Conservation Laws.

Conservation Law + Constitutive Relation $\Rightarrow$ PDE

$\underline{\nabla} \cdot \underline{q} = \sigma$ $\quad\quad$ $\underline{q} = -K\underline{\nabla}U$ $\quad\quad$ $\underline{\nabla} \cdot K\underline{\nabla}U = -\sigma$

q = flux $\equiv$ (Conserved Quantity) / unit time/ unit area

σ = Source terms/unit volume/unit time

Input + generation = Output + accumulation

- Output + Input = accumulation - generation

$$\underline{\nabla} \cdot \underline{q} \quad = \quad \sigma$$

U = many times acts as the scalar surrogate for $\underline{q}$

Physical Examples

q	Conserved Quantity	u	σ
Heat Flux	Thermal Energy	T	Heating rate
	$\nabla \bullet K \nabla T = c\frac{\partial T}{\partial t}$		
Diffusion Flux	Molecules of Species	C	Chem. Rxn Rate
Mass Flux (Porous Media)	Fluid Mass	P	-Evap. Rate (Influx)

Stress	Momentum (F = mA)	δ ↑ displacement strain	Body Forces
Electostatic Field Gravity Field	certain integral properties of force	ϕ	Q/ε_o -kM

Note: σ need not be constant

consider the mass diffusion situation with radioactive decay

σ = - kc and storage $\sigma = -\frac{\partial C}{\partial t}$

(Decay or generation)

$$\nabla \bullet D \nabla C = \frac{\partial C}{\partial t} + kC = -\sigma$$

The conservation law of PDE is a local conservation statement

Globally the conservation law is : $\int (PDE)dv$

a.) $$\int \underline{\nabla} \cdot \underline{q} dv = \int \sigma dv$$

making use of Divergence Theorem

$$\int \underline{\nabla} \cdot (\ ) dv \equiv \oint (\ ) \cdot \underline{\hat{n}} ds$$

$$\oint \underline{q} \cdot \underline{\hat{n}} ds = \int \sigma dv$$

i.e. the rate escape = sum of sources

b.) using constitutive relation

$$\int \nabla \bullet \left(K \nabla U \right) dv = -\int \sigma dv$$

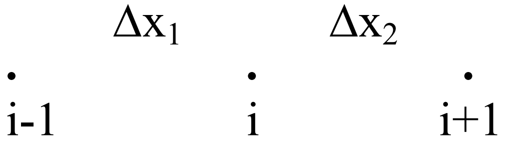
again using divergence

$$\oint K \underline{\nabla} U \cdot \underline{\hat{n}} ds = - \int \sigma dv$$

which is the same as (a) since $\underline{q} = - K \underline{\nabla} U$

Numerical Conservation : $\int (\ \ )\, dv \rightarrow \sum_i (\,)_i \,\Delta v_i$

$$\frac{\partial}{\partial x}\left(K\frac{\partial U}{\partial x}\right) = -\sigma$$

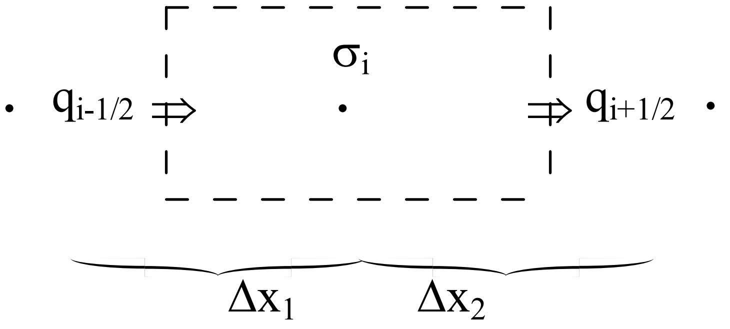


$$\frac{\left(K\frac{\partial U}{\partial x}\right)_{i+1/2} - \left(K\frac{\partial U}{\partial x}\right)_{i-1/2}}{2h} = \frac{\left(K\frac{\partial U}{\partial x}\right)_{i+1/2} - \left(K\frac{\partial U}{\partial x}\right)_{i-1/2}}{x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}}$$

Where $2h = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}$

$$K_{i+\frac{1}{2}}\frac{\left(U_{i+1}-U_i\right)}{x_{i+1}-x_i} - K_{i-\frac{1}{2}}\frac{\left(U_i-U_{i-1}\right)}{x_i-x_{i-1}} = -\sigma_i\left(x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}\right)$$

$$-\,q_{i+1/2} \qquad + \qquad q_{i-1/2} \qquad = -\,\sigma_i\left(\frac{\Delta x_2 - \Delta x_1}{2}\right)$$



