# PHYS-4007/5007: Computational Physics
# Course Lecture Notes
# Section XI

Dr. Donald G. Luttermoser
East Tennessee State University

**Version 5.0**

**Abstract**

These class notes are designed for use of the instructor and students of the course PHYS-4007/5007: Computational Physics taught by Dr. Donald Luttermoser at East Tennessee State University.

# XI. Numerical Solution to Partial Differential Equations

## A. Introduction

**1.** Differential equations involving more than one independent variable are common in physics. Such equations are called **partial differential equations** (PDE). PDEs are typically classified into three categories on the basis of their *characteristics*, or curves of information propagation:

**a)** The **hyperbolic** category has hyperbolic characteristics.

**b)** The **parabolic** category has parabolic characteristics.

**c)** The **elliptic** category has elliptic characteristics.

**2.** The most general form of a PDE involving a function $U$ with two independent variables $x$ and $y$ is

$$A\frac{\partial^2 U}{\partial x^2} + 2B\frac{\partial^2 U}{\partial x \partial y} + C\frac{\partial^2 U}{\partial y^2} + D\frac{\partial U}{\partial x} + E\frac{\partial U}{\partial y} = F \ , \qquad \text{(XI-1)}$$

where the coefficients can be either constant parameters or functions of $x$ and/or $y$.

**a)** If $AC - B^2 < 0$, the PDE is hyperbolic in nature.

**b)** If $AC - B^2 = 0$, the PDE is parabolic in nature.

**c)** If $AC - B^2 > 0$, the PDE is elliptic in nature.

**3.** Examples of these three characteristic categories are:

**a)** The *wave* equation:

$$\frac{\partial^2 U}{\partial t^2} = v^2 \frac{\partial^2 U}{\partial x^2} \ , \qquad \text{(XI-2)}$$

where $t$ is time, $x$ displacement, and $v$ is the <u>constant</u> velocity of the wave propagation $\Longrightarrow$ a *hyperbolic* equation.

**b)** The *diffusion* equation:

$$\frac{\partial U}{\partial t} = -\frac{\partial}{\partial x}\left(D\,\frac{\partial U}{\partial x}\right)\,, \qquad \text{(XI-3)}$$

where $D$ is the diffusion coefficient $\Longrightarrow$ a *parabolic* equation.

**c)** The *Poisson* equation:

$$\nabla^2 U = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} = \rho(x,y)\,, \qquad \text{(XI-4)}$$

where the source term $\rho$ is typically given based on the problem being solved $\Longrightarrow$ an *elliptic* equation.

**i)** For instance in electrostatics, $\rho$ is the charge density.

**ii)** Note that if $\rho = 0$ in Eq. (XI-4), this equation is called *Laplace's equation.*

**4.** Initial Value Problems.

**a)** Eqs. (XI-2) and (XI-3) correspond to an initial value type of problem since the time coordinate $t$ is involved.

**b)** An initial value problem is defined by answers to the following questions:

**i)** What are the variables to be propagated forward in time?

**ii)** What is the evolution equation for each variable? Usually the evolution equations will all be coupled, with more than one dependent variable appearing on the right-hand side of each equation.

**iii)** What is the highest time derivative that occurs in each variable's evolution equation? If possible, this time derivative should be put alone on the left-hand side. Not only the value of a variable, but also the value of all its time derivatives – up to the highest one – must be specified to define the evolution.

**c)** Shooting or iterative methods are typically used for these problems (see §IX.B.1).

**5.** Boundary Value Problems.

**a)** Eq. (XI-4) corresponds to a boundary value problem since boundary conditions need to be supplied to solve the problem. Such a solution is then said to be *static* since it does not change with time due to the lack of time derivatives.

**b)** The questions that define a boundary value problem are:

**i)** What are the variables?

**ii)** What equations are satisfied in the interior of the region of interest?

**iii)** What equations are satisfied by points on the boundary of the region of interest (see Eq. IX-49 and IX-50 for the ODE analogies).

**c)** Marching or relaxation methods are typically used for these types of problems (see §IX.B.1).

## B. Separation of Variables.

**1.** In order to solve partial differential equations, either analytically or numerically, one needs to modify the equation or equations into a set of ordinary differential equations. The method for doing this is described as the method of **Separation of Variables**. To demonstrate this technique, we will first focus on analytic solutions.

**2.** Separation of variables in Cartesian coordinates.

**a)** The best way to describe this method is to use an example from physics using Cartesian coordinates. First we will investigate the Schrödinger equation which describes the physical attributes of a particle's wave function, $\Psi$, in quantum mechanics:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi \ , \qquad \text{(XI-5)}$$

where

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad \text{(XI-6)}$$

(called the **Laplacian**) in Cartesian coordinates. Hence Eq. (XI-5) corresponds to a parabolic equation.

