Computational Physics
(Introduction to) Solving Partial Differential Equations

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Slides available from https://bb.imperial.ac.uk/

Goals

The point of this lecture is to teach you to

- Classify PDEs as elliptic, parabolic or hyperbolic
- Identify them as initial value or boundary-value type problems
- Identify and implement a few common boundary conditions
- Solve some elliptic boundary-value problems with finite difference methods
- Solve some initial value problems with with finite difference methods

Outline

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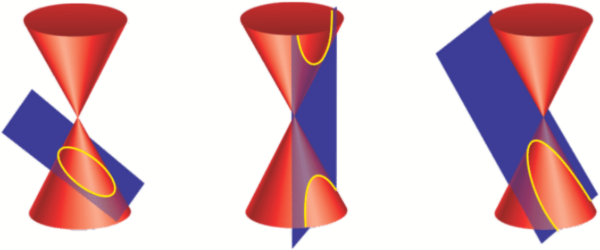
Typical PDEs in physics

Most interesting PDEs in physics are 2nd order linear PDEs:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + f\left(u, x, y, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = G(x, y) \quad (1)$$

We can classify according to A,B,C in analogy with conics:

$$Q \equiv B^2 - 4AC \quad (2)$$



$Q < 0$: Elliptic $Q > 0$: Hyperbolic. $Q = 0$: Parabolic,

Examples

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

$$Q \equiv B^2 - 4AC$$

Poisson Equation (Elliptic):

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x, y) \tag{3}$$

If $\rho(x, y) = 0$ then it's the **Laplace Equation.**
$A = 1$, $B = 0$, $C = 1$ hence $Q = -4 < 0$.

Examples

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

$$Q \equiv B^2 - 4AC$$

Diffusion Equation (Parabolic):

B goes with $\partial^2 u/\partial t \partial x$
C goes with $\partial^2 u/\partial t^2$.

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right) \tag{4}$$

Here, $A = D$, $B = C = 0$ hence $Q = 0$.

Examples

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

$$Q \equiv B^2 - 4AC$$

Wave Equation (Hyperbolic):

B goes with $\partial^2 u / \partial t \partial x$
C goes with $\partial^2 u / \partial t^2$.

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \tag{5}$$

$A = v^2$, $B = 0$, $C = -1$ hence $Q = 4v^2 > 0$.

Do we really care about this conics stuff?

Not so much. What practically matters is whether it's more like an initial value problem (hyperbolic and parabolic PDEs) or a boundary value problem (elliptic PDEs).

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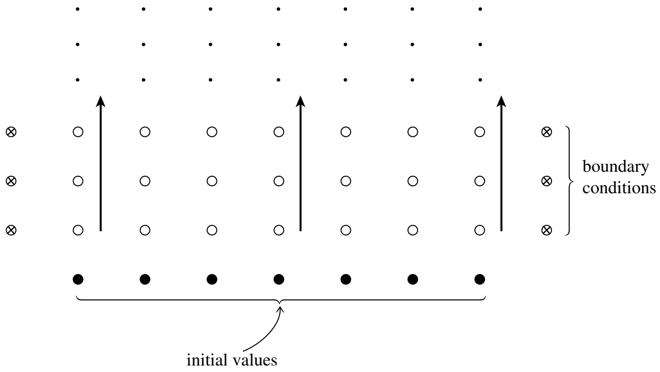

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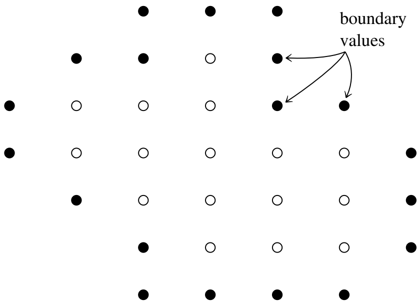


Types of boundary conditions

u defined on boundaries	: Dirichlet
$\vec{\nabla} u$ defined on boundaries	: Neumann
both u and $\vec{\nabla} u$ defined on boundaries	: Cauchy
u or $\vec{\nabla} u$ applied on different parts of a boundary	: mixed

$u(x_r) = u(x_l + L) = u(x_l)$	: periodic (e.g. in x)
$u(-x) = u(x)$	: reflective (e.g. about $x_l = 0$).

