

Topics on PDEs and Numerical Methods



Part 1: Partial Differential Equations (PDEs)

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Partial Differential Equations

Questions:

- What is a PDE?
- Examples of Important PDEs.
- Classification of PDEs.

Goal:

- Formulate PDE:
convert dynamical process into data or equations
- Solve PDE:
find unknown function that satisfies PDE
- Study solutions:
properties of solutions

Lecture on PDE

What is PDE?	Pg 3
Classification of PDEs	Pg 4
Classification of linear 2 nd order PDE: Elliptic, parabolic, hyperbolic	Pg 5
Three fundamental examples of PDE: heat, wave, Laplace	Pg 6
Common but challenging PDEs: diffusion equation, ..., Schrodinger equations, ...	Pg 7
How to solve PDEs: analytically, numerically, combination of both	Pg 8
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Wave equation: 1D, 3D	Pg 11
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Partial Differential Equations

A **partial differential equation (PDE)** is an equation that involves an unknown function and its partial derivatives.

Notation:

□ PDE involves two or more independent variables: x, y, z, t and dependent variables: u, v

□ **Subscripts:** partial derivatives: $u_{xx} = \frac{\partial^2 u(x,t)}{\partial x^2}, u_{xt} = \frac{\partial^2 u(x,t)}{\partial x \partial t}$

□ PDEs are used to **model** many systems in many different fields of science and engineering.

□ **Important examples:**

■ Laplace equation, Heat equation, Wave equation

Linear Second order PDEs are important sets of equations that are used to model many systems in many different fields of science and engineering.

Classifications of PDEs

Classification is important because: Each category relates to specific engineering problems. Different approaches are used to solve these categories.

- Order: 1st, 2nd, 4th

$$2u_{xx} + 2u_{xt}u_t + 3\sqrt{u_t} = 0. \text{ ---2nd order}$$

- Number of independent variables:** $u(x, y, t)$

- Linearity:** linear if it is linear in the unknown functions and its derivatives

$$\text{Linear: } 2u_{xx} + u_{xt} + 3u_{tt} + 4u_x + \cos(2t) = 0$$

$$\text{Nonlinear: } 2u_{xx} + 2u_{xt}u_t + 3\sqrt{u_t} = 0.$$

- Homogeneity**

- Coefficient type:** constant, variable

- Linear 2nd order PDEs:** parabolic, hyperbolic and elliptic

Applications:

Heat conduction

Fluid motion (Navier Stokes equations)

Schrodinger's equations

General relativity (EFE)

Linear 2nd Order PDEs Classification

- A 2nd order linear PDE with 2 independent variables can be written in the form

$$Au_{xx} + Bu_{xy} + Cu_{yy} + D = 0,$$

where A, B, C are functions of x and y , D is a function of x, y, u, u_x, u_y .

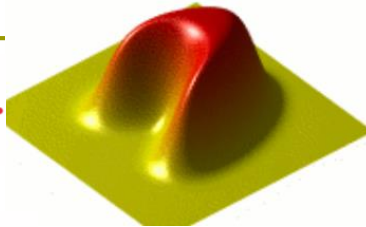
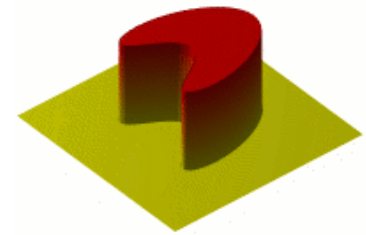
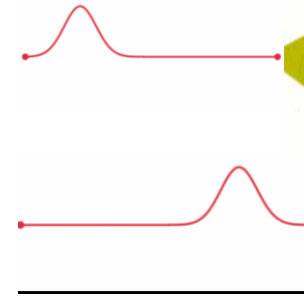
- This kind of equation can be classified based on values of $B^2 - 4AC$ as follows:

Type	Elliptic	Parabolic	Hyperbolic
Condition	$B^2 - 4AC < 0$	$B^2 - 4AC = 0$	$B^2 - 4AC > 0$
Example	Laplace Eqn	Heat Eqn	Wave Eqn
	$u_{xx} + u_{yy} = 0$	$u_t = u_{xx} + u_{yy}$	$u_{tt} = u_{xx} + u_{yy}$

Three fundamental examples of PDE and solutions

Heat equation (parabolic): $u_t = u_{xx}$

- Solution: $u = \frac{1}{2}x^2 + t$
- Challenge: can you find another solution? $u = e^{ax+bt}$
- Fourier, 1800's
- Heat conduction



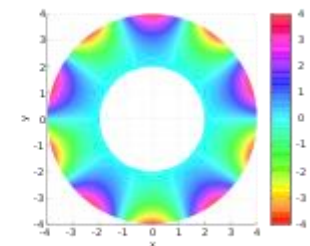
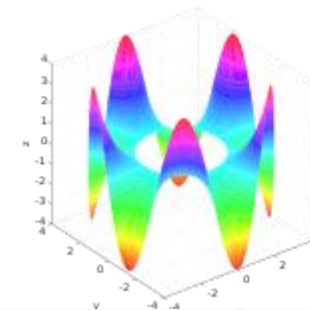
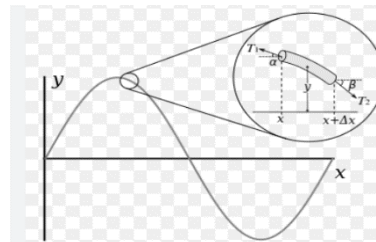
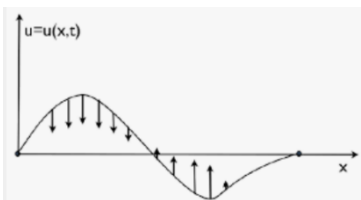
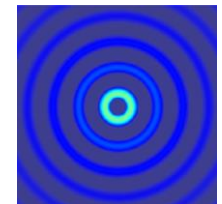
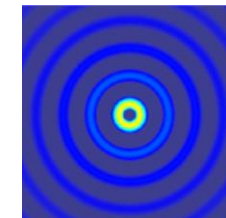
Wave equation (hyperbolic): $u_{tt} = u_{xx}$

