CS601, Lecture 10/10/2022 – Introduction, Partial Differential Equations (PDEs) and their classification

Computation with grids occurs frequently in scientific computing. As part of the frequently occurring patterns or Motifs in scientific computing, the next series of lectures will introduce you to *structured* grids, which appear in application domains such as Finite Difference Methods (FDM) and Finite Element Methods (FEM). Note that the grid in *Grid Computing* is different from the grids that we will be discussing in the next few weeks. The grid in Grid Computing refers to a network of computers, whereas the grid that we discuss in this series of lectures refer to a representation of a physical structure or a process that we intend to model using a computer for the purpose of understanding the properties of the process or structure.

Motivation: *Designing* a mechanical structure, e.g. an airplane component that can withstand a certain temperature or speed etc. is a quite common engineering problem. Once the design is complete, the structure is *manufactured* based on the specifications mentioned in the design drawings / blue print. Later on, the manufactured structure is *tested* in the lab to check if it meets the desired properties. Failure at this stage costs time and money. Hence, to reduce the cost, engineers and scientists use computer modeling to model the structure with the help of graphics software. The question then is to ask how accurately does the computer model describe the structure? Can it withstand certain temp or speed? etc. This is computer simulation. In computer simulations, we are solving certain mathematical equations. While the domain expert (structural engineer) is responsible for formulating, a computer engineer tries to implement and optimize the computations involved. Practical engineering problems can be modeled using Partial Differential Equations (PDEs) and in particular second-order PDEs.

PDEs:

PDEs are mathematical equations that involve two or more *independent* variables and their derivatives. A PDE is of the form:

$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} + D\phi_x + E\phi_y + F\phi + G = 0 \text{ , where} \qquad \textbf{(1)}$$

$$\phi_x = \frac{\partial\phi}{\partial x}, \phi_y = \frac{\partial\phi}{\partial y}, \phi_{xx} = \frac{\partial^2\phi}{\partial x^2}, \phi_{yy} = \frac{\partial^2\phi}{\partial y^2}, \phi_{xy} = \frac{\partial^2\phi}{\partial x \partial y} \text{ and}$$

A to G are coefficients

The above is an example of *second-order* partial differential equation. Practical engineering problems can be modeled using second-order PDEs.

If the coefficients A-C depend on ϕ, x, and y, the PDE is *non-linear* and if the coefficients depend on x, and y only, then the PDE is *linear*. Note that x and y are independent variables here.

Characteristics of PDEs:

If you imagine drawing lines corresponding to the second-order PDE mentioned in (1) previously, the number of lines that you get tells the characteristic of PDE. PDEs are classified into parabolic, elliptic, and hyperbolic based on the number of lines obtained. *But how can we imagine the lines?*

If you consider $D\phi_x + E\phi_y + F\phi + G$ as H in equation (1), then (1) can be rewritten as:

$$A\phi_{xx} + B\phi_{xy} + C\phi_{yy} + H = 0 \qquad \text{———— } \mathbf{(1')}$$

We have the domain or ϕ as a function of independent variables x, and y. We write as: $\phi(x, y)$

the derivative of ϕ w.r.t. x

$$d\phi_x = \frac{\partial\phi_x}{\partial x}dx + \frac{\partial\phi_x}{\partial y}dy \text{ - using chain rule} \qquad \text{———— } \mathbf{(2)}$$

the derivative of ϕ w.r.t. y

$$d\phi_y = \frac{\partial\phi_y}{\partial x}dx + \frac{\partial\phi_y}{\partial y}dy \text{ - using chain rule} \qquad \text{———— } \mathbf{(3)}$$

Equations (2) and (3) can be rewritten using the substitutions for $\phi_{xx} = \frac{\partial^2\phi}{\partial x^2}, \phi_{yy} = \frac{\partial^2\phi}{\partial y^2}, \phi_{xy} = \frac{\partial^2\phi}{\partial x \partial y}$ mentioned previously:

$$d\phi_x = \frac{\partial\phi_x}{\partial x}dx + \frac{\partial\phi_x}{\partial y}dy = \phi_{xx}dx + \phi_{xy}dy \qquad \text{———— } \mathbf{(2')}$$

$$d\phi_y = \frac{\partial\phi_y}{\partial x}dx + \frac{\partial\phi_y}{\partial y}dy = \phi_{yx}dx + \phi_{yy}dy \qquad \text{———— } \mathbf{(3')}$$

Equations (1') (2') and (3') form a system of equations with unknowns $\phi_{xx}, \phi_{yy}, and\ \phi_{xy}$ and can be written in matrix form as:

$$\begin{bmatrix} A & B & C \\ dx & dy & 0 \\ 0 & dx & dy \end{bmatrix} \begin{bmatrix} \phi_{xx} \\ \phi_{xy} \\ \phi_{yy} \end{bmatrix} = \begin{bmatrix} -H \\ d\phi_x \\ d\phi_y \end{bmatrix} \qquad \text{———— } \mathbf{(4)}$$

Equation (4) does not have a solution (and the lines are discontinuous) if the determinant of matrix in (4) is 0. This implies:

$$A(dy)^2 + C(dx)^2 - B(dx)(dy) = 0 \qquad \text{———— } \mathbf{(5)}$$

The roots of the quadratic equation are:

$$\frac{-B \pm \sqrt{B^2 - 4AC}}{2A}$$

For a given PDE, if $\sqrt{B^2 - 4AC} = 0$, there exists one characteristic and the PDE is **parabolic**

For a given PDE, if $\sqrt{B^2 - 4AC} < 0$, there exists No real characteristic and the PDE is **elliptic**

For a given PDE, if $\sqrt{B^2 - 4AC} > 0$, there exist two real characteristics and the PDE is **hyperbolic**

Some examples of Parabolic, Hyperbolic, and Elliptic PDEs:

$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0$ (A=1, B=0, C=1. Therefore, $\sqrt{B^2-4AC}<0$. Hence, this is an elliptic PDE.

The above equation is commonly written as $\nabla^2\phi=0$. Where $\nabla\rightarrow\left(\frac{\partial}{\partial x},\frac{\partial}{\partial y}\right)$

E.g. Boundary value problems. You have a metal plate at uniform temperature and a heat source is applied at the center. The disturbance propagates in all spatial directions.

$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}$ (A=1, B=0, C=0. Therefore, $\sqrt{B^2-4AC}=0$. Hence, this is a parabolic PDE.

E.g. modeling one-dimensional unsteady state e.g. how the temperature varies over time in a one-D rod.

$\frac{\partial^2 u}{\partial t^2}=c^2\frac{\partial^2 u}{\partial x^2}$ (A=$-C^2$, B=0, C=1. Therefore, equation (5) has two real solutions. Hence, this is a hyperbolic PDE.

Suppose you have multiple PDEs to model the system. You can still classify the set of PDEs as parabolic, elliptic, and hyperbolic based on the nature of the characteristic obtained. The characteristic in this case is obtained using an alternative method of computing the eigenvalues of a matrix of system of equations described in class (not written here).

Note that the classification mentioned previously apply to second-order PDEs only.

Boundary Conditions (BC):

Classification of boundary conditions are done as follows:

Essential BC / Dirichlet BC: value of the dependent variable is specified. E.g. the temperature at boundaries of a plate are all at a fixed value of say 50 degrees.

Natural BC / Neumann BC: value of the gradient of dependent variable is specified. E.g. we are given dT/dx.

Mixed BC / Robin BC: value of the dependent variable is expressed as a function of the gradient.

e.g. at the boundaries we write $-K\left(\frac{dT}{dx}\right)_{x=L}=hA(T-T_\infty)$