d^2A}{dx^2}}_{\text{function of } x \text{ only}} = -m$$

makes solution easier later

must be equal for all t and x values $\Rightarrow$ must equal to a const.

time ODE

$$\frac{dB}{dt} = -\alpha m B$$

Space ODE

$$\frac{d^2A}{dt} = -mA$$

$\rightarrow$ two ordinary diff Eq.

- solve space ODE

$$T(x,t) = A(x)B(t)$$

$$\left.\begin{aligned} T(0,t) &= A(0)B(t) \\ T(L,t) &= A(L)B(t) \end{aligned}\right\} \text{Boundary conditions } A(0) = A(L) = 0$$

trivial solution: $B(t) = 0$ for all $T \Rightarrow T(x,t) = 0$

$\Rightarrow$ $A(0) = 0$ and $A(L) = 0$ must hold

$\rightarrow$ found IVP for space ODE

- solve space ODE

$$\frac{d^2A}{dx^2} + mA = 0 \qquad A(0) = 0 \qquad A(L) = 0$$

problem: we do not know m => try cases

$m = 0$

$$\frac{d^2A}{dx^2} = 0 \quad \Rightarrow \quad A(x) = c_1 + c_2 x$$

$$\left.\begin{array}{lll} A(0) = 0 & \Rightarrow c_1 = 0 & \\ A(L) = 0 & \Rightarrow c_2 L = 0 & \Rightarrow c_2 = 0 \end{array}\right\} \text{trivial solution}$$

$m \neq 0 \qquad \frac{d^2A}{dx^2} + mA = 0$

characteristic equation

$\lambda^2 + m = 0 \quad \Rightarrow \quad \lambda_{1,2} = \pm\sqrt{-m}$

Solution: $A(x) = c_1 \exp(\lambda_1 x) + c_2 \exp(\lambda_2 x)$

$m < 0$: $\quad A(0) = c_1 + c_2 = 0 \quad \Rightarrow \quad c_1 = -c_2$

$A(L) = c_1 \exp(\lambda_1 L) + c_2 \exp(\lambda_2 L) = 0$

$\Rightarrow \quad \frac{c_1}{c_2} \exp(\lambda_1 L) = -\exp(\lambda_2 L)$

$\Rightarrow \quad -\exp(\lambda_1 L) = -\exp(\lambda_2 L)$

$\Rightarrow \quad \lambda_1 = \lambda_2 \quad \Rightarrow$ only possible for $m = 0$

$m > 0 \quad \Rightarrow \quad z_{1,2} = \pm\sqrt{m}\, i = 0 \pm \sqrt{m}\, i$

$a \pm b\, i$

$$A(x) = \exp(ax)\,(c_1 \cos(bx) + c_2 \sin(bx))$$

$$A(x) = c_1 \cos(\sqrt{m}\, x) + c_2 \sin(\sqrt{m}\, x)$$

$A(0) = 0 \quad \Rightarrow \quad c_1 = 0$

$A(L) = 0 \quad \Rightarrow \quad c_2 \sin(\sqrt{m}\, L) = 0$

if $c_2 \neq 0 \quad \Rightarrow \quad \sin(\sqrt{m}\, L) = 0$

infinite solutions : $\sin(x) = 0$ for $0, \pi, 2\pi, \dots n\pi$

$\sqrt{m}\, L = n\pi \quad \Rightarrow \quad m_n = \left(\frac{n\pi}{L}\right)^2 \qquad n = 1, 2, \dots,$

$$A_n(x) = c_2 \sin\left(\frac{n\pi}{L} x\right)$$

$\uparrow$ still unknown

- solve time equation

$$\frac{dB}{dt} = -\alpha m_n B \qquad m_n > 0 = \left(\frac{n\pi}{L}\right)^2$$

$$B(t) = c_1 \exp\left(-\alpha \left(\frac{n\pi}{L}\right)^2 t\right)$$

- PDE solution

$$T(x,t) = A(x)\,B(t)$$

$$T(x,t) = c \sin\left(\frac{n\pi}{L}x\right) \exp\left(-\alpha \left(\frac{n\pi}{L}\right)^2 t\right) \qquad \omega = \frac{n\pi}{L}$$

