Advance Mathematical Techniques in ChE.

Saathi

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→ Partial Differential eqⁿ
- → Classification
- → Boundary Conditions.
- → Principle of Linear Superposition.

→ Adjoint Operator & Special ODEs.
- → Properties of Adjoint Operator
- → Properties of eigenvalues of eigen functions

→ Solution of linear homogenous PDEs by separation of variables,
- → Cartesian, Cylindrical, Spherical.

→ Solution of non-homogenous PDES by Green's function.

→ Solⁿ of PDEs by similarity solⁿ.

→ Solⁿ of PDEs by Integral methods

PDEs:

1 independent variable → ODE

>1 " " → PDE

Order of PDE → Highest derivative in the eqⁿ.

$$\frac{\partial u}{\partial t} = \underbrace{\frac{\partial^2 u}{\partial x^2}}_{\text{order 2}}$$

$$\frac{\partial u}{\partial t} = u\frac{\partial u}{\partial x} + \frac{\partial^2 u}{\partial y^2} + \underbrace{\frac{\partial^3 u}{\partial z^3}}_{\text{order 3}}$$

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Linear PDE :

$$\frac{\partial u}{\partial t} = u \frac{\partial^2 u}{\partial x^2}$$ → dependent variable × derivative

$$\frac{\partial u}{\partial t} = \underbrace{u \frac{\partial u}{\partial x}}_{\text{order 1} \to \text{N.L.}} + \underbrace{\frac{\partial u}{\partial x} \cdot \frac{\partial u}{\partial y}}_{\text{order 2} \to \text{N.L.}}$$ ⇒ non-linear

$$\left(\frac{\partial u}{\partial t}\right)^2 = \frac{\partial^2 u}{\partial x^2}$$

(order 1)^2 → non-linear; $\frac{\partial^2 u}{\partial x^2}$ → linear

$$\left(\frac{\partial u}{\partial t}\right)^2 = u \frac{\partial^2 u}{\partial x^2}$$

N.L.

{ linear in 1, u, u', u'', ... }

If a term contains product of dependent variable / it's derivative, or a term with power except 1 → non-linear PDE.

Homogenous PDE :

If a term in governing equation does not contain the dependent variable, it's a non-homogenous variable

$$\frac{\partial u}{\partial t} = \left(\frac{\partial^2 u}{\partial x^2}\right)^2$$ → Homo → non-linear

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 2$$ → no Homo, linear.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + 8x^2$$ → no Homo → linear.

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Boundary Conditions:

Governing eq^n: valid at all points inside a closed volume & on the boundary.

Boundary conditions are specific conditions valid only on boundaries.

Types of BCs $\longrightarrow$ Dirichlet BCs.

If value of dependent variable is specified.

ex. u at $x=1, T=t_0$

$\longrightarrow$ Neumann BCs

If value of derivative of dependent variable is specified

ex. at $x=1, \frac{\partial T}{\partial x} = q$

at $r=0, \frac{\partial u}{\partial r} = 0$

$\longrightarrow$ Robin Mixed BC

Dependent variable & it's derivative are connected by an algebraic eq^n

ex. at $x=1, -k\frac{\partial T}{\partial x} = h(T-T_{\infty})$

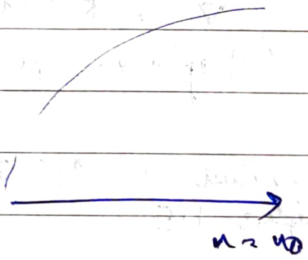
* non-homogenous boundary conditions. whenever the value of dependent variable at boundary condition is not zero.

P.S.: conditions in time aren't boundary conditions, which is why we will split many variable into a time independent & a time dependent part for ex sol^n. (10-08 class)

→ Cauchy's BCs
When more than 1 BCs are specified at the same boundary

At $t = 0$, $T = T_0$,
$-k \frac{\partial T}{\partial x} =$

→ Physical BCs
Comes from the physics of the problem.



