2. Solving Elliptic PDEs with R

Modeling with PDEs

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Warm up

- **Some questions that you can answer:**
  1. What is the order of an/a ODE/PDE?
  2. What is a linear ODE/PDE?
  3. What are the initial conditions?
  4. and boundary conditions?
  5. What is their difference?
  6. Why are they needed?

Introduction

- **Limitations of ODE models**
  - Deviations between an ODE model and data may indicate that its state variables depend on more than one variable
  - It may be appropriate to use PDE models instead

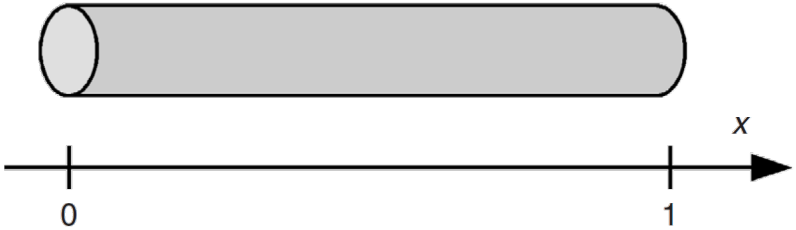
Introduction

- PDE models involve derivatives with respect to at least two independent variables,
- As a whole, PDEs are a really big topic.
- There are many different subtypes of PDEs, which need specifically tailored numerical procedures for their solution.
- In this chapter you will learn the main theoretical concepts about them and how to solve numerically two subtypes: the parabolic and the hyperbolic equations.

Problem 1

- Consider the cylinder in the figure.
- Assuming:
  - a perfect insulation of the cylinder surface in $0 < x < 1$,
  - constant temperatures in the y and z directions at time $t = 0$, that is, no temperature variations across transverse sections,
  - a known initial temperature distribution $T_i(x)$ at time $t = 0$,
  - and constant temperatures T_0 and T_1 at the left and right ends of the cylinder for all times $t > 0$,

What is the temperature $T(x, t)$ for $x \in (0, 1)$ and t $\in (0, T]$?



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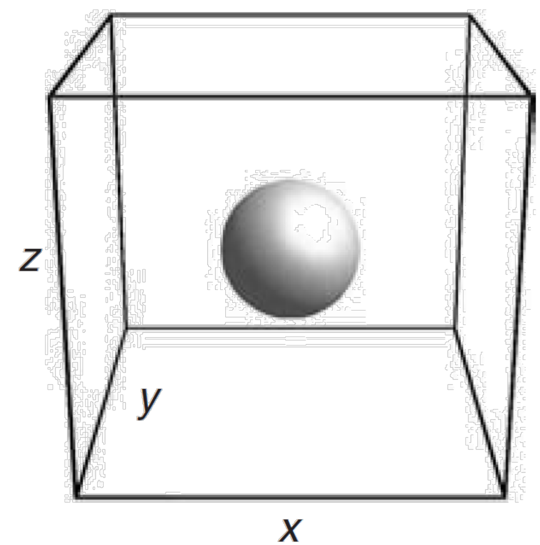
Problem 2

- Referring to the configuration in the figure and assuming:
  - constant temperature T_c at the top surface of the cube ($z = 1$),
  - constant temperature T_s at the sphere surface,
  - and perfect insulation of all other surfaces of the cube,

What is the stationary temperature distribution $T(x, y, z)$ within the cube (i.e. in the domain $[0, 1]^3 \backslash S$ if S is the sphere)?



The heat equation

- To solve these problems, we need an equation that describes the dynamics of temperature as a function of space and time:

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2}\right)$$

Partial Differential Equations

- They involve partial derivatives of a function with respect to at least two independent variables.
- It can be generalized to several unknowns, vector-valued unknowns, and systems of PDEs
- The *order of a PDE* is the degree of the highest derivative appearing in the PDE
- Most PDEs used in science and engineering applications are first- or second-order equations

First-order PDEs

- General form of a first-order PDE in two dimensions:

$$F(x, y, u, u_x, u_y) = 0$$

- Where:
  - x: first dimension
  - y: second dimension
  - u: unknown function
  - u_x: partial derivative of the unknown function with respect to x
  - u_y: partial derivative of the unknown function with respect to y