Outline

Dirichlet boundary conditions

Poisson Equation:

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x, y) \tag{6}$$

We need to use a finite difference rule over a grid in x and y:

$$\begin{array}{ccccc}
C_{0,4} & C_{1,4} & C_{2,4} & C_{3,4} & C_{4,4} \\
* & * & * & * & * \\
C_{0,3} & u_{1,3} & u_{2,3} & u_{3,3} & C_{4,3} \\
* & \circ & \circ & \circ & * \\
C_{0,2} & u_{1,2} & u_{2,2} & u_{3,2} & C_{4,2} \\
* & \circ & \circ & \circ & * \\
C_{0,1} & u_{1,1} & u_{2,1} & u_{3,1} & C_{4,1} \\
* & \circ & \circ & \circ & * \\
C_{0,0} & C_{1,0} & C_{2,0} & C_{3,0} & C_{4,0} \\
* & * & * & * & *
\end{array} \tag{7}$$

where $u_{i,j} \equiv u(x_i, y_j)$, and the BCs are $u_{0,0} = C_{0,0}$, $u_{0,1} = C_{0,1}$, etc.

Dirichlet boundary conditions

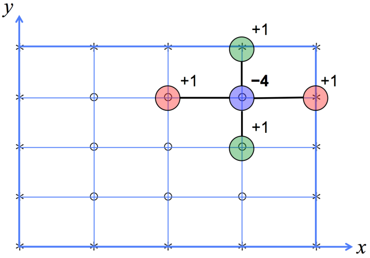
We need a finite difference rule for the second derivatives:

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} \qquad \left\{\mathcal{O}(h^2)\right\}, \tag{8}$$

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{i,j} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{h^2} \qquad \left\{\mathcal{O}(h^2)\right\}, \tag{9}$$

This gives us a finite difference approximation to the Laplacian:

$$\nabla^2 u_{i,j} = \frac{u_{i-1,j} + u_{i,j-1} + u_{i+1,j} + u_{i,j+1} - 4u_{i,j}}{h^2} \qquad \left\{\mathcal{O}(h^2)\right\}. \tag{10}$$



Dirichlet boundary conditions

We can them build a matrix equation $\mathbf{A} \cdot \vec{u} \ = \ \vec{b}$ with all the unknown values of $\vec{u}$ as the solution vector, and the BCs in $\vec{b}$:

$$\left(\begin{array}{ccc|ccc|ccc} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ \hline 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ \hline 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{array}\right) \left(\begin{array}{c} u_{1,1} \\ u_{1,2} \\ u_{1,3} \\ \hline u_{2,1} \\ u_{2,2} \\ u_{2,3} \\ \hline u_{3,1} \\ u_{3,2} \\ u_{3,3} \end{array}\right) = - \left(\begin{array}{c} C_{0,1} + C_{1,0} \\ C_{0,2} \\ C_{0,3} + C_{1,4} \\ \hline C_{2,0} \\ 0 \\ C_{2,4} \\ \hline C_{3,0} + C_{4,1} \\ C_{4,2} \\ C_{4,3} + C_{3,4} \end{array}\right)$$

"All" that remains to do is then solve the matrix equation for $\vec{u}$.

Neumann boundary conditions

What if we have derivatives at the boundaries ($C'_{i,j}$) instead of values ($C_{i,j}$)?

$$
\begin{array}{ccccc}
 & u'_{1,4} = Q_{1,4} & u'_{2,4} = Q_{2,4} & u'_{3,4} = Q_{3,4} & \\
 & * & * & * & \\
C_{0,3} & u_{1,3} & u_{2,3} & u_{3,3} & C_{4,3} \\
* & \circ & \circ & \circ & * \\
C_{0,2} & u_{1,2} & u_{2,2} & u_{3,2} & C_{4,2} \\
* & \circ & \circ & \circ & * \\
C_{0,1} & u_{1,1} & u_{2,1} & u_{3,1} & C_{4,1} \\
* & \circ & \circ & \circ & * \\
 & u'_{1,0} = Q_{1,0} & u'_{2,0} = Q_{2,0} & u'_{3,0} = Q_{3,0} & \\
 & * & * & * &
\end{array}
, \qquad (11)
$$

(This is what you have in Project 4, for example.)

Neumann boundary conditions

We need to introduce some extra fictitious points at the derivative boundaries:

$$
\begin{array}{ccccc}
 & u_{1,5} & u_{2,5} & u_{3,5} & \\
 & * & * & * & \\
C_{0,4} & u_{1,4} & u_{2,4} & u_{3,4} & C_{4,4} \\
* & \circ & \circ & \circ & * \\
C_{0,3} & u_{1,3} & u_{2,3} & u_{3,3} & C_{4,3} \\
* & \circ & \circ & \circ & * \\
C_{0,2} & u_{1,2} & u_{2,2} & u_{3,2} & C_{4,2} \\
* & \circ & \circ & \circ & * \\
C_{0,1} & u_{1,1} & u_{2,1} & u_{3,1} & C_{4,1} \\
* & \circ & \circ & \circ & * \\
C_{0,0} & u_{1,0} & u_{2,0} & u_{3,0} & C_{4,0} \\
* & \circ & \circ & \circ & * \\
 & u_{1,-1} & u_{2,-1} & u_{3,-1} & \\
 & * & * & * &
\end{array}
\tag{12}
$$

We set the 'new' boundary conditions as Dirichlet beyond the fictitious points:

$$
\left.\frac{\partial u}{\partial y}\right|_{i,0} = \frac{u_{i,1} - u_{i,-1}}{2h} = Q_{i,0} \qquad \text{giving} \qquad u_{i,-1} = u_{i,1} - 2h\,Q_{i,0} \tag{13}
$$

(at $y = 0$, for example) and solve for the fictitious points along with the rest.