- d'Alembert, 1740's, vibration of strings

Laplace equation (elliptic): $u_{xx} + u_{yy} = 0$

- Laplace, 1780's,
- gravitation mechanical equilibrium,
- thermal equilibrium

Vibration, [standing waves](#) in a string. The [fundamental](#) and the first 5 [overtones](#) in the [harmonic series](#).



Laplace's equation on an [annulus](#) (inner radius $r = 2$ and outer radius $R = 4$) with Dirichlet boundary conditions $u(r=2) = 0$ and $u(R=4) = 4 \sin(5\theta)$

Common but Challenging PDEs

- Diffusion equation

$$\nabla \cdot D \nabla C + S = 0$$

- Solid-Mechanics

$$\nabla \cdot (\rho \vec{u} \vec{u}^T) = -\nabla P + \nabla \cdot \tau + \rho g$$

- Navier-Stokes

$$\frac{\partial(\rho \vec{u})}{\partial t} + \nabla \cdot (\rho \vec{u} \otimes \vec{u}) + \nabla P = \mu \nabla^2 \vec{u} + \frac{\mu}{3} \nabla(\nabla \cdot \vec{u}) + \rho g$$

- Schrodinger

$$\nabla \cdot \left[-\frac{\hbar^2}{2m^*} \nabla \psi(\vec{r}) \right] + U(\vec{r}) \psi(\vec{r}) = E \psi(\vec{r})$$

- Dynamics Electromagnetic wave equation

$$\frac{\mu \epsilon \partial^2 \vec{E}(\vec{r}, t)}{\partial t^2} + \frac{\mu \sigma \partial \vec{E}(\vec{r}, t)}{\partial t} - \nabla^2 \vec{E}(\vec{r}, t) = -\frac{\mu \partial \vec{j}(\vec{r}, t)}{\partial t}$$

- Boltzmann transport equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{q\mathbf{E}}{\hbar} \cdot \nabla_k f = \left(\frac{\partial f}{\partial t} \right)_c$$

How to solve PDEs?

Analytically:

- Method of characteristic
- Separation of variables
- Fourier analysis---- $\sin(x)$, $\cos(x)$, Bessel's function, Legendre, ..
- Eigenfunction expansion
- Problems:
 - Cannot deal with complicated geometry
 - May not converge with finite terms
 - Hard to deal with nonlinear

Numerically:

Finite difference method (FDM)

Finite element method (FEM)

Finite volume method

Reduce order method, meshless method, etc

Combination of analytical and numerical methods

Laplace Equation

$$3\text{D: } \frac{\partial^2 u(x,y,z)}{\partial x^2} + \frac{\partial^2 u(x,y,z)}{\partial y^2} + \frac{\partial^2 u(x,y,z)}{\partial z^2} = 0$$

$$2\text{D: } \frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = 0$$

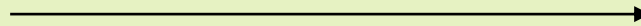
- ❑ Used to describe **the steady state distribution of heat in a body, or the steady state distribution of electrical charge in a body.**
- ❑ $A = 1, B = 0, C = 1 \rightarrow B^2 - 4AC < 0 \rightarrow$ **Elliptic** equation.
- ❑ Possible solution: $u(x, y) = e^x \sin(y)$
- ❑ Temperature is a function of the position (x and y) When no heat source is available in the Poisson equation

$$\frac{\partial^2 T(x,y)}{\partial x^2} + \frac{\partial^2 T(x,y)}{\partial y^2} = f(x, y), f(x, y) = 0$$

Heat Equation

$$3D: \frac{\partial u(x, y, z, t)}{\partial t} = \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$

$$1D: \frac{\partial T(x, t)}{\partial t} = \frac{\partial^2 T(x, t)}{\partial x^2}$$



$$1D \quad \alpha \frac{\partial^2 u(x, t)}{\partial x^2} - \frac{\partial u(x, t)}{\partial t} = 0$$

□ $A = \alpha, B = 0, C = 0 \rightarrow B^2 - 4AC = 0 \rightarrow$ parabolic

□ The function $u(x, y, z, t)$ is used to represent the temperature at time t in a physical body at a point with coordinates (x, y, z)

□ $T(x, t)$ is used to represent the temperature at time t at the point x of the thin rod.

□ α is the thermal diffusivity. It is sufficient to consider the case $\alpha = 1$.

Wave Equation

$$3\text{D: } \frac{\partial^2 u(x,y,z,t)}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right)$$

$$1\text{D: } c^2 \frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial^2 u(x,t)}{\partial t^2} = 0$$

- $A = c^2 > 0, B = 0, C = -1 \rightarrow B^2 - 4AC > 0 \rightarrow$ hyperbolic
- The function $u(x, y, z, t)$ is used to represent the displacement at time t of a particle whose position at rest is (x, y, z) .
- The constant c represents the propagation speed of the wave.