Second-order PDEs

- General form of a second-order PDE in two dimensions:

$$F\left(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}\right) = 0$$

- Where:
  - u_{xx}: partial derivative of the unknown function with respect to x two times
  - u_{xy}: partial derivative of the unknown function with respect to x and to y
  - u_{yy}: partial derivative of the unknown function with respect to y two times

Elliptic, Parabolic, and Hyperbolic Equations

- The general form of a linear second-order PDE in two dimensions is:

$$A \cdot u_{xx} + B \cdot u_{xy} + C \cdot u_{yy} + D \cdot u_x + E \cdot u_y + F = 0$$

- Depending on the sign of the *discriminant*

$$d = A \cdot C - B^2$$

linear second-order PDEs are called:

  - *elliptic* if $d > 0$
  - *parabolic* if $d = 0$
  - *hyperbolic* if $d < 0$

Examples of Parabolic Equations

- Heat equation:

$$\frac{\partial T}{\partial t} - \frac{K}{C\rho}\left(\frac{\partial^2 T}{\partial x^2}\right) = 0$$

$$-\frac{K}{C\rho}\frac{\partial^2 T}{\partial x^2} + 0\frac{\partial^2 T}{\partial x \partial t} + 0\frac{\partial^2 T}{\partial t^2} + 0\frac{\partial T}{\partial x} + \frac{\partial T}{\partial t} + 0 = 0$$

$$A = -\frac{K}{C\rho} \quad B = 0 \quad C = 0 \quad D = 0 \quad E = 1 \quad F = 0$$

$$d = A \cdot C - B^2 = 0 \Rightarrow Parabolic$$

Examples of Parabolic Equations

- Action potential propagation in a fiber:

$$C_m \frac{\partial V_m}{\partial t} - \sigma \frac{\partial^2 V_m}{\partial x^2} + I_{ion} = 0$$

$$-\sigma \frac{\partial^2 V_m}{\partial x^2} + 0 \frac{\partial^2 V_m}{\partial x \partial t} + 0 \frac{\partial^2 V_m}{\partial t^2} + 0 \frac{\partial V_m}{\partial x} + C_m \frac{\partial V_m}{\partial t} + I_{ion} = 0$$

$$A = -\sigma \quad B = 0 \quad C = 0 \quad D = 0 \quad E = C_m \quad F = I_{ion}$$

$$d = A \cdot C - B^2 = 0 \Rightarrow Parabolic$$

Examples of Elliptic Equations

- Laplace Equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

$$\frac{\partial^2 u}{\partial x^2} + 0\frac{\partial^2 u}{\partial x \partial y} + \frac{\partial^2 u}{\partial y^2} + 0\frac{\partial u}{\partial x} + 0\frac{\partial u}{\partial y} + 0 = 0$$

$$A = 1 \quad B = 0 \quad C = 1 \quad D = 0 \quad E = 0 \quad F = 0$$

$$d = A \cdot C - B^2 = 1 \Rightarrow Elliptic$$

Examples of Elliptic Equations

- Bidimensional Heat Equation in equilibrium $\left(\frac{\partial T}{\partial t} = 0\right)$:

$$\frac{\partial T}{\partial t} = \frac{K}{C\rho}\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) \Rightarrow \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$

$$\frac{\partial^2 T}{\partial x^2} + 0\frac{\partial^2 T}{\partial x \partial y} + \frac{\partial^2 T}{\partial y^2} + 0\frac{\partial T}{\partial x} + 0\frac{\partial T}{\partial y} + 0 = 0$$

