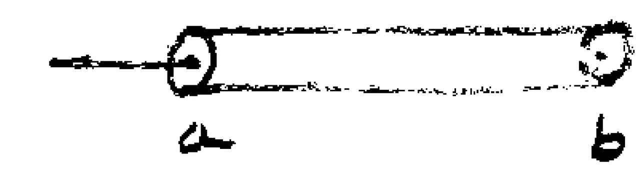
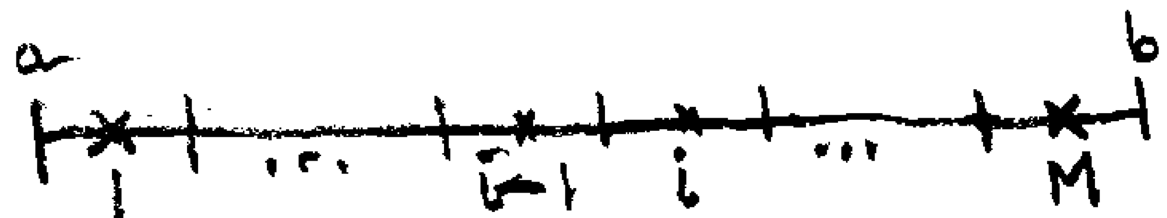
Finite Volume Discretization of $\frac{\partial u}{\partial t} + \frac{\partial F}{\partial x} = 0$ in $\Omega = (a, b)$



mesh:



nodes x_i, $i = 1:M$ (and $x_0 = a$, $x_{M+1} = b$)

faces $x_{i-\frac{1}{2}}$, $i = 1:M+1$

control volumes $V_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times A$

$\Delta V_i = A \cdot \Delta x$

Integrate over V_i and over $[t_n, t_{n+1}]$:

$$\int_{t_n}^{t_{n+1}} \frac{\partial}{\partial t} \int_{V_i} u(x,t)\, A\, dx\, dt + \int_{t_n}^{t_{n+1}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial F}{\partial x} A\, dx\, dt = 0$$

$$\Rightarrow \int_{V_i} u\, A\, dx \Big|_{t=t_n}^{t=t_{n+1}} + \int_{t_n}^{t_{n+1}} \left[AF(x_{i+\frac{1}{2}}, t) - AF(x_{i-\frac{1}{2}}, t) \right] dt = 0$$

Set $U_i^n := \frac{1}{\Delta V_i} \int_{V_i} u(x, t_n)\, dV$ = mean value of u over V_i at time t_n

$AF_{i-\frac{1}{2}}^{n+\theta} := \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} AF(x_{i-\frac{1}{2}}, t)\, dt$ = mean flow rate across face $i-\frac{1}{2}$ during time step

$$\Rightarrow \Delta V_i \left[U_i^{n+1} - U_i^n \right] + \Delta t \left[AF_{i+\frac{1}{2}}^{n+\theta} - AF_{i-\frac{1}{2}}^{n+\theta} \right] = 0 \qquad \begin{array}{l} i = 1:M \\ n = 0, 1, \dots, N_{steps} \end{array}$$

expressing <u>exact</u> discrete conservation over each Control Volume and each time-step.

<u>Explicit scheme</u>: choose $\theta = 0$: assume mean flux during Δt remains $\approx$ flux at time t_n.
Knowing U_i^n and flux law $F = F(u)$, we can compute $F_{i-\frac{1}{2}}^n$, $i = 2:M$
and BCs provide $F_{1/2}^n$, $F_{M+1/2}^n$, so we can update

$$U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta V_i} \left[AF_{i-\frac{1}{2}}^n - AF_{i+\frac{1}{2}}^n \right], \quad i = 1:M, \quad n = 0, 1, \dots, N$$

<u>Implicit schemes</u>: choose $0 < \theta \leq 1$ and $F^{n+\theta} = (1-\theta) F^n + \theta F^{n+1}$

Then we have a coupled system to solve for $\{U_i^{n+1}\}$ at each time step (using some system solver)