Other simple but important PDEs: Transport equation

□ **Transport equation:** $u_t + cu_x = 0$

■ **Other forms:** $\frac{\partial \rho}{\partial t} + \nabla \cdot j = \sigma$, where

□ $\nabla \cdot$ is divergence, ρ is the amount of the quantity q per unit volume per, t is time, σ is the generation of q per unit volume per unit time

■ describe how **water wave transports**

■ **“Relatives”:**

□ volume continuity equation

□ the Navier–Stokes equations

□ the advection equation

□ in physics, Gauss's law of the electric field

Well-posedness?

- A **well-posed initial/boundary condition problem** has a unique solution that depends continuously on the initial/boundary conditions.
- **The specification of proper initial conditions (IC) and boundary conditions (BC)** for a PDE is essential in order to have a well-posed problem.
- **And we can never find a numerical solution of a problem that is ill posed:** the computer will show its disgust by “blowing up”.

What can make PDEs ill post?

- If **too many IC/BC** are specified, there will be no solution.
- If **too few IC/BC** are specified, the solution will not be unique.
- If **the number of IC/BC is right**, but they are specified at the **wrong place or time**, the solution will be unique, but it will not depend smoothly on the IC/BC.
 - This means that small errors in the IC/BC will produce huge errors in the solution.

In any of these cases we have an ill-posed problem.

Types of boundary conditions:

Specify one boundary condition on each point of the spatial boundary:

1. **Dirichlet BC:** specify the value of the function at the borders of a domain

$$u = 0$$

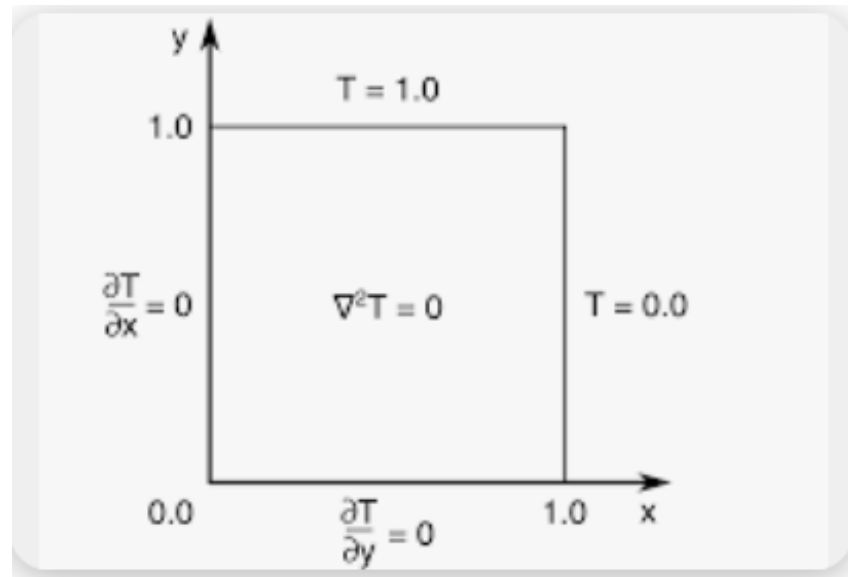
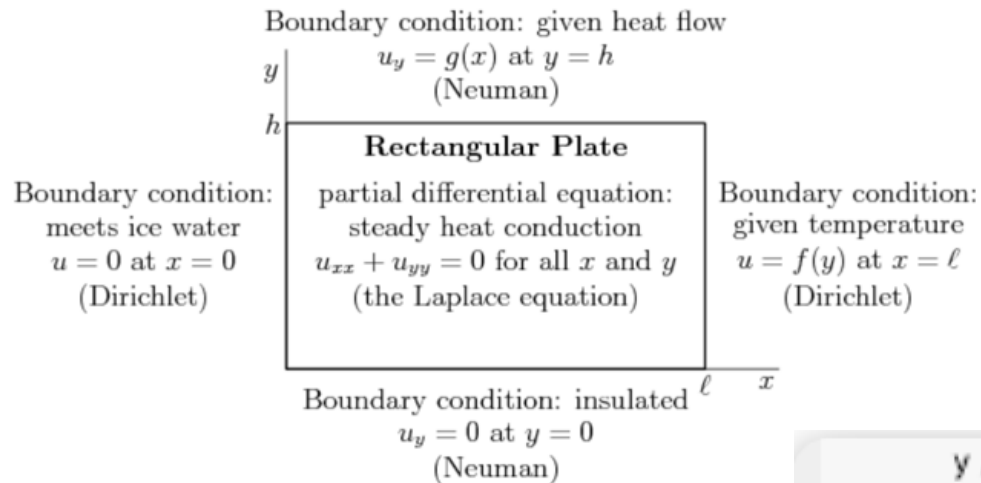
2. **Neumann BC:** specify its normal derivative, e.g., no flux
Neumann BC

$$\frac{\partial u}{\partial x} = 0.$$

3. **Mixed Robin BC:** e.g. flux depends on the temperature

$$\frac{\partial u}{\partial x} = C(u - T).$$

Two examples of Laplace equation with proper boundary conditions in 2D



Two examples of well-posed wave equations:

