EE 3911
數理特論：偏微分方程與數值方法
Partial Differential Equations and Numerical Methods

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Syllabus (Spring 2012):

I. **Basics of Numerical Methods: 4 weeks** (~~2/28~~, 3/6, 3/13, 3/20, 3/27, ~~4/3~~)

1. Floating-Point Representation and Errors, T19.1, N2
2. Roots of Equations, T19.2, N3
3. Interpolations, T19.3, T19.4, N4
4. Numerical Differentiations, T19.5, N4
5. Numerical Integrations, T19.5, N5
6. Numerical Linear Algebra, T20, N7, N8
7. Runge-Kutta methods for ODEs, T21.1, T21.2, T21.3, N10, N11

II. **Numerical Methods for PDEs: 5 weeks** (4/10, 4/17, 4/24, 5/1, 5/8)

1. PDEs and Finite-Difference method, T12, N15, A6
2. Crank-Nicolson method fro Parabolic problems, T21.6, N15.1
3. Lax-Wendroff method for Hyperbolic problems, T21.7, N15.2
4. Gauss-Seidel method for Elliptic Problems, T20.3, T21.4, T21.5, N15.3

PDEs: Definition

- An equation containing partial derivative(s) of an unknown function u with two or more independent variables. E.g.

$$\frac{\partial\, u(t,x)}{\partial t} = \frac{\partial\, u(t,x)}{\partial x^2},$$

or written in short $\quad u_t = u_{xx}.$

- People sense the real world via four (or multiple) dimensions (x, y, z, t), therefore, physical quantities (e.g. electrical field, temperature, electron distribution in an atom) are fully described by four variables.

- Electrostatics (Poisson theory),
- EM waves (Maxwell's equations),
- quantum mechanics (Schrodinger's equation),
- heat transfer (heat equation).

PDEs: Classification

1. Order of PDE: the order of the *highest partial derivative.* E.g.

$$u_t = u_{xx}, \qquad \text{(2nd order)};$$
$$u_t = u\, u_{xxx} + \mathrm{Sin}\, x, \qquad \text{(third order)}.$$

2. Number of variables: the number of independent variables. E.g.

$$u_t = u_{xx}, \qquad \text{(2nd order, two variables: } x \text{ and } t\text{)};$$
$$u_t = u_{rr} + \frac{1}{r} u_r + \frac{1}{r^2} u_{\theta\theta}, \qquad \text{(2nd order, three variables: } r,\ \theta, \text{ and } t\text{)};$$

3. Linearity: PDEs are either *linear* or *nonlinear*,

   - nonlinear ODE: e.g. time-independent nonlinear Schrödinger equation,

$$\frac{-1}{2m} \frac{\mathrm{d}^2}{\mathrm{d}\, x^2} \Psi(x) + V(x)\Psi(x) + |\Psi(x)|^2 \Psi(x) = 0,$$

PDEs: Classification

4. Homogeneity: an equation only containing unknown function u and its derivative(s) is homogeneous. E.g.

$$
\begin{aligned}
&u_t = u_{xx}, && \text{(homogeneous)};\\
&u_x + x\,u_y = e^x u, && \text{(homogeneous)};\\
&u_x + x\,u_y = e^x, && \text{(non-homogeneous)}.
\end{aligned}
$$

5. Kinds of Coefficients: if the coefficients $a_{i,j}(x,y)$ are constants, then the PDE is said to have *constant coefficients* (otherwise, variable coefficients).

PDEs: Big-three PDEs, 2nd-order and linear

Second-order linear PDE with two variables:

$$\boxed{A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + F\,u(x,y) = G,}$$

where A, B, C, D, E, F, and G can be *constants* or given *functions* of x and y.

1. Parabolic PDEs: $B^2 - 4AC = 0$, describe heat flow and diffusion processes, i.e.
$$\frac{\partial}{\partial t}u = \alpha^2 \nabla^2 u = \alpha^2 (\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})u,$$

2. Hyperbolic: $B^2 - 4AC > 0$, describe vibrating systems and wave motion, i.e.
$$\nabla^2 E(x,y,z,t) - \mu_0 \epsilon_0 \frac{\partial^2}{\partial t^2} E = 0$$

3. Elliptic: $B^2 - 4AC < 0$, describe *steady-state phenomena*, i.e. eigenmodes of Laplacian equations,
$$[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}]u(x,y) = f(x,y).$$

PDEs: Big-three PDEs, canonical form

Second-order linear PDE with two variables:

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\frac{\partial u}{\partial x} + E\frac{\partial u}{\partial y} + F\,u(x,y) = G,$$

- Define new coordinates, $\xi = \xi(x,y)$ and $\eta = \eta(x,y)$
- Substitute into the original PDE,

$$\boxed{\bar{A}\,u_{\xi\xi} + \bar{B}\,u_{\xi\eta} + \bar{C}\,u_{\eta\eta} + \bar{D}\,u_{\xi} + \bar{E}\,u_{\eta} + F\,u(\xi,\eta) + G = 0,}$$

where

$$\begin{aligned}
\bar{A} &= A\,\xi_x^2 + B\,\xi_x\xi_y + C\,\xi_y^2 \\
\bar{B} &= 2A\,\xi_x\eta_x + B\,(\xi_x\eta_y + \xi_y\eta_x) + C\,\xi_y\eta_y \\
\bar{C} &= A\,\eta_x^2 + B\,\eta_x\eta_y + C\,\eta_y^2 \\
\bar{D} &= A\,\xi_{xx} + B\,\xi_{xy} + C\,\xi_{yy} + D\,\xi_x + E\,\xi_y \\
\bar{E} &= A\,\eta_{xx} + B\,\eta_{xy} + C\,\eta_{yy} + D\,\eta_x + E\,\eta_y
\end{aligned}$$

PDEs: Big-three PDEs, canonical form, cont.

- Set the coefficients $\bar{A}$ and $\bar{C}$ equal to zero,

$$\begin{aligned} \bar{A} &= A\,\xi_x^2 + B\,\xi_x\xi_y + C\,\xi_y^2 = 0 \\ \bar{C} &= A\,\eta_x^2 + B\,\eta_x\eta_y + C\,\eta_y^2 = 0 \end{aligned}$$

or rewrite these two equations in the form

$$\begin{aligned} A\,[\xi_x/\xi_y]^2 + B\,[\xi_x/\xi_y] + C = 0 \\ A\,[\eta_x/\eta_y]^2 + B\,[\eta_x/\eta_y] + C = 0 \end{aligned}$$

- Solving these equations for $[\xi_x/\xi_y]$ and $[\eta_x/\eta_y]$, we have two *characteristic equations*

$$[\xi_x/\xi_y] = \frac{-B + \sqrt{B^2 - 4AC}}{2A},$$

$$[\eta_x/\eta_y] = \frac{-B - \sqrt{B^2 - 4AC}}{2A},$$

PDEs: Big-three PDEs, canonical form, Example

- For example,

$$\boxed{u_{xx} - 4\,u_{yy} + u_x = 0, \qquad B^2 - 4AC > 0}$$

- the characteristic equations are

$$\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = -[\xi_x/\xi_y] = -2,$$

$$\frac{\mathrm{d}\,y}{\mathrm{d}\,x} = -[\eta_x/\eta_y] = 2,$$

- To find ξ and η, we have

$$\begin{aligned} y &= -2x + c_1, \qquad c_1 = y + 2x \equiv \xi, \\ y &= 2x + c_2, \qquad c_1 = y - 2x \equiv \eta, \end{aligned}$$

PDEs: Big-three PDEs, canonical form, cont.

- Hyperbolic equation: $B^2 - 4AC > 0$

$$u_{\xi\eta} = \Phi(\xi, \eta, u, u_\xi, u_\eta)$$

- By the transformation, $\alpha = \xi + \eta$ and $\beta = \xi - \eta$,

$$u_{\alpha\alpha} - u_{\beta\beta} = \Phi(\alpha, \beta, u, u_\alpha, u_\beta)$$

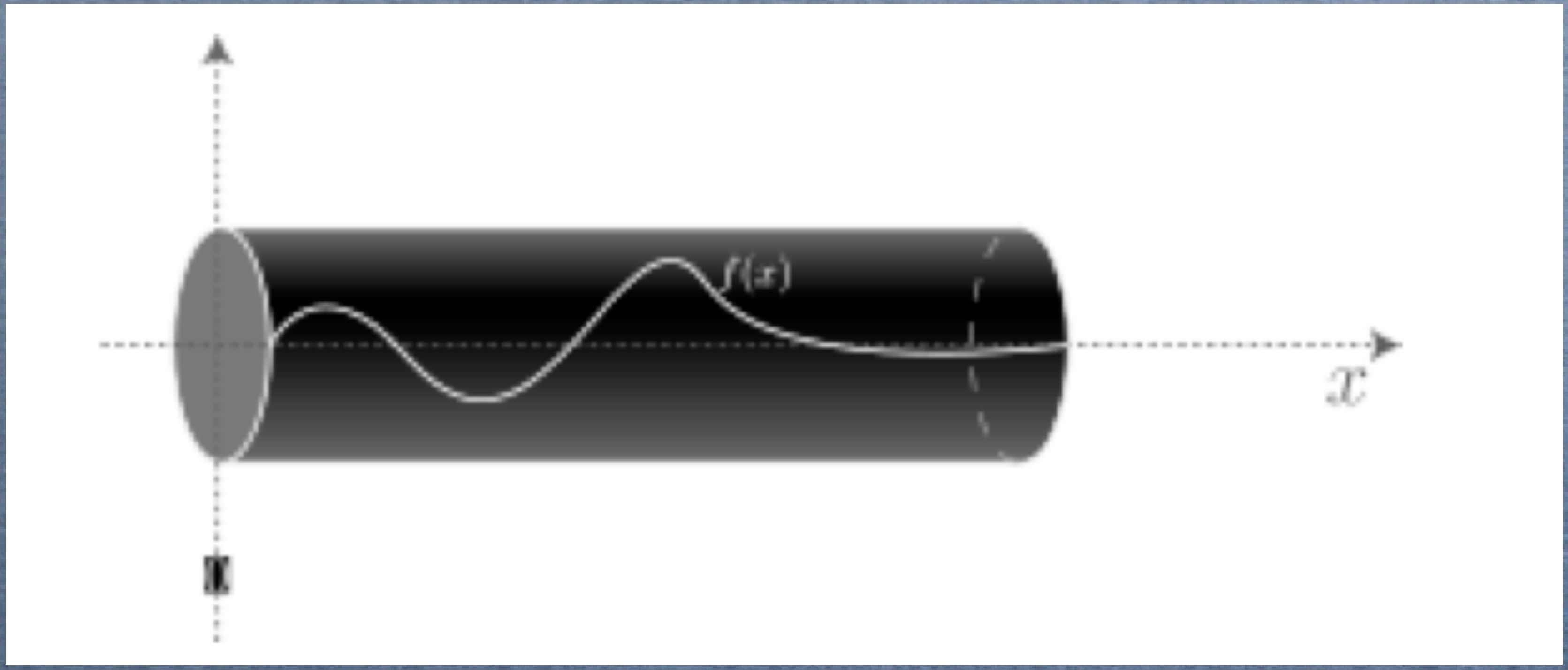
- Parabolic equation: $B^2 - 4AC = 0$

$$u_{\eta\eta} = \Phi(\xi, \eta, u, u_\xi, u_\eta)$$

- Elliptic equation: $B^2 - 4AC < 0$, with the transformation, $\alpha = (\xi + \eta)/2$ and $\beta = (\xi - \eta)/2i$,

$$u_{\alpha\alpha} + u_{\beta\beta} = \Phi(\alpha, \beta, u, u_\alpha, u_\beta)$$

PDEs: Heat Equation, Initial-Boundary-Value Problem



Initial-boundary-value problem:

PDE: $u_t = \alpha^2 u_{xx}, \qquad 0 < x < L, \quad \text{and} \quad 0 < t$

BCs: $\begin{cases} u_x(0,t) = K_1(t) \\ u_x(200,t) = K_2(t) \end{cases}, \quad 0 < t$

IC: $u(x,0) = F(x), \quad 0 \le x \le L$

Divide and Conquer

PDEs: Heat Equation, Separation of Variables

- The basic idea of separation of variables is to break down the *initial conditions* of the problem into simple components, find the response to each component, and the add up these individual responses.

- *Divide and Conquer*

- Separation of variables applies to problems where

  1. The PDE is linear and homogeneous (not necessarily constant coefficients).
  2. The boundary conditions are of the form

$$
\begin{aligned}
\alpha\, u_x(0,t) + \beta\, u(0,t) &= 0, \\
\gamma\, u_x(1,t) + \delta\, u(1,t) &= 0,
\end{aligned}
$$

  where α, β, γ, and δ are constants (boundary conditions of this are called linear homogeneous BCs).

PDEs: Heat Equation, Separation of Variables, Step 1

$$\text{PDE:} \qquad u_t = \alpha^2 u_{xx}, \qquad 0 < x < 1, \quad 0 < t < \infty$$

$$\text{BCs:} \qquad \begin{cases} u(0,t) = 0 \\ u(1,t) = 0 \end{cases}, \qquad 0 < t < \infty$$

$$\text{IC:} \qquad u(x,0) = \phi(x), \quad 0 \le x \le 1$$

- Find elementary solutions to the PDE:

$$\boxed{u(x,t) = X(x)\,T(t), \qquad \text{fundamental solutions}}$$

- substitute this trial solution into the PDE,

$$X(x)\,T'(t) = \alpha^2 X''(x)\,T(t),$$

- divide each side of this equation by $\alpha^2 X(x)\,T(t)$,

$$\frac{T'(t)}{\alpha^2 T(t)} = \frac{X''(x)}{X(x)},$$

and obtain what is call *separated variables*.

PDEs: Heat Equation, Separation of Variables, Step 1

- In this case, x and t are independent of each other, each side must be a fixed constant (say k),

$$\boxed{\frac{T'(t)}{\alpha^2 T(t)} = \frac{X''(x)}{X(x)} = k,}$$

  or two ODEs

$$T'(t) - k\,\alpha^2 T(t) = 0,$$
$$X''(x) - k\,X(x) = 0.$$

- To meet the condition as $t \to \infty$, k must to be *negative*, i.e. $k = -\lambda^2$, where λ is nonzero.

$$T'(t) + \lambda^2\,\alpha^2 T(t) = 0,$$
$$X''(x) + \lambda^2\,X(x) = 0.$$

Review of ODEs

PDEs: Heat Equation, Separation of Variables, Step 2

- For the two ODEs

$$T'(t) + \lambda^2 \alpha^2 T(t) = 0,$$
$$X''(x) + \lambda^2 X(x) = 0.$$

- The corresponding solutions are:

$$\begin{aligned} T(t) &= C_1 e^{-\lambda^2 \alpha^2 t}, && (C_1 \text{ an arbitrary constant}) \\ X(x) &= C_2 \,\mathrm{Sin}(\lambda x) + C_3 \,\mathrm{Cos}(\lambda x), && (C_2 \text{ and } C_3 \text{ arbitrary}) \end{aligned}$$

- The total solution for $u(x, t) = X(x)\, T(t)$ is

$$u(x, t) = e^{-\lambda^2 \alpha^2 t} [A \,\mathrm{Sin}(\lambda x) + B \,\mathrm{Cos}(\lambda x)]$$

PDEs: Heat Equation, Separation of Variables, Step 3

- Find solutions to match the BCs
- The total solution for $u(x,t) = X(x)T(t)$

$$u(x,t) = e^{-\lambda^2\alpha^2 t}[A\,\mathrm{Sin}(\lambda x) + B\,\mathrm{Cos}(\lambda x)]$$

to satisfy the boundary conditions

$$\begin{aligned} u(0,t) &= 0, \\ u(1,t) &= 0, \end{aligned}$$

needs to enforce $B = 0$ and $\mathrm{Sin}\lambda = 0$ (or $\lambda = \pm\pi, \pm 2\pi, \pm 3\pi, \ldots$).

- We have an infinite number of functions,

$$u_n(x,t) = A_n\, e^{-(n\pi\alpha)^2 t}\,\mathrm{Sin}(n\pi x), \qquad n = 1, 2, \ldots$$

which is called the fundamental solution (an infinite number).

