Topic and contents

UNSW, School of Mathematics and Statistics

MATH2089 – Numerical Methods

Week 09 – Partial Differential Equations II

- MATLAB M-files
  - `h1dt.m`
  - `w1dt.m`

Time Dependent Heat Equation

- Domain Space variables $\mathbf{x} \in \Omega \subset \mathbb{R}^3$
- Time $t \in [0, T]$
- Heat equation – Partial Differential Equation (PDE)

$$\frac{\partial u(\mathbf{x},t)}{\partial t} = D\left(\frac{\partial^2 u(\mathbf{x},t)}{\partial x^2} + \frac{\partial^2 u(\mathbf{x},t)}{\partial y^2} + \frac{\partial^2 u(\mathbf{x},t)}{\partial z^2}\right), \mathbf{x} \in \Omega, t \in [0,T]$$

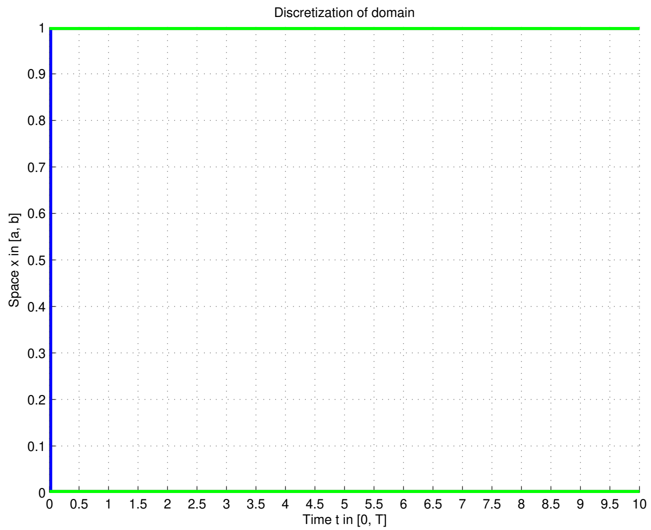
- Boundary conditions: $u(\mathbf{x},t), \mathbf{x} \in \partial\Omega, t \in (0,T]$
- Initial conditions: $u(\mathbf{x},0), \mathbf{x} \in \Omega$
- One-dimensional problem: $\Omega = [a,b] \subset \mathbb{R}$
  - PDE

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^2 u(x,t)}{\partial x^2}, \quad x \in \Omega, \quad t \in (0,T] \tag{1}$$

  - Boundary conditions: $u(a,t) = f_a(t), \quad u(b,t) = f_b(t), \quad t \in (0,T]$
  - Initial conditions: $u(x,0) = u_0(x), \quad x \in \Omega$
  - Consistency at $t = 0$, $x = a, b$

$$u_0(a) = f_a(0), \quad u_0(b) = f_b(0)$$

Domain, IC, BC



Space and Time Discretization

- Space variable discretized by

$$a = x_0 < x_1 < x_2 \cdots < x_{n-1} < x_n < x_{n+1} = b, \tag{2}$$

  - $n + 2$ space points x_j, $j = 0, \ldots, n+1$, including two boundary values
  - equally spaced grid gives

$$\Delta x = (b-a)/(n+1), \qquad x_j = a + j\Delta x \quad j = 0, \ldots, n+1 \tag{3}$$

  - n internal grid points $x_j \in (a,b)$, excluding two boundary values
- Time variable discretized by

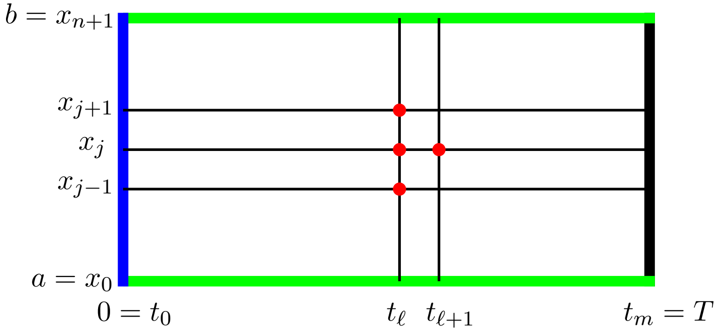
$$0 = t_0 < t_1 < t_2 \cdots < t_{m-1} < t_m = T \tag{4}$$