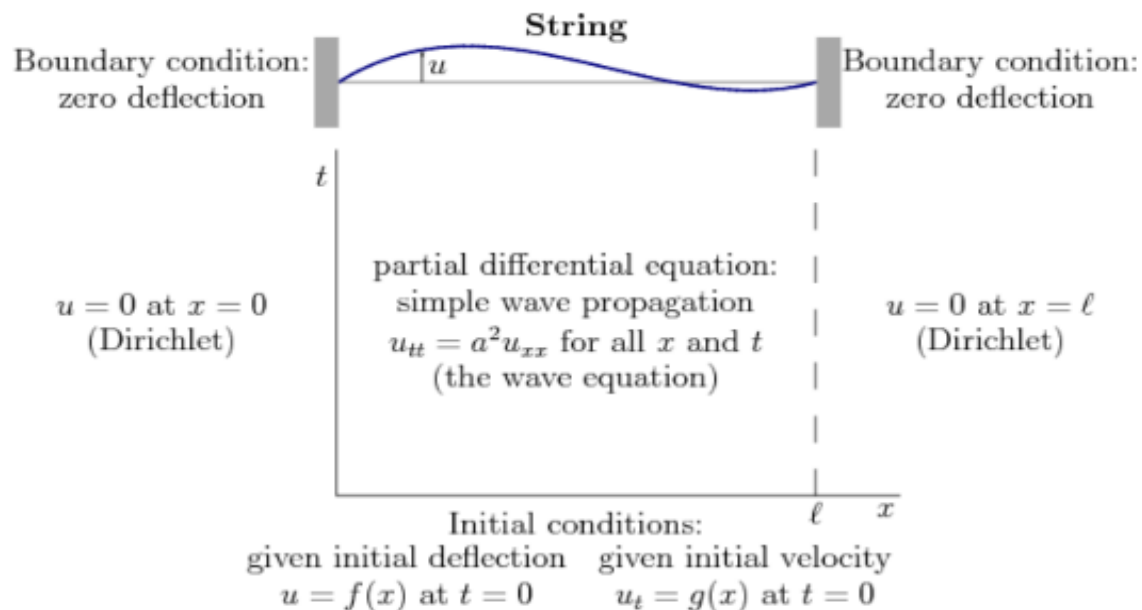
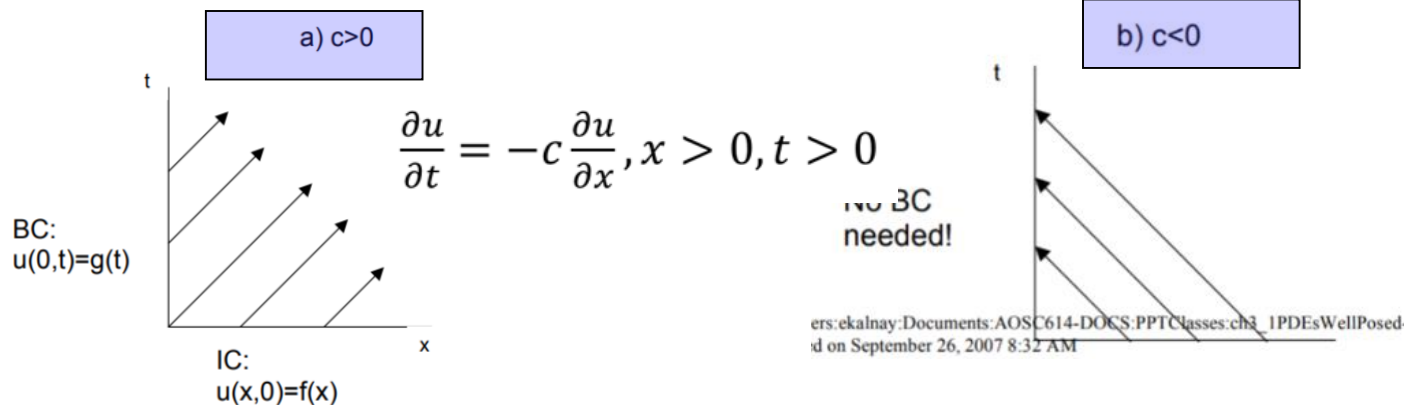


Figure 1.3: An example wave equation problem.



Well post PDEs: an example of heat equation with proper boundary conditions and initial conditions