At $y = 0$, $u = u_0$
At $\boxed{y = \infty, u = 0}$
Physical BC

Classification of PDEs

(PS independent variables are max 4 - x, y, z, t)

i) Consider 3 independent variables (x_1, x_2, x_3)
* Second order PDE
general form
order 0/1 - ish

$$\sum_{i=1}^{3} \sum_{j=1}^{3} a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} = R\left(x_1, x_2, x_3, \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \frac{\partial u}{\partial x_3}\right)$$

L.H.S: $a_{11} \frac{\partial^2 u}{\partial x_1^2} + a_{12} \frac{\partial^2 u}{\partial x_1 \partial x_2} + a_{13} \frac{\partial^2 u}{\partial x_1 \partial x_3}$
$+ a_{21} \frac{\partial^2 u}{\partial x_2 \partial x_1} + a_{22} \frac{\partial^2 u}{\partial x_2^2} + \cdots$

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$$A = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$ Coefficient → matrix

$|A - \lambda I| = 0$
↓
eigenvalue
↓
The eigenvalues give info abt type of PDE.

- If atleast 1 eigenvalue is zero, parabolic PDE
- If all eigenvalues are of same sign, Elliptic PDE
- If eigenvalues are of diff. sign, Hyperbolic PDE

Eg: $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0$

(represented as $\nabla^2 u = 0$, ∇ is known as Laplacian operator)

$$A = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{vmatrix}$$ → eigenvalues all 1, 1, 1
⇒ elliptic PDE.

Eg: $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}$

{PS: understand that this is still a second order eq^n in u with 3 independent variables.}

$$A = \begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{vmatrix}$$ → $\lambda = 1, 1, 0$
⇒ parabolic PDE

Eg: $\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \iff \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \frac{\partial^2 u}{\partial t^2} = 0$

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$ → $\lambda = 1, 1, -1$
⇒ Hyperbolic PDE.

11) For 2 independent variables

$$A \frac{\partial^2 u}{\partial x^2} + 2B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} = f\left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, u\right)$$

Find $(B^2 - AC)$.

$$\begin{cases} B^2 - AC > 0 \Rightarrow \text{Hyperbola PDE} \\ B^2 - AC = 0 \Rightarrow \text{Parabolic PDE} \\ B^2 - AC < 0 \Rightarrow \text{Elliptic PDE} \end{cases}$$

Operator (on a function)

Operators are usually represented by the symbol 'L'.

eg: $Lf = d/dx(f)$

$$Lf = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2} \quad (\rightarrow \nabla f)\ (\rightarrow \text{3-d Laplacian})$$

If $L(f \pm g) = L(f) \pm L(g)$, it's called a linear operator. For ex, $Lf = \frac{d}{dx}(f)$ is linear.

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \rightarrow \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0 \Rightarrow \left\{ L = \frac{\partial}{\partial t} - \frac{\partial^2}{\partial x^2}; \text{ we write } Lu = 0 \right.$$

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

$$0 = \frac{\partial u}{\partial t} - \nabla^2 u \Rightarrow L = \frac{\partial}{\partial t} - \nabla^2; \ Lu = 0$$

If an operator is linear, we can use principle of Linear Superposition in solution of PDE.

Misfortune Saathi COOKIE

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Linear Superposition → non-homogenous components in a PDE may be separated into 3 diff. PDE's that are linearly superposible

$$\frac{d^2u}{dx^2} = x \quad \text{at} \quad x=0, u=1$$
$$x=1, u=2$$

3 sources of N.H.

$u = u_1 + u_2 + u_3$

$u_1 : \frac{d^2u}{dx^2} = x$	$u_2 : \frac{d^2u_2}{dx^2} = 0$	$u_3 : \frac{d^2u_3}{dx^2} = 0$
at $\left.\begin{matrix}x=0\\x=1\end{matrix}\right\} u_1 = 0$	at $x=0, u_2=1$ $x=1, u_2=0$	at $x=0, u_3=0$ $x=1, u_3=2$