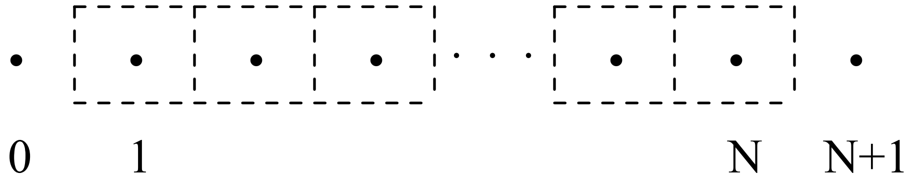
σ_i represents all sources in the two half-boxes:

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

This definition of σ_i is especially important when σ is to be represented as a Dirac Delta Function

$K_{i+1/2}$ embodies all K(x) variations between x_i and x_{i+1}

$$\sum_{i=1}^{N} (FD\ Eqn\ \#i) \Rightarrow$$ All Internal $q_{i+1/2}$ cancel



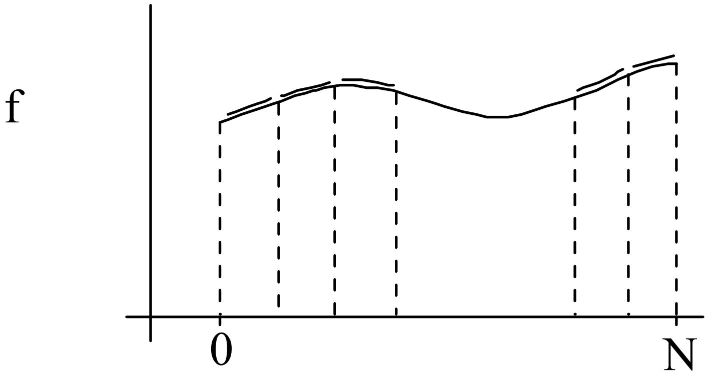
$$q_{\frac{1}{2}} + \left(-\ q_{1\frac{1}{2}} + q_{1\frac{1}{2}}\right) + \left(-\ q_{2\frac{1}{2}} + q_{2\frac{1}{2}}\right) \cdots \left(-\ q_{(N-1)+\frac{1}{2}} + q_{(N+1)+\frac{1}{2}}\right) - q_{N+\frac{1}{2}} =$$

$$= -\sigma_1 \frac{\Delta x_1}{2} - \sum_{i=1}^{N} \frac{\left(\sigma_i + \sigma_{i+1}\right)}{2} \Delta x_{i+1} - \sigma_N \frac{\Delta x_{N+1}}{2}$$

Trapezoidal Rule

Trapezoidal Rule - Hornbeck

$$I = \int_a^b f(x)dx \qquad \text{let } \Delta x = \frac{b - a}{N}$$



Approximate area under curve with straight lines

$$\int_{x_{i-1}}^{x_{i+1}} f(x)dx \cong \frac{f_{i-1} + f_i}{2} \Delta x \;\; ; \;\; \int_{x_i}^{x_{i+1}} f(x)dx \approx \frac{f_i + f_{i+1}}{2} \Delta x$$

or
$$\int_{x_{i-1}}^{x_{i+1}} f(x)dx \cong \frac{\Delta x}{2} \left(f_{i-1} + 2f_i + f_{i+1}\right)$$

and
$$\int_a^b f(x)dx \approx \frac{\Delta x}{2}\left(f_0 + f_N + 2\sum_{i=1}^{N-1} f_i \right)$$

If U_o, U_{N+1} are known → solve problem

(i.e. never wrote PDE on Nodes 0 or N+1)

Note:

- The conservation boundaries are not at 0, N+1
- Conservation is independent of σ_o, σ_{N+1}
- One looses accuracy due to one sided integration near boundaries (i.e. half-cells not evaluated)
- At times one may need the flux at the boundaries

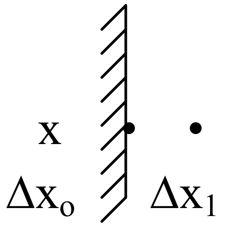
How does one account for the half-cells near the boundary?

Consider type II, III B.C.s
As in PS #2 questions 2 parts c and d.

