Computational Techniques
Module 9: Partial Differential Equations

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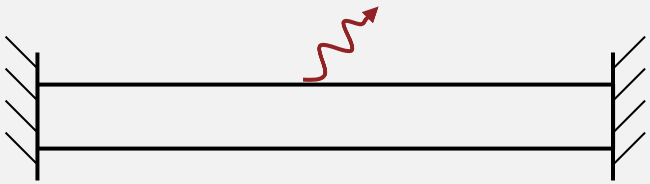
Introduction

- Ordinary Differential Equations
  - States vary in either *time* or one *spatial* dimension
- Partial Differential Equations
  - States vary in:
    - Time *and* space; or
    - More than one spatial dimensions

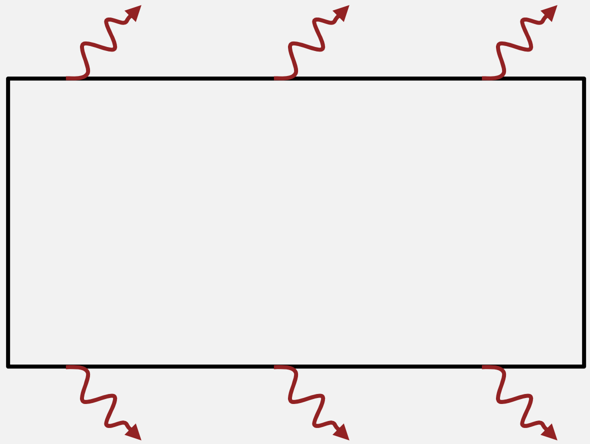
In other words, PDEs represent systems with two or more independent variables

An Example

- A conducting rod

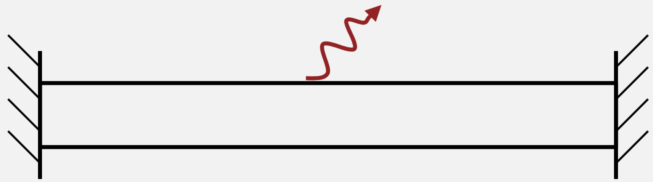


- A conducting block



An Example

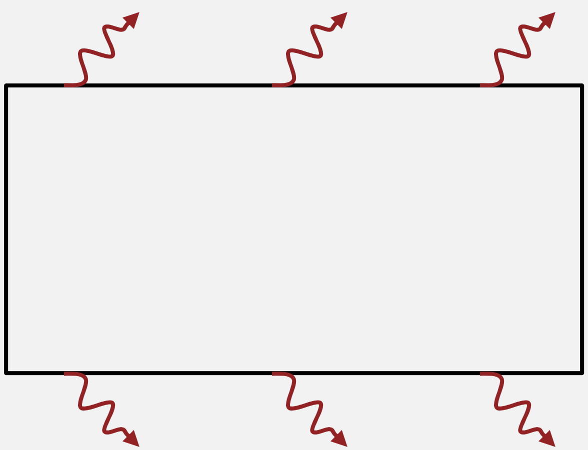
- A conducting rod



$$\frac{d^2T}{dx^2} = \beta(T - T_a)$$

$$T(0) = \gamma$$
$$T(L) = \kappa$$

- A conducting block



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

$$T(0, y) = \gamma$$
$$T(L, y) = \kappa$$

$$T'(x,0) = \lambda(T - T_a)$$
$$T'(x, d) = -\xi(T - T_a)$$

Plug Flow Reactor

- Steady State Model
  - Model: $$\left(\frac{F}{A}\right)\frac{dC_A}{dx} = -r(C_A)$$
  - Initial Condition: $$C_A\Big|_{x=0} = C_0$$
- Unsteady Model
  - Model: $$\frac{\partial C_A}{\partial t} + \left(\frac{F}{A}\right)\frac{\partial C_A}{\partial x} = -r(C_A)$$
  - Initial Conditions: $$C_A\Big|_{(t=0),x} = C_0; \quad C_A\Big|_{t,(x=0)} = C_{in}$$

Typical PDEs of Interest

- First order PDEs

$$D\frac{\partial \phi}{\partial x} + E\frac{\partial \phi}{\partial y} + F\phi + G = 0$$

- Second order PDEs

$$A\frac{\partial^2 \phi}{\partial x^2} + B\frac{\partial^2 \phi}{\partial x \partial y} + C\frac{\partial^2 \phi}{\partial y^2} + D\frac{\partial \phi}{\partial x} + E\frac{\partial \phi}{\partial y} + F\phi + G = 0$$

Linear if (A to G) are functions of x and y only

Homogeneous if G = 0

Overview

- Classification of PDEs
- Method of Lines
  - Convert PDEs to ODEs
- Finite Difference
  - Convert to (non-)linear equations

Parabolic PDEs

- When $B^2 - 4AC = 0$
- Example: Transient Axial Dispersion Reactor
  - $$\frac{\partial C_A}{\partial t} + \left(\frac{F}{A}\right)\frac{\partial C_A}{\partial x} = D\frac{\partial^2 C_A}{\partial x^2} - r(C_A)$$
  - Typically observed when diffusive/conductive terms are present or dominant in the system

Parabolic PDEs: Solution Methods

- Forward in Time, Central in Space (FTCS)
  - Apply forward difference in time: $\mathcal{O}(\Delta t)$
  - Apply central difference in space: $\mathcal{O}(\Delta x^2)$
  - PDE ➔ Algebraic: Solve using NR / Gauss-Siedel
- Crank-Nicholson Method (semi-implicit)
  - Apply "Midpoint Method" in time
  - $\mathcal{O}(\Delta t^2)$ accurate <u>and</u> more stable
- Method of Lines
  - Central difference in space: PDE ➔ ODEs in time

Hyperbolic PDEs

- When $B^2 - 4AC > 0$
- "Wave-like" solution which evolves in one (or more) "*characteristic*" directions
- Example: Transient PFR
  - $$\frac{\partial C_A}{\partial t} + \left(\frac{F}{A}\right)\frac{\partial C_A}{\partial x} = -r(C_A)$$
  - Typically observed when convective terms are dominant in the system

Hyperbolic PDEs: Solution Methods

- Forward in Time, Central in Space (FTCS)
  - Unstable and hence not used
- "Upwind Difference"
  - Apply forward difference in time: $\mathcal{O}(\Delta t)$
  - Apply backward difference in space: $\mathcal{O}(\Delta x)$
  - PDE → Algebraic: Solve using NR / Gauss-Siedel
- Crank-Nicholson Method
  - Semi-implicit, higher accuracy and better stability
- Method of Lines
  - Upwind difference in space: PDE → ODEs in time

Elliptic PDEs

- When $B^2 - 4AC < 0$
- Solution depends on both boundaries
- Example: Heat conduction in a slab
  - $$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$
  - Solution depends on all boundary conditions and the PDEs need to be *solved simultaneously*.

Elliptic PDEs: Solution Methods

- Central difference in all the directions
  - Accuracy: $\mathcal{O}(\Delta x^2)$, $\mathcal{O}(\Delta y^2)$
  - PDE ➔ Algebraic: Solve using NR / Gauss-Siedel

  - Conceptually simple, but implementation is tedious and difficult because all equations are solved simultaneously.

Overview of this Module

- Classification of PDEs
- Method of Lines
  - Convert PDEs to ODEs
- Finite Difference
  - Convert to (non-)linear equations