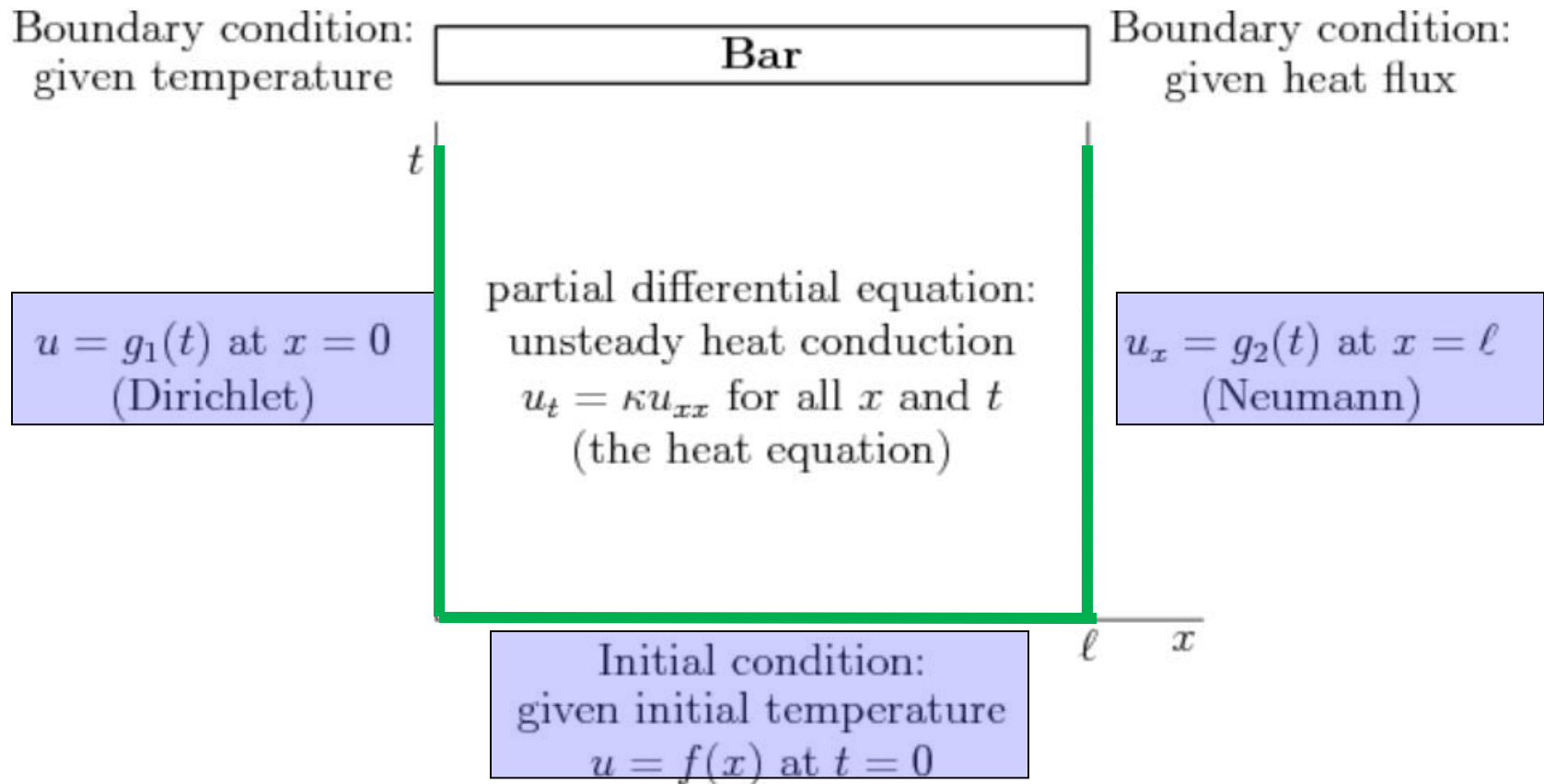
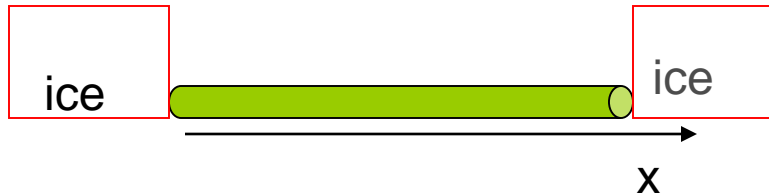


Figure 1.2: An example heat equation problem.

To uniquely specify a solution to the PDE, a set of **boundary conditions** are needed. Both regular and irregular boundaries are possible.

1D Heat Equation



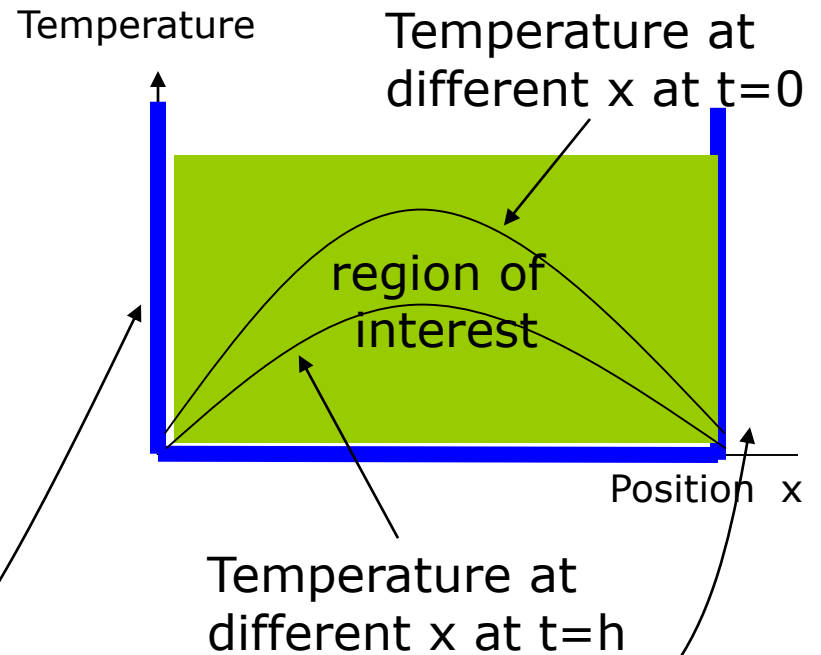
Thin metal rod insulated everywhere except at the edges. At $t = 0$ the rod is placed in ice

$$\frac{\partial^2 T(x, t)}{\partial x^2} - \frac{\partial T(x, t)}{\partial t} = 0$$

$$T(0, t) = T(1, t) = 0$$

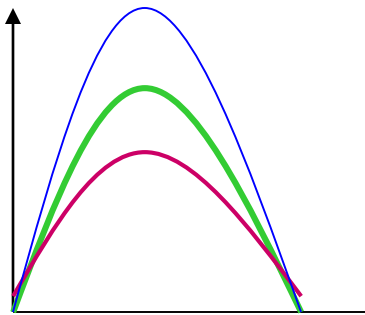
$$T(x, 0) = \sin(\pi x)$$

Different curve is used for each value of t

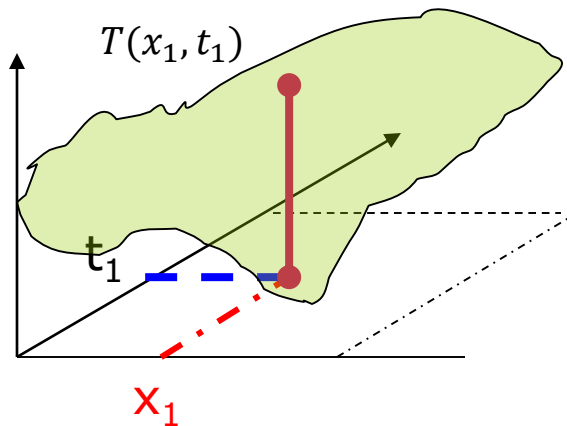


Representing the Solution of a PDE (Two Independent Variables x and t)

