# Topic and contents

**UNSW, School of Mathematics and Statistics**

MATH2089 – Numerical Methods

Week 09 – Partial Differential Equations I



- MATLAB M-files
  - `bvpfd.m`
  - `h1d.m`
  - `lap2d.m`
  - `pdepe.m`





# Partial Differential Equations

- Partial Differential Equation (PDE)
  - Involves functions of more than 1 variable
  - Variables: time $t$, space $x, y, z$
  - Used to model a wide variety of physical problems
  - Order of differential equation is the order of the highest derivative
- Quasi-linear PDE is linear in its highest derivatives
  - Second order quasi-linear PDE for $u(\xi_1, \xi_2)$

$$A\frac{\partial^2 u}{\partial \xi_1^2} + 2B\frac{\partial^2 u}{\partial \xi_1 \partial \xi_2} + C\frac{\partial^2 u}{\partial \xi_2^2} = F\left(\xi_1, \xi_2, u, \frac{\partial u}{\partial \xi_1}, \frac{\partial u}{\partial \xi_2}\right) \qquad (1)$$

  - Two independent variables $\xi_1$ and $\xi_2$
  - Unknown function $u(\xi_1, \xi_2)$
  - $A, B, C$ may be functions of the independent variables $\xi_1$ and $\xi_2$
  - Classify problems based on values of $A, B, C$
  - $\Longrightarrow$ problem characteristics, numerical methods
- Linear PDE
  - Linear in $u$ and all its derivatives





# Classification of PDEs

- Elliptic if $AC - B^2 > 0$
  - Laplace's equation $(A = 1, B = 0, C = 1)$

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad (2)$$

  - Poisson's equation $(A = 1, B = 0, C = 1)$

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f(x, y) \qquad (3)$$

- Parabolic if $AC - B^2 = 0$
  - Heat equation $(A = \alpha, B = 0, C = 0)$

$$\frac{\partial u}{\partial t} = \alpha\frac{\partial^2 u}{\partial x^2} \qquad (4)$$

- Hyperbolic if $AC - B^2 < 0$
  - Wave equation (wave speed $\eta$) $(A = 1, B = 0, C = -1/\eta^2)$

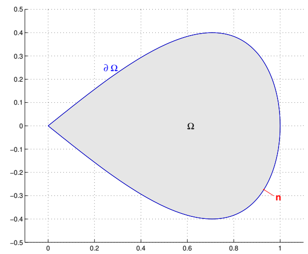
$$\frac{1}{\eta^2}\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \qquad (5)$$





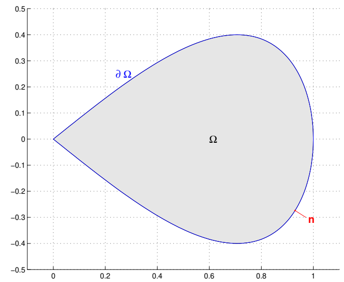
# Complete Problem

- Unknown function $u(\mathbf{x}, t)$
  - Time $t$ and space variables $\mathbf{x} = (x, y, z)^T$
  - Physical problem, symmetry $\Longrightarrow$ fewer space variables $\mathbf{x} \in \mathbb{R}^2$, $\mathbf{x} \in \mathbb{R}$
  - Steady-state $\iff$ no change w.r.t time $t$ $\iff$ time derivatives zero
- Complete problem specification requires
  1. Space domain $\Omega$ and time interval, typically $[0, T]$
  2. Governing partial differential equation
  3. Boundary conditions for $\mathbf{x}$ on boundary $\partial\Omega$ of domain $\Omega$
  4. Initial conditions at $t = 0 \Longrightarrow$ value of $u(\mathbf{x}, 0)$ for $\mathbf{x} \in \Omega$.