$$A = 1 \quad B = 0 \quad C = 1 \quad D = 0 \quad E = 0 \quad F = 0$$

$$d = A \cdot C - B^2 = 1 \Rightarrow Elliptic$$

Re-Cap of the Classification

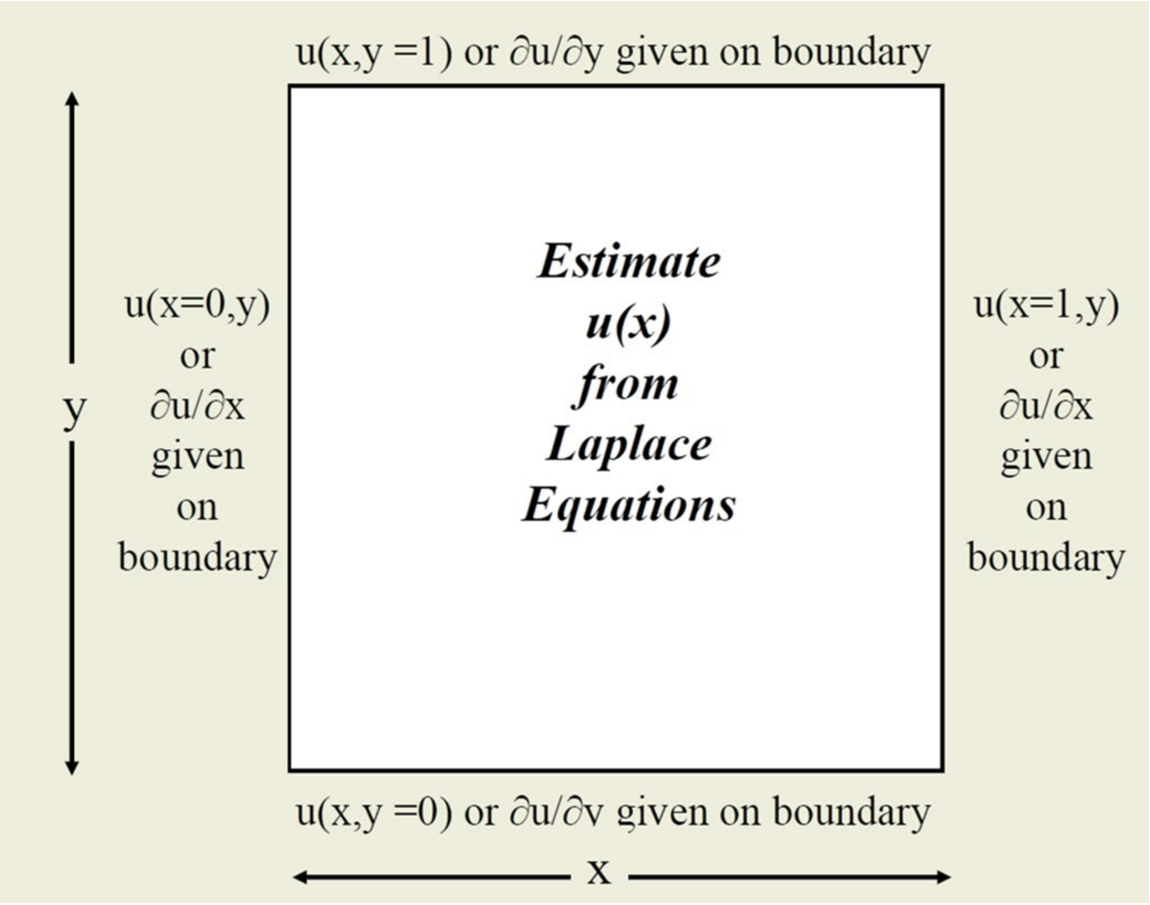
- **Elliptic PDEs:** Contains second-order derivatives with respect to all independent variables, which all have the same sign.
- **Parabolic PDEs:** Involve one second-order derivative and at least one first-order derivative.
- **Hyperbolic PDEs:** Similar to Elliptic but the second-order derivatives have switching signs.

Boundary Conditions for Elliptic PDE's

- **Dirichlet**: u provided along all of edge
- **Neumann**: $\frac{\partial u}{\partial \eta}$ provided along all of the edge $\eta = \{x, y, z, \ldots\}$ (derivative in normal direction)
- **Mixed**: u provided for some of the edge and $\frac{\partial u}{\partial \eta}$ for the remainder of the edge

Elliptic PDE's are analogous to Boundary Value ODE's

Boundary Conditions for Elliptic PDE's



Numerical Methods for Solving PDEs

- The numerical methods used for solving PDE's are different depending on the different character of the problems.
  - Sometimes, the problem is solved at all the positions once for steady state conditions
  - Other times, we need to integrate using the initial conditions forward through time.

