Modelling & Simulation of Chemical Engineering Systems

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LECTURE #11

Partial Differential Equations

Definition of a PDE and Notation

- A PDE is an equation with derivatives of at least two variables in it.
- Let u be a function of x and y. There are several ways to write a PDE, e.g., $u_x + u_y$

  $\delta u / \delta x + \delta u / \delta y$

- The equations above are linear and first order. The order is determined by the maximum number of derivatives of any term.
- A nonlinear PDE has the solution times a partial derivative or a partial derivative raised to some power in it. Most interesting problems are nonlinear and time dependent.

Characterization of Simple Second Order PDE's

- Let

$$au_{xx} + 2bu_{xy} + cu_{yy} + du_x + eu_y + fu = g$$

- Then the type of PDE is determined by the discriminant

$$b^2 - ac$$

  - < 0 elliptic
  - $= 0$ parabolic
  - > 0 hyperbolic

Characterization of n Variable Second Order PDE's

- A general linear PDE of order 2:

$$\Sigma_{i,j=1}^{n} a_{ij}u_{x_i x_j} + \Sigma_{i=1}^{n} b_i u_{x_i} + cu = d.$$

- Assume symmetry in coefficients so that A = [a_{ij}] is symmetric. Eig(A) are real. Let P and Z denote the number of positive and zero eigenvalues of A.
  - Elliptic: Z = 0 and P = n or Z = 0 and P = 0..
  - Parabolic: Z > 0 (det(A) = 0).
  - Hyperbolic: Z=0 and P = 1 or Z = 0 and P = n-1.
  - Ultra hyperbolic: Z = 0 and 1 < P < n-1.

PDE Model Problems

- Laplace's Equation (elliptic):

$$-u_{xx} - u_{yy} = 0$$

- Heat Equation (parabolic):

$$u_t - u_{xx} - u_{yy} = 0$$

- Wave Equations (hyperbolic):

$$u_t - u_x - u_y = 0$$

$$u_{tt} - u_{xx} - u_{yy} = 0$$

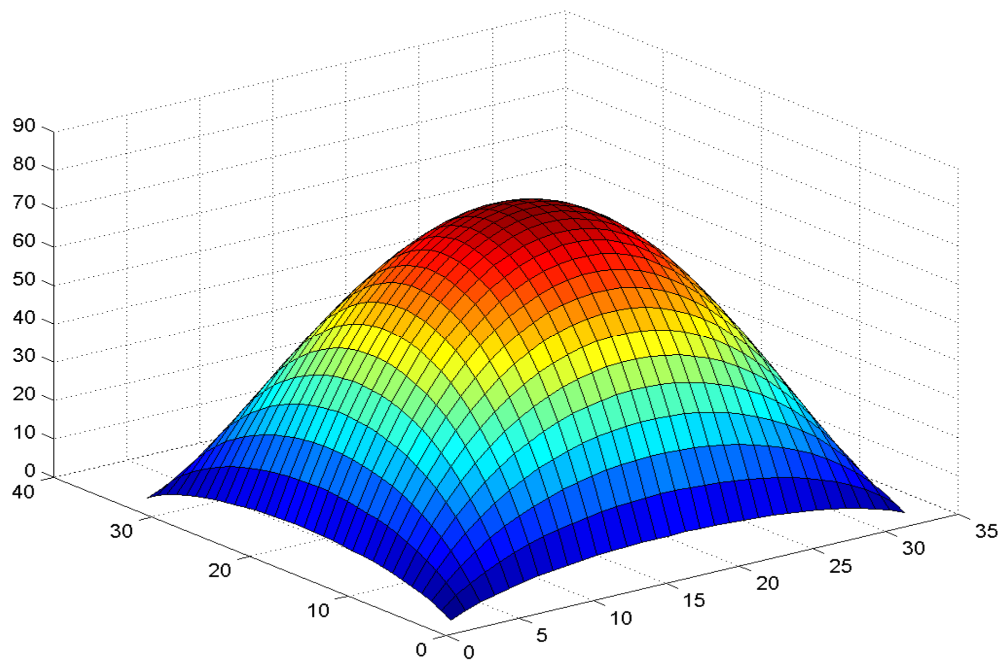
- All problems can be mapped to one of these!... in theory

Boundary and Initial Conditions, Well and Ill Posedness

- Boundary conditions on $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_{R.}$
  - Dirichlet: $u = g$ on Γ_D.
  - Neumann: $u_n = g$ on Γ_N.
  - Robin: $au + b\, u_n = g$ on Γ_R.
- Initial conditions at t=0.
  - $U(t=0,x,y) = u_0(x,y)$.
- Well posed PDE if and only if
  - A solution to the problem exists.
  - The solution is unique.
  - The solution depends continuously on the problem data.
- Ill posed if not well posed.

Example: Poisson Equation in 2D

- $-u_{xx} - u_{yy} = 1$ in $(0,1)^2$; $u = 0$ on $\delta(0,1)^2$.



Methods

- There are three common methods of producing a finite dimensional problem whose solution can be computed, which approximates the solution of the original, infinite dimensional problem:
  - Finite elements
  - Finite differences
  - Finite volumes
- Each has its place, supporters, and detractors.
- There are also other methods, e.g., collocation, spectral methods, pseudo-blah-blah-blah methods, etc.

Finite Differences

- Assume we have a uniform mesh with a point x in the interior..
  - Forward difference: Δ_{+h} u(x) = u(x+h) – u(x).
  - Backward difference: Δ_{-h} u(x) = u(x) – u(x-h).
  - Central difference: δ_x u(x) = u(x+h/2) – u(x-h/2) or δ_ξ^2 u(x) = u(x+h) – 2u(x) + u(x-h).
- Taylor Series and Truncation Error
  - Look at the difference between the approximation and the Taylor series. When they do not match, there is a remainder, which is known as the truncation error. It is usually specified as $O(h^p)$.

Laplace Equation in 2D

$$u_{xx} + u_{yy} = 0$$

Let (x,y) plane be divided into a netwrok of recatngles

$$\Delta x = h, \qquad \Delta y = k$$

$$x = ih, \qquad i = 0,1,2,\ldots$$

$$y = jk, \qquad j = 0,1,2\ldots$$

Finite Difference Form

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{k^2} = 0$$

if k=h

$$\underbrace{u_{ij} = \frac{1}{4}\left[u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right]}_{\text{Standard Five-point Formula}}$$

$$\underbrace{u_{ij} = \frac{1}{4}\left[u_{i\text{-}1,j\text{-}1} + u_{i+1,j\text{-}1} + u_{i+1,j+1} + u_{i\text{-}1,j+1}\right]}_{\text{Diagonal Five-point Formula}}$$