Partial Differential Equations - PDEs

Three main types of PDEs in physics

1) Elliptic - static problems (∇^2, no time)

e.g. Poisson eq^n $\nabla^2 \phi = -\rho/\epsilon_0$

Laplace eq^n $\nabla^2 \phi = 0$

- generally, boundary conditions given around a closed boundary

2) Parabolic (∇^2 and $\partial/\partial t$)

e.g. Diffusion eq^n $\frac{\partial n(\vec{r},t)}{\partial t} - \nabla \cdot (D(\vec{r}) \nabla n(\vec{r},t)) = S(\vec{r},t)$

$n(\vec{r},t)$ - concentration

$D(\vec{r})$ - diffusion coefficient

$S(\vec{r},t)$ - source of matter

if $D = \text{const}$ and $S = 0$ get $\frac{\partial n}{\partial t} = D \nabla^2 n$

3) Hyperbolic - propagation (∇^2 and $\partial^2/\partial t^2$, but not always)

e.g. wave eq^n $\frac{1}{c^2}\frac{\partial^2 u(\vec{r},t)}{\partial t^2} - \nabla^2 u(\vec{r},t) = R(\vec{r},t)$

$\vec{u}$ is a displacement of some sort

R is a source term

Note: Schrödinger's eq^n $\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi(\vec{r},t) = -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi(\vec{r},t)$

can be viewed as a diffusion eq^n with imaginary time.

For a general form

$$a\frac{\partial^2 V}{\partial x^2} + b\frac{\partial^2 V}{\partial x \partial y} + c\frac{\partial^2 V}{\partial y^2} + d\frac{\partial V}{\partial x} + e\frac{\partial V}{\partial y} + fV + g = 0$$

$b^2 < 4ac$ Elliptic (Poisson $b = d = e = f = 0$)

$b^2 = 4ac$ Parabolic (Diff $b = c = d = f = g = 0$)

$b^2 > 4ac$ Hyperbolic (Wave $a = -1$, $b = d = e = f = 0$) $[x \leftrightarrow t]$

These are examples of linear eq$^{\underline{n}}$s – linear in dependent variable (ϕ, n, u, ψ)

Another important eq$^{\underline{n}}$ is the Navier-Stokes eq$^{\underline{n}}$
$\vec{F}=m\vec{a}$ applied to a small volume of fluid

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v}\cdot\nabla)\vec{v} + \frac{1}{\rho}\nabla P - \frac{\eta}{\rho}\nabla^2 v = 0$$

(for incompressible fluid)

$\vec{v}$ – flow velocity $\qquad \eta$ – viscosity
ρ – density $\qquad P$ – pressure

– the (diffusive) term $\frac{\eta}{\rho}\nabla^2 v$ gives a parabolic character.
If this term is negligible, the eq$^{\underline{n}}$ is more hyperbolic.

Also important in fluids is the continuity

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\rho\,\vec{v} = 0$$

The different types of PDEs have different numerical approaches.

We will consider the different approaches in the next lectures.

Do you need a numerical solver?

Separation of Variables

Simplifying PDE analytically can make applying numerical algorithms easier.

E.g. 1-D Wave eq$^{\underline{n}}$ $\quad \dfrac{\partial^2 u}{\partial t^2} - c^2 \dfrac{\partial^2 u}{\partial x^2} = 0$

string with ends fixed at $x = 0$ and $x = L$

c - wave speed $\sqrt{\dfrac{T}{\rho}}$, T - tension, $\rho = \dfrac{M}{L}$

B.C.'s $\quad u(x=0, t) = 0 = u(x=L, t)$

assume $u(x,t) = y(x) f(t)$ - doesn't always work

plug into PDE ...

$\rightarrow y(x) = A \sin(kx) + B\cos(kx)$ $\quad$ B.C. $\rightarrow B = 0$,

$k = k_n = \frac{n\pi}{L}$, $n = 1, 2, \ldots$

$f(t) = C \sin(\omega_n t) + D\cos(\omega_n t)$ $\quad \omega_n^2 = c^2 k_n^2$

...

$$u(x,t) = \sum_{n=1}^{\infty} \left(a_n \sin(\omega_n t) + b_n \cos(\omega_n t) \right) \sin(k_n x)$$

$$a_n = \frac{2}{\omega_n L} \int_0^L v_0(x) \sin(k_n x)\, dx$$

$$b_n = \frac{2}{L} \int_0^L u_0(x) \sin(k_n x)\, dx$$

$u_0(x)$ initial displacement, $v_0(x)$ initial velocity

Problem of solving PDE reduces to evaluating definite integrals numerically, unless $u_0(x)$ and $v_0(x)$ are simple.

Otherwise, if eq$^{\underline{n}}$ not separable, must discretize PDE.