PDEs: Heat Equation, Separation of Variables, Step 4

- Find the solutions to match the IC
- To add the fundamental solutions

$$u(x,t) = \sum_{n=1}^{\infty} A_n \, e^{-(n\pi\alpha)^2 t} \, \mathrm{Sin}(n\pi x),$$

and meet the initial condition, $u(x,0) = \phi(x)$, i.e.

$$\sum_{n=1}^{\infty} A_n \, \mathrm{Sin}(n\pi x) = \phi(x),$$

- Luckily, $\mathrm{Sin}(n\pi x)$ is **orthogonal** for different n, i.e.

$$\int_0^1 \mathrm{Sin}(m\pi x)\mathrm{Sin}(n\pi x)\mathrm{d}\,x = \frac{1}{2}\delta_{mn}, \quad \text{by} \quad \mathrm{Sin}(x)\mathrm{Sin}(y) = \frac{1}{2}[\mathrm{Cos}(x-y) - \mathrm{Cos}(x+y)].$$

- By multiply $\mathrm{Sin}(m\pi x)$, we obtain

$$A_m = 2\int_0^1 \phi(x)\mathrm{Sin}(m\pi x)\mathrm{d}\,x$$

Power Series: Sturm-Liouville Problem

- Sturm-Liouville Problem:

$$[p(x)y']' + [q(x) + \lambda r(x)]y = 0, \qquad \text{with the boundary conditions}$$

$$\begin{cases} k_1 y(a) + k_2 y'(a) = 0 \\ l_1 y(b) + l_2 y'(b) = 0 \end{cases}$$

- λ is a parameter.
- For the interval $a \leq x \leq b$, $p(x)$, $q(x)$, $r(x)$, and $p'(x)$ are *continuous*.
- k_1, k_2 are given constants, not both zero, and so are l_1, l_2 , not both zero.
- If $k_2 = l_2 = 0$, one has Dirichlet B.C.
- If $k_1 = l_1 = 0$, one has Neumann B.C.
- If $k_1 = l_2 = 0$ or $k_2 = l_1 = 0$, one has Mixed (Robin) B.C.

Power Series: Orthogonality of Eigenfunctions

- For a given number λ, eigen-value, a solution to satisfy the Sturm-Liouville Problem is called eigen-function.

- Functions $y_1(x), y_2(x), \ldots$ defined on some interval $a \le x \le b$ are called orthogonal on this interval with respect to the *weight function* $r(x) > 0$ if

$$\boxed{(y_m(x), y_n(x)) \equiv \int_a^b r(x) y_m(x) y_n(x)\, \mathrm{d}x = \delta_{mn},}$$

where we introduce Kronecker's delta δ_{mn} which gives the value

$$\delta_{mn} = \begin{cases} 0 & ; \quad \text{if} \quad m \neq n \\ 1 & ; \quad \text{if} \quad m = n \end{cases}$$

- The norm $\| y_m \|$ of $y_m(x)$ is defined by

$$\boxed{\| y_m(x) \| = \sqrt{\int_a^b r(x) y_m^2(x)\, \mathrm{d}x},}$$

Power Series: Orthogonality, Example 1

- The functions $y_m(x) = \sin mx$, $m = 1, 2, \ldots,$ form an orthogonal set on the interval $-\pi \le x \le \pi$, for

$$\boxed{\int_{-\pi}^{\pi} \sin mx \sin nx \, \mathrm{d}x = 0, \qquad m \neq n}$$

i.e. $2 \sin\alpha \sin\beta = \cos(\alpha - \beta) - \cos(\alpha + \beta)$.

- The norm $\| y_m \|$ of $\sin mx$ is

$$\boxed{\| y_m(x) \| = \sqrt{\int_{-\pi}^{\pi} \sin^2 mx \, \mathrm{d}x} = \sqrt{\pi}.}$$

Power Series: Orthogonality, Example 2

- The Legendre Polynomials form an orthogonal set on the interval $-1 \leq x \leq 1$, for

$$\boxed{\int_{-1}^{1} P_m(x) P_n(x)\, \mathrm{d}x = 0, \qquad m \neq n}$$

- The Bessel's functions form an orthogonal set on the interval $0 \leq x \leq R$, for

$$\boxed{\int_{0}^{R} x J_\nu(k_{\nu,m} x) J_\nu(k_{\nu,n} x)\, \mathrm{d}x = 0, \qquad m \neq n}$$

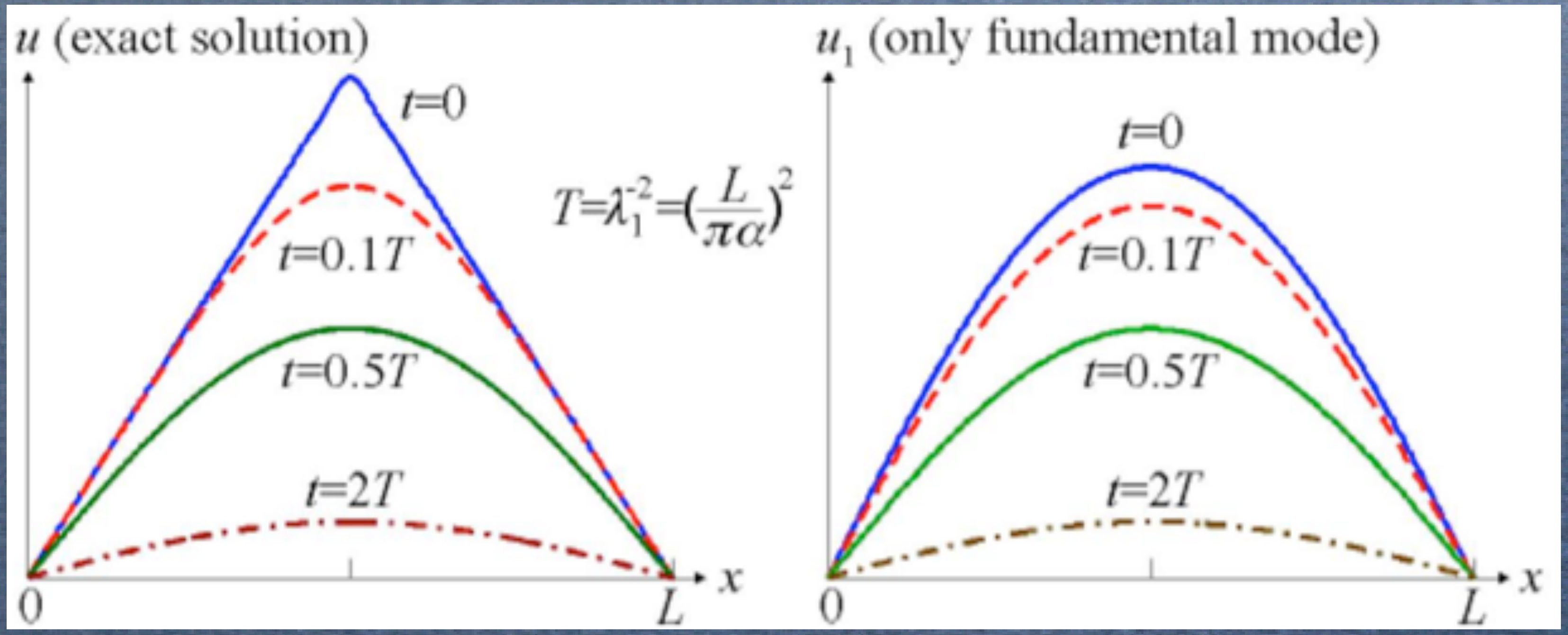
PDEs: Heat Equation, Separation of Variables, Dirichlet BCs

Example:

PDE: $u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad 0 < t < \infty$

BCs: $u(0,t) = 0$ and $u(L,t) = 0, \quad 0 < t < \infty$

IC: $$u(x,0) = \begin{cases} x & ; \text{ for } 0 \le x \le L/2 \\ L - x & ; \text{ for } L/2 \le x \le L \end{cases}$$



Solution:

$$u(x,t) = \sum_{n=1} A_n e^{-(n\pi/L)^2\alpha^2 t} \mathrm{Sin}(\frac{n\pi}{L}x),$$

$$A_n = [\frac{4L}{n^2\pi^2}]\mathrm{Sin}(\frac{n\pi}{2}) = \begin{cases} (-1)^{(n-1)/2}\left[\frac{4L}{n^2\pi^2}\right] & ; \text{ if } n \text{ is odd} \\ 0 & ; \text{ if } n \text{ is even} \end{cases}$$

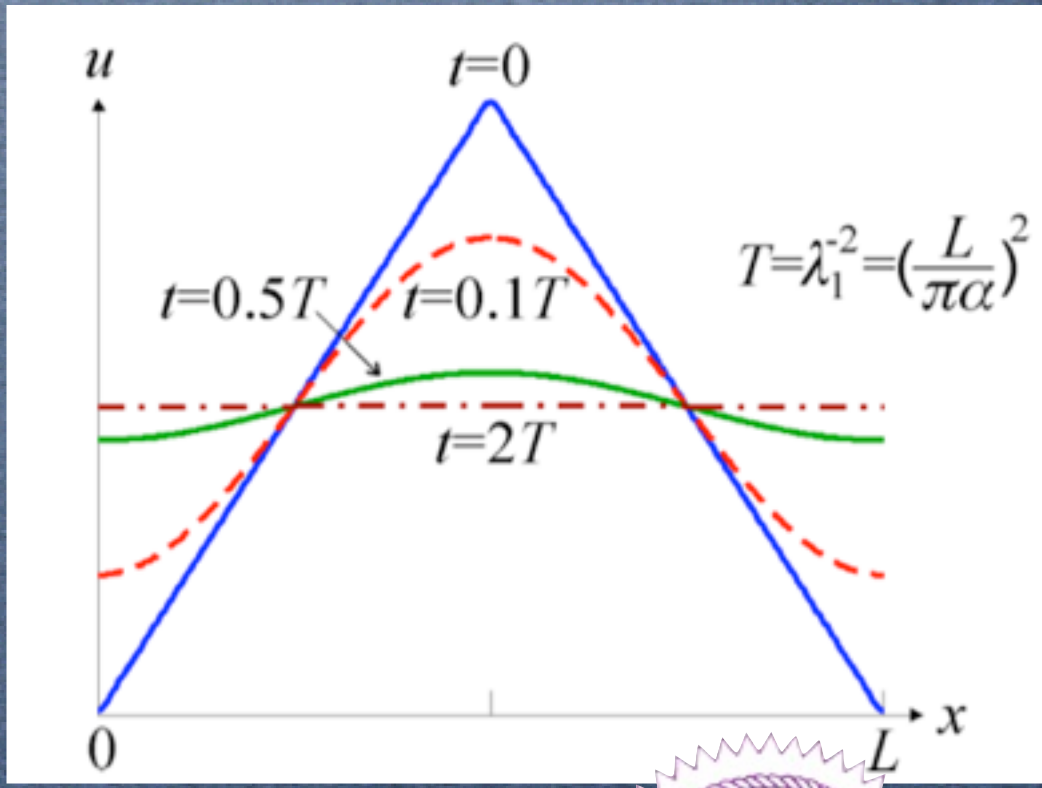
PDEs: Heat Equation, Separation of Variables, Neumann BCs

Example:

PDE: $u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad 0 < t < \infty$

BCs: $u_x(0,t) = 0 \quad \text{and} \quad u_x(L,t) = 0, \quad 0 < t < \infty$

IC: $u(x,0) = \begin{cases} x & ; \quad \text{for} \quad 0 \le x \le L/2 \\ L - x & ; \quad \text{for} \quad L/2 \le x \le L \end{cases}$



Solution:

$$u(x,t) = \sum_{n=0} A_n e^{-(n\pi/L)^2\alpha^2 t}\mathrm{Cos}(\frac{n\pi}{L}x),$$

$$A_n = \begin{cases} L/4 & ; \quad \text{for} \quad n = 0 \\ \frac{2L}{n^2\pi^2}[2\mathrm{Cos}(\frac{n\pi}{2}) - \mathrm{Cos}(n\pi) - 1] & ; \quad \text{for} \quad n \neq 0 \end{cases}$$

PDEs: Heat Equation, Separation of Variables, Mixed BCs

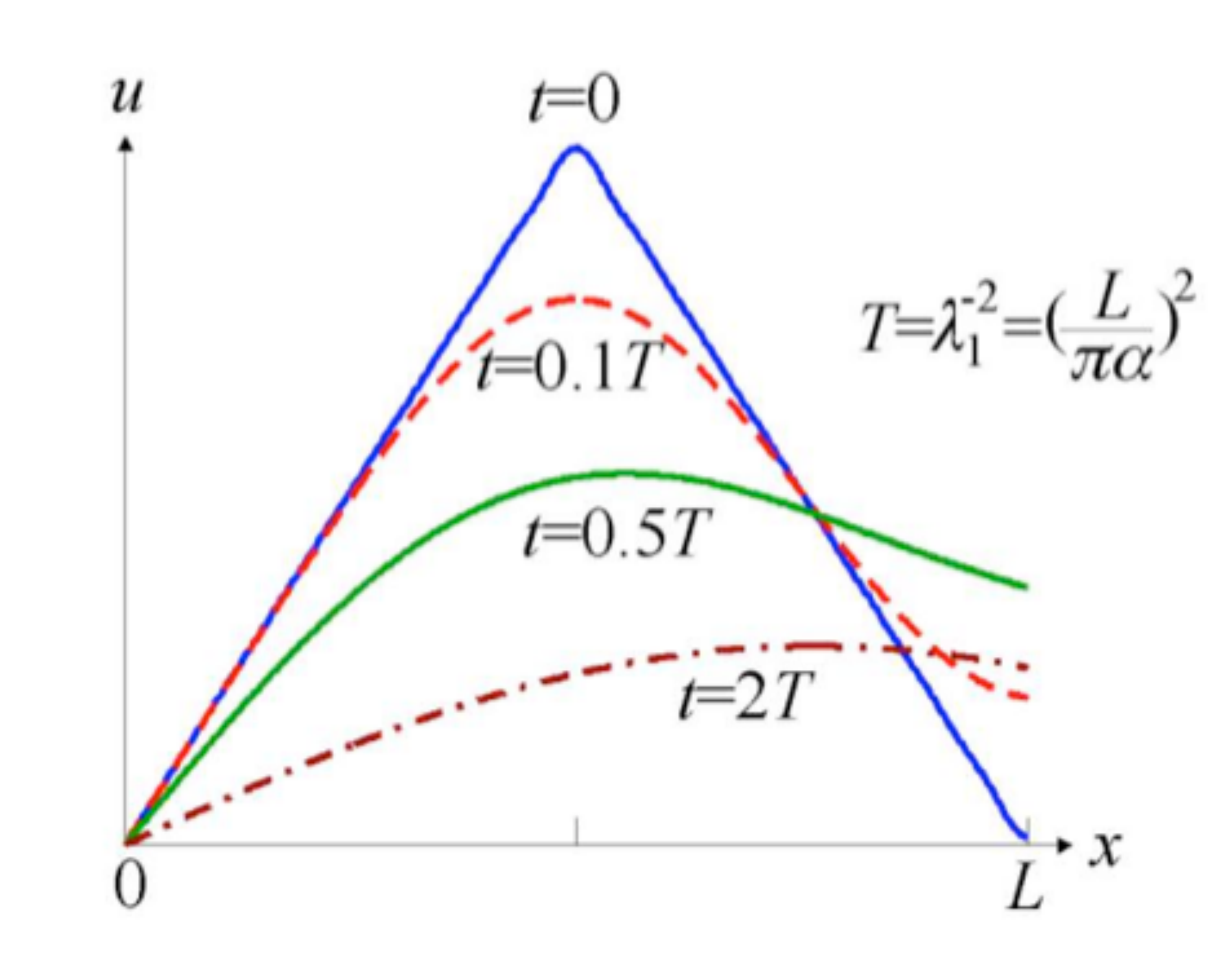
Example:

PDE: $u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad 0 < t < \infty$

BCs: $u(0,t) = 0 \quad \text{and} \quad u_x(L,t) + h\,u(L,t) = 0, \quad 0 < t < \infty$