Numerical Methods for Solving PDEs

- **Methods**
  - **Finite Difference Method (FDM):** Based on approximating solution at a finite # of points, usually arranged in a regular grid.
  - **Finite Element Method (FEM):** Based on approximating solution on an assemblage of simply shaped (triangular, quadrilateral) finite pieces or "elements".
  - **Method of Lines**: valid for PDEs that are formulated as an initial-value problem in one of its variables. Based on a reformulation of the PDE in terms of a system of ODEs or differential-algebraic equations.

Finite Difference Method

- Based on approximating solution at a finite # of points, usually arranged in a regular grid.

- Similar to the Forward Euler integration: derivatives are approximated using the difference between two points with an small separation

Solving Elliptic PDE's

- Solve all at once
- Liebmann Method:
  - Based on Boundary Conditions (BCs) and finite difference approximation to formulate system of equations
  - Solve the system of equations

Solving Elliptic PDE's

- Discretize domain into grid of evenly spaced points
- For nodes where u is unknown:

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{\Delta x^2}$$

$$\frac{\partial^2 u}{\partial y^2} \approx \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\Delta y^2}$$

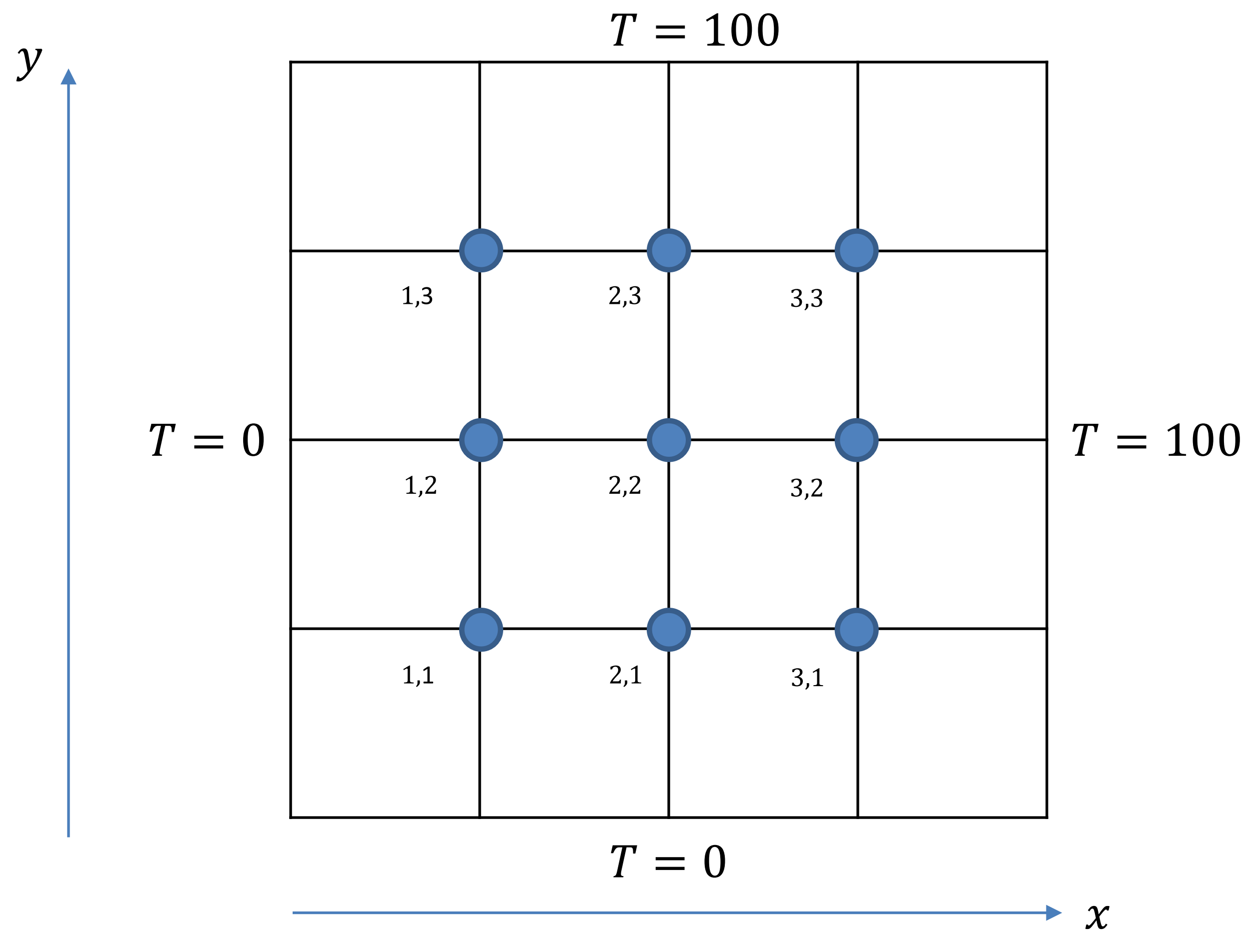
  – with Δx=$\Delta y = h$, substitute into main equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \approx \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j} + u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{\mathrm{h}^2}$$