  - $m + 1$ time points t_ℓ, $\ell = 0, \ldots, m$
  - equally spaced grid gives

$$\Delta t = T/m, \qquad t_\ell = \ell\Delta t \quad \ell = 0, \ldots, m \tag{5}$$

- u_j^ℓ approximation to $u(x_j, t_\ell)$, $\quad j = 0, \ldots, n+1, \quad \ell = 0, \ldots, m$

Space and Time discretization



- Initial conditions $u_0(x)$
- Boundary conditions $f_a(t),\ f_b(t)$
- Want $u(x, T)$ for $x \in (a, b)$

Derivative approximations

- At the point $(x_j,\, t_\ell)$, $\quad u_j^\ell \approx u(x_j, t_\ell)$
- Forward difference approximation to time derivative

$$\frac{\partial u(x_j, t_\ell)}{\partial t} = \frac{u(x_j, t_\ell + \Delta t) - u(x_j, t_\ell)}{\Delta t} + O(\Delta t)$$

- Central difference approximation to space derivative

$$\frac{\partial^2 u(x_j, t_\ell)}{\partial x^2} = \frac{u(x_j - \Delta x, t_\ell) - 2u(x_j, t_\ell) + u(x_j + \Delta x, t_\ell)}{(\Delta x)^2} + O((\Delta x)^2)$$

- $t_\ell + \Delta t = t_{\ell+1}, \quad x_j - \Delta x = x_{j-1}, \quad x_j + \Delta x = x_{j+1}$
- Approximations

$$\frac{\partial u(x_j, t_\ell)}{\partial t} \approx \frac{u_j^{\ell+1} - u_j^\ell}{\Delta t}$$

$$\frac{\partial^2 u(x_j, t_\ell)}{\partial x^2} \approx \frac{u_{j-1}^\ell - 2u_j^\ell + u_{j+1}^\ell}{(\Delta x)^2}$$

Explicit method

- Substitute approximations into PDE (1): Explicit FTCS scheme

$$\frac{u_j^{\ell+1} - u_j^\ell}{\Delta t} = D \frac{u_{j-1}^\ell - 2u_j^\ell + u_{j+1}^\ell}{(\Delta x)^2}$$

  - Forward difference approximation for Time derivative
  - Central difference approximation for the Space derivative
- Important quantity

$$s = \frac{D\ \Delta t}{(\Delta x)^2} > 0 \tag{6}$$

- Time stepping from $t_0 = 0$ where $u(x, 0)$ given by initial conditions
- Known values u_j^ℓ, Unknown values $u_j^{\ell+1}$
- Explicit method: explicit formula for unknown values

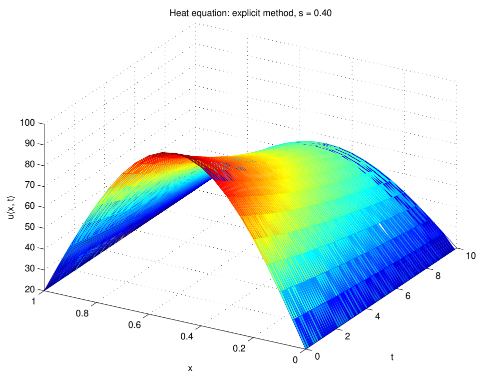
$$u_j^{\ell+1} = s u_{j-1}^\ell + (1 - 2s) u_j^\ell + s u_{j+1}^\ell, \quad j = 1, \ldots, n, \quad \ell = 1, \ldots, m \tag{7}$$

- Each time step ℓ requires $5n$ flops $\Longrightarrow$ total $5mn$ flops

Example

Example (One dimensional heat equation)

$a = 0,\ b = 1$, Boundary conditions $f_a(t) = 20,\ f_b(t) = 20,\ D = 0.008$
Initial conditions $u_0(x) = 20 + 80\sin(\pi x),\ T = 10$ and 20
MATLAB `h1dt.m`



