Lecture 11/10/2022 – Computing Partial Derivatives and Approximations

In the previous lecture, we saw two methods to classify partial differential equations (PDEs) and example problems that can be modeled using PDEs. We also saw the types of boundary conditions—The method used to specify the values that the dependent variable can attain at e.g. time=0 or at boundaries of a domain etc. This lecture discusses the broad steps involved in solving a PDE via a computer.

Introduction: any structure to be modeled is inherently 3D. If the structure is made up of homogeneous material, then it will have the same properties at all points within and on the body. Hence, for the purpose of analyzing the properties, a 2D cross-section can be representative of the original 3D domain. This reasoning can be further extended to *approximate* a 2D domain with a representative 1D domain, on which the properties can be analyzed. The approximation is done to simplify the mathematical formulation of the original structure and reduce the computations involved while solving the equations that help us understand the properties of the structure that is modeled. It is important to note that not all problems or processes admit such simplification/approximation e.g. a majority of aerospace structures.

Some problem types:

Boundary Value Problems: these problems are modeled with the help of PDEs, where the independent variables are only spatial in nature (e.g. x, y, z coordinates). Time is not an independent variable in these PDEs. E.g. $\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$

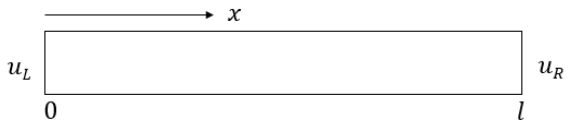
Initial Boundary Value Problems: these problems are modeled with the help of PDEs, where the set of independent variables contain both time and spatial variables. E.g. $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$

Example problem: consider the problem of analyzing the conduction of heat through a rod modeled as a 1D structure. The problem can be modeled using the PDE $\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}$**,** where α is thermal diffusivity, a is constant if the material is homogeneous and *isotropic*. Goal is to find the temperature at different points on the rod at different times. The dependent variable, temperature, is a function of both time t and distance x along the rod i.e. the dependent variable is $u(x,t)$. The initial and boundary conditions as follows:

$u(0,t) = u_L$, //temperature at the left end of the rod (at distance=0) at any time is a constant u_L

$u(l,t) = u_R$, //temperature at the right end of the rod (at distance=l) at any time is a constant u_R

$u(x,0) = f(x)\ 0 < x < l$ //temperature at any point on the rod at time=0 is some function f of the distance of the point from the left end of the rod.



i.e. given the four equations (3 mentioned previously and the PDE), a solution to find the temperature at any point x at time t i.e. $u(x,t)$, could look like:

$u(x,\ t) \quad = \sum_{m=1}^{\infty} Bme^{-m2\alpha\pi 2t/l2}\sin\left(\frac{m\pi x}{l}\right)$, where, $B_m = 2/l \int_0^l f(s)\sin\left(\frac{m\pi s}{l}\right) ds$

The above is called an *analytical solution* and is expensive to compute. Moreover, we *cannot find* such analytical solutions for all problems. Hence, approximate or *numerical* solutions are employed.

Steps involved in computing a numerical solution:

1) *Discretization*: a given domain is divided into a number of sub-domains. This division is represented using *grid points*.

2) The PDEs are approximated by finding an equivalent algebraic equation that is computed at *every* grid point. The algebraic equations are relatively easier to solve via computer when compared to analytical solutions of the PDEs.

3) Assemble the equations of step 2 (you will get one at each grid point), possibly represent in matrix form, and solve the system of equations. The solution to the system of equations tells the values of the dependent variable.

Steps 1 and 2 are called *preprocessing stage* and step 3 is the *solution stage*. There could be a *post processing* stage as well: in some problems, once the solution is computed, e.g. stress or strain may have to be computed.

How do we approximate the PDEs?

Taylor series tells us that if a function $f(x)$ is infinitely differentiable at $x = a$ (i.e. the derivatives exist at $x = a$) then it can be written as:

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)(x-a)^2}{2!} + \frac{f'''(a)(x-a)^3}{3!} + \ldots \text{ up to infinity}$$

applying this in the heat conduction through the rod problem: suppose we know the temperature at point i i.e. u_i. Can we compute the temperature u_{i+1} at point $i+1$ based on the value of u_i? Note that the first step (discretization) has given us points $i, i+1, i+2$, and so on. These points are equally spaced at a programmer chosen step size: Δx.

$$u_{i+1} = u_i + u'(\mathrm{i})\ (\Delta x) + \frac{u''(i)(\Delta x)^2}{2!} + \frac{u'''(i)(\Delta x)^3}{3!} + \ldots \qquad \text{(1)}$$

Rearranging terms and rewriting, the first-order derivative $u'(i)$ at point i:

$$u'(i) = (u_{i+1} - u_i)/\Delta x - 1/\Delta x\left(\frac{u''(i)(\Delta x)^2}{2!} + \frac{u'''(i)(\Delta x)^3}{3!} + \cdots\right)$$

If we choose to approximate the first derivative of u at point i by ignoring the highlighted expression, then the *truncation error* is of the order $O(\Delta x)$. We say that the solution is first-order accurate. The approximation of the first order derivative of u is therefore:

$$u'(i) = (u_{i+1} - u_i)/\Delta x \qquad \text{(2)}$$

Because we are moving forward (from the left end of the rod) relative to point i, we call the above formula *forward difference formula*. Similarly, you can compute the value of function u at point $i-1$ i.e. u_{i-1} based on the value of the function u at point i:

$$u_{i-1} = u_i - u'(\mathrm{i})\,(\Delta x) + \frac{u''(i)(\Delta x)^2}{2!} - \frac{u'''(i)(\Delta x)^3}{3!} + \ldots \qquad \textbf{(3)}$$

Rearranging terms and rewriting, the first-order derivative $u'(i)$ at point i:

$$u'(i) = (u_i - u_{i-1})/\Delta x + 1/\Delta x\left(\frac{u''(i)(\Delta x)^2}{2!} - \frac{u'''(i)(\Delta x)^3}{3!} + \cdots\right)$$

If we choose to approximate the first derivative of u at point i by ignoring the highlighted expression, the approximation of the first order derivative of u is therefore:

$$u'(i) = (u_i - u_{i-1})/\Delta x \qquad \textbf{(4)}$$

Because we are moving backward relative to point i, we call the above formula *backend difference formula*.

If you subtract equation (3) from equation (1), you get the *central difference approximation to the first derivative of u* as:

$$u'(i) = (u_{i+1} - u_{i-1})/2\Delta x \qquad \textbf{(5)}$$

If you add equations (3) and (1), you get the *central difference approximation to the second derivative of u* as:

$$u''(i) = (u_{i+1} - 2u_i + u_{i-1})/(\Delta \mathrm{x})^2 \qquad \textbf{(6)}$$

Equations (2), (4), (5), and (6) are important and tell us how to approximate the derivatives using different methods. Now we know how derivatives of u can be approximated, we can compute the numerical solution. This is the topic of the next lecture.