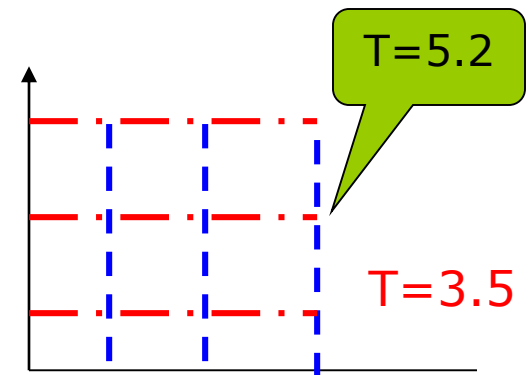
- Three main ways to represent the solution



Different curves are used for different values of one of the independent variable



Three dimensional plot of the function $T(x, t)$



The axis represent the independent variables. The value of the function is displayed at grid points

2D Heat Equation

$$\frac{\partial T(x, y, t)}{\partial t} = 1.2 \left(\frac{\partial^2 T(x, y, t)}{\partial x^2} + \frac{\partial^2 T(x, y, t)}{\partial y^2} \right), 0 < x, y < 1, t > 0$$

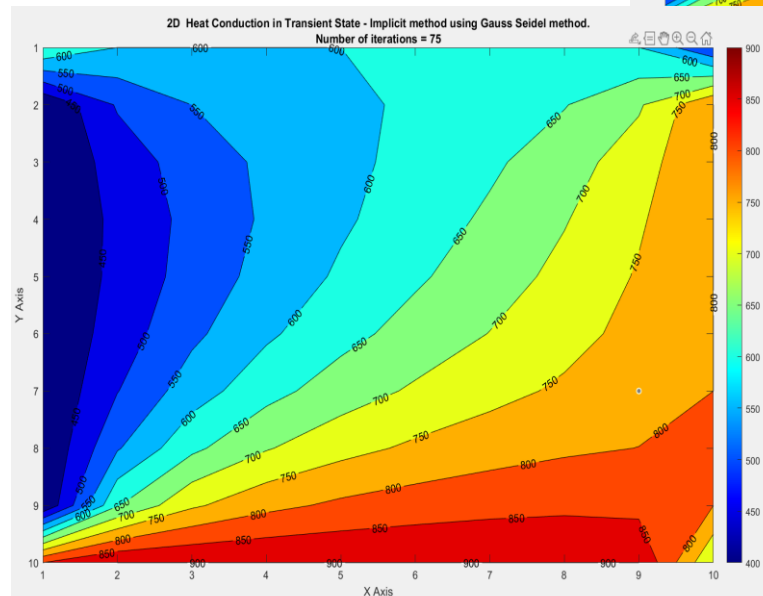
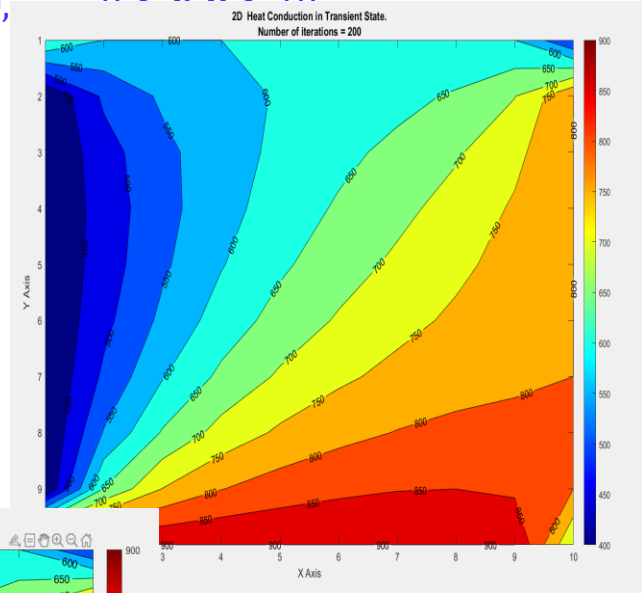
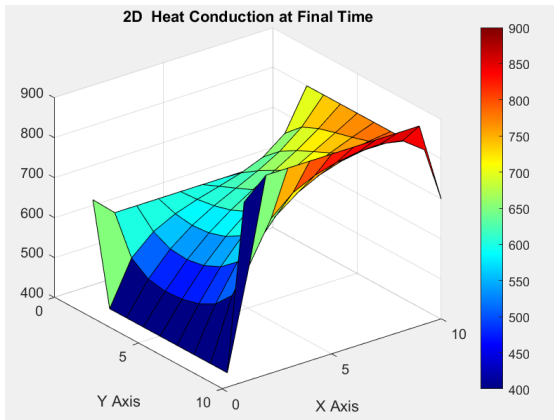
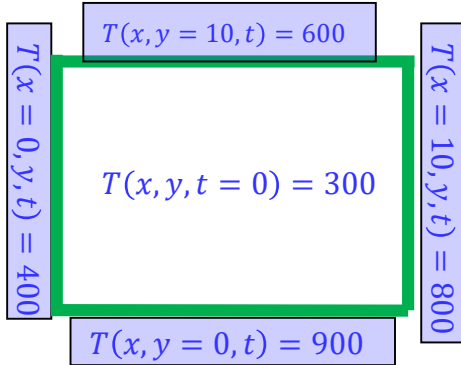
$$T(x = 0, y, t) = 400, \quad 0 \leq y \leq 10, t > 0$$