Stability Analysis

- Initial condition $u_j^0 = e^{ikx_j}$, $\quad i = \sqrt{-1}$, $\quad$ wave number k
- Substituting into the difference equation (7)

$$\begin{aligned} u_j^1 &= se^{ikx_{j-1}} + (1-2s)e^{ikx_j} + se^{ikx_{j+1}} \\ &= \left(se^{-ik\Delta x} + (1-2s) + se^{ik\Delta x}\right) e^{ikx_j} \\ &= \left(1 - 2s + 2s\cos(k\Delta x)\right) e^{ikx_j} \\ &= G_k u_j^0 \end{aligned}$$

  - $\cos(\theta) = (e^{i\theta} + e^{-i\theta})/2$
- Amplification factor G_k

$$G_k = 1 + 2s(\cos(k\Delta x) - 1) = 1 - 4s\sin^2(k\Delta x/2) \qquad (8)$$

  - $\cos(2\theta) = 1 - 2\sin^2(\theta)$
- Working forwards through time gives

$$u_j^1 = G_k u_j^0, \quad u_j^2 = G_k u_j^1 = G_k^2 u_j^0, \quad \ldots \quad u_j^\ell = G_k^\ell u_j^0$$

Stability Analysis cont

- Unstable $|G_k| > 1$
  - unwanted components can grow and dominate the solution
  - every initial solution has rounding errors
- Stable $|G_k| \le 1$
  - amplitudes do not grow
- Stability for explicit method

$$|G_k| = |1 - 4s\sin^2(k\Delta x/2)| \le 1$$

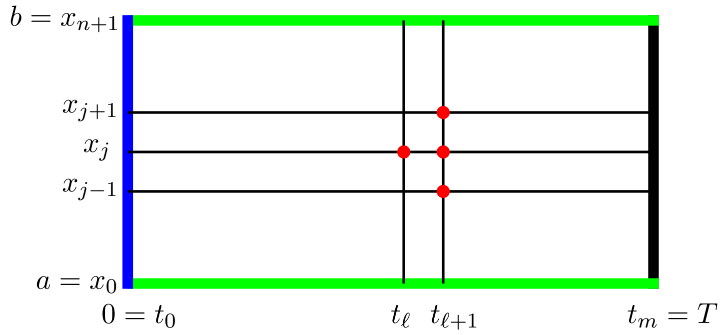
- Hold for all wave numbers k

$$s = \frac{D\,\Delta t}{(\Delta x)^2} \le \frac{1}{2} \qquad (9)$$

  - Stability $\Longrightarrow$ large number of time steps $\Longrightarrow$ computationally expensive
  - $D = 1$, $\Delta x = 10^{-3} \Longrightarrow \Delta t \le \frac{1}{2}10^{-6}$
  - $T = 10 \Longrightarrow 2 \times 10^7$ time steps

Fully Implicit Method

- Approximate space derivative at $t_{\ell+1}$



Fully Implicit Method

- Discretize space derivative at time step $t_{\ell+1}$, rather than t_ℓ

$$\frac{\partial^2 u(x_j, t_{\ell+1})}{\partial x^2} \approx \frac{u_{j-1}^{\ell+1} - 2u_j^{\ell+1} + u_{j+1}^{\ell+1}}{(\Delta x)^2}$$

- Backward difference approximation for time derivative

$$\frac{\partial u(x_j, t_{\ell+1})}{\partial t} \approx \frac{u_j^\ell - u_j^{\ell+1}}{-\Delta t} = \frac{u_j^{\ell+1} - u_j^\ell}{\Delta t}$$

- Substitute in PDE (1): Implicit BTCS scheme

$$\frac{u_j^{\ell+1} - u_j^\ell}{\Delta t} = D\frac{u_{j-1}^{\ell+1} - 2u_j^{\ell+1} + u_{j+1}^{\ell+1}}{(\Delta x)^2}.$$

- Unknowns $u_j^{\ell+1}$ satisfy system of linear equations, $\quad s$ given by (6)

$$-su_{j-1}^{\ell+1} + (1+2s)u_j^{\ell+1} - su_{j+1}^{\ell+1} = u_j^\ell \qquad (10)$$

