FD Conservation

- Conservation Law + Constitutive Relation $\Rightarrow$ PDE

$$\underbrace{\nabla \cdot q}_{\text{Flux}} = \underbrace{\sigma}_{\text{source/volume}} \qquad q = -K\nabla u \qquad \nabla \cdot K \nabla u = -\sigma$$

Flux source/volume Scalar Surrogate for q

eg:

q	Conserved	u	σ
Heat Flux	Thermal Energy	T	Heating rate
Diffusion Flux	Molecules of species	C	Reaction Rate
Mass Flux	Fluid mass	P	Evaporation Rate
⋮	⋮	⋮	⋮

Note: σ need not be constant

- radioactive decay : $\sigma = -kC$
  Storage : $\sigma = -\frac{\partial C}{\partial t}$

$$\Rightarrow \quad \nabla \cdot D \nabla C = \underbrace{\frac{\partial C}{\partial t} + kC}_{-\sigma} \qquad \text{(Parabolic More later)}$$

- PDE is <u>local</u> conservation Statement

– Global Conservation:

$$\int (\text{PDE})\, dV \Rightarrow \int \nabla \cdot q \, dV = \int \sigma \, dV$$

Divergence Theorem: $\oint q \cdot \hat{n}\, ds = \int \sigma \, dV$

Rate of escape = sum of sources

<u>or</u> $\oint -K \nabla u \cdot \hat{n}\, ds = \int \sigma \, dV$

$$\oint -K \frac{\partial u}{\partial n}\, ds = \int \sigma \, dV$$

- Numerical Conservation $\Rightarrow \int (\ )\, dV = \sum (\ )_i \Delta V_i$

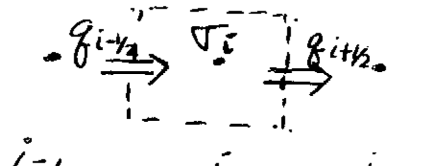
e.g. 1-D ... $\sum_i \int_{i-1/2}^{i+1/2} (\ )_i \, dx$

$\frac{\partial}{\partial x} K \frac{\partial u}{\partial x} = -\sigma$ for 1 box:

$$\int_{i-1/2}^{i+1/2} \left(\frac{\partial}{\partial x} K \frac{\partial u}{\partial x}\right)_i dx = -\int_{i-1/2}^{i+1/2} \sigma \, dx$$

$$\underbrace{K \frac{\partial u}{\partial x}\Big|_{i+1/2}} - \underbrace{K \frac{\partial u}{\partial x}\Big|_{i-1/2}} = -\sigma_i h$$

$$-q_{i+1/2} \quad + \quad q_{i-1/2} = -\sigma_i h$$



So σ_i represents all sources in the box associated w/ Node i

$$\sigma_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \sigma \, dx \Big/ \left(x_{i+1/2} - x_{i-1/2}\right)$$

Now: $-q_{i+1/2} + q_{i-1/2} = K_{i+1/2}\left(\frac{u_{i+1} - u_i}{h}\right) - K_{i-1/2}\left(\frac{u_i - u_{i-1}}{h}\right)$

$$= -\sigma_i h$$

Or

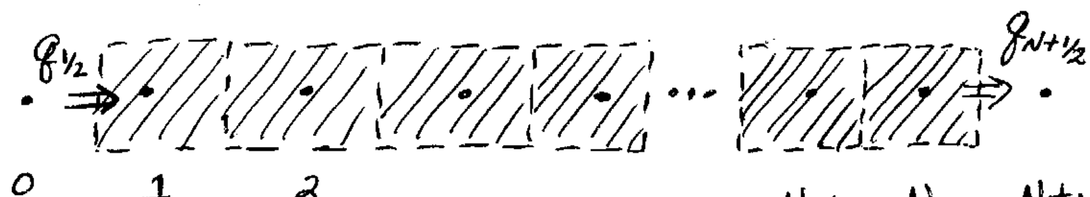
$$\frac{K_{i+1/2}\left(\frac{u_{i+1} - u_i}{h}\right) - K_{i-1/2}\left(\frac{u_i - u_{i-1}}{h}\right)}{h} = -\sigma_i$$

But left-hand side is exactly our FD approximation at node i ... so to conserve we must view σ_i as average of sources in box

$$\text{i.e.}\quad \sigma_i = \int_{x_{i-1/2}}^{x_{i+1/2}} \sigma\, dx \Big/ \left(x_{i+1/2} - x_{i-1/2}\right)$$

Then $\sum_{i=1}^{N}$ (FD equation #i) :

$$-q_{N+1/2} + q_{1/2} = -\sum_{i=1}^{N} \sigma_i h \qquad \text{Internal } q_{i+1/2} \text{ cancel}$$



- Type I BCs at 0, N+1 $\Rightarrow$ Can solve ...
  - Conservation boundaries <u>not</u> at 0, N+1
  - Conservation independent of σ_0 + σ_{N+1}