## Boundary Conditions

- Dirichlet boundary conditions
  - Function values $u(\mathbf{x}, t)$ are specified for $\mathbf{x} \in \partial\Omega$
  - eg boundary of the body is held at a specified temperature
- Neumann boundary conditions
  - normal derivatives $\frac{du(\mathbf{x},t)}{d\mathbf{n}} = \mathbf{n} \cdot \nabla u(\mathbf{x}, t)$ for $\mathbf{x} \in \partial\Omega$ are specified.
  - $\mathbf{n}$ = outward normal vector to surface of domain at point $\mathbf{x}$
  - eg body insulated $\Longrightarrow$ no heat flow into or out of body across boundary $\Longrightarrow \frac{du(\mathbf{x},t)}{d\mathbf{n}} = 0$












## Diffusion

- Heat conduction, Chemical concentration (Fick's second Law), ...
- Domain $\Omega \subset \mathbb{R}^3$
- Temperature $u(\mathbf{x}, t)$ at $\mathbf{x} = (x, y, z) \in \Omega$, time $t \geq 0$
- Partial differential equation

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = D\left(\frac{\partial^2 u(\mathbf{x},t)}{\partial x^2} + \frac{\partial^2 u(\mathbf{x},t)}{\partial y^2} + \frac{\partial^2 u(\mathbf{x},t)}{\partial z^2}\right) \qquad (6)$$

- Diffusion coefficient $D > 0$
  - Conductivity of the body
  - Uniform material $\Longrightarrow$ constant $D$
  - Non-uniform material $\Longrightarrow D(\mathbf{x})$ may depend on position $\mathbf{x}$ in body
- Steady state $\Longrightarrow$ no change with time $\Longrightarrow u(\mathbf{x}, t) = u(\mathbf{x})$
  - Derivatives with respect to $t$ are zero
  - Laplace's equation

$$\nabla^2 u(\mathbf{x}) \equiv \frac{\partial^2 u(\mathbf{x})}{\partial x^2} + \frac{\partial^2 u(\mathbf{x})}{\partial y^2} + \frac{\partial^2 u(\mathbf{x})}{\partial z^2} = 0 \qquad (7)$$





## Finite Difference Methods

- Based on Taylor series for $f \in C^{n+1}$

$$f(x+h) = f(x) + \sum_{k=1}^{n} \frac{h^k}{k!} f^{(k)}(x) + \frac{h^{n+1}}{(n+1)!} f^{(n+1)}(\xi), \quad \xi \in (x, x+h)$$

- Standard finite difference approximations

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x)}{h} + O(h) \\ f'(x) &= \frac{f(x+h) - f(x-h)}{2h} + O(h^2) \\ f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + O(h^2) \end{aligned}$$

- Functions of more than one variable $\Longrightarrow$ partial derivatives
  - ONLY change variable in derivative, eg

$$\frac{\partial u(x,t)}{\partial x} = \frac{u(x+h,t) - u(x-h,t)}{2h} + O(h^2)$$

## 1-D Steady State Heat Equation

- One-dimensional steady state heat equation
- Single space variable $\mathbf{x} = x \in \Omega = [a, b]$
- No variation with time $\Longrightarrow u(\mathbf{x}, t) \equiv u(\mathbf{x})$, $\quad \frac{\partial u(\mathbf{x},t)}{\partial t} = 0$
- Heat equation reduces to ODE

$$\frac{d^2u(x)}{dx^2} = 0 \quad x \in (a, b)$$

- Dirichlet boundary conditions $\Longrightarrow$ BVP $\quad u(a) = U_a, \quad u(b) = U_b$
- Analytic solution $u(x) = \alpha x + \beta$
- Constants $\alpha$ and $\beta$ determined by boundary conditions

$$u(a) = \alpha a + \beta = U_a, \qquad u(b) = \alpha b + \beta = U_b$$

- Solving for $\alpha$, $\beta$

$$u(x) = \frac{U_b - U_a}{b - a}x + \frac{bU_a - aU_b}{b - a}.$$

- Line through $(a, U_a)$ and $(b, U_b)$
- Analytic solution provides important check for numerical method





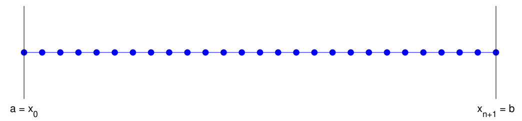
## 1-D discretization

- Divide domain $[a, b]$ into $n + 1$ equal length subintervals

$$a = x_0 < x_1 < x_2 < \cdots < x_{n-1} < x_n < x_{n+1} = b$$

- Grid points

$$x_j = a + j\,h, \quad j = 0, \ldots, n + 1, \qquad h = \frac{b - a}{n + 1}$$




  - End points $\quad x_0 = a, \quad x_{n+1} = b$
  - Internal grid points $x_j$ for $j = 1, \ldots, n$
- $u_j$ approximate value of $u(x_j)$ at grid point $x_j$
  - Boundary values $\quad u_0 = u(x_0) = U_a, \quad u_{n+1} = u(x_{n+1}) = U_b$
  - Unknowns $u_j = u(x_j)$ for $j = 1, \ldots, n$