**b)** From quantum mechanics, the probability of finding the particle in an infinitesimal volume $d^3\boldsymbol{r} = dx\,dy\,dz$ is $|\Psi(\boldsymbol{r}, t)|^2\, d^3\boldsymbol{r}$. To account for all real particles in this box, the probability for finding all real particle wave functions is 100% – this is referred to as the condition of normalization, hence

$$\int |\Psi|^2\, d^3\boldsymbol{r} = 1 \ , \qquad \text{(XI-7)}$$

with the integral taken over all space.

**c)** For our example here, we will use separation of variables in Cartesian coordinates to determine the wave function for a "particle in a box" – a particle located in an infinite cubical potential well:

$$V(x,y,z) = \begin{cases} 0, & \text{if } x,\ y, \text{ and } z \text{ are all between 0 and } a; \\ \infty, & \text{otherwise.} \end{cases} \qquad \text{(XI-8)}$$

**d)** Since the potential is independent of time, there will be a complete set of stationary states,

$$\Psi_n(\boldsymbol{r},t) = \psi_n(\boldsymbol{r})\, e^{-iE_nt/\hbar}, \qquad \text{(XI-9)}$$

where the spatial wave function $\psi_n$ satisfies the time-*independent* Schrödinger equation (TISE):

$$-\frac{\hbar^2}{2m}\,\nabla^2\psi_n + V\psi_n = E_n\psi_n\ , \qquad \text{(XI-10)}$$

where $n$ is an integer labeling the various energy ($E$) states. As can be seen in this equation, time-independent wave functions are written with a lowercase psi, $\psi$, whereas the time-dependent wave functions are written with an uppercase Psi, $\Psi$.

**e)** The separable solution is: $\psi(x,y,z) = X(x)Y(y)Z(z)$. Put this in the above equation (Eq. XI-9) and divide by $XYZ$:

$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = -\frac{2m}{\hbar^2}\,E = -(k_x^2 + k_y^2 + k_z^2),$$

where

$$E \equiv \frac{(k_x^2 + k_y^2 + k_z^2)\hbar^2}{2m},$$

and $k_x$, $k_y$, and $k_z$ are three constants. The three terms on the left of this equation are functions of $x$, $y$, and $z$, respectively, so each must be a constant, where $k_x^2$, $k_y^2$, and $k_z^2$ are the three separation constants.

**f)** This leads to three separate differential equations:

$$\frac{d^2X}{dx^2} = -k_x^2\,X, \qquad \frac{d^2Y}{dy^2} = -k_y^2\,Y, \qquad \frac{d^2Y}{dz^2} = -k_z^2\,Z.$$

**g)** The solution to these three equations are

$$\begin{aligned} X(x) &= A_x \sin k_x x + B_x \cos k_x x \ , \\ Y(y) &= A_y \sin k_y y + B_y \cos k_y y \ , \\ Z(z) &= A_z \sin k_z z + B_z \cos k_z z \ , \end{aligned}$$

(prove this to yourself by taking the double derivative of each to see that they satisfy this differential equations above).

**h)** But $X(0) = 0$, so $B_x = 0$; $Y(0) = 0$, so $B_y = 0$; $Z(0) = 0$, so $B_z = 0$. Likewise, $X(a) = 0 \Rightarrow \sin(k_x a) = 0 \Rightarrow k_x = n_x \pi/a$, $(n_x = 1, 2, 3, ...)$ (note that negative values of $k$ are redundant with the positive values and $n_x \neq 0$ since this would give us no wave function). Likewise, $k_y = n_y \pi/a$ and $k_z = n_z \pi/a$. So

$$E = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} \left(n_x^2 + n_y^2 + n_z^2\right),$$

and

$$\psi(x, y, z) = A_x A_y A_z \sin\left(\frac{n_x \pi}{a} x\right) \sin\left(\frac{n_y \pi}{a} y\right) \sin\left(\frac{n_z \pi}{a} z\right).$$

**i)** We can normalize the three independent solutions separately, giving $A_x = A_y = A_z = \sqrt{2/a}$. So the final solution is

$$\begin{aligned} \psi(x, y, z) &= \left(\tfrac{2}{a}\right)^{\frac{3}{2}} \sin\left(\tfrac{n_x \pi}{a} x\right) \sin\left(\tfrac{n_y \pi}{a} y\right) \sin\left(\tfrac{n_z \pi}{a} z\right) \\ E &= \tfrac{\pi^2 \hbar^2}{2ma^2} \left(n_x^2 + n_y^2 + n_z^2\right) \\ n_x, n_y, n_z &= 1, 2, 3, ... \end{aligned}$$

**3.** Separation of variables in spherical coordinates.

**a)** Now we will investigate the Schrödinger equation in spherical coordinates. Here the Laplacian is written as

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right) . \tag{XI-11}$$

**b)** Typically, the potential $V$ is a function only of the distance from the origin. In that case it is natural to adopt spherical coordinates, to determine the wave equation for $\Psi(r, \theta, \phi, t)$.