Fully Implicit Method II

- Boundary values at $j = 0, \quad j = n+1$
- Linear system

$$\begin{array}{rl} j = 1 & (1+2s)u_1^{\ell+1} - s u_2^{\ell+1} = u_1^\ell + s f_a(t_{\ell+1}) \\ 1 < j < n & -s u_{j-1}^{\ell+1} + (1+2s)u_j^{\ell+1} - s u_{j+1}^{\ell+1} = u_j^\ell \\ j = n & -s u_{n-1}^{\ell+1} + (1+2s)u_n^{\ell+1} = u_n^\ell + s f_b(t_{\ell+1}) \end{array}$$

- Coefficient matrix

$$A = \begin{bmatrix} 1+2s & -s & & & \\ -s & 1+2s & -s & & \\ & \ddots & \ddots & \ddots & \\ & & -s & 1+2s & -s \\ & & & -s & 1+2s \end{bmatrix}$$

- Exploit structure of the n by n matrix $A \Longrightarrow$ solve in $O(n)$ flops
  - Tridiagonal, symmetric, Toeplitz, strictly diagonally dominant

Fully Implicit Method – Stability

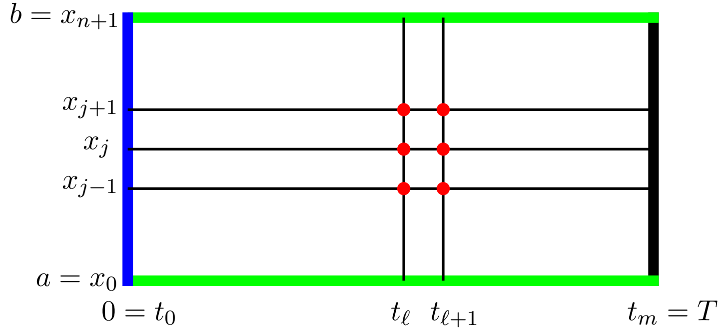
- Use $u_j^\ell = e^{ikx_j}, \quad u_j^{\ell+1} = G_k e^{ikx_j}$
- $-s u_{j-1}^{\ell+1} + (1+2s)u_j^{\ell+1} - s u_{j+1}^{\ell+1} = u_j^\ell$
- $-s G_k e^{ikx_{j-1}} + (1+2s)G_k e^{ikx_j} - s G_k e^{ikx_{j+1}} = e^{ikx_j}$
- $G_k e^{ikx_j}\left(-s e^{-ik\Delta x} + (1+2s) - s e^{ik\Delta x}\right) = e^{ikx_j}$

$$G_k = \frac{1}{1+2s-2s\cos(k\Delta x)} = \frac{1}{1+4s\sin^2(k\Delta x/2)}$$

- $0 \le G_k \le 1$ for all $s > 0$ and $k = 0, 1, 2, \ldots$
- Unconditional stable
- Only possible for implicit methods
- No restrictions on the time step Δt or space step Δx
- Exploiting structure of linear system $\Longrightarrow$ efficient

Crank-Nicolson Method

- Crank-Nicolson discretization (1947)



Crank-Nicolson Method

- Explicit method: Space $O(\Delta x^2)$, Time $O(\Delta t)$

$$u_j^{\ell+1} = u_j^\ell + s\left[u_{j-1}^\ell - 2u_j^\ell + u_{j+1}^\ell\right],$$

- Fully implicit method: Space $O(\Delta x^2)$, Time $O(\Delta t)$

$$u_j^{\ell+1} = u_j^\ell + s\left[u_{j-1}^{\ell+1} - 2u_j^{\ell+1} + u_{j+1}^{\ell+1}\right].$$

- Crank-Nicolson: Average

$$u_j^{\ell+1} = u_j^\ell + \frac{s}{2}\left[\left(u_{j-1}^\ell - 2u_j^\ell + u_{j+1}^\ell\right) + \left(u_{j-1}^{\ell+1} - 2u_j^{\ell+1} + u_{j+1}^{\ell+1}\right)\right] \tag{11}$$

  - Space $O(\Delta x^2)$, Time $O((\Delta t/2)^2) = O(\Delta t^2)$
  - Implicit: Solve tridiagonal linear system for unknowns $u_j^{\ell+1}$
  - Unconditionally stable

Hyperbolic PDE – Wave Equation

- Domain Space variables $\mathbf{x} \in \Omega \subset \mathbb{R}^3$
- Time $t \in [0, T]$
- Wave equation – Hyperbolic Partial Differential Equation (PDE)