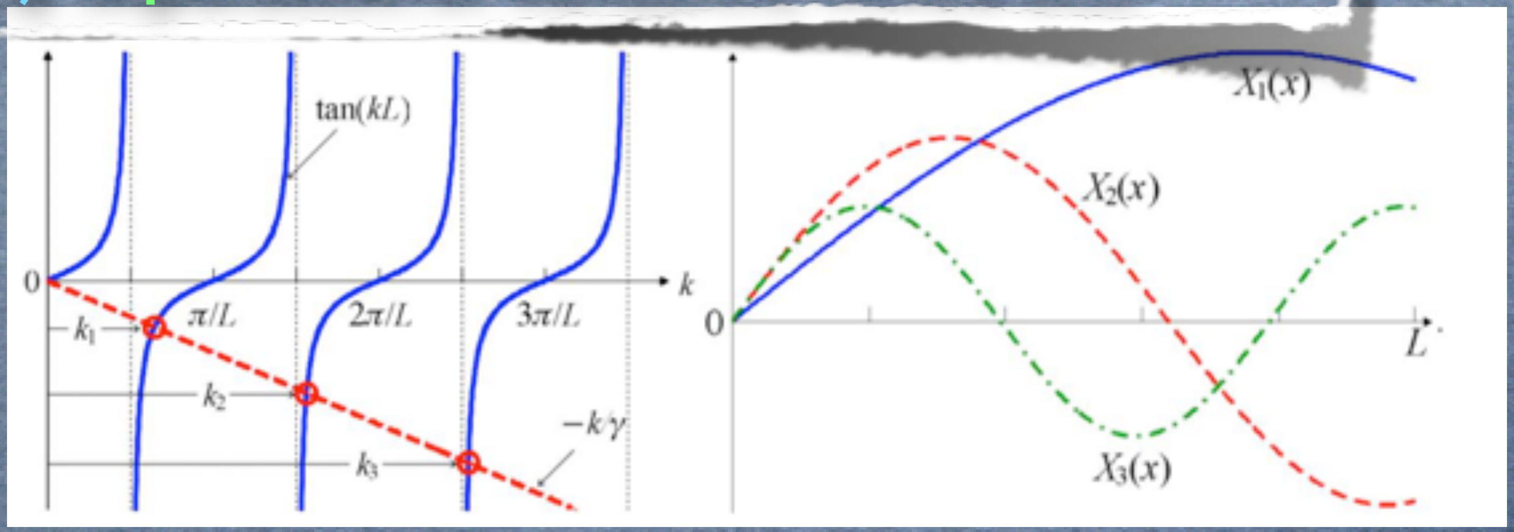
IC: $u(x,0) = \begin{cases} x & ; \quad \text{for} \quad 0 \le x \le L/2 \\ L - x & ; \quad \text{for} \quad L/2 \le x \le L \end{cases}$

Solution:



PDEs: Heat Equation, Separation of Variables, Mixed BCs

Solution:



- From the BCs:

$$X_n(x) = \mathrm{Sin}(k_n x), \quad \text{where} \quad \tan(k_n L) = -\frac{k_n}{h}.$$

- The total solution:

$$\boxed{u(x,t) = \sum_{n=1}^{\infty} A_n\, e^{-(k_n \alpha)^2 t}\,\mathrm{Sin}(k_n x),}$$

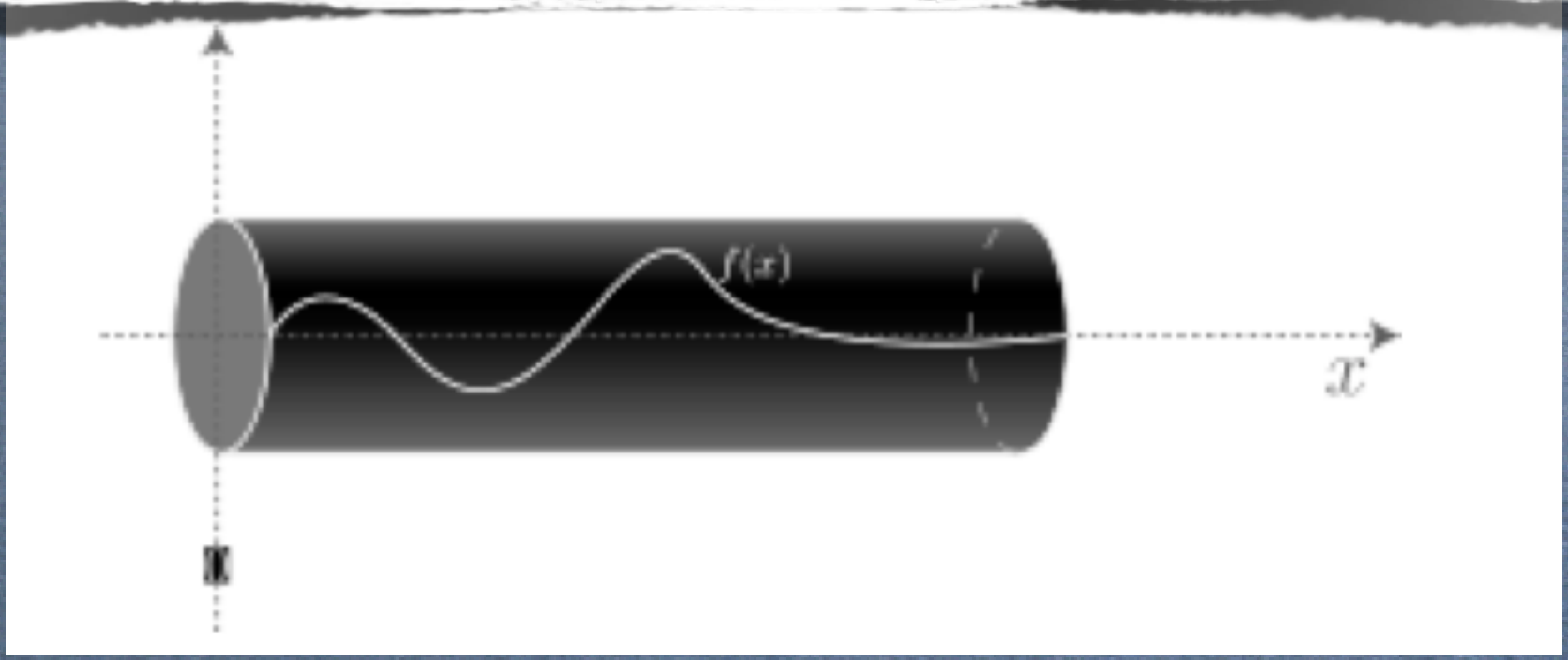
- By the orthogonality of $X_n(x)$ in $[0, L]$ (for the spatial ODE is a Sturm-Liouville problem):

$$\int_0^L \mathrm{Sin}(k_n x)\mathrm{Sin}(k_m x)\mathrm{d}\,x = [\frac{L}{2} - \frac{\mathrm{Sin}(2k_n L)}{4k_n}]\delta_{mn} \equiv \frac{L}{2}[1 - \mathrm{Sinc}(2k_n L)]\delta_{mn},$$

where

$$A_n = \frac{2}{L[1 - \delta_{mn}\mathrm{Sinc}(2k_n L)]}\int_0^L \phi(x)\mathrm{Sin}(k_m x)\mathrm{d}\,x.$$

PDEs: Heat Equation, Initial-Boundary-Value Problem



Initial-boundary-value problem:

PDE: $$u_t = \alpha^2 u_{xx}, \qquad 0 < x < L, \quad \text{and} \quad 0 < t$$

BCs: $$\begin{cases} u_x(0,t) = K_1(t) \\ u_x(200,t) = K_2(t) \end{cases}, \quad 0 < t$$

IC: $$u(x,0) = F(x), \quad 0 \le x \le L$$

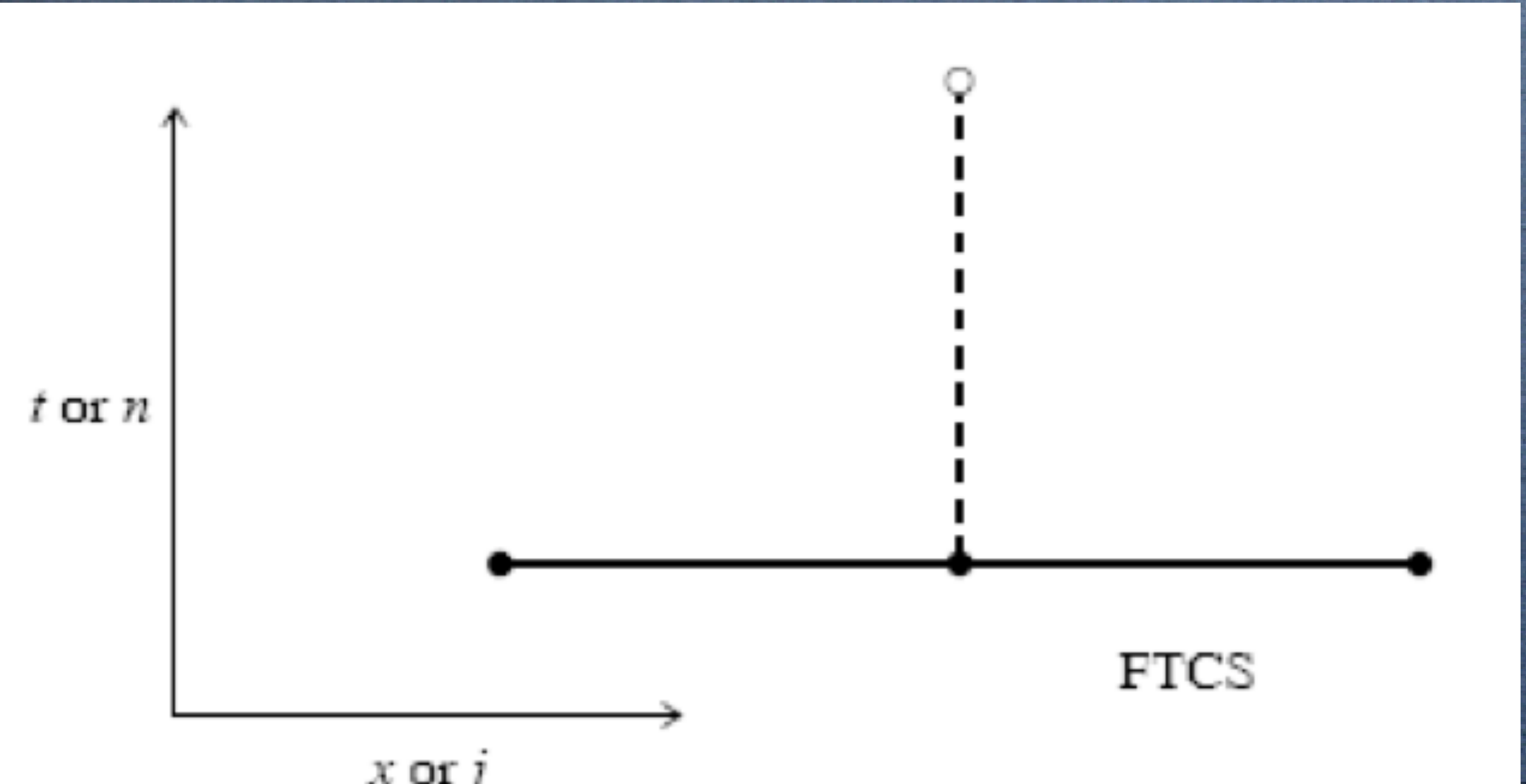
PDEs: Forward Time Centered Space

For a 1st-order PDE:

$$\frac{\partial}{\partial t}A(x,t) = \kappa \frac{\partial}{\partial x}A(x,t),$$

this equation can be approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^n - A_{j-1}^n}{2\Delta x} + \mathbf{O}(\Delta x^2).$$



PDEs: Forward Time Centered Space

For diffusion equation:

$$\frac{\partial}{\partial t}A(x,t) = \kappa \frac{\partial^2}{\partial x^2}A(x,t)$$

which is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^n - 2A_j^n + A_{j-1}^n}{\Delta x^2} + \mathbf{O}(\Delta x^2).$$

This is a explicit scheme.

PDEs: Implicit Forward Time Centered Space

By finite difference,

$$\frac{\partial}{\partial t}A(x,t) = \kappa \frac{\partial}{\partial x}A(x,t)$$

this equation is approximated by

(b) Fully Implicit

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^{n+1} - A_{j-1}^{n+1}}{2\Delta x} + \mathbf{O}(\Delta x^2).$$

For diffusion equation:

$$\frac{\partial}{\partial t}A(x,t) = \kappa \frac{\partial^2}{\partial x^2}A(x,t)$$

which is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^{n+1} - 2A_j^{n+1} + A_{j-1}^{n+1}}{\Delta x^2} + \mathbf{O}(\Delta x^2).$$

This is a implicit scheme, but also with first-order accuracy.

PDEs: Implicit Crank-Nicholson mehtod

For diffusion equation:

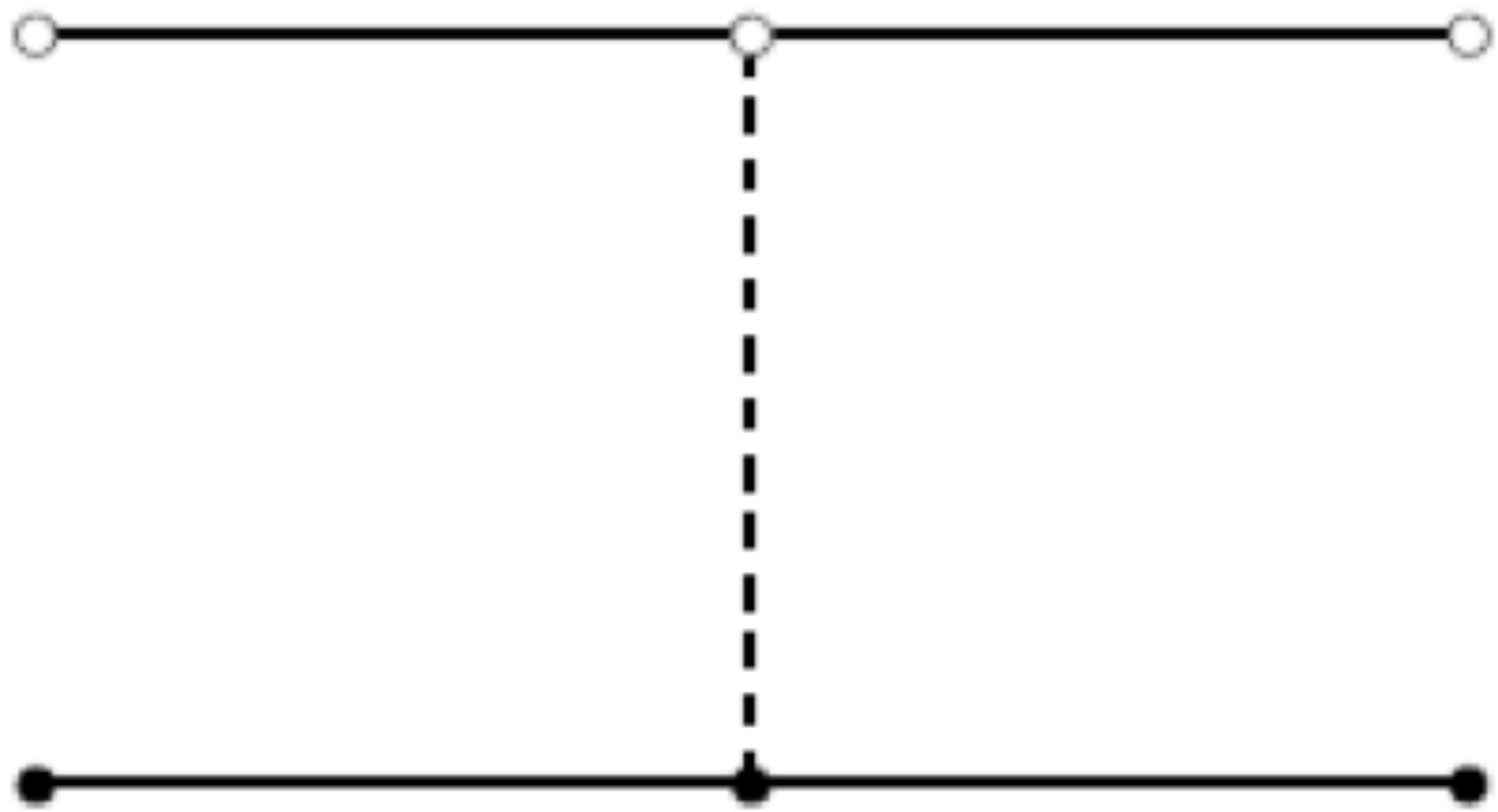
$$\frac{\partial}{\partial t}A(x,t) = \kappa \frac{\partial^2}{\partial x^2}A(x,t)$$

which is approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} \approx \frac{\kappa}{2}\left(\frac{A_{j+1}^n - 2A_j^n + A_{j-1}^n}{\Delta x^2} + \frac{A_{j+1}^{n+1} - 2A_j^{n+1} + A_{j-1}^{n+1}}{\Delta x^2}\right)$$

This is a implicit scheme, but also with *second-order* accuracy.

