# Chapter 7: Numerical Solutions of Partial Differential Equations

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Course Name: Introduction to Numerical Analysis (PH 307)

# Partial Differential Equations

- In the previous chapter we discussed various approaches for solving the ODEs numerically
- ODEs are those differential equations which involve only one variable, generally called $x$.
- However, when the differential equation involves more than one variable, say $(x,t)$, $(x,y)$, $(x,y,z)$, $(x,y,z,t)$, etc., it is called a partial differential equation (PDE).
- Above variables $x$, $y$, and $z$ normally refer to the spatial variables, while $t$ denotes the time variable.
- A PDE is a differential equation involving more than one variable
- Therefore, in principle, it will consist of partial derivatives
- If $u$ is the function that we want to solve for, the PDE will consist of partial derivatives $u$, such as $\frac{\partial u}{\partial t}$, $\frac{\partial u}{\partial x}$, $\frac{\partial^2 u}{\partial x^2}, \frac{\partial^2 u}{\partial y^2}, \frac{\partial^2 u}{\partial x \partial y}$, etc.

# PDEs (contd.)...

- Occasionally, we will use the following short notations to denote the partial derivatives of various orders

$$u_t = \frac{\partial u}{\partial t}; u_x = \frac{\partial u}{\partial x}$$
$$u_{xx} = \frac{\partial^2 u}{\partial x^2}; u_{xy} = \frac{\partial^2 u}{\partial x \partial y}$$

- PDEs are normally boundary value problems
- But, in some cases, they can be a combination of boundary value and initial value problems
- Some famous PDEs in 3+1 dimensions (3 denotes space dimensions, while +1 is the time dimension) are

$$\begin{aligned} u_{xx} + u_{yy} + u_{zz} - u_{tt} &= 0 \quad \text{wave equation} \\ u_{xx} + u_{yy} + u_{zz} - u_t &= 0 \quad \text{heat/diffusion equation} \\ u_{xx} + u_{yy} + u_{zz} &= 0 \quad \text{Laplace equation} \\ -\frac{h^2}{2m}(\psi_{xx} + \psi_{yy} + \psi_{zz} + V\psi) &= i\hbar\psi_t \quad \text{Schrödinger equation} \end{aligned}$$

# Heat Equation

- There are several other important PDEs such as the Navier-Stokes equation of fluid mechanics that we have not mentioned here
- Let us first discuss the heat equation, which is also a special form of the diffusion equation.
- Diffusion equation is used quite extensively in modeling financial markets
- Our aim is to solve the heat equation subject to some general boundary and initial condition
- Here we consider the heat equation in 1+1 dimensions with the specified boundary conditions

$$\begin{aligned} \frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{\partial u(x,t)}{\partial t} \\ u(0,t) = u(1,t) &= 0 \\ u(x,0) &= \sin \pi x \end{aligned} \tag{1}$$

we want the solution of the equation in the linear region $0 \leq x \leq 1$

# Solution of Heat Equation

- As it turns out, Eq. 1 with the given boundary and initial conditions has exact solutions
- We will first obtain its exact solution using the method of separation of variables, using the conjecture

$$u(x,t) = X(x)T(t) \tag{2}$$

- We substitute this in Eq. 1 and divide both sides by $X(x)T(t)$ to obtain

$$\frac{1}{X}\frac{d^2X}{dx^2} = \frac{1}{T}\frac{dT}{dt} \tag{3}$$

- Given that the left-hand side of the equation is a function only of $x$, while the right-hand side is that of only $t$, both sides must be equal to the same constant, say, $-k^2$

$$\begin{aligned} \frac{d^2X}{dx^2} + k^2X = 0 \\ \frac{dT}{dt} + k^2T = 0 \end{aligned} \tag{4}$$

- Eq. 4 admits the solutions

$$\begin{aligned} X(x) &= A\sin kx + B\cos kx \\ T(t) &= Ce^{-k^2 t} \end{aligned} \tag{5}$$

- However, the given the initial value $u(x,0) = \sin \pi x$ implies that $X(x) = \sin \pi x$, which means that in Eq. 5 we must have $A = 1$; $B = 0$; $k = \pi$, and we can choose $C = 1$, leading to the final solution

$$u(x,t) = e^{-\pi^2 t} \sin \pi x \tag{6}$$

  which clearly satisfies the boundary conditions $u(0,t) = u(1,t) = 0$ as well implying that this is the exact solution of our PDE

- Let us next develop finite-difference based numerical methods for solving Eq. 1, and we can judge the accuracy of the numerical results against the exact solution.