At $x=0$, $u = u_1 + u_2 + u_3 = 1$
$x=1$, $u = u_1 + u_2 + u_3 = 2$

$$u_1 : \frac{du_1}{dx} = \frac{x^2}{2} + C_1$$

$$u_1 = \frac{x^3}{2} + C_1 x + C_2$$

$x=0, x=1 \rightarrow u_1 = 0$
$\Rightarrow C_2 = 0 \; ; \; C_1 = -1/2$

[PS: Sources of NH get split:
$$\frac{d^2u}{dx^2} = x + 0 + 0 .$$
At $x=0$, $u = 0 + 1 + 0$.
At $x=1$, $u = 0 + 0 + 2$]

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$u_2 : u_2 = c_1 x + c_2$; $(0,1)$; $(1,0)$

$c_2 =$

$c_2 = 1$; $c_1 = -1$

$u_2 = -x + 1$

$u_3 : u_3 = c_1 x + c_2$; $(0,0)$; $(1,2)$.

$u_3 = 2x$

$$u = \left(\frac{x^2}{2} - \frac{x}{2}\right) + (-x+1) + (2x)$$

$$= \frac{x^2}{2} + \frac{x}{2} + 1$$

Parabolic PDE

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

At $t = 0$, $u = u_0$ →
At $x = 0$, $u = 0$
At $x = 1$, $u = 1$ →

2 sources of non-homogenity

$\therefore u = u_1 + u_2$

u_1 :	$\frac{\partial u_1}{\partial t} = \frac{\partial^2 u_1}{\partial x^2}$	$t = 0$, $u_1 = u_0$ (doesn't matter) $x = 0, x = 1$, $u_1 = 0$	well-posed
u_2 :	$\frac{\partial u_2}{\partial t} = \frac{\partial^2 u_2}{\partial x^2}$	$t = 0$, $u_2 = 0$ $x = 0$, $u_2 = 0$ $x = 1$, $u_2 = 1$	ill-posed problem

well-posed is for boundary conditions.
Time → ∞

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If IC's are 0, BC's are 0, it's a 'well behaved' problem & can be solved directly

In previous example, u_1 is well-posed;
u_2 is ill-posed.

Ill-posed problems need to be split into 2 subproblems → Time dependent → transient part
Time independent → steady state part

u_2 : $\frac{\partial u_2}{\partial t} = \frac{\partial^2 u_2}{\partial x^2}$

At $t=0$, $u_2 = 0$
At $x=0$, $u_2 = 0$
$x=1$, $u_2 = 1$

$u_2(x,t) = u_2^s(x) + u_2^t(x,t)$

$\frac{\partial}{\partial t}(u_2^s + u_2^t) = \frac{\partial^2}{\partial x^2}(u_2^s + u_2^t)$

$\Rightarrow \frac{\partial u_2^t}{\partial t} = \frac{d^2 u_2^s}{dx^2} + \frac{\partial^2 u_2^t}{\partial x^2}$

$u_2 = u_2^s + u_2^t$

$\frac{d^2 u_2^s}{dx^2} = 0$ $\qquad$ $\frac{\partial u_2^t}{\partial t} = \frac{\partial^2 u_2^t}{\partial x^2}$

At $x=0$, $u_2^s = 0$ $\qquad$ At $x=0$, $u_2^t = 0$
At $x=1$, $u_2^s = 1$ $\qquad$ At $x=1$, $u_2^t = 0$

At $t=0$, $u_2^t = -u_2^s(x)$

Can't be assigned a value as this is a steady-state thingy.

} As independent of t / steady-state

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(★) We technically have three BCs:

At $x=0$, $u_2^t + u_2^s = 0$

At $x=1$, $u_2^t + u_2^s = 1$

These can be split in *ANY* way & give the same solⁿ nonetheless.

At $x=0$, $u_2^t = -8$; $u_2^s = 8$ ✓

At $x=1$, $u_2^t = -69$; $u_2^s = 70$

At $x=0$, $u_2^t = 0$; $u_2^s = 0$ ✓

At $x=1$, $u_2^t = 1$; $u_2^s = 0$

We are choosing the value of $u_2^t = 0$ at $x=0$ & $x=1$, so it becomes a well-posed problem.

Abt the cannot assign: At $x=0$, $u_2^s(x)$ *HAS* to have some fixed value. Hence, it just may be assigned some value.

Linear Superposition

$\therefore$ $u_2^t(0,t)$ will just take the value of $0 - u_2^s(0)$ at $x=0$, $\forall t$.