1.) Write the PDE at boundary. Computational molecule will spill over onto a “shadow” or image mode

2.) Write the BC at boundary. Use this formulation to eliminate shadow node in PDE

3.) Synthesis of PDE + BC give FD equation at the boundary



$$\frac{\partial}{\partial x}\left(K\frac{\partial U}{\partial x}\right) = -\sigma$$

a.) Write PDE at boundary

$$K_{i+\frac{1}{2}}\frac{\left(U_{i+1}-U_{i}\right)}{x_{i+1}-x_{i}}-K_{i-\frac{1}{2}}\frac{\left(U_{i}-U_{i-1}\right)}{x_{i}-x_{i-1}}=-\sigma_{i}\left(x_{i+\frac{1}{2}}-x_{i-\frac{1}{2}}\right)$$

$$\mathrm{K}_{\mathrm{i}+\frac{1}{2}}\left(\mathrm{U}_{\mathrm{i}+1} - \mathrm{U}_{\mathrm{i}}\right) - \mathrm{K}_{\mathrm{i}+\frac{1}{2}}\left(\mathrm{U}_{\mathrm{i}} - \mathrm{U}_{\mathrm{i}-1}\right) = - \sigma_{\mathrm{i}}\left(\frac{\Delta \mathrm{x}_{\mathrm{i}+1} + \Delta \mathrm{x}_{\mathrm{i}}}{2}\right)$$

on Boundary i = 0 ; $\Delta x_o = \Delta x_1$ $K_{\frac{1}{2}} = K_{-\frac{1}{2}}$

$$K_{i+\frac{1}{2}}\frac{\left(U_{1}-2U_{0}+U_{x}\right)}{\Delta x_{0}}=-\sigma_{0}\left(x_{\frac{1}{2}}-x_{-\frac{1}{2}}\right)$$

b.) B.C. $-K\frac{\partial u}{\partial x}=q_{0} \quad \Rightarrow \quad q_{0}=-K_{0}\frac{\left(U_{1}-U_{x}\right)}{2\Delta x_{0}}$

due to symmetry $K_o = K_{1/2}$

∴

$$U_x = U_1 + \frac{2\Delta x_1}{K_{\frac{1}{2}}} q_o$$

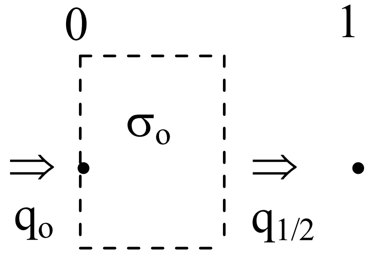
c.)

$$\frac{K_{1/2}\left(\frac{2\Delta x_1}{K_{\frac{1}{2}}} q_o - 2U_o + 2U_1\right)}{\Delta x_1} = - \sigma_o \Delta x_1$$

$$q_o + K_{1/2}\frac{(U_1 - U_o)}{\Delta x_1} = -\frac{\sigma_o \Delta x_1}{2}$$

or $$q_o - q_{\frac{1}{2}} = -\frac{\sigma_o \Delta x_1}{2}$$

This is the missing link in Conservation



A similar conservation statement is obtained at node N+1

$$-q_{N+1} + q_{N+1/2} = -\sigma_{N+1}\frac{\Delta x_{N+1}}{2}$$

Add these 2 B.C. entries into original PDE and get a F.D. conservation statement

$$-q_{N+1} + q_0 = -\sum_{i=0}^{N}\left(\frac{\sigma_i + \sigma_{i+1}}{2}\right)\Delta x_{i+1}$$

If node 0 is a Type I boundary $\Rightarrow$ U_o given

The flux at 0 is determined from the boundary molecule, i.e.

$$q_o - q_{1/2} = - \sigma_o \frac{\Delta x_i}{2}$$

Essentially difference between Δ and δ at boundary

$$q_o = \underbrace{- K_{\frac{1}{2}}\left(\frac{U_1 - U_o}{\Delta x_i}\right)} - \frac{\sigma_o \Delta x_i}{2}$$

$\Uparrow$

this intuitive way; in general use looks like

$O(h)$

makes

This correction term balances the heat/mass

Goes away as $h \to 0$

$q_o \; O(h^2)$

Conservation in 2-D is a direct extension of the 1-D results

$$\underline{\nabla} \cdot K \underline{\nabla} U = - \sigma$$

$$\frac{1}{\Delta x}\left[K_{i+1/2}\left(\frac{U_{i+1} - U_i}{\Delta x_{i+1}}\right) - K_{i-1/2}\left(\frac{U_i - U_{i-1}}{\Delta x_i}\right)\right]_j +$$

$$\frac{1}{\Delta y}\left[K_{j+1/2}\left(\frac{U_{j+1} - U_j}{\Delta y_{j+1}}\right) - \underbrace{K_{j-1/2}\left(\frac{U_j - U_{j-1}}{\Delta y_j}\right)}_{q^y_{j-1/2}}\right]_i = - \sigma_{ij}$$

Multiply by $\Delta x \Delta y$

$$\Delta y\left[- q^{x}_{i+1/2} + q^{x}_{i-1/2}\right] + \Delta x\left[- q^{y}_{j+1/2} + q^{y}_{j-1/2}\right] = - \Delta x \Delta y \sigma_{ij}$$

σ_{ij} is the 2-D average of sources
$K_{j+1/2}$ is the K average in the y direction