$$T(x,t) = c \sin(\omega x) \exp(-\alpha \omega^2 t)$$

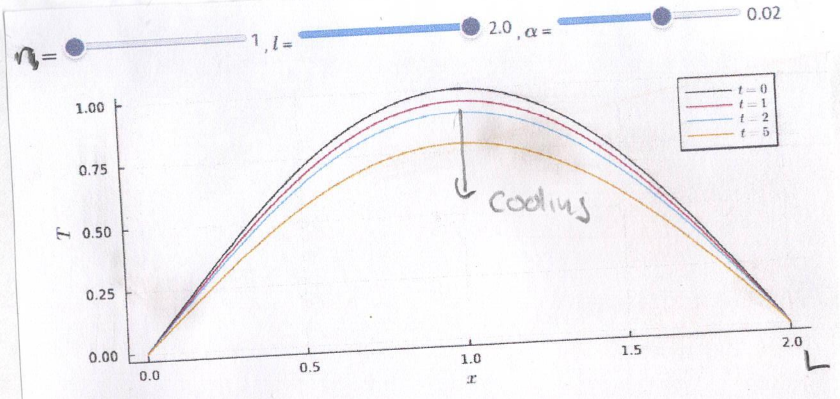
IVP $\quad T(x,0) = f(x) = c \sin(\omega x)$

$$= c \sin\left(\frac{n\pi}{L}x\right) \qquad \text{original } f(x) = \sin\left(\frac{\pi}{L}x\right)$$

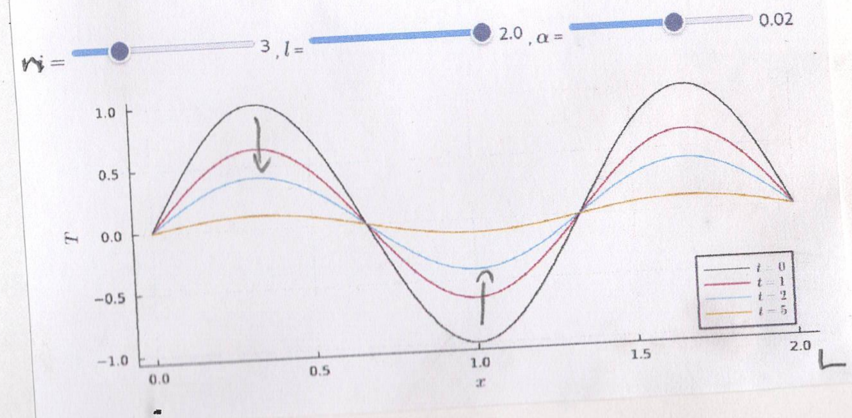
$$n = 1$$

$$\Rightarrow c = 1$$

$$\boxed{T(x,t) = \sin\left(\frac{\pi}{L}x\right) \exp\left(-\alpha \left(\frac{\pi}{L}\right)^2 x\right)}$$



$$\alpha \uparrow \Rightarrow \frac{\partial T}{\partial t} \uparrow$$



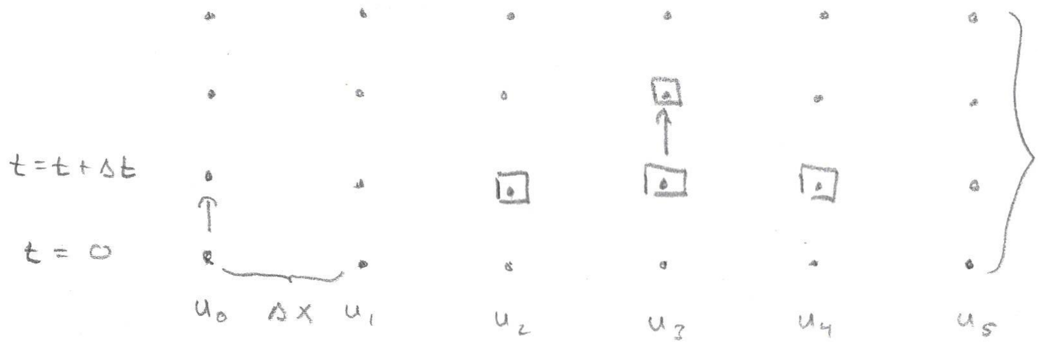
$$T(x,t) = \sin\left(\frac{3\pi}{L}x\right)\exp\left(-\alpha\left(\frac{3\pi}{L}\right)^2 t\right)$$