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

  - Wave speed c
- Boundary conditions: $u(\mathbf{x},t), \quad \mathbf{x} \in \partial\Omega, \quad t \in (0,T]$
- Two Initial conditions:
  - Initial displacement:

$$u(\mathbf{x},0) = f(\mathbf{x}), \quad \mathbf{x} \in \Omega$$

  - Initial velocity:

$$\frac{\partial u(\mathbf{x},0)}{\partial t} = g(\mathbf{x}), \quad \mathbf{x} \in \Omega$$

One-Dimensional Wave Equation

- One-dimensional problem: $\Omega = [a,b] \subset \mathbb{R}$
- PDE

$$\frac{\partial^2 u(x,t)}{\partial t^2} = c^2 \frac{\partial^2 u(x,t)}{\partial x^2}, \quad x \in \Omega, \quad t \in (0,T] \tag{12}$$

- Boundary conditions: $u(a,t) = f_a(t), \quad u(b,t) = f_b(t), \quad t \in (0,T]$
- Initial conditions:
  - Initial displacement

$$u(x,0) = f(x), \quad x \in \Omega$$

  - Initial velocity

$$\frac{\partial u(x,0)}{\partial t} = g(x), \quad x \in \Omega$$

Space and Time Discretization

- Space variable discretized by

$$a = x_0 < x_1 < x_2 \cdots < x_{n-1} < x_n < x_{n+1} = b \tag{13}$$

  - $n+2$ space points x_j, $j = 0, \ldots, n+1$, including two boundary values
  - equally spaced grid gives

$$\Delta x = (b-a)/(n+1), \qquad x_j = a + j\Delta x \quad j = 0, \ldots, n+1 \tag{14}$$

  - n internal grid points $x_j \in (a,b)$, excluding two boundary values
- Time variable discretized by

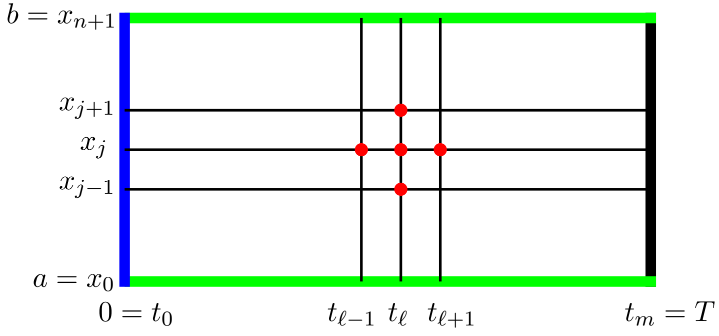
$$0 = t_0 < t_1 < t_2 \cdots < t_{m-1} < t_m = T \tag{15}$$

  - $m+1$ time points t_ℓ, $\ell = 0, \ldots, m$
  - equally spaced grid gives

$$\Delta t = T/m, \qquad t_\ell = \ell \Delta t \quad \ell = 0, \ldots, m \tag{16}$$

- u_j^ℓ approximation to $u(x_j, t_\ell)$, $\quad j = 0, \ldots, n+1, \quad \ell = 0, \ldots, m$

Space and Time Stencil



- Initial conditions $u(x,0) = f(x)$, $u_t(x,0) = g(x)$
- Boundary conditions $f_a(t)$, $f_b(t)$
- Want $u(x,t)$ for $x \in (a,b)$, $t \in (0,T]$

Derivative Approximations

- At the point (x_j, t_ℓ), $\quad u_j^\ell \approx u(x_j, t_\ell)$
- Central difference approximation to time derivative

$$\frac{\partial^2 u(x_j,t_\ell)}{\partial t^2} = \frac{u(x_j,t_\ell-\Delta t) - 2u(x_j,t_\ell) + u(x_j,t_\ell+\Delta t)}{(\Delta t)^2} + O((\Delta t)^2)$$

- Central difference approximation to space derivative

$$\frac{\partial^2 u(x_j,t_\ell)}{\partial x^2} = \frac{u(x_j-\Delta x,t_\ell) - 2u(x_j,t_\ell) + u(x_j+\Delta x,t_\ell)}{(\Delta x)^2} + O((\Delta x)^2)$$