Consider another example:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$

At $t=0$, $u = \underline{u_{01}}$ $\longrightarrow$ 3 sources of N.H.

At $x=0$, $\frac{\partial u}{\partial x} + \alpha u = \underline{\underline{u_{02}}}$ $\longrightarrow$

At $x=1$, $\frac{\partial u}{\partial x} = \underline{u_{03}}$ $\longrightarrow$ [P.S. not αu]

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$u_1 \Rightarrow \frac{\partial u_1}{\partial t} = \frac{\partial^2 u_1}{\partial x^2}$

At $t=0$, $u_1 = u_{01}$

At $x=0$, $\frac{\partial u_1}{\partial x} + \alpha u_1 = 0$

At $x=1$, $\frac{\partial u_1}{\partial x} = 0$

Well-posed problem

$u_2 \Rightarrow \frac{\partial u_2}{\partial t} = \frac{\partial^2 u_2}{\partial x^2}$

At $t=0$, $u_2 = 0$

At $x=0$, $\frac{\partial u_2}{\partial x} + \alpha u_2 = u_{02}$

At $x=1$, $\frac{\partial u_2}{\partial x} = 0$

Ill-posed

$\downarrow$

$u_2 = u_2^s(x) + u_2^t(x,t)$

$u_3 \Rightarrow \frac{\partial u_3}{\partial t} = \frac{\partial^2 u_3}{\partial x^2}$

At $t=0$, $u_3 = 0$

At $x=0$, $\frac{\partial u_3}{\partial x} + \alpha u_3 = 0$

At $x=1$, $\frac{\partial u_3}{\partial x} = u_{03}$

Ill-posed

$u_3 = u_3^s(x) + u_3^t(x,t)$

$u_2 s : \frac{\partial u_2^t(x,t)}{\partial t} = \frac{d^2 u_2^s}{dx^2} + \frac{\partial^2 u_2^t(x,t)}{\partial x^2}$

$\therefore$ Governing eq^n

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$u_2 s$: $\frac{d^2 u_2^s}{dx^2} = 0$

At $x=0$, $\frac{d u_2^s}{dx} + \alpha u_2^s = u_{02}$

At $x=1$, $\frac{d u_2^s}{dx} = 0$

$u_2 t$: $\frac{\partial u_2 t}{\partial t} = \frac{\partial^2 u_2^t}{\partial x^2}$

At $x=0$, $\frac{\partial u_2^t}{\partial x} + \alpha u_2^t = 0$

At $x=1$, $\frac{\partial u_2^t}{\partial x} = 0$

$\boxed{\text{At } t=0,\ u_2^t = -u_2^s(x)}$ *

(Associating non-homogenity with steady state / time independent part to get well-posed problem again.)

(While this does hold for both, it's use as a BC is in 2nd; transient part of eqn)

11-08 Consider an ODE of the form

$\frac{d^2 y}{dx^2} + \lambda y = 0$, where λ is scalar.

$\Rightarrow$ $\boxed{Ly = -\lambda y}$, where L is d^2/dx^2

This may be thought of as analogous to

$\boxed{AX = \lambda X}$, a standard eigenvalue problem.

square matrix — vector — eigenvalue

Any eqn $Ly = \lambda y$ with homogenous boundary conditions is a standard eigenvalue problem.

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In solving, we consider 3 cases!

$\lambda = 0 \rightarrow$ trivial solⁿ $(y=0)$ | $\lambda < 0 \rightarrow \lambda = -\alpha^2$ | $\lambda > 0 \rightarrow \lambda = \alpha^2$

Consider again: (1) $\frac{d^2y}{dx^2} + \lambda y = 0$; at $x=0, y=0$; $x=1, y=0$

$\lambda = -\alpha^2 \rightarrow \frac{d^2y}{dx^2} = \alpha^2 y \rightarrow y = c_1 e^{\alpha x} + c_2 e^{-\alpha x}$

Using B.C., $y=0$:(

$\lambda = \alpha^2 \rightarrow \frac{d^2y}{dx^2} + \alpha^2 y = 0 \rightarrow y = c_1 \sin(\alpha x) + c_2 \cos(\alpha x)$