Numerical Solution to PDEs

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

"Method of Lines" : RHS as finite difference approximation

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$



boundary values $T(L, t)$

"initial values

$$du_0 = 0 = u_0 (t + \Delta t)$$

$$du_1 = u_1 (t+\Delta t) = \alpha \frac{u_2 - 2u_1 + u_0}{\Delta x^2} = \frac{\alpha}{\Delta x^2} (u_2 - 2u_1 + u_0$$

⋮

$$d\vec{u} = \begin{bmatrix} du_0 \\ du_1 \\ du_2 \\ du_3 \\ du_4 \\ du_5 \end{bmatrix} = \frac{\alpha}{\Delta x^2} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}$$

$$d\vec{u} = \frac{\alpha}{\Delta x^2} A \vec{u} \qquad \Delta x^2 = \frac{L}{n-1}$$

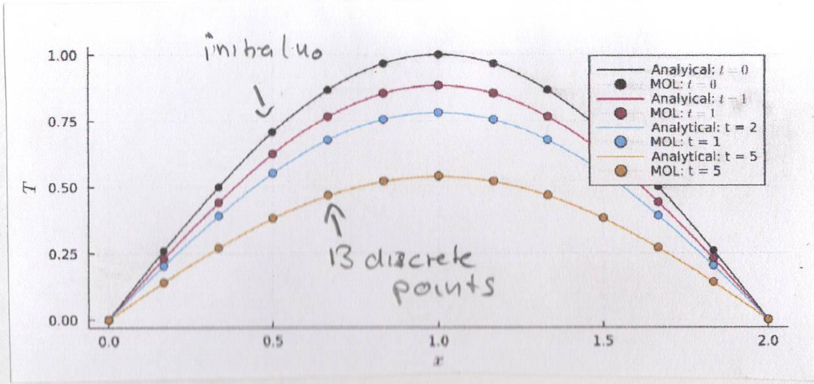
$$A \in R^{n \times n}$$

System of first order ODEs => use ODE solver

$$\left.\begin{array}{l} du_0 = 0 \\ du_{n-1} = 0 \end{array}\right\} \text{Dirichlet Boundary Condition}$$

u_0, u_{n-1} - can take on other values than zero
- picked zero to compare to analytical solution

Numerical Solution



function f(u, p, t)

$\alpha = p[1]$

$\Delta x = p[2]$

$A = p[3]$

$du = \frac{\alpha}{\Delta x^2} A u$

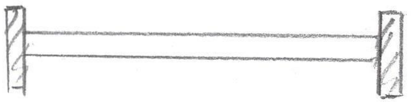
return du

end

n is length of u

and A is size(n, n)

Other Boundary conditions



Dirichlet: fixed value

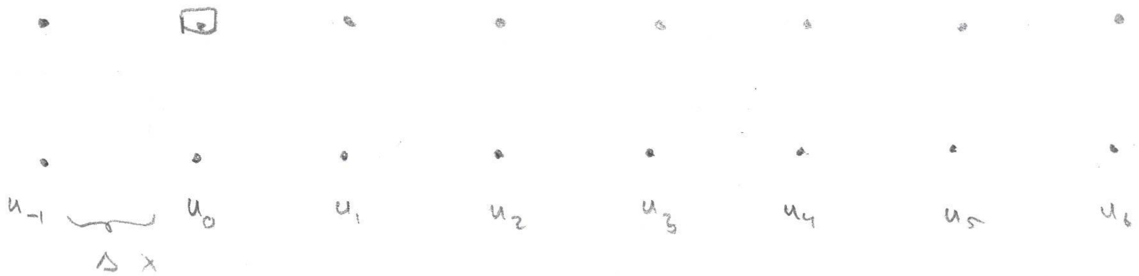
$$\Rightarrow \frac{du_0}{dt} = \frac{du_L}{dt} = 0$$

Neumann: fixed gradient / flux

$$\frac{du_0}{dx} = \frac{du_L}{dx} = c$$

constant

often $c=0$: zero flux $\Rightarrow$ "adiabatic"



$$\frac{u_1 - u_{-1}}{2\Delta x} = C \qquad \Rightarrow \qquad u_{-1} = u_1 - 2\Delta x\, C$$