- $t_\ell - \Delta t = t_{\ell-1}, \quad t_\ell + \Delta t = t_{\ell+1}, \qquad x_j - \Delta x = x_{j-1}, \quad x_j + \Delta x = x_{j+1}$
- Finite difference approximations

$$\frac{\partial^2 u(x_j,t_\ell)}{\partial t^2} \approx \frac{u_j^{\ell-1} - 2u_j^\ell + u_j^{\ell+1}}{(\Delta t)^2}$$

$$\frac{\partial^2 u(x_j,t_\ell)}{\partial x^2} \approx \frac{u_{j-1}^{\ell} - 2u_j^\ell + u_{j+1}^{\ell}}{(\Delta x)^2}$$

Explicit Central Difference Method

- Substitute approximations into PDE (12):

$$\frac{u_j^{\ell-1} - 2u_j^\ell + u_j^{\ell+1}}{(\Delta t)^2} = c^2 \frac{u_{j-1}^{\ell} - 2u_j^\ell + u_{j+1}^{\ell}}{(\Delta x)^2}$$

  - Central difference approximation for Time derivative
  - Central difference approximation for Space derivative
- Important quantity

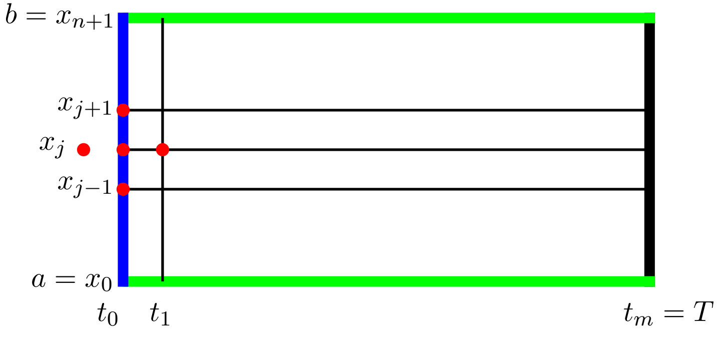
$$r = \frac{c^2\,(\Delta t)^2}{(\Delta x)^2} > 0 \tag{17}$$

- Time stepping from $t_0 = 0$ where have initial conditions
- Known values $u_j^{\ell-1}$, u_j^ℓ, $\quad$ Unknown values $u_j^{\ell+1}$
- Explicit method: $j = 1, \ldots, n, \quad \ell = 1, \ldots, m-1$

$$u_j^{\ell+1} = r u_{j-1}^\ell + 2(1-r)u_j^\ell + r u_{j+1}^\ell - u_j^{\ell-1} \tag{18}$$

- Each time step ℓ requires $6n$ flops $\Longrightarrow$ total $6mn$ flops

Initial Conditions



- Initial conditions
  - $u(x,0) = f(x)$
  - $u_t(x,0) = g(x)$
- First time step $\ell = 0$ has u_j^{-1}

First Time Step

- Time step $\ell = 0$

$$u_j^1 = r u_{j-1}^0 + 2(1-r)u_j^0 + r u_{j+1}^0 - u_j^{-1}$$

  - Values u_j^{-1} at time step $t_{-1} = -\Delta t$ not known
- Central difference approximation to first derivative

$$g(x_j) = \frac{\partial u(x,0)}{\partial t} \approx \frac{u_j^1 - u_j^{-1}}{2\Delta t}$$

- Fictitious values

$$u_j^{-1} = u_j^1 - 2\Delta t g(x_j), \quad j = 1, \ldots, n$$

- First time step $\ell = 0$, (18) becomes

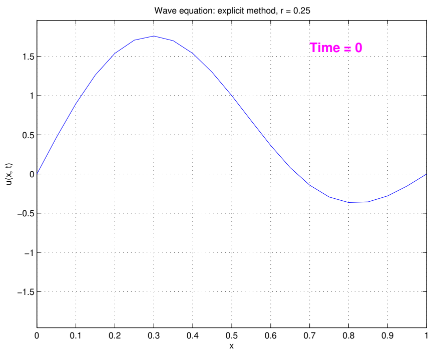
$$u_j^1 = \frac{1}{2}\left(r f_{j-1} + 2(1-r) f_j + r f_{j+1}\right) + \Delta t g_j$$