PDEs: Implicit Crank-Nicholson mehtod



(c) Crank-Nicholson

PDEs: Implicit Crank-Nicholson mehtod

By introducing $\gamma = \frac{\kappa \Delta t}{\Delta x^2}$, the original Crank-Nicolson method,

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} \approx \frac{\kappa}{2}\left(\frac{A_{j+1}^n - 2A_j^n + A_{j-1}^n}{\Delta x^2} + \frac{A_{j+1}^{n+1} - 2A_j^{n+1} + A_{j-1}^{n+1}}{\Delta x^2}\right)$$

becomes

$$\boxed{(2 + 2\,\gamma)A_j^{n+1} - \gamma(A_{j+1}^{n+1} + A_{j-1}^{n+1}) = (2 - 2\,\gamma)A_j^n + \gamma(A_j^{n+1} + A_j^{n-1}).}$$

PDEs: Implicit Crank-Nicholson mehtod

In the matrix form:

$$
\begin{bmatrix}
 & & \ddots & & \\
\ddots & -\gamma & (2+2\gamma) & -\gamma & \ddots \\
 & & \ddots & &
\end{bmatrix}
\begin{pmatrix}
A_0^{n+1} \\ \vdots \\ A_{j-1}^{n+1} \\ A_j^{n+1} \\ A_{j+1}^{n+1} \\ \vdots \\ A_N^{n+1}
\end{pmatrix}
=
$$

$$
\begin{bmatrix}
 & & \ddots & & \\
\ddots & +\gamma & (2-2\gamma) & +\gamma & \ddots \\
 & & \ddots & &
\end{bmatrix}
\begin{pmatrix}
A_0^{n+1} \\ \vdots \\ A_{j-1}^{n} \\ A_j^{n} \\ A_{j+1}^{n} \\ \vdots \\ A_N^{n+1}
\end{pmatrix}
.
$$

PDEs: Implicit Crank-Nicholson mehtod

Boundary conditions

Homework 6: Heat equation

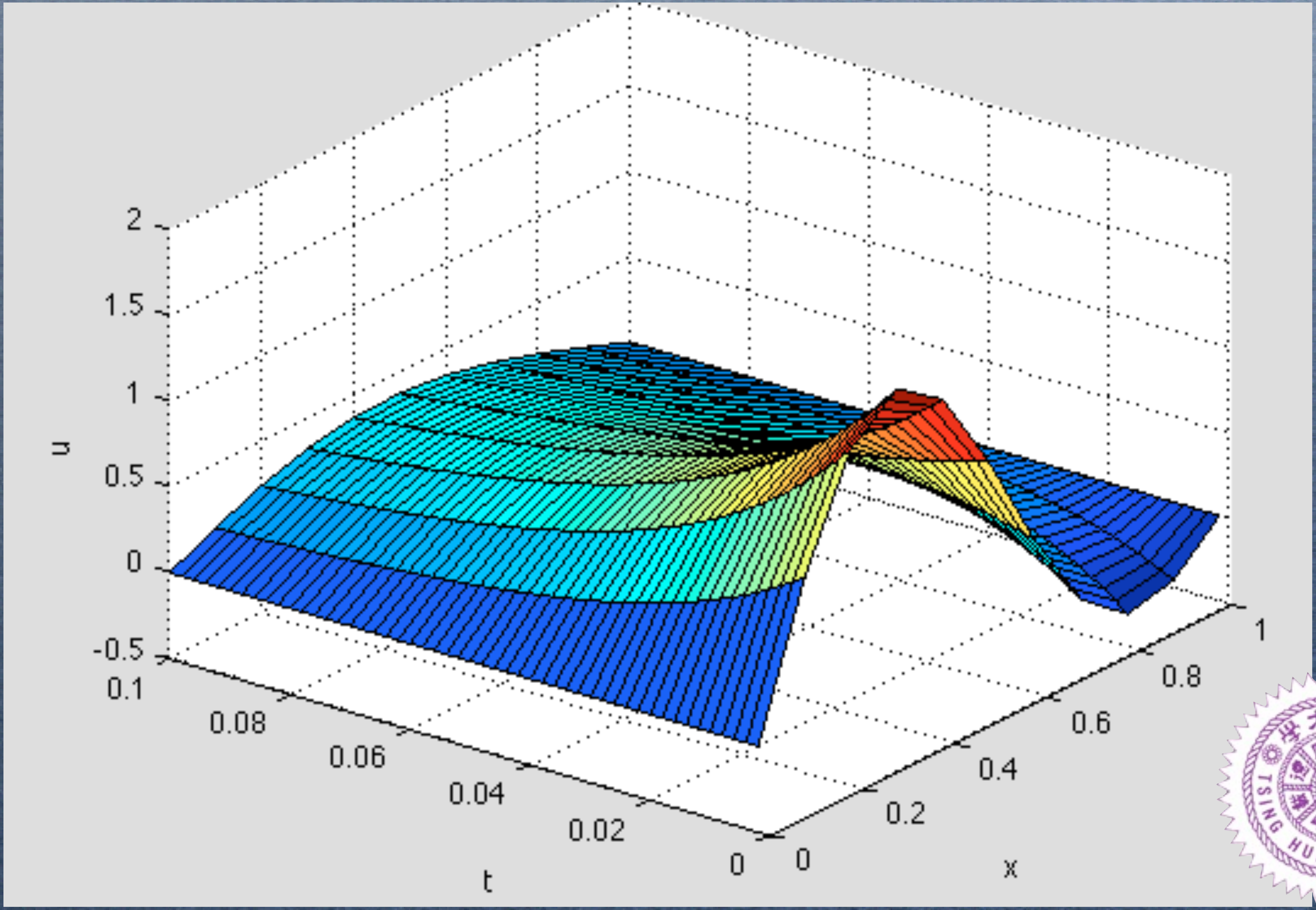
Initial-boundary-value problem:

PDE: $u_t = u_{xx}, \qquad 0 < x < 1, \quad \text{and} \quad 0 < 0.1$

BCs: $\begin{cases} u(0,t) = 0 \\ u(1,t) = 0 \end{cases}, \quad 0 < t$

IC: $u(x,0) = \mathrm{Sin}(\pi x) + \mathrm{Sin}(2\pi x), \quad 0 \le x \le 1$

PDEs: Heat Equation, Initial-Boundary-Value Problem



PDEs: Heat Equation, with Lateral Heat Loss

Example:

$$\begin{array}{lll} \text{PDE:} & u_t = \alpha^2 u_{xx} - \beta u, & 0 < x < L, \quad 0 < t < \infty \\ \text{BCs:} & u(0,t) = 0 \quad \text{and} \quad u(L,t) = 0, & 0 < t < \infty \\ \text{IC:} & u(x,0) = \phi(x), & 0 \le x \le L \end{array}$$

Hits: where $-\beta u$ represents heat flow across the lateral boundary.

By means of the transformation

$$\boxed{u(x,t) = e^{-\beta t} w(x,t),}$$

then the original heat equation with lateral loss becomes,

$$\begin{array}{lll} \text{PDE:} & w_t = \alpha^2 w_{xx}, & 0 < x < L, \quad 0 < t < \infty \\ \text{BCs:} & w(0,t) = 0 \quad \text{and} \quad w(L,t) = 0, & 0 < t < \infty \\ \text{IC:} & w(x,0) = \phi(x), & 0 \le x \le L \end{array}$$

with the solutions already known, i.e.

$$w(x,t) = \sum_{n=1} \left[\frac{2}{L} \int_{-L}^{L} \phi(s) \mathrm{Sin}(\frac{n\pi}{L} s) \mathrm{d}\, s \right] e^{-(\frac{n\pi\alpha}{L})^2 t} \mathrm{Sin}(\frac{n\pi}{L} x).$$

PDEs: Heat Equation, Non-homogeneous Boundary Conditions

Example:

PDE: $$u_t = \alpha^2 u_{xx}, \qquad 0 < x < L, \quad 0 < t < \infty$$

BCs: $$\begin{cases} u(0,t) = k_1 \\ u(L,t) = k_2 \end{cases}, \quad 0 < t < \infty$$

IC: $$u(x,0) = \phi(x), \quad 0 \le x \le L$$

Hits:

Transforming non-homogeneous BCs to homogeneous ones:

$$\begin{aligned} u(x,t) &= \text{steady state} + \text{transient} \\ &= [k_1 + \frac{x}{L}(k_2 - k_1) + U(x,t)], \end{aligned}$$

where

PDE $$U_t = \alpha^2 U_{xx}, \qquad 0 < x < L, \quad 0 < t < \infty$$

BCs $$\begin{cases} U(0,t) = 0 \\ U(L,t) = 0 \end{cases}, \quad 0 < t < \infty$$

IC $$U(x,0) = \phi(x) - [k_1 + \frac{x}{L}(k_2 - k_1)], \quad 0 \le x \le L$$

PDEs: Heat Equation, More

- Lateral heat loss proportional to the temperature difference:

$$\boxed{u_t = \alpha^2 u_{xx} - \beta(u - u_0), \qquad \beta > 0.}$$

  Heat loss ($u > u_0$) or gain ($u < u_0$) is proportional to the difference between the temperature $u(x,t)$ of the rod and the surrounding medium u_0 (with β the proportionality constant).

- Internal heat source:

$$\boxed{u_t = \alpha^2 u_{xx} + f(x,t), \qquad \text{the nonhomogeneous equation.}}$$

  The rod is supplied with an internal heat source (everywhere along the rod and for all time t).

- Diffusion-convection equation:

$$\boxed{u_t = \alpha^2 u_{xx} - \nu u_x.}$$

  E.g. a pollutant is carried along in a stream moving with velocity ν.

- Nonhomogeneous material: $u_t = \alpha^2(x) u_{xx} + \text{f(x,y)}$.

PDEs: Heat Equation, Non-homogeneous

Example:

$$\begin{array}{rll} \text{PDE:} & u_t = \alpha^2 u_{xx} + f(x,t), & 0 < x < 1, \quad 0 < t < \infty \\ \text{BCs:} & u(0,t) = 0 \quad \text{and} \quad u(1,t) = 0, & 0 < t < \infty \\ \text{IC:} & u(x,0) = \phi(x), & 0 \le x \le 1 \end{array}$$

Hits:

- For $f(x,t) = 0$, we have solutions for the homogeneous problem, i.e.

$$u(x,t) = \sum_{n=1} a_n e^{-(\lambda_n \alpha)^2 t} X_n(x),$$

  where λ_n and $X_n(x)$ are the eigenvalues and the eigenfunctions of the Sturm-Liouville problem, i.e.

$$X'' + \lambda^2 X = 0, \quad \text{and} \quad X(0) = 0, X(1) = 0,$$

- For non-homogeneous problem, $f(x,t) \neq 0$, we try the slightly more general form,

$$\boxed{u(x,t) = \sum_{n=1} T_n(t) X_n(x),}$$

PDEs: Heat Equation, Non-homogeneous, Example

Example:

PDE: $u_t = \alpha^2 u_{xx} + \text{Sin}(3\pi x), \quad 0 < x < 1, \quad 0 < t < \infty$

BCs: $u(0,t) = 0 \quad \text{and} \quad u(1,t) = 0, \quad 0 < t < \infty$

IC: $u(x,0) = \text{Sin}(\pi x), \quad 0 \le x \le 1$

Hits:

- Since the BCs support $\text{Sin}(n\pi x)$ eigenfunctions,

$$\boxed{u(x,t) = \sum_{n=1} T_n(t) X_n(x) = \sum_{n=1} T_n(t)\text{Sin}(n\pi x),}$$

- Substitute this expansion into the problem,

PDE: $$\sum_{n=1} [T_n' + (n\pi\alpha)^2 T_n]\text{Sin}(n\pi x) = \text{Sin}(3\pi x),$$

IC: $$\sum_{n=1} T_n(0)\text{Sin}(n\pi x) = \text{Sin}(\pi x),$$

PDEs: Heat Equation, Non-homogeneous, Example, cont.

- With the orthogonality for $\mathrm{Sin}(n\pi x)$, we have,

$$\text{PDE:} \qquad T_n' + (n\pi\alpha)^2 T_n = 2\int_0^1 \mathrm{Sin}(n\pi x)\mathrm{Sin}(3\pi x)\mathrm{d}\,x = \begin{cases} 1 & ; \quad \text{for} \quad n = 3 \\ 0 & ; \quad \text{for} \quad n \neq 3 \end{cases}$$

$$\text{IC:} \qquad T_n(0) = 2\int_0^1 \mathrm{Sin}(n\pi x)\mathrm{Sin}(\pi x)\mathrm{d}\,x = \begin{cases} 1 & ; \quad \text{for} \quad n = 1 \\ 0 & ; \quad \text{for} \quad n \neq 1 \end{cases}$$

- Writing out these equations for $n = 1, 2, \ldots,$, wee see

$$(n=1) \qquad \left.\begin{array}{l} T_1' + (\pi\alpha)^2 T_1 = 0 \\ T_1(0) = 1 \end{array}\right\} \Rightarrow T_1(t) = e^{-(\pi\alpha)^2 t},$$

$$(n=2) \qquad \left.\begin{array}{l} T_2' + (2\pi\alpha)^2 T_2 = 0 \\ T_2(0) = 0 \end{array}\right\} \Rightarrow T_2(t) = 0,$$

$$(n=3) \qquad \left.\begin{array}{l} T_3' + (3\pi\alpha)^2 T_3 = 1 \\ T_3(0) = 0 \end{array}\right\} \Rightarrow T_3(t) = \frac{1}{(3\pi\alpha)^2}[1 - e^{-(3\pi\alpha)^2 t}],$$

$$(n \geq 4) \qquad \left.\begin{array}{l} T_n' + (n\pi\alpha)^2 T_n = 0 \\ T_n(0) = 0 \end{array}\right\} \Rightarrow T_n(t) = 0,$$

PDEs: Heat Equation, Non-homogeneous, Example

Solution:

- The total solution for our problem is

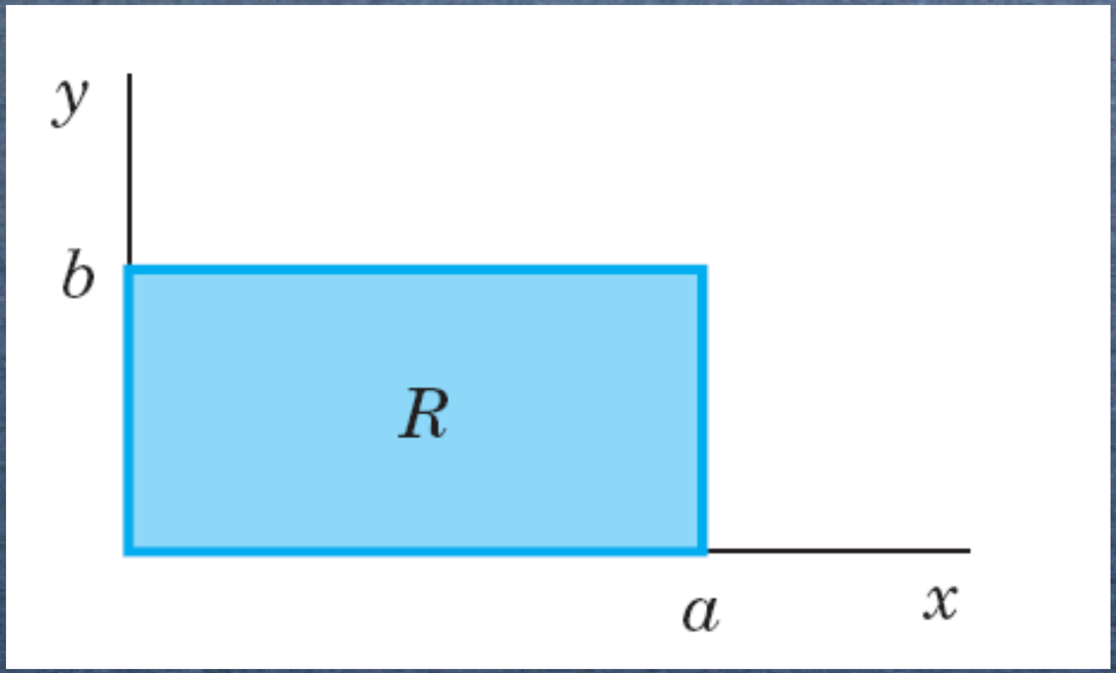
$$\begin{aligned} u(x,t) &= e^{-(\pi\alpha)^2 t}\mathrm{Sin}(\pi x) + \frac{1}{(3\pi\alpha)^2}[1 - e^{-(3\pi\alpha)^2 t}]\mathrm{Sin}(3\pi x) \\ &= \quad \text{transient} \quad + \quad \text{steady state} \end{aligned}$$

- The first term represents transient behavior, due to the initial conditions.
- The second term represents steady state behavior, due to the right-hand side of the PDE (non-homogeneous term).

PDEs: 2D Heat Equation,

PDE:	$u_t = \alpha^2 (u_{xx} + u_{yy}) \equiv \alpha^2 \nabla_{\perp}^2,$	$0 < x < a, \quad 0 < y < b, \quad 0 < t < \infty$
BCs:	$u(0, y, t) = u(a, y, t) = 0$ and $u(x, 0, t) = u(x, b, t) = 0,$	$0 < t < \infty$
IC:	$u(x, y, 0) = c_0,$	$0 < x < a, \quad 0 < y < b.$

where α and c_0 are both constants.