$x=0, y=0 \rightarrow c_2 = 0$

$x=1, y=0 \rightarrow c_1 \sin\alpha = 0$

Again, $c_1 = 0$ gives trivial solⁿ $\Rightarrow \sin\alpha = 0$

$\alpha_n = n\pi, n \in I$

$y = c\sin(n\pi x)$

(2) $\frac{d^2y}{dx^2} + \lambda y = 0$, subject to: $x=0, dy/dx = 0$; $x=1, y=0$

$\lambda = 0 \rightarrow y = c_1 x + c_2 \quad dy/dx = c_1 \rightarrow$ trivial :(

$\lambda = -\alpha^2 \rightarrow y = c_1 e^{\alpha x} + c_2 e^{-\alpha x} \rightarrow c_2 = -c_1$

$dy/dx = \alpha(c_1 e^{\alpha x} - c_2 e^{-\alpha x}) \rightarrow \alpha(c_1 e^{\alpha} - c_2 e^{-\alpha}) = 0$

$\Rightarrow \underbrace{\alpha c_1}_{>0} \underbrace{(e^{\alpha} + e^{-\alpha})}_{>0} = 0 \rightarrow c_1 = 0$ (trivial)

$\lambda = \alpha^2 \rightarrow y = c_1\sin(\alpha x) + c_2\cos(\alpha x) \rightarrow c_2\cos\alpha = 0$

$dy/dx = \alpha[c_1\cos(\alpha x) - c_2\sin(\alpha x)] \rightarrow c_1 = 0$

$c_2 \neq 0 \rightarrow \alpha = (2n-1)\pi/2$

$y = c\cos\left(\frac{(2n-1)\pi}{2} x\right)$

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(8) $\frac{d^2y}{dx^2} + \lambda y = 0$, subject to: $x=0,\ y=0$
$x=1,\ dy/dx = -\beta y$

$\lambda = 0 \rightarrow y = c_1 x + c_2 \rightarrow c_2 = 0;\ c_1 = 0 \rightarrow$ trivial.

$\lambda = -\alpha^2 \rightarrow y = c_1 e^{\alpha x} + c_2 e^{-\alpha x} \longrightarrow c_2 = -c_1$

$dy/dx = \alpha(c_1 e^{\alpha x} - c_2 e^{-\alpha x})$

$= -\beta c_1 e^{\alpha x} - \beta c_2 e^{-\alpha x}$ at $x=1$

$\Rightarrow [(\alpha+\beta) e^{\alpha} + (\alpha-\beta) e^{-\alpha}] c_1 = 0$

If $c_1 \neq 0 \rightarrow e^{2\alpha} = \frac{\beta - \alpha}{\beta + \alpha}$

At $\alpha = 0,\ 1 = 1$

$\alpha > 0 \rightarrow >1 = <1$ ✗

$\alpha < 0 \rightarrow <1 = >1$ ✗

$\therefore c_1 = 0 \rightarrow$ trivial.

$\lambda = \alpha^2 \rightarrow y = c_1 \sin(\alpha x) + c_2 \cos(\alpha x) \rightarrow c_2 = 0$

$\frac{dy}{dx} = \alpha c_1 \cos(\alpha x) = -\beta c_1 \sin(\alpha x)$ at $x = 1$

$\Rightarrow c_1(\alpha \cos\alpha + \beta \sin\alpha) = 0$

$\Rightarrow \alpha + \beta \tan\alpha = 0$

$\Rightarrow \frac{\alpha}{\tan\alpha} = -\beta$

↳ transcendental eqn. solvable w/ Newton Raphson

Boundary Condition	Evalue	Efn
Dirchlet	$n\pi$	$\sin(n\pi x)$
Neuman + Dirchlet	$(2n-1)\pi/2$	$\cos\left((2n-1)\frac{\pi}{2} x\right)$
Dirchlet + Robin	$\alpha_n + \beta \tan\alpha_n = 0$	$\sin(\alpha_n x)$

Transformation of co-ordinates, e.g., $x' = 1 - x$ can be used to convert seemingly tough problem into a standard eigenvalue problem like above 3 forms.