$\theta = \frac{1}{2}$ is Crank-Nicolson scheme

$\theta = 1$ is Fully Implicit (Backward Euler) scheme

Note: Cross-sectional area A cancels out in 1D, but <u>not</u> in 2D, 3D

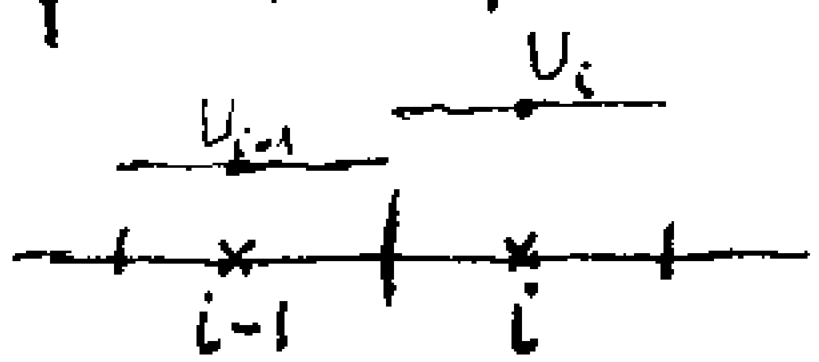
Flux for diffusion / heat conduction

The conservation law $u_t + \mathcal{F}_x = S$ conserves u for <u>any</u> $\mathcal{F}$

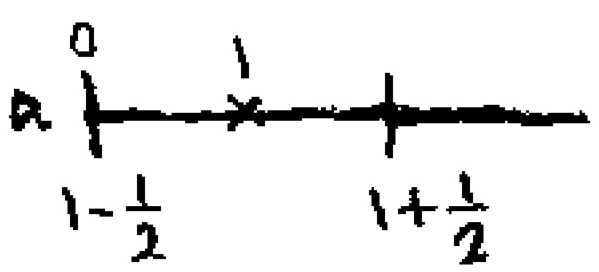
$\mathcal{F}$ is specified by a <u>constitutive Law</u> expressing particular physical phenomena.

<u>Diffusion</u>: Fick's law: $\mathcal{F} = -D u_x$, D = diffusivity $[cm^2/sec]$
u = consentration $[gr/cm^3]$

($\Rightarrow$ diffusion equation: $u_t = (D u_x)_x = D u_{xx}$ if $D \equiv$ constant
a most important PDE, more later...)



Flux Discretization: $F_{i-\frac{1}{2}} \approx -D \dfrac{U_i - U_{i-1}}{\Delta x}$, $i = 2:M$ (at internal faces)



$F_{1-\frac{1}{2}} \approx -D \dfrac{U_1 - U_0}{\Delta x/2}$, $F_{M+\frac{1}{2}} \approx -D \dfrac{U_{M+1} - U_M}{\Delta x/2}$

boundary fluxes $F_{\frac{1}{2}}$, $F_{M+\frac{1}{2}}$ from Boundary Conditions

e.g. <u>impermeable boundary means Flux = 0</u> (so nothing goes through the bry)
so $F_{\frac{1}{2}} = 0$ and $F_{M+\frac{1}{2}} = 0$

Boundary Conditions in FV scheme for diffusion

A **PDE Problem** consists of: for $u(x,t)$

PDE e.g. $u_t = D u_{xx}$, $x \in \Omega$, $t_0 < t < t_{end}$

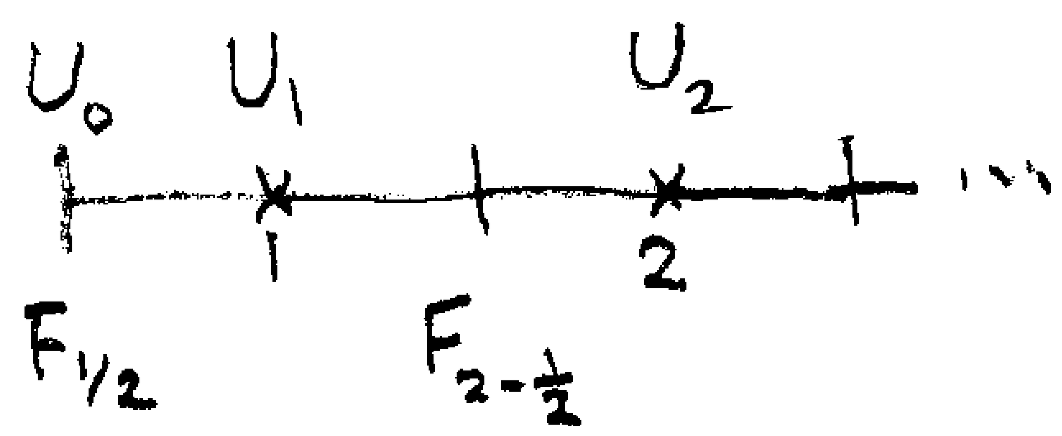
IC $u(x,0) = u_{init}(x)$, $x \in \Omega$