PDEs: 2D Heat Equation, solution

- Find elementary solutions to the PDE:

$$\boxed{u(x,y,t) = X(x)\,Y(y)\,T(t),}$$

- Fundamental solutions to match the BCs:

$$u(x,y,t) = \sum_m \sum_n A_{mn} e^{-[(\frac{m\pi}{a})^2 + (\frac{n\pi}{b})^2]\alpha^2 t} \sin(\frac{m\pi}{a}x)\sin(\frac{n\pi}{b}y),$$

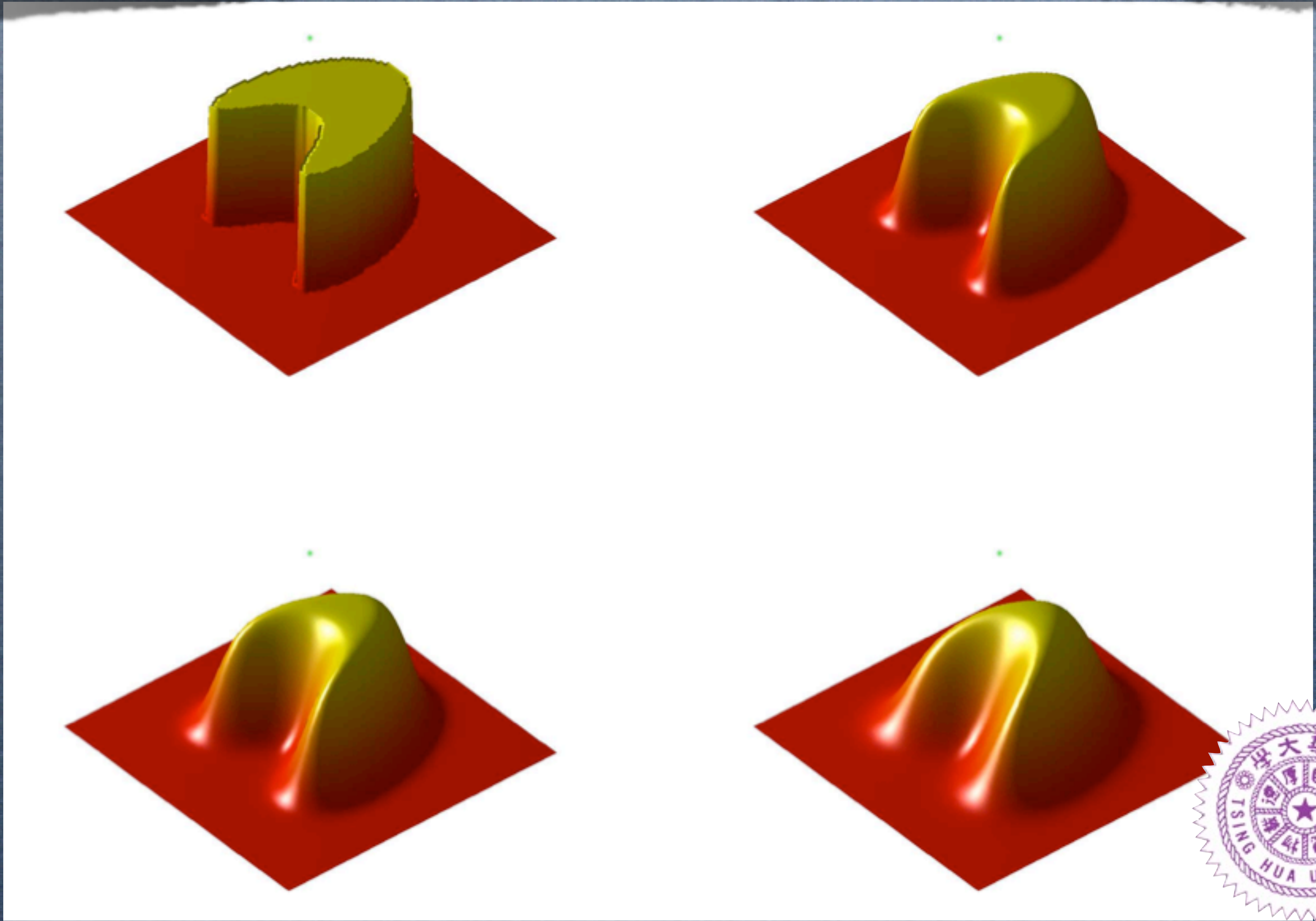
- For the IC:

$$u(x,y,0) = c_0 = \sum_m \sum_n A_{mn} \sin(\frac{m\pi}{a}x)\sin(\frac{n\pi}{b}y),$$

where the *double* Sine series coefficient A_{mn} is

$$A_{mn} = \frac{4}{ab}\int_0^b \int_0^a c_0 \sin(\frac{m\pi}{a}x)\sin(\frac{n\pi}{b}y)\,dxdy.$$

PDEs: Heat Equation, Separation of Variables, 2D



Homework 6: Heat equation

$$\text{PDE:} \quad u_t = u_{xx} + \text{Sin}(3\pi x), \quad 0 < x < 1, \quad 0 < t < 1$$

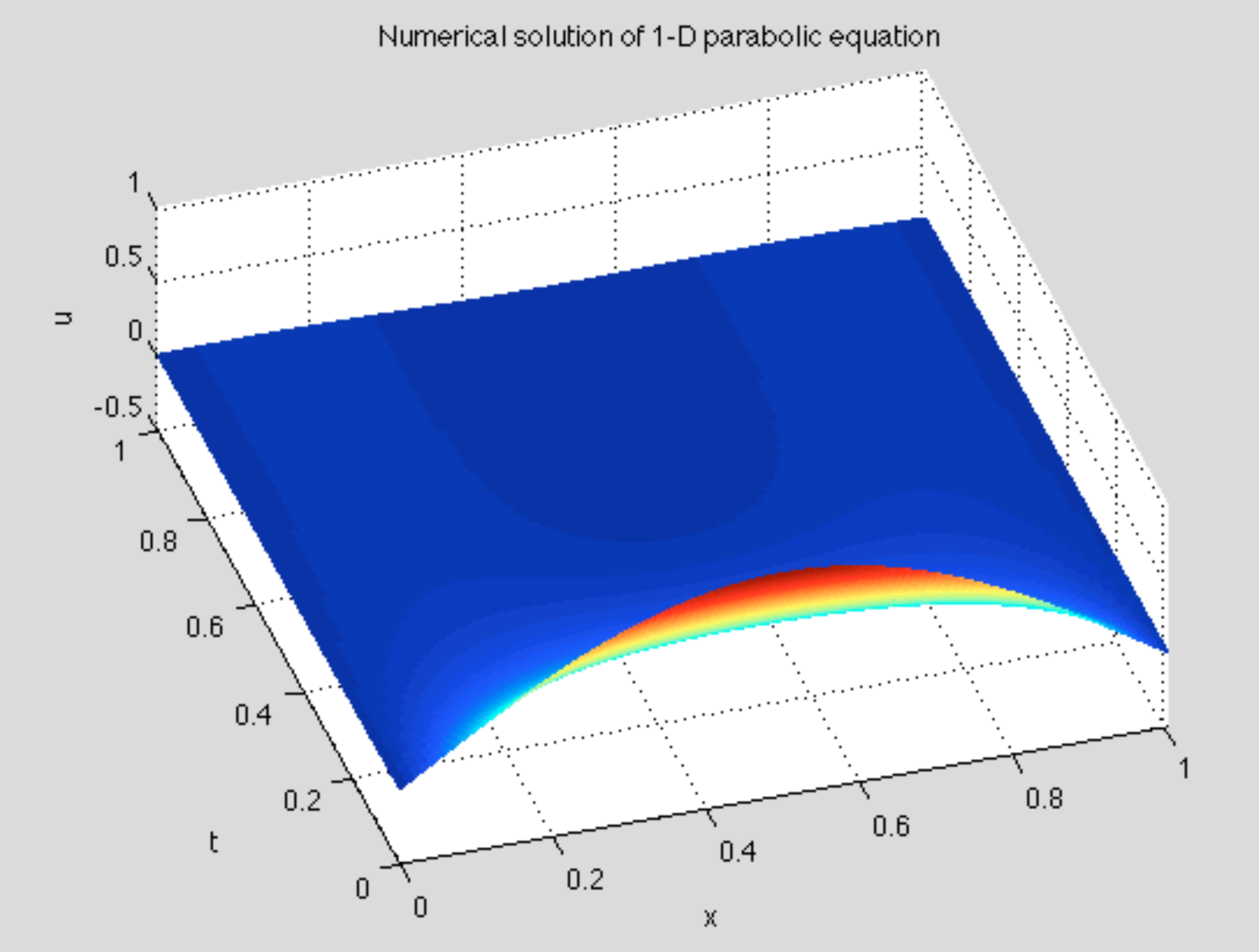
$$\text{BCs:} \quad u(0,t) = 0 \quad \text{and} \quad u(1,t) = 0, \quad 0 < t < 1$$

$$\text{IC:} \quad u(x,0) = \text{Sin}(\pi x), \quad 0 \le x \le 1$$

The total solution for our problem is

$$\begin{aligned} u(x,t) &= e^{-(\pi\alpha)^2 t}\text{Sin}(\pi x) + \frac{1}{(3\pi\alpha)^2}[1 - e^{-(3\pi\alpha)^2 t}]\text{Sin}(3\pi x) \\ &= \quad \text{transient} \quad + \quad \text{steady state} \end{aligned}$$

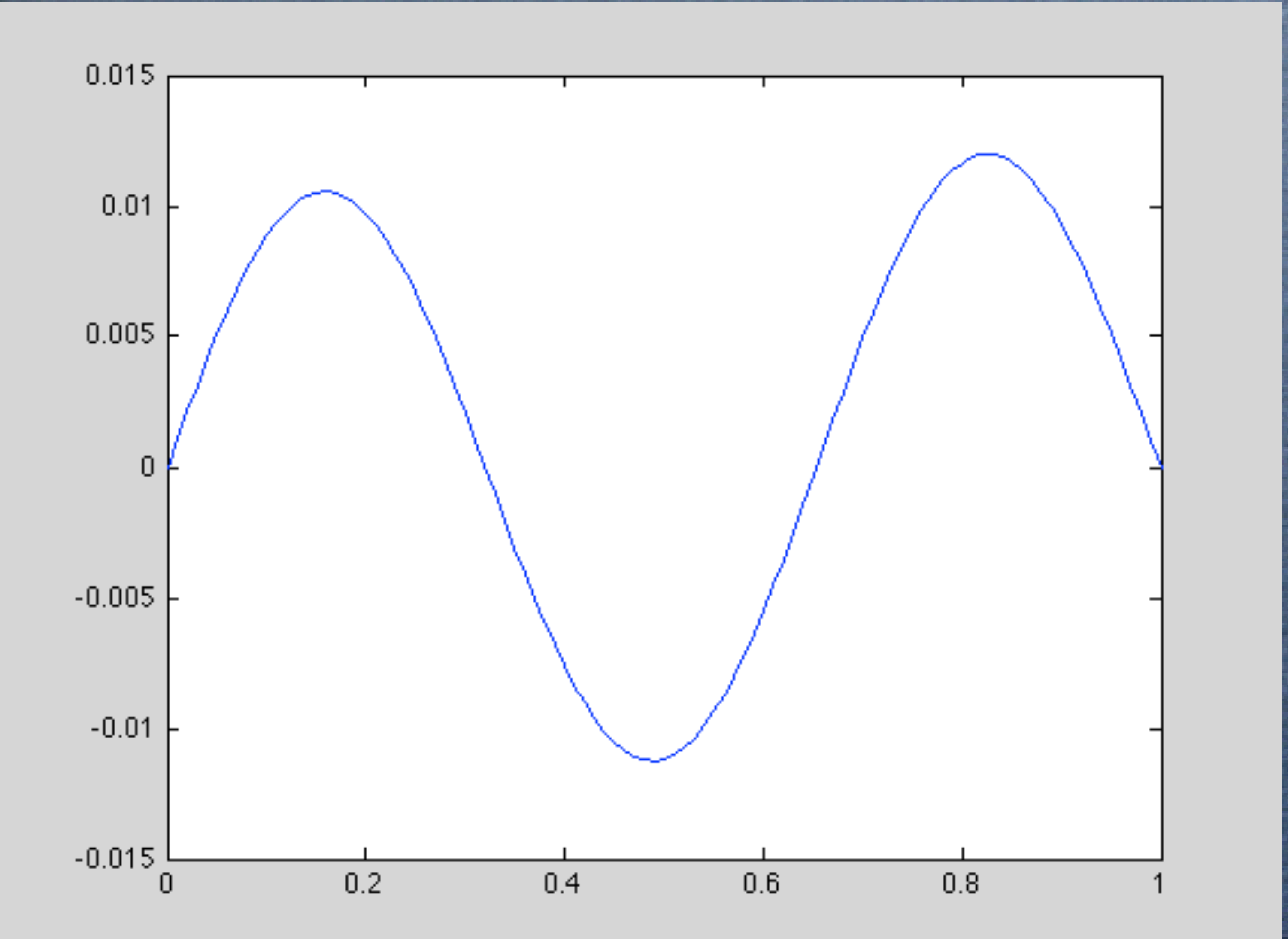
PDEs: Heat Equation, Initial-Boundary-Value Problem



Homework 6: Heat equation

The total solution for our problem is

$$\begin{aligned} u(x,t) &= e^{-(\pi\alpha)^2 t}\mathrm{Sin}(\pi x) + \frac{1}{(3\pi\alpha)^2}[1 - e^{-(3\pi\alpha)^2 t}]\mathrm{Sin}(3\pi x) \\ &= \quad \text{transient} \quad + \quad \text{steady state} \end{aligned}$$



t = 1

Homework 6: **Heat equation**

PDE: $u_t = u_{xx} + \mathrm{Sin}(3\pi x), \qquad 0 < x < 1, \quad 0 < t < 1$

BCs: $u_x(0,t) = 0 \quad \text{and} \quad u_x(1,t) = 0, \quad 0 < t < 1$

IC: $u(x,0) = \mathrm{Sin}(\pi x), \qquad 0 \le x \le 1$

Non-homogeneous and with Neumann BCs

PDEs: Heat Equation, Non-homogeneous, Example

Example:

PDE: $u_t = u_{xx} + \text{Sin}(3\pi x), \qquad 0 < x < 1, \quad 0 < t < 1$

BCs: $u_x(0,t) = 0 \quad \text{and} \quad u_x(1,t) = 0, \quad 0 < t < 1$

IC: $u(x,0) = \text{Sin}(\pi x), \qquad 0 \le x \le 1$

Hits:

- Since the BCs support $\text{Cos}(n\pi x)$ eigenfunctions,

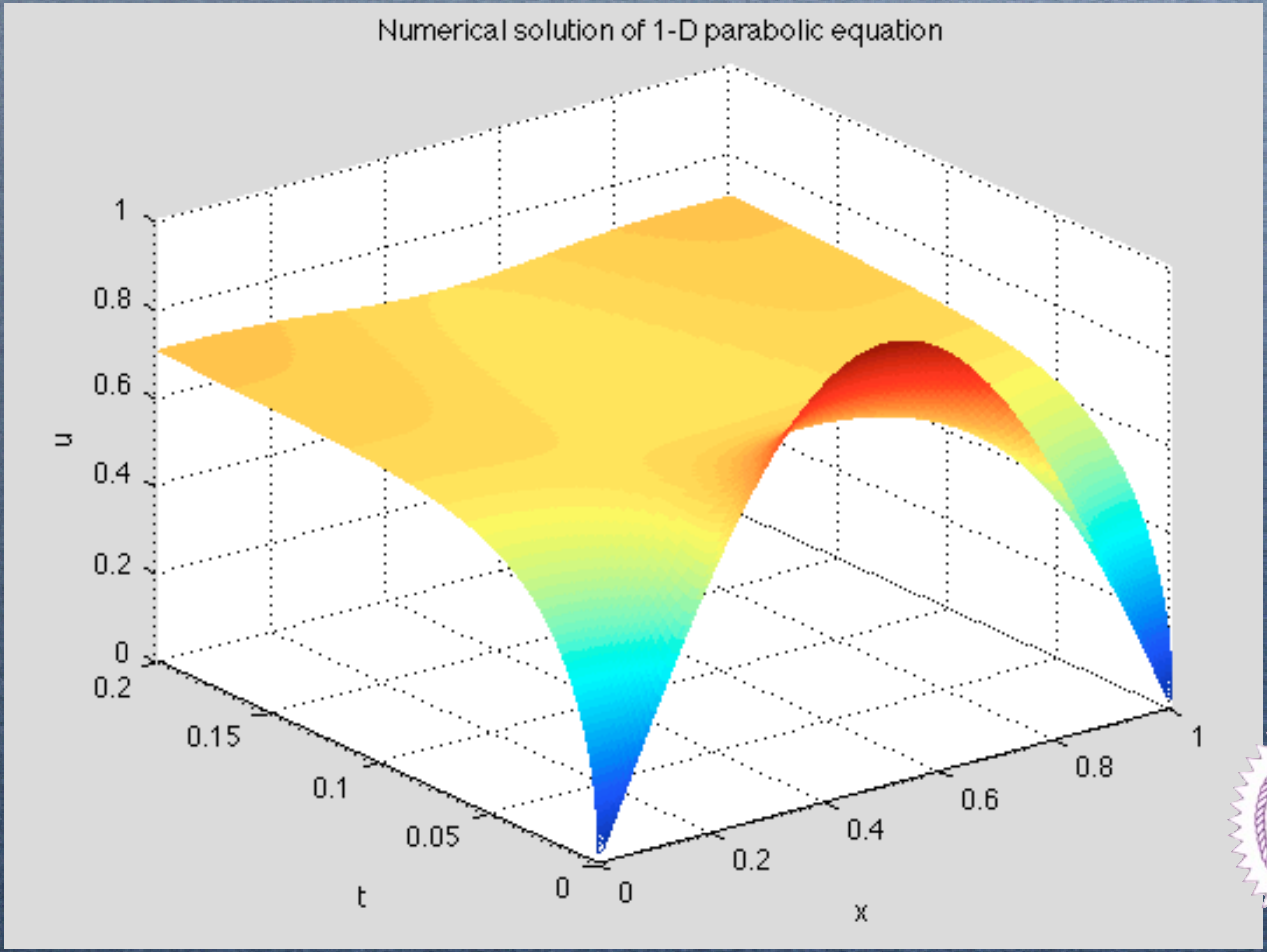
$$\boxed{u(x,t) = \sum_{n=1} T_n(t) X_n(x) = \sum_{n=1} T_n(t)\text{Cos}(n\pi x),}$$