- Using Boundary Conditions, write, n*m equations for u($x_{i=1:m}$, $y_{j=1:n}$) or n*m unknowns.
- Solve this banded system with an efficient scheme.

Solving Elliptic PDE's

- **Example**: Heat equation under steady-state conditiosn



Solving Elliptic PDE's

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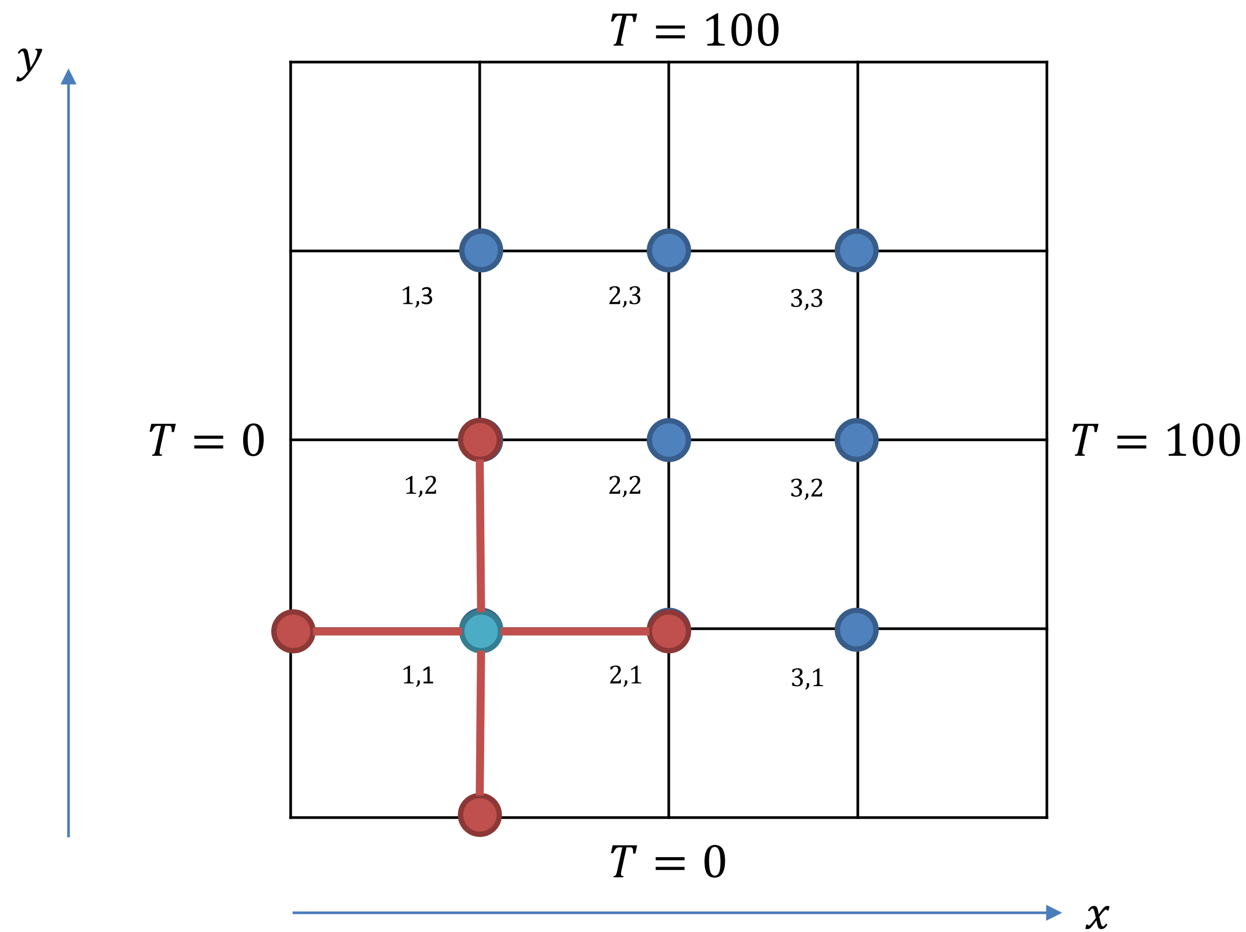