## BVP Discretization I

- At grid point $x_j$: $O(h^2)$ central difference approximation

$$u''(x) = \frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} + O(h^2)$$

- Substitute in DE $u''(x) = 0$

$$\frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} = 0$$

- Multiply by $-h^2$

$$-u_{j-1} + 2u_j - u_{j+1} = 0$$

- Boundary values $\quad u_0 = U_a, \quad u_{n+1} = U_b$
- System of linear equations

$$\begin{aligned} &2u_1 - u_2 = U_a \\ &-u_{j-1} + 2u_j - u_{j+1} = 0, \quad j = 2, ..., n-1 \\ &-u_{n-1} + 2u_n = U_b \end{aligned}$$

## BVP Discretization II

- Linear system $A\mathbf{u} = \mathbf{b}$, $\quad A \in \mathbb{R}^{n\times n}$, $\quad \mathbf{u}, \mathbf{b} \in \mathbb{R}^n$

$$\begin{bmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -1 & 2 & -1 & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{n-2} \\ u_{n-1} \\ u_n \end{bmatrix} = \begin{bmatrix} U_a \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ U_b \end{bmatrix}$$

- Coefficient matrix $A$: MATLAB `h1d.m`
  - Tridiagonal lower bandwidth $m_\ell = 1$, upper bandwidth $m_u = 1$
  - Symmetric $A^T = A$, Positive definite as
  - Diagonally dominant

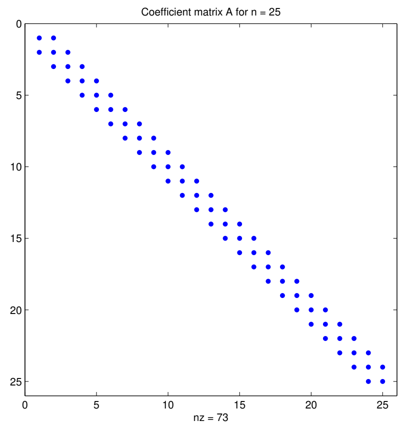
$$a_{ii} \geq \sum_{\substack{j=1 \\ j\neq i}}^{n} |a_{ij}| \quad \text{for all } i = 1, \ldots, n$$

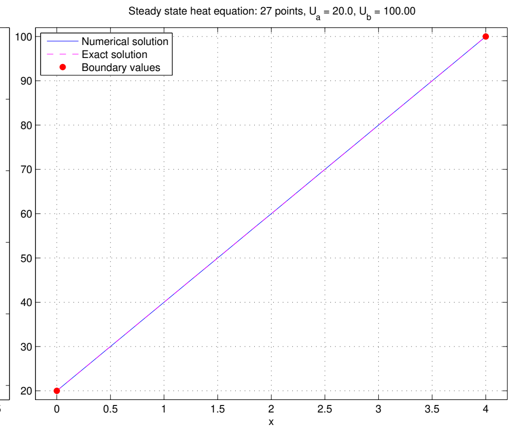
with strict inequality for at least one $i$





## BVP Discretization III




1. Spy plot of non-zero elements in sparse coefficient matrix $A$
2. Numerical and exact solution for steady state heat equation in 1-D





## BVP Example

**Example (BVP)**

$$y'' - \frac{y'}{t} + \frac{y}{t^2} = 0, \qquad y(1) = 2, \quad y(2) = 6$$

1. Show exact solution is $y(t) = 2t + \dfrac{t\log(t)}{\log(2)}$
2. Set up linear system using central difference approximations of $O(h^2)$

**Solution**

- *Derivatives* $\quad y' = 2 + \dfrac{\log(t)}{\log(2)} + \dfrac{1}{\log(2)}, \quad y'' = \frac{1}{t\log(2)}$
- *Substitute to check* $y'' - \dfrac{y'}{t} + \dfrac{y}{t^2} = 0$
- *BCs* $\quad t = 1 \implies y(1) = 2, \quad t = 2 \implies y(2) = 6$