BCs some BC at each pt of $\partial\Omega$ for all time

Scheme needs fluxes

Standard BCs at $x=a$ or $x=b$ coded in FLUX routine

I. Dirichlet (or 1st kind): impose value at $x=a$: $u(a,t) = u_a(t)$ given



so $U_0^n \approx u(a,t_n) = u_a(t_n)$ known bry value

$$\Rightarrow F_{1/2}^n \simeq -D \frac{U_1^n - U_0^n}{\Delta x/2}, \quad F_{M+\frac{1}{2}}^n = -D \frac{U_{M+1}^n - U_M^n}{\Delta x/2}$$

II. Neumann (or 2nd kind): impose flux at $x=a$: $\mathcal{F}(a,t) = F_a(t)$ given

so $F_{1/2}^n = F_a(t_n)$ known bry flux

then bry value U_0^n can be found from $F_{1/2} \simeq -D \frac{U_1 - U_0}{\Delta x/2} \doteq F_a(t_n)$

solve for U_0

$$\Rightarrow U_0^n = U_1^n + \frac{\Delta x}{2D} F_{1/2}^n, \quad U_{M+1}^n = U_M^n - \frac{\Delta x}{2D} F_{M+\frac{1}{2}}^n$$

In particular, impermeable/insulated bry: $\mathcal{F}(a,t) = F_a(t) \equiv 0$

$$\Rightarrow U_0^n = U_1^n, \quad U_{M+1}^n = U_M^n$$

Note: FV scheme needs only fluxes. Boundary values U_0, U_{M+1} (consistent with BCs) are for outputing (to plot profiles).

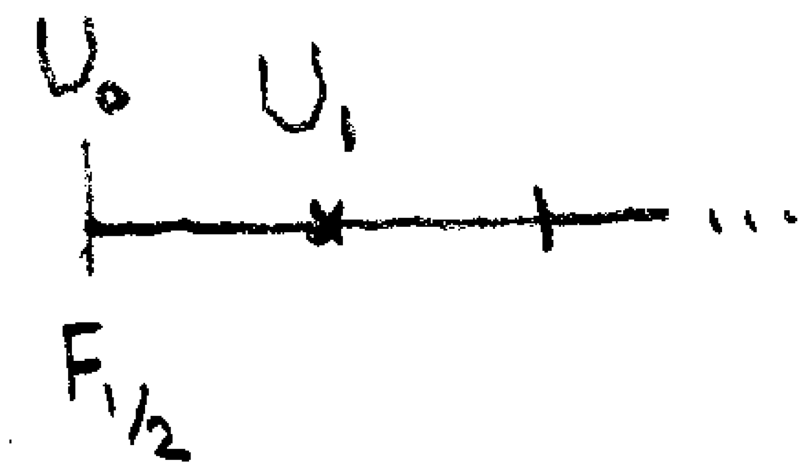
BCs ...

III. Convective BC (or Robin or 3rd kind):

most realistic BC physically

h = film coeff, heat transfer coeff,

$u_{amb}(t)$ = ambient u, given



$$\mathcal{F}(a,t) = h\left[u_{amb}(t) - u(a,t)\right]$$

$$F^n_{1/2} = h\left[u_{amb}(t_n) - U^n_0\right] \overset{\text{want}}{=} -D\,\frac{U^n_1 - U^n_0}{\Delta x/2}$$

solve for U_0: $$U^n_0 = \frac{U_1 + \frac{h\Delta x}{2D}\,u_{amb}(t_n)}{1 + \frac{h\Delta x}{2D}}$$ for Output

$$\Rightarrow F^n_{1/2} = -D\,\frac{U^n_1 - u_{amb}(t_n)}{\frac{D}{h} + \frac{\Delta x}{2}}$$

so u_{amb} plays role of U_0 but with $\frac{D}{h} + \frac{\Delta x}{2}$ instead of $\frac{\Delta x}{2}$

Note: $h \to \infty \Rightarrow u(a,t) = u_{amb}(t)$ (for $\mathcal{F}$ to be finite).
Dirichlet BC!

$h = 0 \Rightarrow \mathcal{F} = 0$, insulated bry
homogeneous Neumann BC