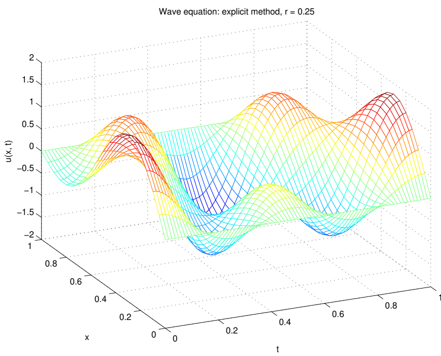
  - $f_j \equiv f(x_j) = u(x_j, 0), \quad g_j \equiv g(x_j) = \frac{\partial u(x_j,0)}{\partial t}$

Example 1

Example (MATLAB `w1dt.m` – Example 1)

$a = 0$, $b = 1$, Boundary conditions $f_a(t) = 0$, $f_b(t) = 0$, $c = 2$
Initial displacement $f(x) = \sin(\pi x) + \sin(2\pi x)$, $g(x) = 0$
Different times: $T = 1, 2, 2.1$





Stability Analysis

- Trial solution $u_j^\ell = \lambda^\ell e^{ikx_j}$, $i = \sqrt{-1}$, wave number k
- Difference equation

$$u_j^{\ell+1} = r u_{j-1}^\ell + 2(1-r) u_j^\ell + r u_{j+1}^\ell - u_j^{\ell-1},$$

- Substitute trial solution

$$\lambda^{\ell+1} e^{ikx_j} = r\lambda^\ell e^{ikx_{j-1}} + 2(1-r)\lambda^\ell e^{ikx_j} + r\lambda^\ell e^{ikx_{j+1}} - \lambda^{\ell-1} e^{ikx_j}$$

- Divide through by $\lambda^{\ell-1} e^{ikx_j}$

$$\lambda^2 = r\lambda e^{-ik\Delta x} + 2(1-r)\lambda + r\lambda e^{ik\Delta x} - 1$$

- Using $\cos(\theta) = (e^{i\theta} + e^{-i\theta})/2$

$$\lambda^2 + 2(r(1 - \cos(k\Delta x)) - 1)\lambda + 1 = 0$$

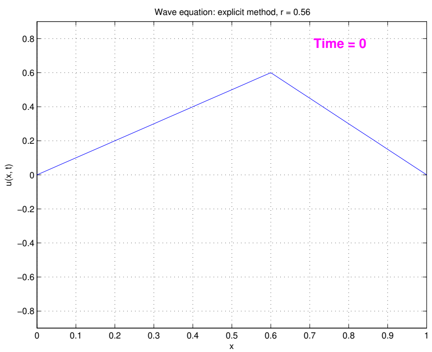
- Stability

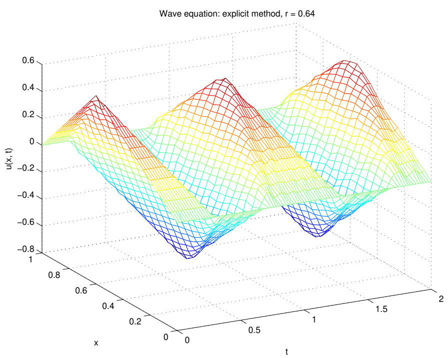
$$|\lambda| \le 1 \iff r \le \frac{2}{1 - \cos(k\Delta x)} \iff r = \frac{c^2 \Delta t^2}{\Delta x^2} \le 1$$

Example 2

Example (MATLAB `w1dt.m` – Example 2)

$a = 0$, $b = 1$, Boundary conditions $f_a(t) = 0$, $f_b(t) = 0$, $c = 2$, $T = 2$
Initial displacement $f(x)$ piecewise linear, $g(x) = 0$, Different grids





Example 3

Example (MATLAB `w1dt.m` – Example 3)

$a = 0$, $b = 1$, Boundary conditions $f_a(t) = 0$, $f_b(t) = 0$, $c = 2$, $T = 2$
Initial displacement $f(x) = c_1 \sin(\pi x)$, Velocity $g(x) = 2\pi c_2 \sin(\pi x)$
Exact solution $u(x,t) = \sin(\pi x)(c_1 \cos(2\pi t) + c_2 \sin(2\pi t))$, Error