Computational Physics

Partial Differential Equations

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Spring 2014

Introduction

- A differential equation involving more than one independent variable is called a partial differential equation (PDE)
- Many problems in applied science, physics and engineering are modeled mathematically with PDE.
- We will mostly focus on finite-difference methods to solve numerically PDEs.
- PDEs are classified as one of three types, with terminology borrowed from the conic sections on the basis of their characteristics, or curves of information propagation.
- In geometry, we represent conic sections for a 2nd-degree polynomial in x and y

$$Ax^2 + Bxy + Cy^2 + D = 0$$

  the graph is a quadratic curve, and when

  - $B^2 - 4AC < 0$ the curve is a ellipse,
  - $B^2 - 4AC = 0$ the curve is a parabola
  - $B^2 - 4AC > 0$ the curve is a hyperbola

Similarly, given

$$A\frac{\partial^2\psi}{\partial x^2} + B\frac{\partial^2\psi}{\partial x\partial y} + C\frac{\partial^2\psi}{\partial y^2} + D\left(x, y, \psi, \frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial x}\right) = 0$$

where A, B and C are constants. There are 3 types of equations:

- If $B^2 - 4AC < 0$, the equation is called elliptic,
- If $B^2 - 4AC = 0$, the equation is called parabolic
- If $B^2 - 4AC > 0$, the equation is called hyperbolic

The classification can be extended to PDEs in more than two dimensions.

Two classic examples of elliptic PDEs are the Laplace and Poisson equations:

$$\nabla^2\phi = 0 \quad \text{and} \quad \nabla^2\phi = \rho$$

where in 3D

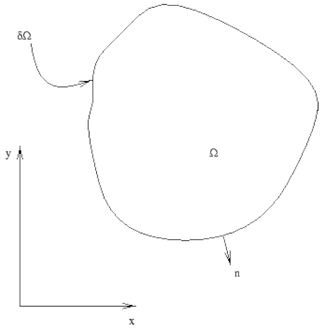
$$\begin{aligned}
\nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \\
\nabla^2 &= \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \\
\nabla^2 &= \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\sin\theta\frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \phi^2}
\end{aligned}$$

Boundary-value Problem

$$\nabla^2 \phi = \rho \quad \text{in a domain } \Omega$$

Boundary Conditions

- Dirichlet: $\phi = b_1$ on $\partial\Omega$
- Neumann: $\frac{\partial \phi}{\partial n} = \hat{n} \cdot \nabla \phi = b_2$ on $\partial\Omega$
- Robin: $\frac{\partial \phi}{\partial n} + \alpha\, \phi = \hat{n} \cdot \nabla \phi = b_3$ on $\partial\Omega$



Classic examples of hyperbolic PDEs are:

$$
\begin{aligned}
-\frac{1}{v^2}\frac{\partial^2\phi}{\partial t^2} + \nabla^2\phi &= 0 \quad \text{wave equation} \\
\frac{\partial\phi}{\partial t} + \vec{V}\cdot\nabla\phi &= 0 \quad \text{advection equation}
\end{aligned}
$$

where v is the speed of the wave propagation ($v = c$ for light waves). For advection, a scalar field, ϕ, is advected by a velocity field $\vec{V}$.

Classic example of parabolic PDEs are

$$\frac{\partial \phi}{\partial t} - \nabla \cdot (D \nabla \phi) = 0 \quad \text{diffusion equation}$$

$$\frac{\partial \phi}{\partial t} - \alpha \nabla^2 \phi = 0 \quad \text{heat equation}$$

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \vec{J} = 0 \quad \text{continuity equation}$$

$$\vec{J} = -D \nabla \phi \quad \text{Fick's first law}$$

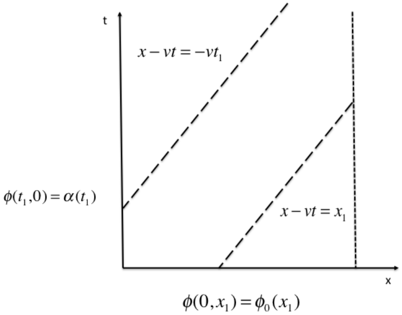
where $\vec{J}$ is the diffusion flux, the amount of substance that flows through a small area of a small time interval. D is the diffusion coefficient, ψ is the concentration and x is the position. Ficke's first law tells us about diffusion in a steady state, i.e. flux goes from regions of high concentration to regions of low concentration proportional to the concentration gradient.

Advection or Convection Equation

- Let's consider the 1D case

$$\partial_t \phi + v\,\partial_x \phi = 0$$

  with $v = \text{const} > 0$, $t \geq 0$ and $x \in [0, 1]$
- Initial data: $\phi(0, x) = \phi_0(x)$
- Boundary conditions: $\phi(t, 0) = \alpha(t)$ and $\phi(t, 1) = \beta(t)$
- Solutions to this equation have the form $\phi(t, x) = \phi(x - v\,t)$
- Therefore, the solution $\phi(t, x)$ is constant along the lines $x - v\,t = \text{const}$ called characteristics



Forward-Time Center-Space (FTCS) Discretization

- Let's consider the following discretization of the differential operators

$$\begin{aligned} \partial_t \phi_i^n &= \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + O(\Delta t) \\ \partial_x \phi_i^n &= \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\,\Delta x} + O(\Delta x^2) \end{aligned}$$

  where we have used the notation $\phi_i^n \equiv \phi(t^n, x_i)$

- Therefore, the finite difference approximation to $\partial_t \phi + v\,\partial_x \phi = 0$ is

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v\,\frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)}{2\,\Delta x} = 0$$

- Notice that we are making a distinction between the solution $\phi(t, x)$ to the continuum equation and $\bar{\phi}_i^n$ the solution to the discrete equation.

Solving

$$\frac{(\bar{\phi}_i^{n+1} - \bar{\phi}_i^n)}{\Delta t} + v\,\frac{(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n)}{2\,\Delta x} = 0$$

for $\bar{\phi}_i^{n+1}$, one gets the following relationship to update the solution

$$\bar{\phi}_i^{n+1} = \bar{\phi}_i^n - \frac{1}{2} C\,\left(\bar{\phi}_{i+1}^n - \bar{\phi}_{i-1}^n\right)$$

where $C \equiv \Delta t\, v / \Delta x$