Partial Differential Equation (PDE's)

Real world applications:
1) recovering oil from the ground
2) modeling blood flow in the heart
3) modeling fluid (current) of ions through protein channels

The Continuity Equation

Illustrate in 2D

\[ \text{For flow into (control) point } (i,j): \]

\[ a \tilde{p}_{i,j} = (\frac{\partial x}{\partial x})_{i,j} - (\frac{\partial x}{\partial y})_{i,j} \]

\[ -\tilde{f}_y(i,j) = \tilde{f}_x(i,j) \]

\[ \rho \frac{\partial x}{\partial t} = \frac{\partial (\rho x \tilde{u})}{\partial x} + \frac{\partial (\rho y \tilde{v})}{\partial y} \]

\[ \text{In 3D:} \]

\[ \frac{\partial (\rho x \tilde{u})}{\partial x} + \frac{\partial (\rho y \tilde{v})}{\partial y} + \frac{\partial (\rho z \tilde{w})}{\partial z} \]

Application to Diffusion: Fick's Law:

\[ \tilde{j}(x,t) = -D \nabla \tilde{g}(x,t) \]

† diffusion content
Solving PDE's via finite difference (real-space lattice) methods

Illustrate 1D Diffusion \[ \frac{\partial p(x,t)}{\partial t} = \frac{1}{2} \frac{\partial^2 p(x,t)}{\partial x^2} \]

\[
\frac{j_i}{a} = \frac{1}{a^2} \left( j_{i+\frac{1}{2}} - j_{i-\frac{1}{2}} \right)
\]

Thus, for point \( i \):

\[
\frac{\partial p(x,t)}{\partial x} = \frac{D}{a^2} \left[ p_{i+1} - 2p_i + p_{i-1} \right]
\]
at \( G \)

What about points next to the boundary?

For convenience, consider absorbing \( r_j \) (boundary condition)

\[
\begin{align*}
1 & 2 & 3 & \ldots & N (\text{in}) \\
0 & 0 & 0 & \ldots & 0 (\text{out}) \\
\end{align*}
\]

\[
N_0 \phi_0 = 0 = N_{N1} \phi_1
\]

Thus,

\[
\begin{align*}
\hat{p}_i &= \frac{D}{a^2} \left[ \phi_{i-2} - 2 \phi_i + \phi_{i+2} \right] \\
\phi_i &= \frac{D}{a^2} \left[ -2 \phi_i + \phi_{i-2} + \phi_{i+2} \right]
\end{align*}
\]

Put all this together:

\[
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\vdots \\
\phi_N
\end{pmatrix}
= a^2
\begin{pmatrix}
-2 & 1 & 0 & \cdots & 0 \\
1 & -2 & 0 & \cdots & 0 \\
0 & 1 & -2 & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & -2
\end{pmatrix}
\begin{pmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\vdots \\
\phi_N
\end{pmatrix}
\]

Reduction to ordinary ODE's

Note: special techniques for \( \phi \) solution.

\[
\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial \phi}{\partial t}
\]

Comment on multi-dimensional finite difference. For convenience,

In 2D:

- \( (1,1) \) to \( (1,0) \) extended boundary points. Take the derivative there.
- \( (1,1) \) to \( (1,0) \) exterior boundary points. Considered on internal boundary points or fixed.
- \( (1,1) \) to \( (0,0) \) and for simplicity, \( \phi = 0 \) interior source/sink.

Extended boundary points.
The flux at completely isolated points like 0:

\[
\frac{\partial}{\partial t} \rho_j^{(0)} = \begin{bmatrix} \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \\ \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \end{bmatrix}
\]

For a point on the edge, e.g., 0:

\[
\frac{\partial}{\partial x} \rho_j^{(0)} = \begin{bmatrix} \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \\ \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \end{bmatrix}
\]

For a point in one of the centers, e.g., 0:

\[
\frac{\partial}{\partial x} \rho_j^{(0)} = \begin{bmatrix} \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \\ \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \end{bmatrix}
\]

**Diffusion-Diffusion**: When there is a systematic (external) force \( F(x) \),

there is a drift flux:

\[
\frac{\partial}{\partial x} \rho_j^{(0)} &= \begin{bmatrix} \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \\ \rho_{i+1}^{(0)} - 2\rho_j^{(0)} + \rho_{i-1}^{(0)} \end{bmatrix}
\]

Total flux in \( j \)th:

\[
\frac{\partial}{\partial t} \rho_j^{(0)} + \frac{\partial}{\partial x} \rho_j^{(0)} = -\nabla \cdot \mathbf{F} - \frac{\partial}{\partial j} \rho_j^{(0)} = -D \nabla \nabla \mathbf{F} - \frac{\partial}{\partial j} \rho_j^{(0)}
\]

Then:

\[
\frac{\partial}{\partial x} \rho_j^{(0)} = -\nabla \cdot \mathbf{F} = -\nabla \nabla \mathbf{F} - \frac{\partial}{\partial j} \rho_j^{(0)}
\]