- **Method 1: Explicit Method:** In this approach we use the central-difference approach to compute the second derivate, while the forward-difference formula is used to compute the first derivative
- Therefore

$$\frac{\partial u(x,t)}{\partial t} \approx \frac{1}{k}\Delta_t(u(x,t)) = \frac{u(x,t+k)-u(x,t)}{k} \tag{7}$$

- And

$$\begin{aligned}\frac{\partial^2 u(x,t)}{\partial x^2} \approx \frac{1}{h^2}\delta_x^2 u(x,t) \quad &= \frac{1}{h^2}\delta_x\left(u\left(x+\frac{h}{2},t\right)-u\left(x-\frac{h}{2},t\right)\right)\\ \frac{\partial^2 u(x,t)}{\partial x^2} &\approx \frac{1}{h^2}\left(\delta_x u\left(x+\frac{h}{2},t\right)-\delta_x u\left(x-\frac{h}{2},t\right)\right)\\ &\approx \frac{u(x+h,t)-2u(x,t)+u(x-h,t)}{h^2}\end{aligned} \tag{8}$$

Note that above $h$ is the grid size for $x$, while $k$ is the grid size for $t$.

# Heat Eqn., finite difference explicit approach

- Substituting Eqs. 7 and 8 in the heat eqn (1), we obtain

$$\frac{u(x+h,t)-2u(x,t)+u(x-h,t)}{h^2}=\frac{u(x,t+k)-u(x,t)}{k} \tag{9}$$

- Which can be rewritten as

$$u(x,t+k)=\sigma u(x+h,t)+(1-2\sigma)u(x,t)+\sigma u(x-h,t),$$

where $\sigma=\frac{k}{h^2}$.

- Because both $x$ and $t$ have been discretized, we can write $x=x_n=nh$, $t=t_m=mk$, and $u(x,t)=u(x_n,t_m)=u(n,m)$, so that the previous difference equation becomes

$$u(n,m+1)=\sigma u(n+1,m)+(1-2\sigma)u(n,m)+\sigma u(n-1,m) \tag{10}$$

- We are looking for solutions in the region $0 \leq x \leq 1$, and $0 \leq t \leq t_{max}$ so that with total $N$ bins in the $x$ directions and $M$ in the $t$ direction, we have

$$x_N = Nh = 1$$
$$t_M = Mk = t_{max}$$

- The finite difference form of heat equation (Eq. 10) is general, and independent of the boundary conditions.
- However, for the boundary condition given here $u(x,0) = \sin \pi x$, we basically need to obtain $u(x,t)$, for $0 \leq t \leq t_{max}$, where $t_{max}$ is user defined.
- The difference equation above (Eq. 10) is a simple recursion relation which can be used be used to give us solution for all $t$ values if we use the initial conditions $u(x_n,0) = u(n,0) = \sin \pi (nh)$.

# Heat Eqn; explicit approach

- One can show that the procedure of obtaining the solutions using Eq. 10 are stable, provided $(1-2\sigma) \geq 0$
- The choice $\sigma = 1/2$ so that $(1-2\sigma) = 0$, simplifies the recursion relations further.
- Next we discuss an alternative finite difference method called the Crank-Nicholson approach

# Heat Equation; Crank-Nicholson Algorithm

- **Crank-Nicholson Approach:** This approach differs from the previous one in that we adopt a backward difference approach to compute the time derivative, i.e.,

$$\frac{\partial u(x,t)}{\partial t} \approx \frac{u(x,t) - u(x,t-k)}{k}$$

- If we substitute this on the right-hand side of Eq. 9, while keeping the left-hand side the same, we obtain

$$\frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2} = \frac{u(x,t) - u(x,t-k)}{k} \tag{11}$$

- This equation is written as

$$-u(x-h,t) + ru(x,t) - u(x+h,t) = su(x,t-k),$$

where $r = 2 + s$ and $s = \frac{h^2}{k}$

- We can rewrite above also as

$$-u(n-1,m) + ru(n,m) - u(n+1,m) = su(n,m-1) \tag{12}$$

# Crank-Nicholson Method...

- In the previous equation, if we adopt the notations $u_n = u(n,m)$ and $b_n = su(n,m-1)$, and use the boundary conditions $u(0,m) = u(N,m)$, where $Nh = 1$, it reduces to the following tridiagonal matrix equation

$$\begin{pmatrix} r & -1 & & & & \\ -1 & r & -1 & & & \\ & -1 & r & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & r & -1 \\ & & & & -1 & r \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_{N-2} \\ b_{N-1} \end{pmatrix}$$

- This $N-1$ dimensional linear tridiagonal system of equations needs to be solved using a library routine which we will discuss in the next chapter.