- Substitute this expansion into the problem,

PDE: $$\sum_{n=1} [T_n' + (n\pi\alpha)^2 T_n]\text{Cos}(n\pi x) = \text{Sin}(3\pi x)$$

IC: $$\sum_{n=1} T_n(0)\text{Cos}(n\pi x) = \text{Sin}(\pi x),$$

PDEs: Heat Equation, Initial-Boundary-Value Problem



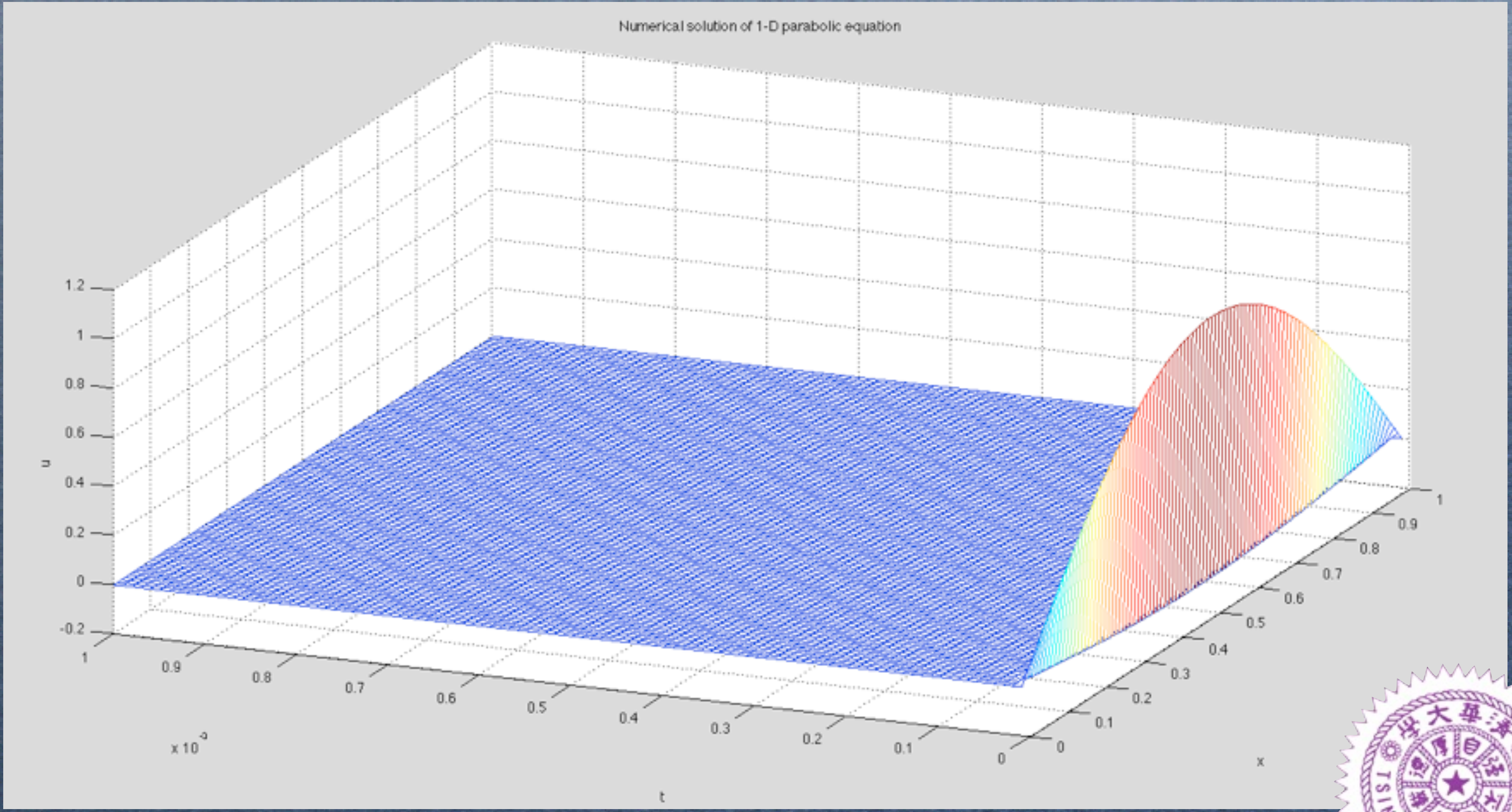
PDEs: Implicit Crank-Nicholson mehtod

In the matrix form:

$$
\begin{bmatrix}
 & & \ddots & & \\
\ddots & -\gamma & (2+2\gamma) & -\gamma & \ddots \\
 & & \ddots & &
\end{bmatrix}
\begin{pmatrix}
A_0^{n+1} \\ \vdots \\ A_{j-1}^{n+1} \\ A_j^{n+1} \\ A_{j+1}^{n+1} \\ \vdots \\ A_N^{n+1}
\end{pmatrix}
=
$$

$$
\begin{bmatrix}
 & & \ddots & & \\
\ddots & +\gamma & (2-2\gamma) & +\gamma & \ddots \\
 & & \ddots & &
\end{bmatrix}
\begin{pmatrix}
A_0^{n+1} \\ \vdots \\ A_{j-1}^{n} \\ A_j^{n} \\ A_{j+1}^{n} \\ \vdots \\ A_N^{n+1}
\end{pmatrix}
.
$$

Homework 6: Heat equation



PDEs: Wave Equation, Semi-infinite media, Ch. 12.11

PDE: $w_{tt} = c^2 w_{xx}, \quad 0 < x < \infty, \quad \text{and} \quad 0 < t < \infty$

BCs: $w(0,t) = f(t) = \begin{cases} \sin t & ; \quad \text{for} \quad 0 \le t \le 2\pi \\ 0 & ; \quad \text{otherwise} \end{cases}$

AC: $\lim_{x \to \infty} w(x,t) = 0, \quad t \ge 0 \quad$ Asymptotic Condition.

Laplace Transform: ODE with IVP, Example

t-space

Given problem

$$y'' - y = t$$
$$y(0) = 1$$
$$y'(0) = 1$$

s-space

Subsidiary equation

$$(s^2 - 1)Y = s + 1 + 1/s^2$$

Solution of subsidiary equation

$$Y = \frac{1}{s-1} + \frac{1}{s^2-1} - \frac{1}{s^2}$$

Solution of given problem

$$y(t) = e^t + \sinh t - t$$

Laplace Transform: Definition

- If $f(t)$ is a function defined for all $t \geq 0$, its Laplace transform is defined as

$$\boxed{F(s) = \mathcal{L}(f) \equiv \int_0^\infty e^{-st} f(t)\,\mathrm{d}t.}$$

- Here we must assume that $f(t)$ is such that the integral exists (that is, has some finite value).
- This assumption is usually satisfied in applications.

Laplace Transform: Derivatives

- The transform of first derivative of f satisfies

$$\boxed{\mathcal{L}[f'(t)] = s\mathcal{L}[f(t)] - f(0).}$$

- The transform of second derivative of f satisfies

$$\boxed{\mathcal{L}[f''(t)] = s^2\mathcal{L}[f(t)] - sf(0) - f'(0).}$$

- The transform of nth-derivative of f satisfies

$$\boxed{\mathcal{L}[f^{(n)}(t)] = s^n\mathcal{L}[f(t)] - s^{n-1}f(0) - s^{n-2}f'(0) - \cdots - f^{(n-1)}(0).}$$

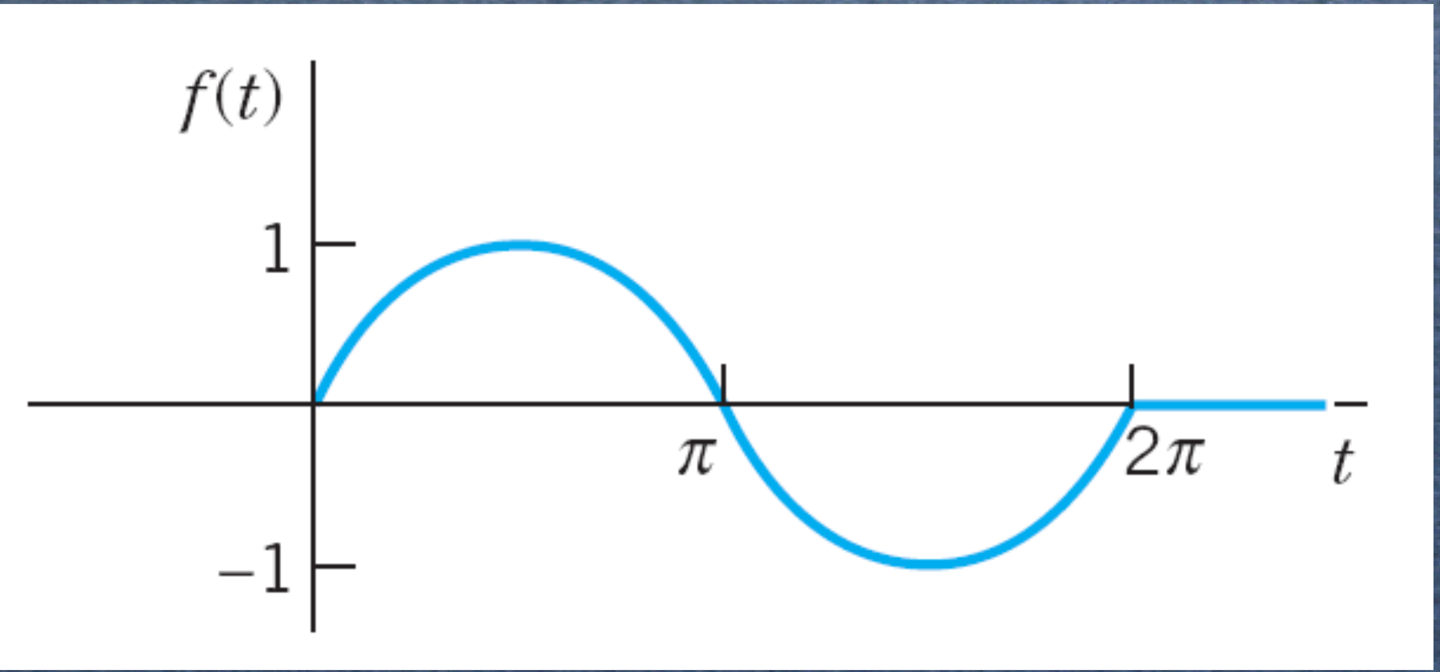
PDEs: Wave Equation, Semi-infinite media, Ch. 12.11

PDE: $w_{tt} = c^2 w_{xx}, \quad 0 < x < \infty, \quad \text{and} \quad 0 < t < \infty$

BC: $w(0,t) = f(t) = \begin{cases} \sin t & ; \quad \text{for} \quad 0 \le t \le 2\pi \\ 0 & ; \quad \text{otherwise} \end{cases}$

ICs: $w(x,0) = w_t(x,0) = 0, \quad 0 \le x \le \infty$

AC: $\lim_{x\to\infty} w(x,t) = 0, \quad t \ge 0$ Asymptotic Condition.



PDEs: Wave Equation, Semi-infinite media, cont.

- Transform t-variable via the Laplace transform, i.e. $\mathcal{L}[w(x,t)] = W(x)$,

$$\mathcal{L}[w_{tt}] = s^2 W(x,s) - sw(x,0) - w_t(x,0),$$

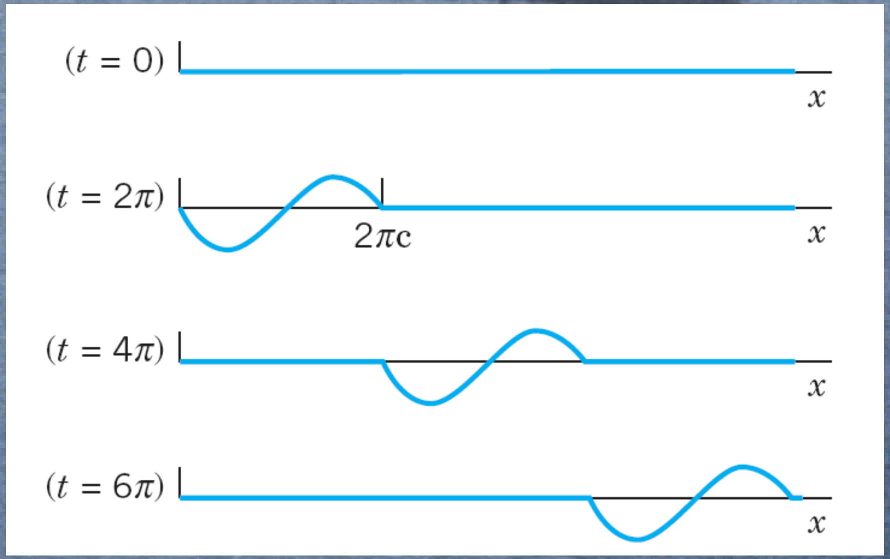
- For the ODE,

$$s^2 W(x) = c^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} W(x),$$

we have the general solution (homogeneous),

$$W(x,s) = c_1 e^{sx/c} + c_2 e^{-sx/c},$$

PDEs: Wave Equation, Semi-infinite media, cont.



Solution:

- From the AC, we have $c_1 = 0$.
- From the BS:

$$W(0,s) = c_2 = \mathcal{L}[f(t)] \equiv F(s)$$

we have the coefficients,

$$W(x,s) = F(s)e^{-sx/c}.$$

- By the inverse Laplace transform, i.e., $\boxed{\mathcal{L}^{-1}[e^{-as}F(s)] = f(t-a)u(t-a).}$

$$\begin{aligned} u(x,t) &= f(t-\frac{x}{c})u(t-\frac{x}{c}) \\ &= \sin(t-\frac{x}{c}). \end{aligned}$$

PDEs: Wave Equation, Semi-infinite media, cont.

- For the another general solution,

$$W(x,s) = G(s)\, e^{sx/c},$$

- By the inverse Laplace transform, i.e., $\boxed{\mathcal{L}^{-1}[e^{-as}F(s)] = f(t-a)u(t-a).}$

$$u(x,t) \quad = \quad g(t+\frac{x}{c})\, u(t+\frac{x}{c}).$$

Backward wave !

Fourier Integral !

PDEs: Wave Equation, d'Alembert Solution, Ch. 12.4

- For the diffusion problems (the parabolic case), we solve the bounded case $(0 \le x \le L)$ by separation of variables while solve the unbounded case $(-\infty < x < \infty)$ by the Fourier transform.

- For the wave problems (the hyperbolic case), we will do the **opposite**.

$$\text{PDE:} \qquad u_{tt} = \alpha^2 u_{xx}, \qquad -\infty < x < \infty, \quad 0 < t < \infty$$

$$\text{ICs:} \qquad \begin{cases} u(x,0) = f(x) \\ u_t(x,0) = g(x) \end{cases}, \qquad -\infty < x < \infty$$

- Replace (x, t) by new canonical coordinates (ξ, η), i.e. the moving-coordinate,

$$\xi = x + \alpha t \qquad \eta = x - \alpha t$$

- the PDE becomes

$$\boxed{u_{\xi\eta} = 0,}$$

with the solution of arbitrary functions of ξ or η, i.e.

$$\boxed{u(\xi, \eta) = \phi(\eta) + \psi(\xi).}$$

PDEs: Wave Equation, d'Alembert Solution, cont.