Solving Elliptic PDE's

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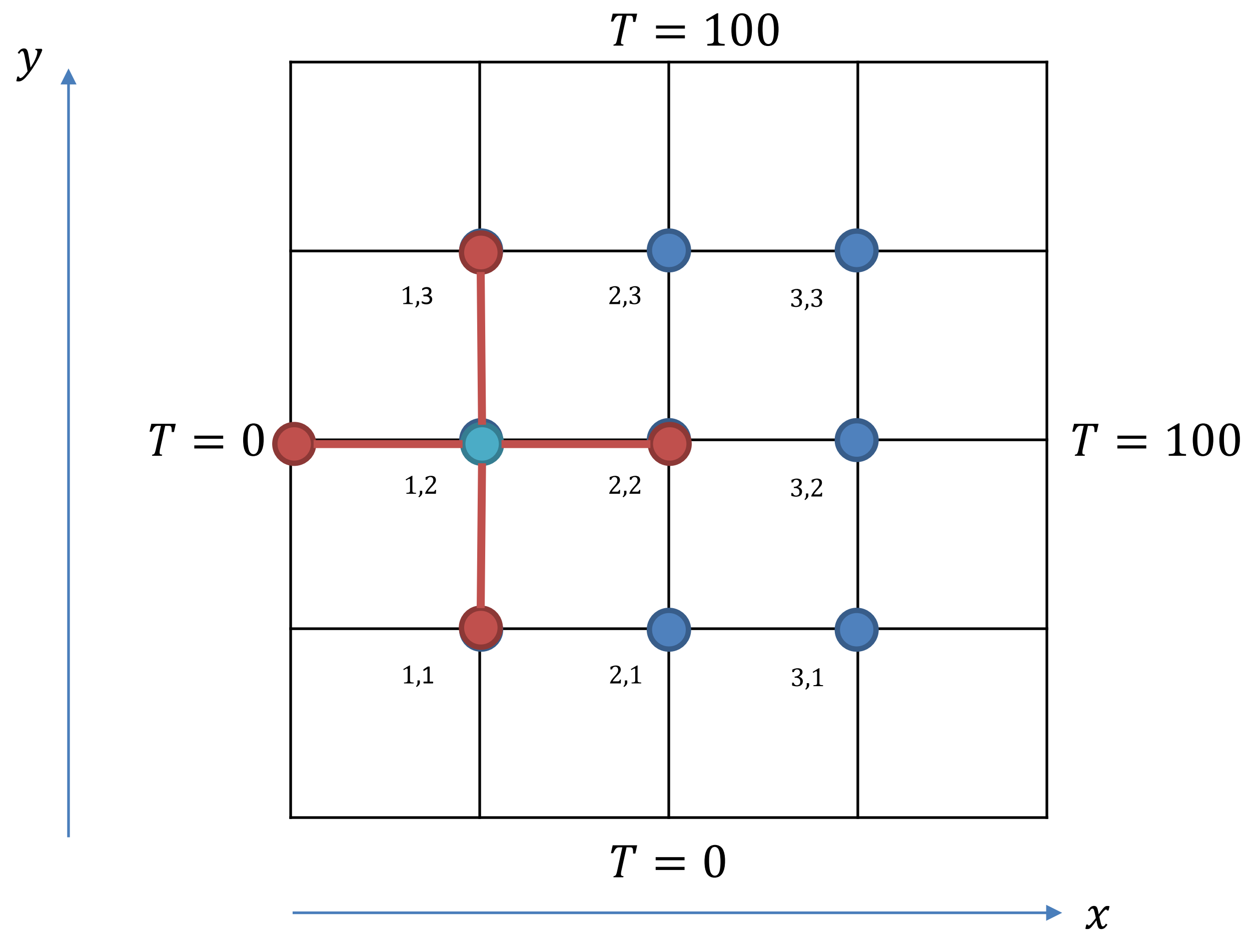