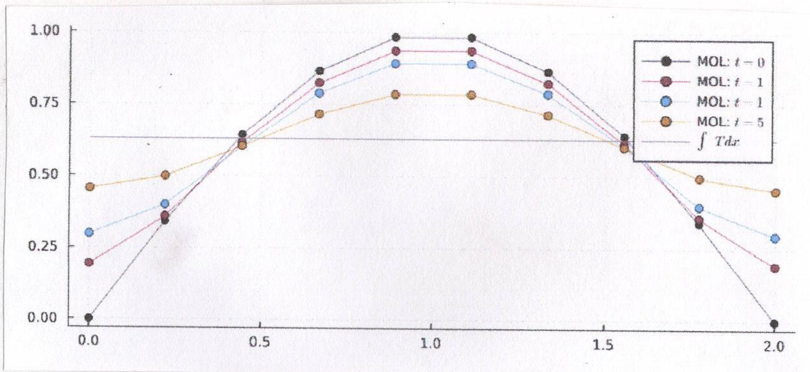
$$du_0 = u(t+\Delta t) = \alpha \frac{u_1 - 2u_0 + u_{-1}}{\Delta x^2} = \frac{\alpha}{\Delta x^2}(u_1 - 2u_0 + u_{-1} - 2\Delta x\, C)$$

for $c = 0$

$$du_0 = \frac{\alpha}{\Delta x^2}(2u_1 - 2u_0)$$

$$A = \begin{bmatrix} -2 & 2 & 0 & 0 & \cdots & & 0 \\ 1 & -2 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & \\ 0 & 0 & \cdots & & & -2 & 2 \end{bmatrix}$$

$$d\vec{u} = \frac{\alpha}{\Delta x^2} A \vec{u}$$



Numerical Solution Stability

Integration through Euler's Method

u_i^j ← time (j), ← space (i)

$$du = \frac{u_i^{j+1} - u_i^j}{\Delta t} = \alpha \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}$$

- could use this to get u_i^{j+1}

system is stable if $\frac{2\alpha \Delta t}{\Delta x^2} \leq 1$ "CFL condition" (Courant-Friedrich-Lewy)

$\Rightarrow \Delta t$ must be sufficiently small

note $\tau_{cond} = \frac{\Delta x^2}{\alpha}$ time scale of conduction

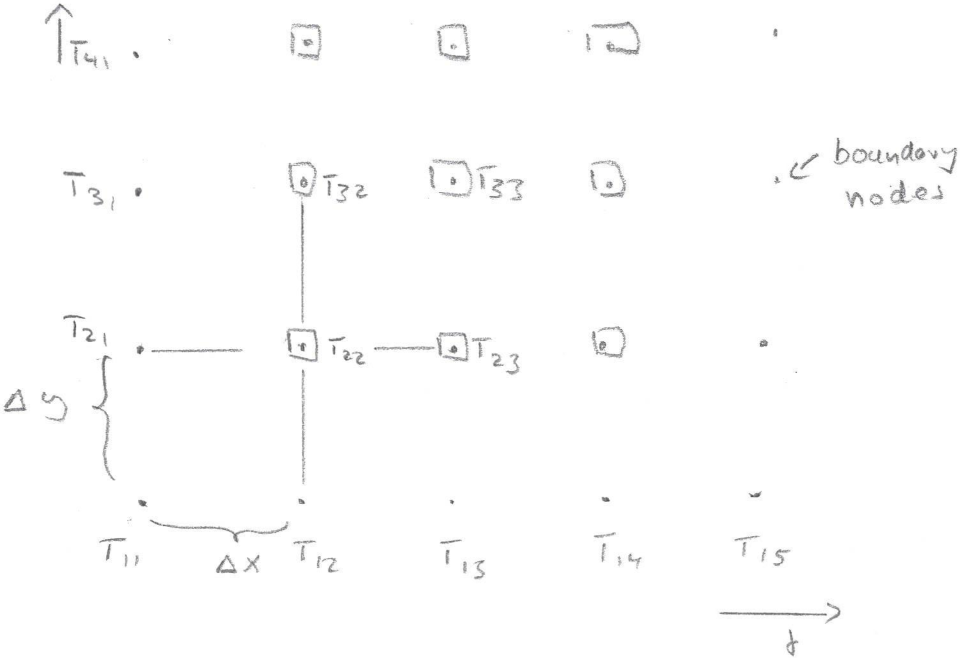
$$\Rightarrow \Delta t < \frac{1}{2} \tau_{cond}$$

