Conservation Laws.

Conservation Law + Constitutive Relation $\Rightarrow$ PDE

$$\nabla \cdot q = \sigma \quad q = -K\nabla U \quad \nabla \cdot K\nabla U = -\sigma$$

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

$\sigma =$ Source terms/unit volume/unit time

Input + generation = Output + accumulation

- Output + Input = accumulation - generation

$$\nabla \cdot q = \sigma$$

$U =$ many times acts as the scalar surrogate for $q$

Physical Examples

$q$ Conserved Quantity $u$ $\sigma$

Heat Flux Thermal Energy $T$ Heating rate

$$\nabla \cdot K\nabla T = c\frac{\partial T}{\partial t}$$

Diffusion Molecules of Species $C$ Chem. Rxn Rate

Mass Flux Fluid Mass $P$ -Evap. Rate (Influx)
Stress \hspace{1cm} Momentum \hspace{1cm} \delta \hspace{1cm} Body

\[ F = mA \]
\[ \uparrow \]
\[ \text{displacement} \]
\[ \text{strain} \]

Electostatic Field \hspace{1cm} certain integral \hspace{1cm} \phi \hspace{1cm} Q/\varepsilon_0

Gravity Field \hspace{1cm} properties of force \hspace{1cm} -kM

Note: \( \sigma \) need not be constant

consider the mass diffusion situation with radioactive decay

\[ \sigma = -kc \hspace{1cm} \text{and storage} \]
\[ \sigma = -\frac{\partial C}{\partial t} \]

(Decay or generation)

\[ \nabla \cdot D \nabla C = \frac{\partial C}{\partial t} + kC = -\sigma \]
The conservation law of PDE is a local conservation statement. Globally the conservation law is:
\[ \int (PDE)dv \]

\[ \int \nabla \cdot q dv = \int \sigma dv \]

a.) making use of Divergence Theorem

\[ \int \nabla \cdot (\ )dv \equiv \int (\ ) \cdot \hat{n}ds \]

\[ \int q \cdot \hat{n}ds = \int \sigma dv \]

i.e. the rate escape = sum of sources

b.) using constitutive relation

\[ \int \nabla \cdot (K \nabla U) dv = -\int \sigma dv \]

again using divergence

\[ \int K \nabla U \cdot \hat{n}ds = -\int \sigma dv \]

which is the same as (a) since \[ q = -K \nabla U \]
Numerical Conservation: \[ \int(\ )d\nu \to \sum_i (\ )\Delta v_i \]

\[
\frac{\partial}{\partial x} \left( K \frac{\partial U}{\partial x} \right) = -\sigma \cdot \Delta x_1 \cdot \Delta x_2
\]

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

Where \[ 2h = x_{i+1/2} - x_{i-1/2} \]

\[
K \left( U_{i+1} - U_i \right)_{x_{i+1} - x_i} - K \left( U_i - U_{i-1} \right)_{x_i - x_{i-1}} = -\sigma_i \left( x_{i+1/2} - x_{i-1/2} \right)
\]

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

\[
\begin{array}{c}
\text{\( \Delta x_1 \)}
\end{array}
\begin{array}{c}
\text{\( \Delta x_2 \)}
\end{array}
\]

ME 515 (Sullivan) Numerical Soln of PDEs - Conservation Issues - Lecture 8
\( \sigma_i \) represents all sources in the two half-boxes:

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

This definition of \( \sigma_i \) is especially important when \( \sigma \) is to be represented as a Dirac Delta Function

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

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

\[
q_{1/2} + (-q_{11/2} + q_{11/2}) + (-q_{21/2} + q_{21/2}) \cdots (-q_{(N-1)+1/2} + q_{(N+1)+1/2}) - q_{N+1/2} =
\]

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

Trapezoidal Rule
Trapezoidal Rule - Hornbeck

\[ I = \int_a^b f(x) \, dx \]
let \( \Delta x = \frac{b - a}{N} \)

Approximate area under curve with straight lines

\[ \int_{x_{i-1}}^{x_i} f(x) \, dx \approx \frac{f_{i-1} + f_i}{2} \Delta x \]
\[ \int_{x_i}^{x_{i+1}} f(x) \, dx \approx \frac{f_i + f_{i+1}}{2} \Delta x \]

or

\[ \int_{x_{i-1}}^{x_i} f(x) \, dx \approx \frac{\Delta x}{2} (f_{i-1} + 2f_i + f_{i+1}) \]

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 $U_0$, $U_{N+1}$ 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 $\sigma_o$, $\sigma_{N+1}$
- One loses 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

\[ K \frac{U_{i+1} - U_i}{x_{i+1} - x_i} - K \frac{U_i - U_{i-1}}{x_i - x_{i-1}} = -\sigma_i \left( x_{\frac{i+1}{2}} - x_{\frac{i-1}{2}} \right) \]

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

on Boundary \( i = 0 \); \( \Delta x_0 = \Delta x_1 \) \( K_{\frac{1}{2}} = K_{\frac{1}{2}} \)

\[ K \frac{U_1 - 2U_0 + U_x}{\Delta x_0} = -\sigma_0 \left( \frac{1}{2} x_1 - \frac{1}{2} x_\frac{1}{2} \right) \]

b.) B.C. \(-K \frac{\partial u}{\partial x} = q_0 \quad \Rightarrow \quad q_0 = -K_0 \frac{(U_1 - U_x)}{2\Delta x_0} \)

due to symmetry \( K_0 = K_{1/2} \)

\( \therefore U_x = U_1 + \frac{2\Delta x_1}{K_\frac{1}{2}} q_0 \)

\( K_{1/2} \left( \frac{2\Delta x_1}{K_\frac{1}{2}} q_0 - 2U_0 + 2U_1 \right) \)

\[ \frac{\Delta x_1}{\Delta x_1} = -\sigma_0 \Delta x_1 \]
\[ q_0 + K_{1/2} \frac{(U_1 - U_0)}{\Delta x_1} = - \frac{\sigma_o \Delta x_1}{2} \]

or

\[ q_0 - q_{1/2} = - \frac{\sigma_o \Delta x_1}{2} \]

This is the missing link in Conservation

\[ \begin{array}{ccc}
0 & \sigma_o & 1 \\
\hline 
q_0 & \sigma_o & q_{1/2} \\
\end{array} \]

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 \( \Rightarrow U_0 \) given
The flux at 0 is determined from the boundary molecule, i.e.

$$q_0 - q_{1/2} = -\sigma_0 \frac{\Delta x_i}{2}$$

Essentially difference between $\Delta$ and $\delta$ at boundary

$$q_0 = -K \frac{U_1 - U_0}{\Delta x_i} - \frac{\sigma_0 \Delta x_i}{2}$$

This intuitive way; in general this correction term balances the heat/mass use looks like: Goes away as $h \to 0$

$$O(h)$$ makes $$q_0 \sim O(h^2)$$

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

$$\nabla \cdot KVU = -\sigma$$

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

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

$$q_{j-1/2}^y$$
Multiply by $\Delta x \Delta y$

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

$\sigma_{ij}$ is the 2-D average of sources

$K_{j+1/2}$ is the $K$ average in the $y$ direction