Comment on the discretization procedure when \( F(x) = -\nabla \nabla \mathbf{F} \)

\[
\frac{\partial}{\partial t} \rho_j^{(0)} + \frac{\partial}{\partial x} \rho_j^{(0)} = -D \nabla \nabla \mathbf{F} - \frac{\partial}{\partial j} \rho_j^{(0)}
\]

\[
\rho_j^{(0)} = -\nabla \cdot \mathbf{F} - \frac{\partial}{\partial j} \rho_j^{(0)}
\]

\[
\frac{\partial}{\partial j} \rho_j^{(0)} = -D \nabla \nabla \mathbf{F} - \frac{\partial}{\partial j} \rho_j^{(0)}
\]
Applying the exercise. \( \dot{J}_0 = \text{interesting} \) to the given Eq.

In the special case of steady state: \( \nabla \cdot \mathbf{J} = 0 \). For diffusion: \( \dot{N} = -\nabla \cdot \mathbf{J} \). Example:

1. Only 1D problem: \( J = \frac{\partial N}{\partial x} \). Physically:

\[
J(x) = -\frac{\partial N}{\partial x}.
\]

What is? \( p(x) + 2 \alpha \equiv p(x) \); what is? \( \lim_{x \to -\infty} N = 0 \).

\[
O = \frac{1}{2} \left( \frac{\partial p}{\partial x} + \frac{\partial f}{\partial x} \right) ; \ \text{let} \ \theta = \frac{-\partial f}{\partial x} \text{ constant!}
\]

\[
-\frac{\partial f}{\partial x} = \text{constant!}
\]

\[
f' = -\int_x^\infty \frac{\partial f}{\partial x'} \, dx' + f_x^{\infty}
\]

\[
f_0 = \int_0^\infty \frac{\partial f}{\partial x} \, dx'
\]

Note: In Fig.3, \( \infty \) asymptotic state to \( \mathbf{D} \infty \).

\[
\text{Note:} \quad \frac{\partial f}{\partial x} = \frac{1}{2} (1 - \frac{\partial f}{\partial x})
\]

Finally, geometric for:

\[
j = \frac{\partial f}{\partial x} \frac{\partial f}{\partial x} \, dx
\]

\[
n_0 \frac{\partial f}{\partial x} \, dx = \frac{1}{2} (1 - \frac{\partial f}{\partial x})
\]

Fig.3
In the case of 2, 3,... Dim., use "Relaxation" principle. In 2D, the Diff-Diff Eq:

\[ 0 = \sum_{j=1}^{3} (j^2 + 3j + j^3) \sum_{k=1}^{2} D \Rightarrow \]

\[ 0 = (x_0 - y_0) + \varepsilon (x_0 - y_1) \frac{\phi(x_0)}{\phi(x_1)} + (x_1 - y_0) + \varepsilon (x_1 - y_1) \frac{\phi(x_1)}{\phi(x_0)} \]

\[ + (x_0 - y_3) + \varepsilon (x_0 - y_4) \frac{\phi(x_0)}{\phi(x_4)} + (x_1 - y_3) + \varepsilon (x_1 - y_4) \frac{\phi(x_1)}{\phi(x_4)} \]

\[ 0 = \frac{4}{\varepsilon} \left( \frac{(\phi(x_0)}{\phi(x_1)} - \frac{(\phi(x_1))}{\phi(x_4)} \right) \]

\[ \phi_0 = \frac{1}{2} \sum_{k=1}^{N} \left[ 1 + \varepsilon (\phi(x_k) - \phi(x_{k+1})) \right] \]

\[ = \frac{1}{2} \sum_{k=1}^{N} \left[ 1 + \varepsilon (\phi(x_k) - \phi(x_{k-1})) \right] \]

\[ = \frac{1}{2} \sum_{k=1}^{N} \frac{\phi(x_k)}{\phi(x_{k+1})} \]

\[ \text{Relaxation Method} \]

In practice: \[ \phi_{\text{new}} = (1 - \alpha) \phi_{\text{old}} + \alpha \phi \]

\[ 0 < \alpha < 2 \]

points i up date them one by one.

\[ \text{Find vector on the PDE Relaxation scheme: Poisson Eq.} \]

\[ \nabla^2 \phi = -4 \pi j_0 \]

\[ \phi(x) = \text{dielectric potential} \]

Consider the discretized 2-D version:

\[ \frac{1}{a^2} \left( \nabla^2 + \frac{1}{2} \frac{\phi(x_0) + \phi(x_1)}{\phi(x_0) + \phi(x_1)} \right) = -4 \pi j_0 \]

\[ \left[ \frac{4n^2 \phi}{\phi_0} + \frac{\phi(x_1)}{\phi(x_0)} \right] = \frac{1}{a^2} \]

\[ \text{in a vacuum (using Gaussian/CGS units)} \]
Chapter 16: Solving Differential Equations

Partial differential equations

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