$$T(x = 10, y, t) = 800, \quad 0 \leq y \leq 10, t > 0$$

$$T(x, y = 10, t) = 600, \quad 0 \leq x \leq 10, t > 0$$

$$T(x, y = 0, t) = 900, \quad 0 \leq x \leq 10, t > 0$$

$$T(x, y, t = 0) = 300, \quad 0 \leq x, y \leq 10$$



2D Laplace Equation

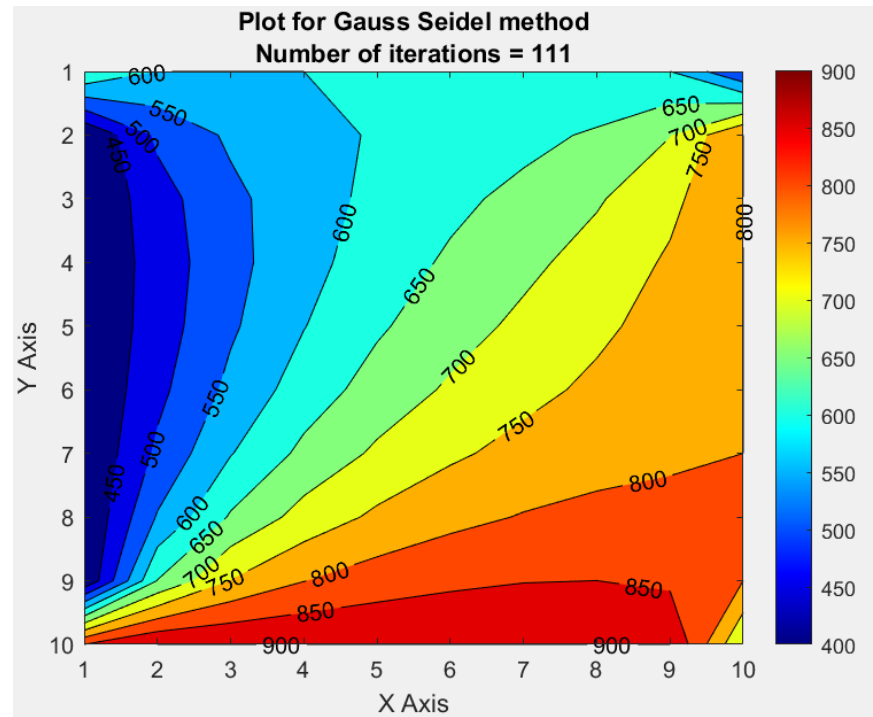
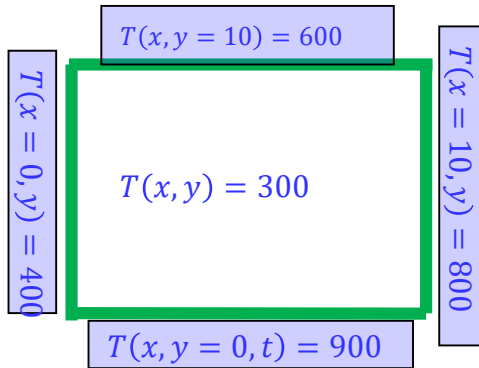
$$\frac{\partial^2 T(x, y, t)}{\partial x^2} + \frac{\partial^2 T(x, y, t)}{\partial y^2} = 0, \quad 0 < x, y < 10$$