- In the original coordinates x and t, we have

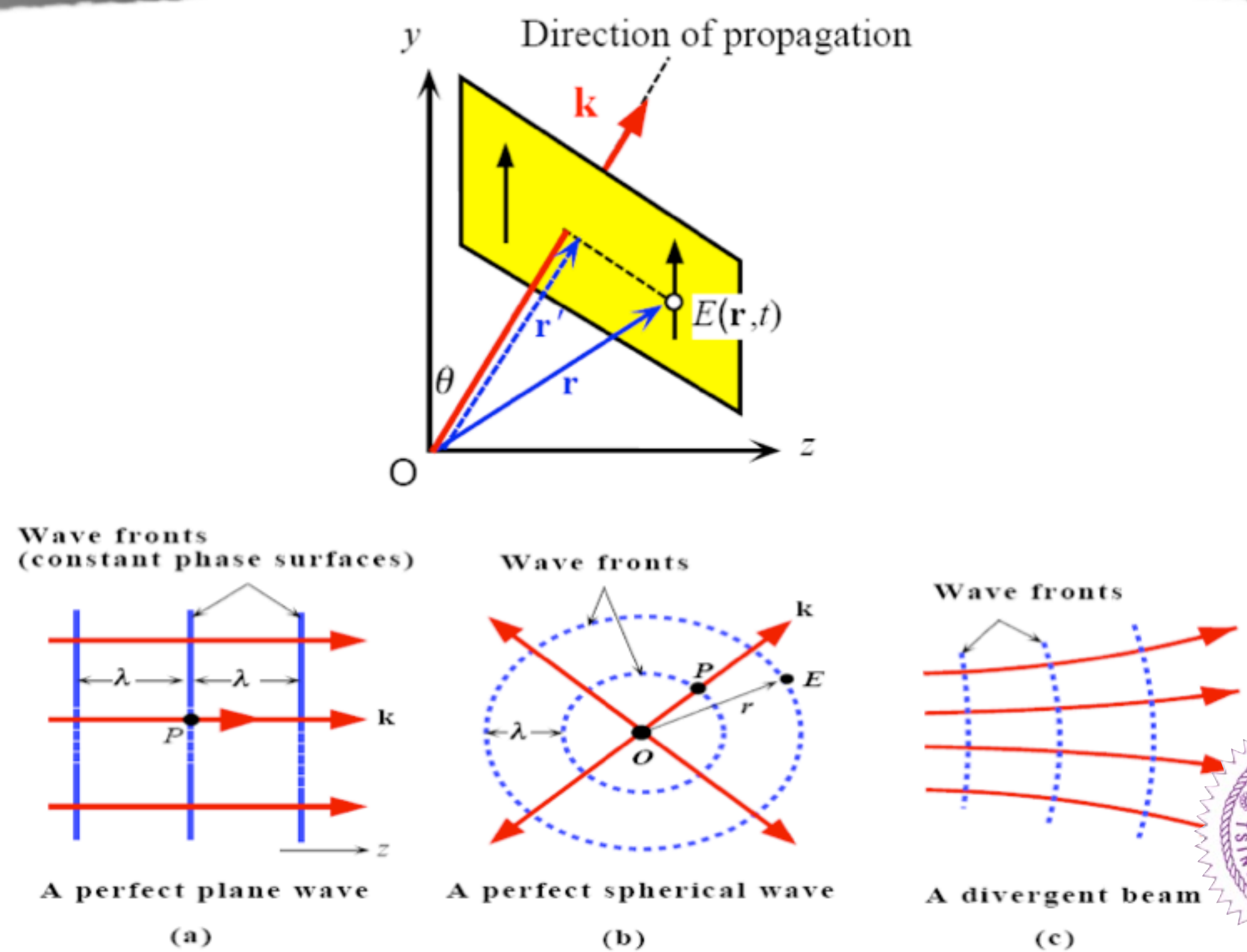
$$\boxed{u(x,t) = \Phi(x - \alpha\, t) + \Psi(x + \alpha\, t),}$$

  this is the general solution of the wave equation.

- Physically it represents the sum of any two moving waves, each moving in opposite direction with the velocity α. Eg.

$$\begin{aligned} u(x,t) &= Sin(x - \alpha\, t), && \text{(one right-moving wave)} \\ u(x,t) &= (x + \alpha\, t)^2, && \text{(one left-moving wave)} \\ u(x,t) &= Sin(x - \alpha\, t) + (x + \alpha\, t)^2, && \text{(two oppositely moving waves)} \end{aligned}$$

PDE: Wave equation



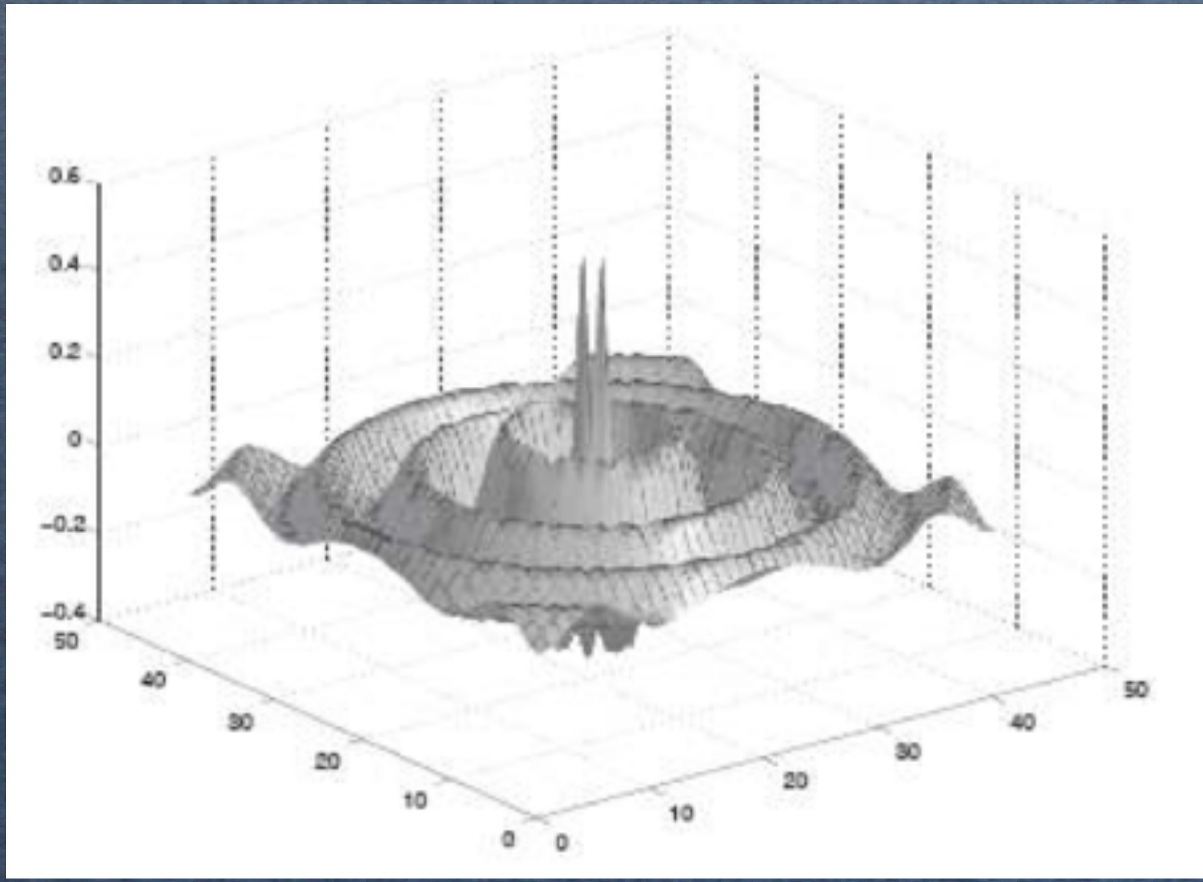
PDE: Wave equation, Spherical wave

- spherical wave:

$$\boxed{U(r) = \frac{A}{|r-r_0|}\exp(-ik|r-r_0|),}$$

where $k|r-r_0| =$ constant, wavefronts resemble sphere surfaces,

- intensity:



$$I(r) = \frac{|A|^2}{r^2},$$

PDEs: Wave Equation, d'Alembert Solution, IC

- Substitute the general solution into the two ICs,

$$\text{ICs:} \qquad \begin{cases} u(x,0) = f(x) \\ u_t(x,0) = g(x) \end{cases},$$

- for arbitrary functions ϕ and ψ, we have

$$\begin{aligned} \phi(x) + \psi(x) &= f(x), \\ -\alpha\,\phi'(x) + \alpha\,\psi'(x) &= g(x), \end{aligned}$$

- then by integrating from x_0 to x,

$$-\alpha\,\phi(x) + \alpha\,\psi(x) = \int_{x_0}^{x} g(\xi)\mathrm{d}\,\xi + K,$$

where K is an integration constant.

PDEs: Wave Equation, d'Alembert Solution

- The solutions for ϕ and ψ are

$$\begin{aligned}\phi(x) &= \frac{1}{2}f(x) - \frac{1}{2\alpha}\int_{x_0}^{x} g(\xi)\mathrm{d}\,\xi,\\ \psi(x) &= \frac{1}{2}f(x) + \frac{1}{2\alpha}\int_{x_0}^{x} g(\xi)\mathrm{d}\,\xi,\end{aligned}$$

- The D'Alembert solution,

$$\boxed{u(x,t) = \frac{1}{2}[f(x-\alpha, t) + f(x+\alpha\, t)] + \frac{1}{2\alpha}\int_{x-\alpha\, t}^{x+\alpha\, t} g(\xi)\mathrm{d}\,\xi.}$$

PDEs: Wave Equation, d'Alembert Solution, Example

Example 1:

Motion of an initial Sine wave,

$$\text{PDE:} \qquad u_{tt} = \alpha^2 u_{xx}, \qquad -\infty < x < \infty, \quad 0 < t < \infty$$

$$\text{ICs:} \qquad \begin{cases} u(x,0) = Sin(x) \\ u_t(x,0) = 0 \end{cases}, \qquad -\infty < x < \infty$$

Solution:

- D'Alembert's solution:

$$u(x,t) = \frac{1}{2}[Sin(x - \alpha\, t) + Sin(x + \alpha\, t)].$$

PDEs: Wave Equation, d'Alembert Solution, Example

Example 2:

Motion of an initial Sine wave,

$$\text{PDE:} \qquad u_{tt} = \alpha^2 u_{xx}, \qquad -\infty < x < \infty, \quad 0 < t < \infty$$

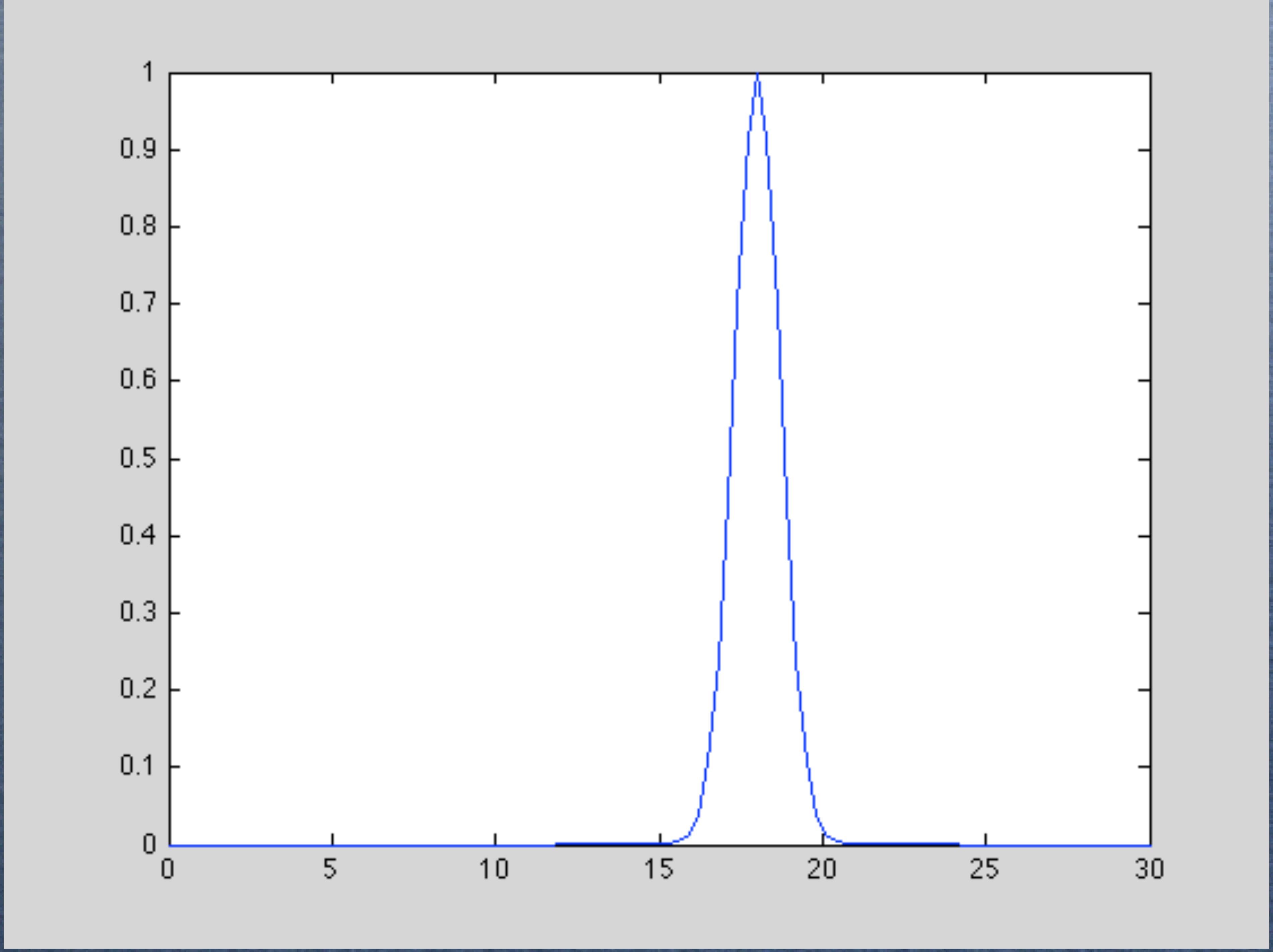
$$\text{ICs:} \qquad \begin{cases} u(x,0) = 0 \\ u_t(x,0) = Sin(x) \end{cases}, \qquad -\infty < x < \infty$$

Initial velocity is given.

Solution:

$$\begin{aligned} u(x,t) &= \frac{1}{2\alpha}\int_{x-\alpha\, t}^{x+\alpha\, t} Sin(\xi)\mathrm{d}\,\xi \\ &= \frac{1}{2\alpha}[Cos(x+\alpha\, t) - \mathrm{Cos}(x-\alpha\, t)]. \end{aligned}$$

PDEs: Wave Equation,



PDEs: Wave Equation, 1D

One-dimensional scalar wave equation:

$$\frac{\partial^2}{\partial t^2}u(x,t) = c^2\frac{\partial^2}{\partial x^2}u(x,t),$$

has the solution

$$u(x,t) = F(x+ct) + G(x-ct),$$

where F and G are arbitrary function.
Finite-difference approximation:

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} + \mathbf{O}(\Delta t^2) = c^2\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} + \mathbf{O}(\Delta x^2),$$

for the latest value of u at grid point i,

$$\boxed{u_i^{n+1} = (c\Delta t)^2[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}] + 2u_i^n - u_i^{n-1} + \mathbf{O}(\Delta t^2) + \mathbf{O}(\Delta x^2).}$$

PDEs: Wave Equation, FD-TD scheme

- This is a *fully explicit* second-order accurate expression for u_i^{n+1}.
- All wave quantities on the RHS are known, obtained during the previous time steps, n and $n-1$.
- Upon performing FDTD approximation for all space points, yielding the complete set of u_i^{n+1}.

PDEs: Wave Equation, magic time step

For the **magic time step**:

$$\boxed{c\Delta t/\Delta x = 1,}$$

$$\begin{aligned} u_i^{n+1} &= (u_{i+1}^n - 2u_i^n + u_{i-1}^n) + 2u_i^n - u_i^{n-1} \\ &= u_{i+1}^n + u_{i-1}^n - u_i^{n-1}, \end{aligned}$$

note that there is *no* remainder (error) term here.