- Type II + Type III ... bring PDE molecule to boundary e.g. $-K\frac{\partial u}{\partial x} = q_0$ specified ... then

FD molecule at node 0:

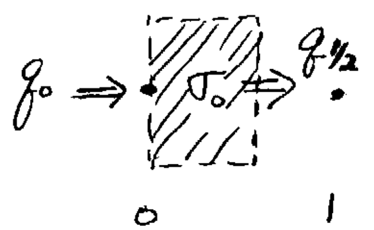
$$K_{1/2}\left(\frac{U_{-1}-2U_0+U_1}{h}\right) = -\sigma_0 h \qquad (K_{1/2}=K_{-1/2})$$

But BC says: $K_0\frac{U_{-1}-U_1}{2h} = q_0$

$$\Rightarrow U_{-1} = \frac{2hq_0}{K_0}+U_1 = \frac{2hq_0}{K_{1/2}}+U_1 \qquad \left(K_0=\frac{K_{1/2}+K_{-1/2}}{2} \text{ average!}\right)$$

So we get $2q_0 + 2\left(\frac{U_1-U_0}{h}\right)K_{1/2} = -\sigma_0 h$

or $$q_0 + \underbrace{K_{1/2}\left(\frac{U_1-U_0}{h}\right)}_{-q_{1/2}} = -\sigma_0 h/2$$



This provides the missing half box!

Similarly at node N+1: $-q_{N+1}+q_{N+1/2} = -\sigma_{N+1}h/2$

So For Global conservation add in the two boundary molecules ...

$$-q_{N+1} + q_0 = -\sum_{i=1}^{N} \sigma_i h - \frac{\sigma_0 h}{2} - \frac{\sigma_{N+1} h}{2}$$

$$= \underbrace{-\sum_{i=0}^{N} (\sigma_i + \sigma_{i+1}) \frac{h}{2}}_{\text{Trapezoidal Rule Integration}}$$

This is the FD Conservation Statement !

- At Type I boundaries need to use <u>all</u> molecules to conserve ... use the unused (in sol'n) molecules at boundary to compute fluxes

$$q_0 = \underbrace{-K_{1/2}\left(\frac{U_1 - U_0}{h}\right)}_{\substack{\text{This is the}\\ \text{intuitive FD}\\ \text{expression ...}\\ \text{looks } O(h)}} \underbrace{- \frac{\sigma_0 h}{2}}_{\substack{\text{Correction term to}\\ \text{account for half box}\\ \text{makes everything } O(h^2)}}$$

Similar at node N+1 :

$$-q_{N+1} = K_{N+1/2}\left(\frac{U_{N+1} - U_N}{h}\right) - \sigma_{N+1} h/2$$

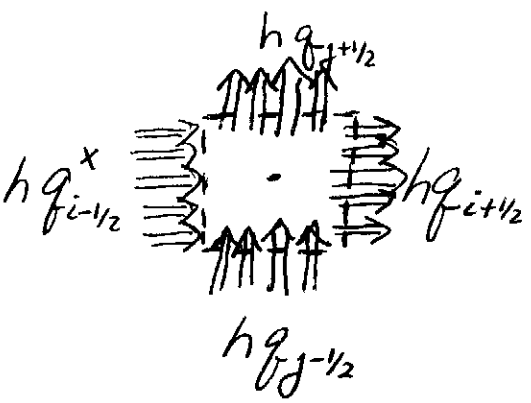
In 2-D:

$$\frac{1}{h}\left[K_{i+1/2}\left(\frac{U_{i+1,j}-U_{i,j}}{h}\right) - K_{i-1/2}\left(\frac{U_{i,j}-U_{i-1,j}}{h}\right)\right]$$

$$+ \frac{1}{h}\left[K_{j+1/2}\left(\frac{U_{i,j+1}-U_{i,j}}{h}\right) - K_{j-1/2}\left(U_{i,j}-U_{i,j-1}\right)\right]$$

$$= -\sigma_{ij}$$

$$-hq^x_{i+1/2} + hq^x_{i-1/2} - hq^y_{j+1/2} + hq^y_{j-1/2} = -\sigma_{ij}h^2$$



σ_{ij} is 2D average

i.e. $$\sigma_{ij} = \frac{\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i-1/2}}^{x_{i+1/2}} \sigma \, dx\, dy}{(x_{i+1/2}-x_{i-1/2})(y_{j+1/2}-y_{j-1/2})}$$

- Note: if $\sigma = Q\delta(x-x_0, y-y_0)$ then for Node ij corresponding to (x_0, y_0)

$$\sigma_{ij} = \frac{\iint Q\delta(x-x_0, y-y_0)\, dx\, dy}{h^2} = \underbrace{Q/h^2}$$

Source Strength divided by area of 1 Box !!