# Wave Equation in 1+1 Dimensions

- The wave equation in $1+1$ dimension can be written as

$$\begin{aligned} \frac{\partial^2 u(x,t)}{\partial x^2} &= \frac{\partial^2 u(x,t)}{\partial t^2} \\ u(x,0) &= f(x) \\ u_t(x,0) &= 0 \\ u(0,t) &= u(1,t) = 0 \end{aligned} \tag{13}$$

  we want the solution of the equation in the region $0 \leq x \leq 1$ and $0 \leq t \leq t_{max}$.
- In principle, the wave equation (Eq. 13) describes the propagating or standing waves in 1 space dimension
- For the boundary conditions given above, it describes standing waves
- Above the shape function $f(x)$ must be doubly differentiable for the obvious reasons, and must satisfy $f(x) = -f(-x)$

- It is easy to verify that the exact analytic solution of Eq. 13 is

$$u(x,t) = \frac{f(x+t)+f(x-t)}{2}. \tag{14}$$

- To verify this solution, we take its derivatives with respect to $x$ and $t$ using the chain rule

$$\begin{aligned} u_x &= \frac{f'(x+t)+f'(x-t)}{2} \implies & u_{xx} &= \frac{f''(x+t)+f''(x-t)}{2} \\ u_t &= \frac{f'(x+t)-f'(x-t)}{2} \implies & u_{tt} &= \frac{f''(x+t)+f''(x-t)}{2} \end{aligned}$$

$$\implies u_{xx} = u_{tt}$$

- Next, we develop the finite difference approach for solving this wave equation

# Finite Difference approach for 1+1 wave equation

- We note that the wave equation in 1+1 dimensions involves second derivatives w.r.t. both $x$ and $t$

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial^2 u(x,t)}{\partial t^2}$$

- We represent them using the central difference formula for both

$$\frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2} = \frac{u(x,t+k) - 2u(x,t) + u(x,t-k)}{k^2}, \tag{15}$$

where, as in the case of heat equation, $h$, $k$ respectively represent the bin sizes for the $x$, and $t$, respectively.

- Again, as in case of the heat equation, we are looking for solutions in the region $0 \leq x \leq 1$, and $0 \leq t \leq t_{max}$ so that with total $N$ bins in the $x$ directions and $M$ in the $t$ direction, we have

$$
\begin{aligned}
x_N &= Nh = 1 \\
t_M &= Mk = t_{max}
\end{aligned}
$$

- Using the earlier discrete notation, Eq. 15 becomes

$$\rho \{u(n+1,m) - 2u(n,m) + u(n-1,m)\} = u(n,m+1) - 2u(n,m) + u($$

where $\rho = k^2/h^2$

- This leads to the final recursion relation which can be programmed

$$
\begin{aligned}
u(n,m+1) = \rho u(n+1,m) + 2(1-\rho)u(n,m) + \rho u(n-1,m) \\
- u(n,m-1) \qquad (16)
\end{aligned}
$$

- The values of $u(n,m)$ are initialized subject to the boundary conditions

$$\begin{aligned} u(n,0) &= f(x_n) \\ \frac{u(n,1)-u(n,0)}{k} &= 0 \\ u(0,m) &= u(N,m) = 0 \end{aligned} \tag{17}$$

## Laplace Equation in two dimensions

- Here our aim is to set up a numerical scheme for solving the Laplace equation in 2D

$$\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = 0. \tag{18}$$

- Note that above there is no time coordinate, but second derivatives are there with respect to the two space coordinates
- A numerical scheme, subject to the specified boundary conditions, can be set up by using the central-difference representation of the second derivatives, as before

$$\frac{u(x+h_1,y) - 2u(x,y) + u(x-h_1,y)}{h_1^2} + \frac{u(x,y+h_2) - 2u(x,y) + u(x,y+h_2)}{h_2^2} = 0 \tag{19}$$

we have assumed a general anisotropic system so that the grid sizes are different in $x$ and $y$ directions.

- However, if the system is anisotropic in the two Cartesian directions, we can take the grid size to be the same in both the directions, i.e., $h_1 = h_2 = h$
- With this, we get a simplified version of Eq. 19

$$\frac{u(x+h,y)-2u(x,y)+u(x-h,y)}{h^2} + \frac{u(x,y+h)-2u(x,y)+u(x,y+h)}{h^2} = 0 \qquad (20)$$

- This formula involves five space points $(x, y)$, $(x \pm h, y)$, and $(x, y \pm h)$, therefore, it is called the "five-point formula". Note that Eq. 19 is also a five-point formula.
- This equation can be solved numerically once the boundary conditions are specified

# 2D Laplace Eqn; discretized version

- We can also write down the discretized recursion-relation form of Eq. 20 by adopting the usual notations

$$x = x_n = nh \equiv n$$
$$y = y_m = mh \equiv m$$

leading to

$$u(n+1,m) + u(n,m+1) = 4u(n,m) - u(n-1,m) - u(n,m-1) \tag{21}$$

note that the terms on the left-hand side of this relation are the unknown quantities while those on the right-hand side of the recursion relation are known from previous iterations, or boundary conditions.

- Clearly, Eq. 21 is a system of linear equations of tridiagonal form, with the main diagonal elements being zero, while the two neighboring diagonal elements being 1.