$\Rightarrow$ may need small Δt and solution is slow

2D case

$$\frac{\partial T}{\partial t} = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right)$$

$$\frac{\partial T_{ij}}{\partial t} = \alpha \frac{T_{i,j+1} - 2T_{ij} + T_{i,j-1}}{\Delta x^2} + \alpha \frac{T_{i+1,j} - 2T_{ij} + T_{i-1,j}}{\Delta y^2}$$



Puff Dispersion

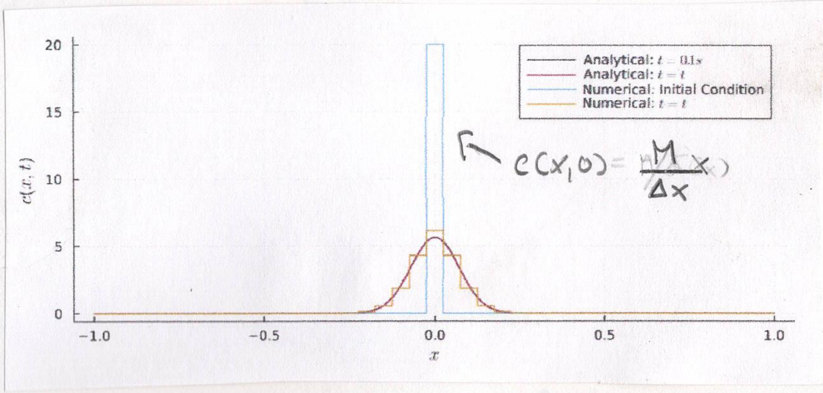
$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

$c(x,0) = M\delta(x)$ $\qquad$ $c(x,t) \to 0 \quad x \to \infty$

solution identical to heat problem

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

$$c(x,t) = \frac{M}{\sqrt{4\pi D t}} \exp\left(-\frac{x^2}{4Dt}\right)$$

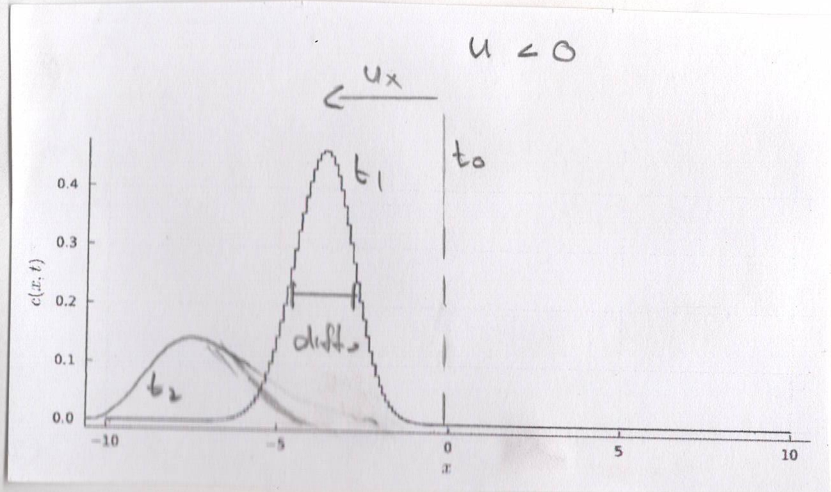


Puff Dispersion + Advection

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

MOL: $$\frac{\partial c_i}{\partial t} = D \left(\frac{T_{i+1} - 2T_i + T_{i-1}}{\Delta x^2} \right) - u_x \left(\frac{c_{i+1} - c_{i-1}}{2 \Delta x} \right)$$

Forward time centered difference (FTSC)



- even for good CFL condition solution will develop oscillations
- need more sophisticated scheme for advection problem
  - -> upwind scheme / Fromm's method
  - -> better to solve c_i through loop instead of ODE Solver