**c)** To simplify matters for our illustrative purposes, let's assume the wave function doesn't change in time. Then in spherical coordinates the TISE reads

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right]+V\psi = E\psi . \tag{XI-12}$$

**d)** To solve this equation, we will assume that the solution can be represented as the product of separable terms composed of a radial part ($R$) and an angular part ($Y$):

$$\psi(r, \theta, \phi) = R(r)\,Y(\theta, \phi) . \tag{XI-13}$$

**e)** Putting this into Eq. (XI-12) we get

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{R}{r^2\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\phi^2}\right)\right]+VRY = ERY . \tag{XI-14}$$

**f)** Dividing by $RY$ and multiplying by $-2mr^2/\hbar^2$ we get

$$\left\{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left[V(r) - E\right]\right\} + \frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\phi^2}\right)\right\} = 0 \ . \quad \text{(XI-15)}$$

**g)** As can be seen, the term in the first curly bracket depends only upon the radial parameter $r$, hence the partial derivative can be rewritten as an ordinary derivative.

**h)** The second curly bracket term depends on $\theta$ and $\phi$, hence we still have to use partial derivatives.

**i)** With Eq. (XI-15) written in this manner each curly bracket term must be equal to the negative of the other term, hence each term must be constant. We will write this separation constant as $\ell(\ell+1)$ (the reason for choosing this form of the constant is explained in the Quantum Physics course), as such

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left[V(r) - E\right] = \ell(\ell+1) \ , \quad \text{(XI-16)}$$

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\left(\frac{\partial^2 Y}{\partial\phi^2}\right)\right\} = -\ell(\ell+1) \ . \quad \text{(XI-17)}$$

**j)** To solve the angular equation (*e.g.*, Eq. XI-18), multiply each side by $Y\sin^2\theta$ gives

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1)Y\sin^2\theta \ . \quad \text{(XI-18)}$$

**k)** Once again, use separation of variables:

$$Y(\theta,\phi) = \Theta(\theta)\,\Phi(\phi) \ . \quad \text{(XI-19)}$$

Plugging this into Eq. (XI-17) and dividing by $\Theta\Phi$ gives

$$\begin{aligned}
\sin\theta \frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial}{\partial\theta}(\Theta\Phi)\right] + \frac{\partial^2}{\partial\phi^2}(\Theta\Phi) &= -\ell(\ell+1)\Theta\Phi\sin^2\theta \\
\Phi\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \Theta\frac{\partial^2\Phi}{\partial\phi^2} &= -\ell(\ell+1)\Theta\Phi\sin^2\theta \\
\frac{1}{\Theta}\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \frac{1}{\Phi}\frac{\partial^2\Phi}{\partial\phi^2} &= -\ell(\ell+1)\sin^2\theta\ ,
\end{aligned}$$

or

$$\left\{\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right] + \ell(\ell+1)\sin^2\theta\right\} + \frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = 0\ . \qquad \text{(XI-20)}$$

**l)** The first term of Eq. (XI-20) is a function only of $\theta$, and the second is a function only of $\phi$, so each must be constant. Let's choose the separation constant $m^2$ ($m$ is called the **magnetic quantum number**), then

$$\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right] + \ell(\ell+1)\sin^2\theta = m^2, \qquad \text{(XI-21)}$$

and

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2. \qquad \text{(XI-22)}$$

**m)** The equation for $\phi$ is easy with the solution

$$\Phi(\phi) = e^{im\phi} \qquad \text{(XI-23)}$$

(actually, there are two solutions: $e^{im\phi}$ and $e^{-im\phi}$, but we will fold the negative exponents into the positive solution by letting $m$ be negative as well as positive). We also will fold the integration constant into the solution for $\Theta$.

**n)** Since Eq. (XI-23) is nothing more than trigonometric functions in complex space, note that

$$\Phi(\phi + 2\pi) = \Phi(\phi)\ . \qquad \text{(XI-24)}$$

In other words, $\mathbf{exp}[im(\phi+2\pi)] = \mathbf{exp}(im\phi)$, or $\mathbf{exp}(2\pi im) = 1$. From this it follows that $m$ must be an integer:

$$m = 0, \pm 1, \pm 2, ... \qquad \text{(XI-25)}$$

**o)** The equation for $\theta$ becomes

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + [\ell(\ell+1)\sin^2\theta - m^2]\,\Theta = 0\,. \qquad \text{(XI-26)}$$

The analytic solution to this differential equation and radial equation are not trivial. These 'Separation of Variables' analytic solutions are covered in the Quantum Physics course.