Example: Time-Dependent Schrödinger Equation

$$H\psi(\vec{r},t) = i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t)$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)\right)\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

- for simplicity, set $m = 1/2$, $\hbar = 1$

1-D

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{\partial^2}{\partial x^2}\psi(x,t) + V(x)\psi(x)$$

- parabolic eq$^{\underline{n}}$ - ψ complex - $|\psi|^2$ probability density that particle is at x

B.C. $\psi \to 0$ at $x = \pm\infty$

normalization $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$

In discretized system: $\psi(x,t) \to \vec{\psi}^{\,n}$ or ψ_j^n

n - time index

j - spatial index

- magnitude of $\vec{\psi}$ is fixed

$\therefore$ want an algorithm equivalent to $\vec{\psi}^{\,n+1} = P\vec{\psi}^{\,n}$

where P is unitary

$P^\dagger = P^{-1}$

$$\vec{\psi} = \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_N) \end{pmatrix}$$

$$H = -\partial^2/\partial x^2 + V(x)$$

Formal sol$^{\underline{n}}$ to $i\frac{\partial}{\partial t}\psi = H\psi$ is $\psi(x,t) = \psi(x,0)\,e^{-iHt}$

For $t \to \Delta t$, approximate $e^{-iH\Delta t} \doteq 1 - iH\Delta t$

So might use $\psi_j^{n+1} = (1 - iH\Delta t)\,\psi_j^n$

but $1 - iH\Delta t$ is not unitary, so probability won't be conserved.

Instead, use Cayley's form for finite difference expression

$$e^{-iH\Delta t} \simeq \frac{1 - \frac{1}{2} i H \Delta t}{1 + \frac{1}{2} i H \Delta t}$$ (2^{nd} order accurate)

which is unitary

Aside

$P = e^{-iH\Delta t}$, $P^{+} = e^{iH^{+}\Delta t} = e^{iH\Delta t}$ H Hermitian $H = H^{+}$

$P P^{+} = 1$

$$\tilde{P}\tilde{P}^{+} = \frac{1 - \frac{1}{2} i H \Delta t}{1 + \frac{1}{2} i H \Delta t} \cdot \frac{1 + \frac{1}{2} i H \Delta t}{1 - \frac{1}{2} i H \Delta t} = 1$$

so we get $\psi_j^{n+1} = \dfrac{1 - \frac{1}{2} i H \Delta t}{1 + \frac{1}{2} i H \Delta t} \psi_j$

or $\left(1 + \frac{1}{2} i H \Delta t\right) \psi_j^{n+1} = \left(1 - \frac{1}{2} i H \Delta t\right) \psi_j = b$

↑ complex tridiagonal matrix because of $\dfrac{\partial^2}{\partial x^2}$

$$H\psi_j^{n+1} = -\frac{\left(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}\right)}{\Delta x^2} + V_j \psi_j^{n+1}$$

$$\left(1 + \tfrac{1}{2} H i \Delta t\right)\psi_j^{n+1} = \frac{-i\Delta t}{2\Delta x^2}\left(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j-1}^{n+1}\right) + \frac{i\Delta t}{2} V_j \psi_j^{n+1} + \psi_j^{n+1}$$

$$= \frac{-i\Delta t}{2\Delta x^2}\psi_{j+1}^{n+1} + \left(\frac{i\Delta t}{\Delta x^2} + \frac{i\Delta t}{2} V_j + 1\right)\psi_j^{n+1} - \frac{i\Delta t}{2\Delta x^2}\psi_{j-1}^{n+1}$$

$$= \frac{i\Delta t}{2\Delta x^2}\left[-\psi_{j+1}^{n+1} + \left(2 + \Delta x^2 V_j - \frac{i2\Delta x^2}{\Delta t}\right)\psi_j^{n+1} - \psi_{j-1}^{n+1}\right]$$

Similarly $(1 - \tfrac{1}{2} H i \Delta t)\psi_j^n$

$$= \frac{-i\Delta t}{2\Delta x^2}\left[-\psi_{j+1}^n + \left(2 + \Delta x^2 V_j + i\,2\frac{\Delta x^2}{\Delta t}\right)\psi_j^n - \psi_{j-1}^n \right]$$

call

$$T = \begin{pmatrix} \left(2 + V_1\Delta x^2 - i\,2\frac{\Delta x^2}{\Delta t}\right) & -1 & 0 & 0 & \cdots \\ -1 & \left(2 + V_2\Delta x^2 - i\,2\frac{\Delta x^2}{\Delta t}\right) & -1 & 0 & \cdots \\ 0 & -1 & (\ldots V_3 \ldots) & -1 & \cdots \\ 0 & 0 & -1 & \ddots & \\ & \vdots & & & \end{pmatrix}$$

$$T^* = \begin{pmatrix} \left(2 + V_1\Delta x^2 + i\,2\frac{\Delta x^2}{\Delta t}\right) & -1 & 0 & \cdots \\ -1 & \left(2 + V_2\Delta x^2 + i\,2\frac{\Delta x^2}{\Delta t}\right) & -1 & 0 & \cdots \\ 0 & -1 & (\ldots V_3 \ldots) & -1 & \cdots \\ 0 & 0 & -1 & & \\ & \vdots & & \ddots & \end{pmatrix}$$

get $$T\vec{\psi}^{n+1} = -T^*\vec{\psi}^n$$

$$\vec{b} = -T^*\psi^n$$

$$T\vec{\psi}^{n+1} = \vec{b}$$

solve for unknown wave fn at next time step or $\quad T \vec{\psi}^{\,n+1} = \vec{b}$

solve for unknown wave function at next time step

$\vec{b} = -T^{*} \vec{\psi}^{\,n}$

$$\vec{\psi} = \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_J) \end{pmatrix}$$

Boundary conditions imply $\psi_0 = 0 = \psi_{J+1}$