## BVP Examples - Discretization

**Solution**

- *Central difference approximations of $O(h^2)$ at $t_j$ with $y_j \approx y(t_j)$*

$$\begin{aligned} y'(t_j) &= \frac{y_{j+1} - y_{j-1}}{2h} + O(h^2) \\ y''(t_j) &= \frac{y_{j-1} - 2y_j + y_{j+1}}{h^2} + O(h^2) \end{aligned}$$

- *DE* $\quad y'' - \frac{y'}{t} + \frac{y}{t^2} = 0$

$$\frac{y_{j-1} - 2y_j + y_{j+1}}{h^2} - \frac{1}{t_j}\frac{y_{j+1} - y_{j-1}}{2h} + \frac{y_j}{t_j^2} = 0$$

- *Multiply through by $-h^2$ and collect terms*

$$y_{j-1}\left(-1 - \frac{h}{2t_j}\right) + y_j\left(2 - \frac{h^2}{t_j^2}\right) + y_{j+1}\left(-1 + \frac{h}{2t_j}\right) = 0$$

## BVP Example - Discretization cont

**Solution (Cont)**

- *Coefficients of equation $j$ for $j = 1, \dots, n$*

$$\alpha_j = \left(-1 - \frac{h}{2t_j}\right), \quad \beta_j = \left(2 - \frac{h^2}{t_j^2}\right), \quad \gamma_j = \left(-1 + \frac{h}{2t_j}\right)$$

- *Boundary values determine $y_0$ and $y_{n+1}$*
- *Linear system $\alpha_j y_{j-1} + \beta_j y_j + \gamma_j y_{j+1} = 0$*

$$\begin{array}{rl} j = 1 & \beta_1 y_1 + \gamma_1 y_2 = -\alpha_1 y_0 \\ j = 2, \dots, n-1 & \alpha_j y_{j-1} + \beta_j y_j + \gamma_j y_{j+1} = 0 \\ j = n & \alpha_n y_{n-1} + \beta_n y_n = -\gamma_n y_{n+1} \end{array}$$

- *Linear system with coefficient matrix $A$:* MATLAB `bvpfd.m`
  - *Tridiagonal $\Longrightarrow$ Thomas algorithm $O(n)$ flops*
  - *Not symmetric $\alpha_{j+1} \neq \gamma_j$,*









## 2-D Steady State Heat Equation

- 2-D $\Longrightarrow$ variables $\mathbf{x} = (x, y)^T \in \Omega \subset \mathbb{R}^2$
- Steady state $\Longrightarrow$ time derivative zero, $u(\mathbf{x}, t) = u(\mathbf{x})$
- PDE

$$\frac{\partial^2 u(\mathbf{x})}{\partial x^2} + \frac{\partial^2 u(\mathbf{x})}{\partial y^2} = 0 \qquad \mathbf{x} \in \Omega \tag{8}$$

- Domain

$$\Omega = \left\{\mathbf{x} \in \mathbb{R}^2 : 0 \le x \le L_x,\ 0 \le y \le L_y\right\}.$$

- Boundary conditions on $\partial\Omega$

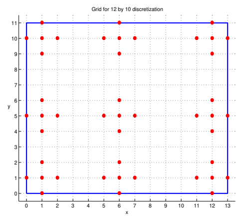
$$\begin{array}{rcl} \partial\Omega & = & \{(0, y), \quad (L_x, y), \quad 0 \le y \le L_y; \\ & & (x, 0), \quad (x, L_y), \quad 0 \le x \le L_x\} \end{array}$$





## Discretization of domain

- Domain



- Divide $x$ interval $[0, L_x]$ into $m + 1$ equal length subintervals

$$0 = x_0 < x_1 < x_2 < \cdots < x_{m-1} < x_m < x_{m+1} = L_x,$$

$$x_i = i\ h_x, \quad i = 0, \dots, m+1, \qquad h_x = \frac{L_x}{m+1}.$$

- Divide $y$ interval $[0, L_y]$ into $n + 1$ equal length subintervals

$$0 = y_0 < y_1 < y_2 < \cdots < y_{n-1} < y_n < y_{n+1} = L_y,$$

$$y_j = j\ h_y, \quad j = 0, \dots, n+1, \qquad h_y = \frac{L_y}{n+1}.$$

## Discretization of Laplacian

- At the grid point $(x_i, y_j)$
- $u_{i,j}$ approximates $u(x_i, y_j)$
- Central difference approximations of $O(h^2)$ to second derivative

$$\frac{\partial^2 u(x_i,y_j)}{\partial x^2} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h_x^2} + O(h_x^2),$$
$$\frac{\partial^2 u(x_i,y_j)}{\partial y^2} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{h_y^2} + O(h_y^2)$$