## C. PDE Numerical Solution Techniques

**1.** How does one solve these problems involving partial differential equations (PDEs)? Basically, it depends on the type of problem being solved and whether it is a boundary value type of problem or an initial conditions type of problem.

### 2. Numerical solutions using Fourier Series.

**a)** As an example, we will calculate the electrostatic potential $U$ in a square box with each side of length $L$ such that $U = 0$ at the boundaries $x = 0$, $x = L$, and $y = 0$; and $U = U_{\rm max}$ at $y = L$.

**b)** The electrostatic potential can then be found using the 2-D Laplace equation:

$$\nabla^2 U = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} = 0\,. \qquad \text{(XI-27)}$$

**c)** It is fairly straight forward to show using separation of variables that the solution for $U$ involves an infinite Fourier

Series of the form

$$U(x,y) = \sum_{n=1}^{\infty} E_n \sin\left(\frac{n\pi}{L}x\right) \sinh\left(\frac{n\pi}{L}y\right) . \qquad \text{(XI-28)}$$

**d)** Here the $E_n$ values are arbitrary constants and are fixed by requiring the solution to satisfy the $y = L$ boundary condition

$$\sum_{n=1}^{\infty} E_n \sin\left(\frac{n\pi}{L}x\right) \sinh\left(n\pi\right) = U_{\rm max} . \qquad \text{(XI-29)}$$

**e)** However, how many terms will we need until the converged numerical solution is reached? Since the sine term in this sum oscillates, we might have to use a large number of terms which will increase roundoff error significantly.

**f)** Also, the hyperbolic sine function will overflow as $n$ becomes large. As such, a Fourier Series numerical solution is not very practical for this type of problem.

## 3. Numerical solutions using the Finite-Difference Method.

**a)** Here we will numerically solve our 2-D PDE by dividing the space up into a 2-D grid called a **lattice**.

**b)** This Finite-Difference Method essentially follows the same techniques described for differentiation in §VII.A. We start by adding two Taylor expansions of the potential to the right and left of $(x,y)$:

$$U(x+\Delta x, y) = U(x,y) + \frac{\partial U}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(\Delta x)^2 + \cdots \qquad \text{(XI-30)}$$

$$U(x-\Delta x, y) = U(x,y) - \frac{\partial U}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 U}{\partial x^2}(\Delta x)^2 - \cdots \qquad \text{(XI-31)}$$

**c)** All odd terms cancel when we add these two equations together resulting in a central-difference approximation for the second partial derivative (with error of order $(\Delta x)^4$:

$$\frac{\partial^2 U}{\partial x^2} \simeq \frac{U(x+\Delta x, y) + U(x-\Delta x, y) - 2U(x,y)}{(\Delta x)^2} + \mathcal{O}\left(\Delta x^4\right) , \tag{XI-32}$$

and doing the same thing for the $y$ derivatives:

$$\frac{\partial^2 U}{\partial y^2} \simeq \frac{U(x, y+\Delta y) + U(x, y-\Delta y) - 2U(x,y)}{(\Delta y)^2} + \mathcal{O}\left(\Delta y^4\right) . \tag{XI-33}$$

**d)** Substituting both these approximations into Laplace's PDE (*i.e.*, Eq. XI-27) leads to the finite-difference form of the equation:

$$\begin{aligned} \frac{U(x+\Delta x, y) + U(x-\Delta x, y) - 2U(x,y)}{(\Delta x)^2} \quad &+ \qquad \text{(XI-34)} \\ \frac{U(x, y+\Delta y) + U(x, y-\Delta y) - 2U(x,y)}{(\Delta y)^2} \quad &= \; 0 \; . \end{aligned}$$

**e)** If the $x$ and $y$ grids are of equal spacings, this equation takes the simple form

$$\begin{aligned} U(x+\Delta x, y) + U(x-\Delta x, y) \; + & \qquad \text{(XI-35)} \\ U(x, y+\Delta y) + U(x, y-\Delta y) - 4U(x,y) \; &= \; 0 \; . \end{aligned}$$

**f)** When $U(x,y)$ is evaluated for the $N_x$ $x$ values on the lattice and the $N_y$ $y$ values, there results a set of $N_x \times N_y$ simultaneous linear algebraic equations for U[i][j]. The most direct approach to solve these linear equations numerically is to use one of the matrix techniques discussed in §VIII of these notes.

**g)** Unfortunately this direct solution typically requires a great deal of memory and book keeping to carry out.

**4.** There are other techniques that can be used for PDEs which we won't describe here. One of these is the **relaxation method** which was described in §XI.B.4 in these notes.