Neumann boundary conditions

We need to introduce some extra fictitious points at the derivative boundaries:

$$\begin{array}{ccccc}
 & u_{1,5} & u_{2,5} & u_{3,5} & \\
 & * & * & * & \\
C_{0,4} & u_{1,4} & u_{2,4} & u_{3,4} & C_{4,4} \\
* & \circ & \circ & \circ & * \\
C_{0,3} & u_{1,3} & u_{2,3} & u_{3,3} & C_{4,3} \\
* & \circ & \circ & \circ & * \\
C_{0,2} & u_{1,2} & u_{2,2} & u_{3,2} & C_{4,2} \\
* & \circ & \circ & \circ & * \\
C_{0,1} & u_{1,1} & u_{2,1} & u_{3,1} & C_{4,1} \\
* & \circ & \circ & \circ & * \\
C_{0,0} & u_{1,0} & u_{2,0} & u_{3,0} & C_{4,0} \\
* & \circ & \circ & \circ & * \\
 & u_{1,-1} & u_{2,-1} & u_{3,-1} & \\
 & * & * & * &
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We set the 'new' boundary conditions as Dirichlet beyond the fictitious points:

$$\left.\frac{\partial u}{\partial y}\right|_{i,0} = \frac{u_{i,1} - u_{i,-1}}{2h} = Q_{i,0} \qquad \text{giving} \qquad u_{i,-1} = u_{i,1} - 2h\,Q_{i,0} \tag{13}$$

But now $\mathbf{A}$ in $\mathbf{A} \cdot \vec{u} = \vec{b}$ is an $[n_x \times (n_y + 2)]^2$ matrix instead of $[n_x n_y]^2$

Outline

Wave equation

Wave Equation:

$$\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2} \tag{14}$$

Can try to solve it directly by using second order finite difference approximations in both the space and time derivatives.
$\rightarrow$ end up with a multi-point method.

This is fine, but we can do better by using a bit of insight: the Wave Eqn splits into two uncoupled 1st order "advection" PDEs:

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} = 0 \qquad , \qquad \frac{\partial g}{\partial t} - v \frac{\partial g}{\partial x} = 0, \tag{15}$$

They have solutions $f(x,t) = F(x - vt)$ and $g(x,t) = G(x + vt)$, such that

$$u(x,t) = F(x - vt) + G(x + vt) \tag{16}$$

So actually we only need to solve one of the 1st order PDEs in (15).

Upwind method

We take a finite difference approximation to $\partial u/\partial x$ in the *direction from which information propagates*. For $v_x > 0$, choose backwards difference scheme:

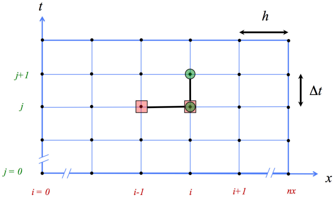
$$\left.\frac{\partial u}{\partial x}\right|_i^j = \frac{u_i^j - u_{i-1}^j}{h} \qquad \{\, \mathcal{O}(h) \,\} \tag{17}$$

For t we choose the forward difference scheme:

$$\left.\frac{\partial u}{\partial t}\right|_i^j = \frac{u_i^{j+1} - u_i^j}{\Delta t} \qquad \{\, \mathcal{O}(\Delta t) \,\} \tag{18}$$

The resulting FD scheme (for $v_x > 0$) is

$$u_i^{j+1} = u_i^j - |v_x| \Delta t/h \left(u_i^j - u_{i-1}^j \right) \tag{19}$$



Upwind method

The "advection number"

$$a = \frac{|v_x|\Delta t}{h} \tag{20}$$

determines stability.

$a > 1 \implies$ instability
$a < 1 \implies$ stability, but smaller a introduces more *numerical diffusion*.

Let's look at an example...

Housekeeping

- This is my last lecture
- Upcoming:
  - Tues Nov 27: Anders Kvellestad (LHC Monte Carlo simulations)
  - Tues Dec 4: Eliel Camargo-Molina (advanced methods for high energy theory)
  - Tues Dec 11: Revision Lecture (Yoshi)