Solving Elliptic PDE's

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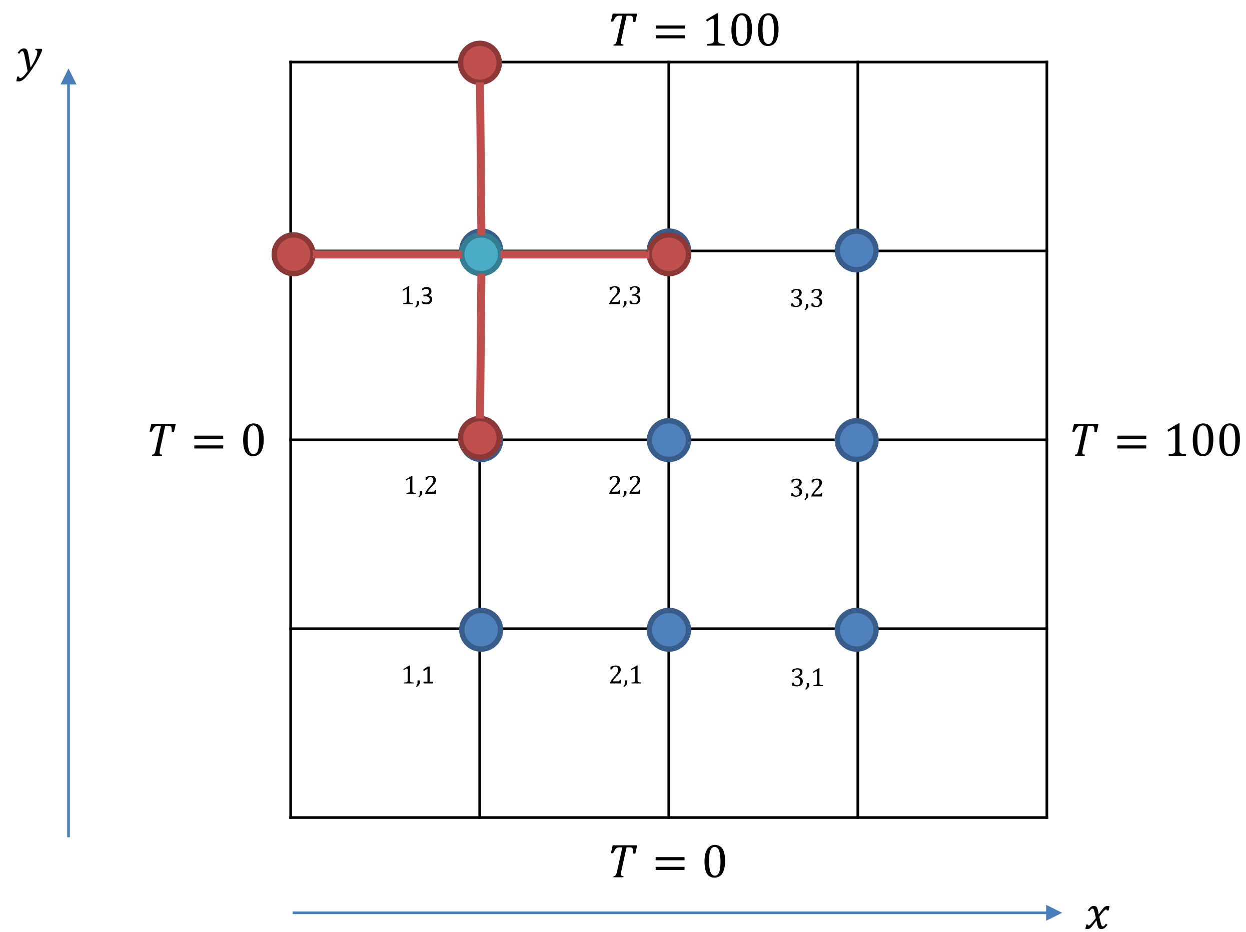

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