- Substituting into PDE

$$\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h_x^2} + \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{h_y^2} = 0$$

- Assume $h_x = h_y = h$ and multiply through by $-h^2$

$$4u_{i,j} - u_{i-1,j} - u_{i+1,j} - u_{i,j-1} - u_{i,j+1} = 0 \quad i = 1, \ldots, m,\ j = 1, \ldots, n$$





## Converting into a linear system

- $2-D$ array of variables $u_{i,j}$ for $i = 1, \ldots, m, \quad j = 1, \ldots, n$
- Convert into vector of variables $\mathbf{v} \in \mathbb{R}^{mn}$
- Row-ordering goes across the rows ($x$ variable, $i$ subscript) first

$$v_{(j-1)m+i} = u_{i,j} \qquad i = i, \ldots, m, \quad j = 1, \ldots, n$$

$$\mathbf{v} = \begin{array}{l} [u_{1,1}, u_{2,1}, \cdots, u_{m,1},\ u_{1,2}, u_{2,2}, \cdots, u_{m,2}, \\ u_{1,3}, u_{2,3}, \cdots, u_{m,3},\ \cdots,\ u_{1,n}, u_{2,n}, \cdots u_{m,n}]^T \end{array}$$

- Column ordering goes up a column ($y$ variable, $j$ subscript) first

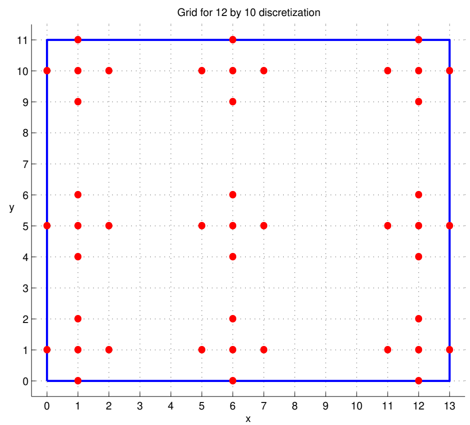
$$v_{(i-1)n+j} = u_{i,j} \qquad j = 1, \ldots, n, \quad i = i, \ldots, m.$$

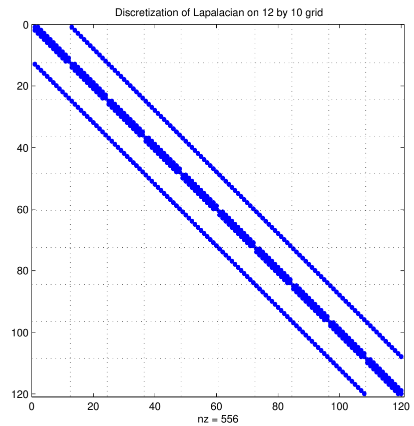
- Other orderings possible
  - Red-Black ordering
  - Diagonal ordering





## Linear system from row-ordering




- Boundary values $u_{0,j}$, $u_{m+1,j}$, $u_{i,0}$, $u_{i,n+1}$ known $\Longrightarrow$ RHS
- Coefficient matrix $A$: banded, sparse, ...
- MATLAB `lap2d.m`





## MATLAB function pdepe

- MATLAB pdepe: Parabolic and elliptic equations of the form

$$c\left(x,t,u,\frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^m f\left(x,t,u,\frac{\partial u}{\partial x}\right)\right) + s\left(x,t,u,\frac{\partial u}{\partial x}\right)$$

- Geometry parameter $m$
  - $m = 0$ "slab" geometry
  - $m = 1$ cylindrical geometry
  - $m = 2$ spherical geometry
- Space domain $x \in [a, b]$, Time domain $t \in [t_0, t_f]$
- Boundary conditions: For $x = a$ or $x = b$

$$p(x,t,u) + q(x,t)f\left(x,t,u,\frac{\partial u}{\partial x}\right) = 0.$$

- Initial conditions: $u(x, t_0) = u_0(x), \quad x \in (a, b)$
- pdepe uses space discretization to create a system of ODEs in time, then uses ODE solver
- MATLAB: `doc pdepe`