$$T(x = 0, y) = 400, \quad 0 \leq y \leq 10$$

$$T(x = 10, y) = 800, \quad 0 \leq y \leq 10$$

$$T(x, y = 10) = 600, \quad 0 \leq x \leq 10$$

$$T(x, y = 0) = 900, \quad 0 \leq x \leq 10$$



2D Wave Equation

$$u_{tt} = c^2(u_{xx} + u_{yy}), 0 < x, y < 1, t > 0$$

$$\text{BC: } u(0, y, t) = u(1, y, t) = u(x, 0, t) = u(x, 1, t) = 0, t > 0$$

$$\text{IC: } T(x, y, t = 0) = \sin(p\pi x) \sin(q\pi y), 0 \leq x, y \leq 1$$

$$T(x, 1, t) = 0$$

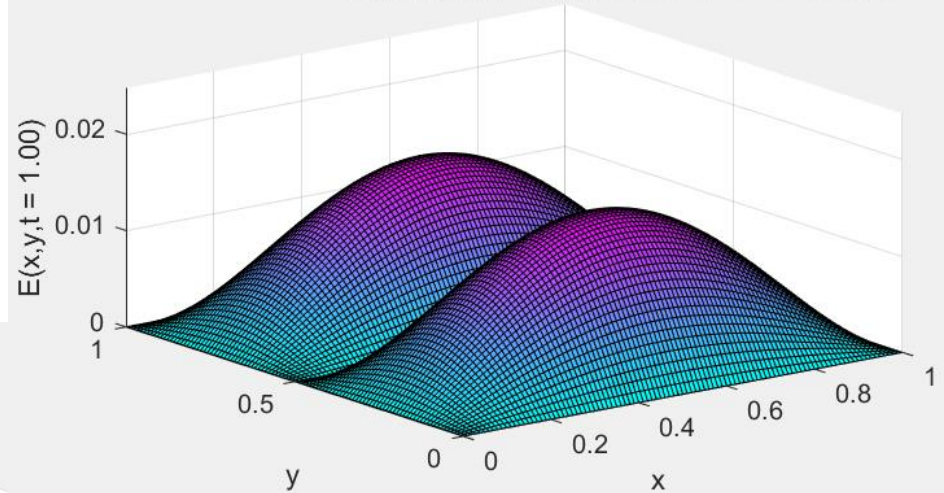
$$T(0, y, t) = 0$$

$$T(x, y, 0) = \sin(p\pi x) \sin(q\pi y)$$

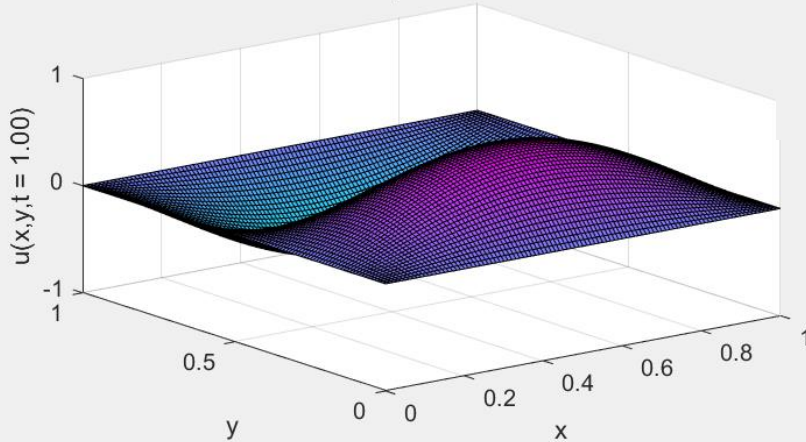
$$T(1, y, t) = 0$$

$$T(x, 0, t) = 0$$

Absolute error at t = 1.00



2D wave equation at t = 1.00



2D Wave Equation

$$u_{tt} = c^2(u_{xx} + u_{yy}), 0 < x, y < 1, t > 0$$

$$\text{BC: } u(0, y, t) = u(1, y, t) = u(x, 0, t) = u(x, 1, t) = 0, t > 0$$

$$\text{IC: } T(x, y, t = 0) = \sin(p\pi x) \sin(q\pi y), 0 \leq x, y \leq 1$$

$$T(x, 1, t) = 0$$

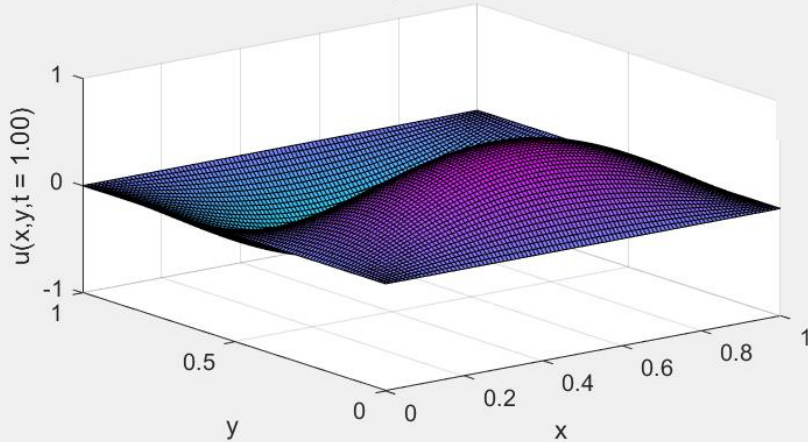
$$0 = (T', 0) \perp$$

$$T(x, y, 0) = \sin(p\pi x) \sin(q\pi y)$$

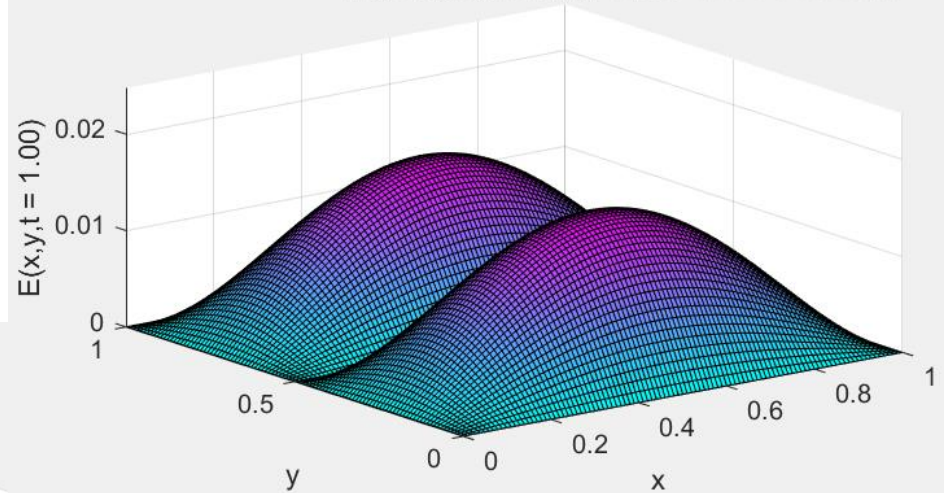
$$0 = (T', t) \perp$$

$$T(x, 0, t) = 0$$

2D wave equation at t = 1.00



Absolute error at t = 1.00



THANK YOU!

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