PDEs: Wave Equation, magic time step

Consider the exact propagating-wave solutions to the 1D scalar wave equation,

$$u_j^n = F(x_i + ct_n) + G(x_i - ct_n),$$

where $x_i = i\Delta x$ and $t_n = n\Delta t$. Then

$$\begin{aligned} u_i^{n+1} &= u_{i+1}^n + u_{i-1}^n - u_i^{n-1} \\ \left[\begin{array}{c} F(x_i + ct_{n+1}) \\ +G(x_i - ct_{n+1}) \end{array}\right] &= \left[\begin{array}{c} F(x_{i+1} + ct_n) \\ +G(x_{i+1} - ct_n) \end{array}\right] + \left[\begin{array}{c} F(x_{i-1} + ct_n) \\ +G(x_{i-1} - ct_n) \end{array}\right] - \left[\begin{array}{c} F(x_i + ct_{n-1}) \\ +G(x_i - ct_{n-1}) \end{array}\right] \end{aligned}$$

$$\begin{aligned} \text{RHS} &= \left\{\begin{array}{c} F[(i+1)\Delta x + cn\Delta t] \\ +G[(i+1)\Delta x - cn\Delta t] \end{array}\right\} + \left\{\begin{array}{c} F[(i-1)\Delta x + cn\Delta t] \\ +G[(i-1)\Delta x - cn\Delta t] \end{array}\right\} \\ &- \left\{\begin{array}{c} F[i\Delta x + c(n-1)\Delta t] \\ +G[i\Delta x - c(n-1)\Delta t] \end{array}\right\} \\ &= \left\{\begin{array}{c} F[(i+1+n)\Delta x] \\ +G[(i-1-n)\Delta x] \end{array}\right\} = \text{LHS} \end{aligned}$$

PDEs: Wave Equation, dispersion, velocity

For a continuous sinusoidal-travelling-wave solution

$$u(x,t) = e^{j(\omega t - kx)},$$

we have

- dispersion relation:

$$\omega^2 = c^2 k^2,$$

- phase velocity:

$$v_p = \frac{\omega}{k} = \pm c,$$

- group velocity:

$$v_g = \frac{\mathrm{d}\omega}{\mathrm{d}k} = \pm c.$$

PDEs: Wave Equation, Numerical dispersion

Finite-difference approximation:

$$u_i^{n+1} \approx (c\Delta t)^2 [\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}] + 2u_i^n - u_i^{n-1},$$

and at the discrete space-time point (x_i, t_n),

$$u_i^n = u(x_i, t_n) = e^{j(\omega n \Delta t - \bar{k} i \Delta x)},$$

where $\bar{k}$ is the numerical wavenumber.

$$\begin{aligned} e^{j[\omega(n+1)\Delta t - \bar{k} i \Delta x]} &= (\frac{c\Delta t}{\Delta x})^2 \{ e^{j[\omega n \Delta t - \bar{k}(i+1)\Delta x]} - 2e^{j[\omega n \Delta t - \bar{k} i \Delta x]} + e^{j[\omega n \Delta t - \bar{k}(i-1)\Delta x]}) \\ &+ (2e^{j[\omega n \Delta t - \bar{k} i \Delta x]} - e^{j[\omega(n-1)\Delta t - \bar{k} i \Delta x]}) \end{aligned}$$

After factoring out the complex expoential term,

$$\begin{aligned} e^{j\omega\Delta t} &= (\frac{c\Delta t}{\Delta x})^2 \cdot (e^{-j\bar{k}\Delta x} - 2 + e^{j\bar{k}\Delta x}) + (2 - e^{-j\omega\Delta t} \\ \rightarrow \cos(\omega\Delta t) &= (\frac{c\Delta t}{\Delta x})^2 \cdot [\cos(\bar{k}\Delta x) - 1] + 1. \end{aligned}$$

PDEs: Wave Equation, Numerical velocity

- Very Fine Mesh: $\Delta t \to 0, \Delta x \to 0,$

$$1 - \frac{(\omega \Delta t)^2}{2} \approx (\frac{c\Delta t}{\Delta x})^2 \cdot [1 - \frac{(\bar{k}\Delta x)^2}{2} - 1] + 1$$

then

$$\omega^2 = c^2 \bar{k}^2.$$

- Magic Time Step: $c\Delta t = \Delta x,$

$$\cos(\omega \Delta t) = 1 \cdot [\cos(\bar{k}\Delta x) - 1] + 1 = \cos(\bar{k}\Delta x),$$

then

$$\bar{k}\Delta x = \pm \omega \Delta t.$$

PDEs: Wave Equation, Dispersive wave

The general solution for FD dispersion relation is

$$\bar{k} = \frac{1}{\Delta x}\cos^{-1}\{1 + (\frac{c\Delta t}{\Delta x})^2 \cdot [\cos(\omega\Delta t) - 1]\}.$$

For example, $c\Delta t = \Delta x/2$, and $\Delta x = \lambda_0/10$, one has

$$\begin{aligned}\bar{k} &= \frac{1}{\Delta x}\cos^{-1}\{1 + 4\cdot[\cos(\frac{2\pi}{\lambda_0}\cdot\frac{\Delta x}{2}) - 1]\} \\ &= \frac{1}{\Delta x}\cos^{-1}(0.8042) = \frac{0.63642}{\Delta x},\end{aligned}$$

Then the numerical phase velocity

$$\begin{aligned}\bar{v}_p &= \omega/\bar{k} \\ &= \frac{2\pi(c/\lambda_0)\Delta x}{0.63642} = 0.9873c.\end{aligned}$$

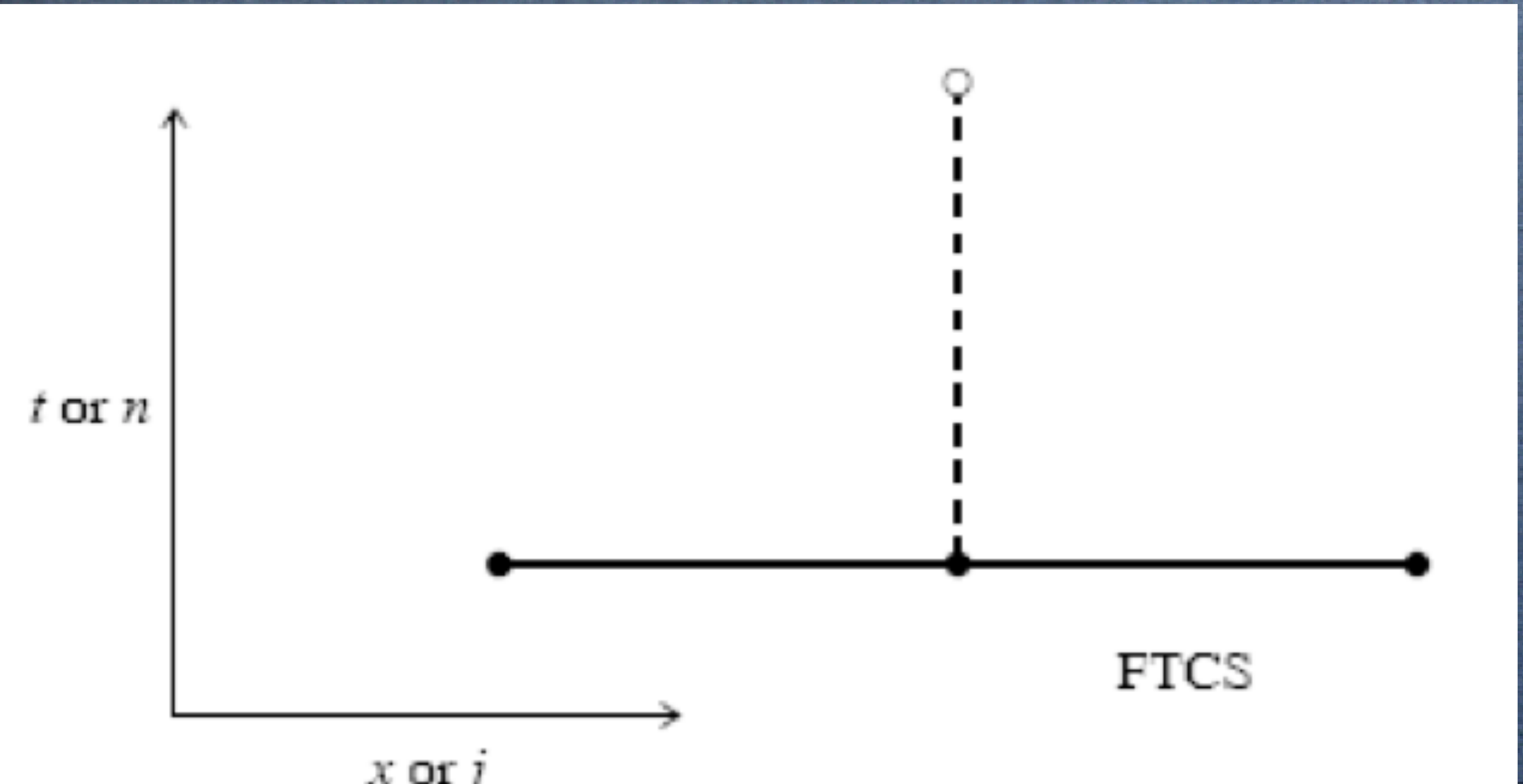
PDEs: Forward Time Centered Space

For a 1st-order PDE:

$$\frac{\partial}{\partial t}A(x,t) = \kappa \frac{\partial}{\partial x}A(x,t),$$

this equation can be approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^n - A_{j-1}^n}{2\Delta x} + \mathbf{O}(\Delta x^2).$$



PDEs: Wave Equation, Advection equation

$$\boxed{\frac{\partial}{\partial t}A(x,t) = \kappa \frac{\partial}{\partial x}A(x,t),}$$

The advection equation can be approximated by

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} + \mathbf{O}(\Delta t) \approx \kappa \frac{A_{j+1}^n - A_{j-1}^n}{2\Delta x} + \mathbf{O}(\Delta x^2).$$

By using $A_j^n = \lambda^n e^{i\,k\,j\,\Delta x}$, i.e., von Neumann technique, we obtain the amplification factor,

$$\lambda \equiv \lambda(k) = 1 + \kappa \frac{\Delta t}{\Delta x}\, i\, sin\, k \Delta x.$$

PDEs: Stability, Advection equation

- Center difference scheme:

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} = \kappa \frac{A_{j+1}^n - A_{j-1}^n}{2\Delta x},$$

is unconditional unstable,

$$|\lambda|^2 = 1 + (\kappa \frac{\Delta t}{\Delta x})^2 > 1.$$

- Upwind scheme:

$$\frac{A_j^{n+1} - A_j^n}{\Delta t} = \kappa \frac{A_j^n - A_{j-1}^n}{\Delta x},$$

is conditional stable only for $|\kappa \frac{\Delta t}{\Delta x}| \leq 1$, i.e.,

$$\lambda \equiv \lambda(k) = 1 + \kappa \frac{\Delta t}{\Delta x}(1 - e^{-i\,k\,\Delta x}),$$

and

$$|\lambda|^2 = (1+\mu)^2 - 2\mu(1+\mu)\cos k\Delta x + \mu^2,$$

where $\mu \equiv \kappa \frac{\Delta t}{\Delta x}$.

PDEs: Lax-Wendroff scheme, Advection equation

Lax-Wendroff scheme:

$$\begin{aligned} A(x, t+\Delta t) &= A(x,t) + \Delta t A_t + \frac{\Delta t^2}{2} A_{tt} + \mathbf{O}(\Delta t)^3, \\ &= A(x,t) + \kappa \Delta t A_x + \kappa^2 \frac{\Delta t^2}{2} A_{xx} + \mathbf{O}(\Delta t)^3, \end{aligned}$$

with the central difference,

$$A_j^{n+1} = A_j^n + \mu(A_{j+1}^n - A_{j-1}^n) + \mu^2(A_{j+1}^n - 2A_j^n + A_{j-1}^n).$$

The corresponding amplification factor is

$$\lambda(k) = 1 + i\mu \sin k\Delta x + 2\mu^2 \sin^2 \frac{1}{2} k\Delta x,$$

which is stable when $|\mu| \leq 1$.

PDEs: Leap-Frog scheme, Advection equation

Leap-Frog scheme:

$$\frac{A_j^{n+1} - A_j^{n-1}}{2\Delta t} = \kappa \frac{A_{j+1}^{n} - A_{j-1}^{n}}{2\Delta x},$$

with the truncation error $\mathbf{O}(\Delta t^2 + \Delta x^2)$. By von Neumann stability we have

$$\lambda^2 - i2\mu\lambda \sin k\Delta x - 1 = 0,$$

which gives

$$\lambda = i\mu \sin k\Delta x \pm \sqrt{1 - \mu^2 \sin^2 k\Delta x}$$

i.e. the leap-frog scheme is stable when $|\mu| \leq 1$.

Homework 7: Wave equation

Advection equation with a variable coefficient:

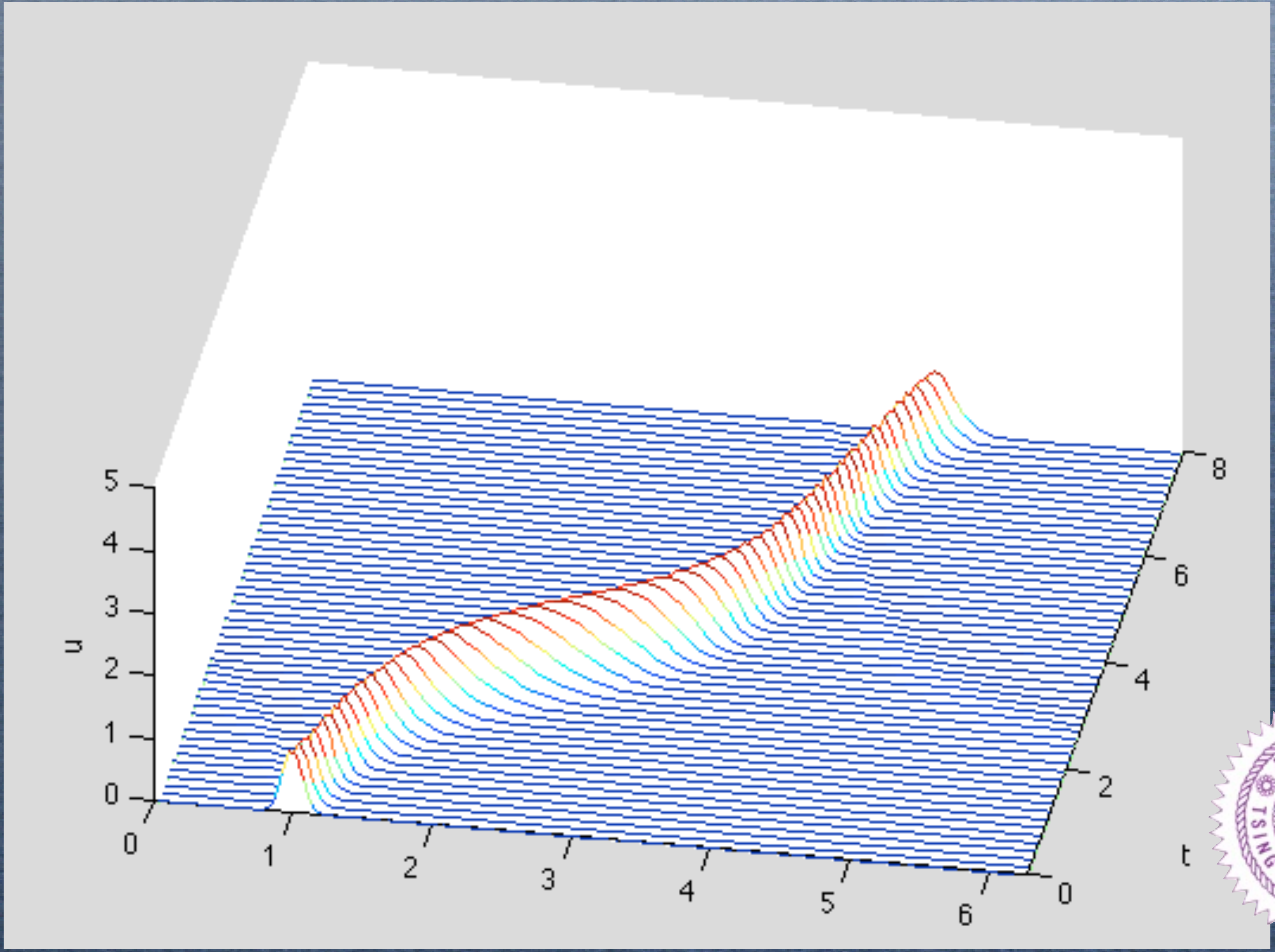
PDE: $u_t = -c(x) u_x, \qquad 0 < x < 2\pi, \quad \text{and} \quad 0 < t < 10$

IC: $u(x,0) = \mathrm{Exp}(-100(x - x_0)^2),$

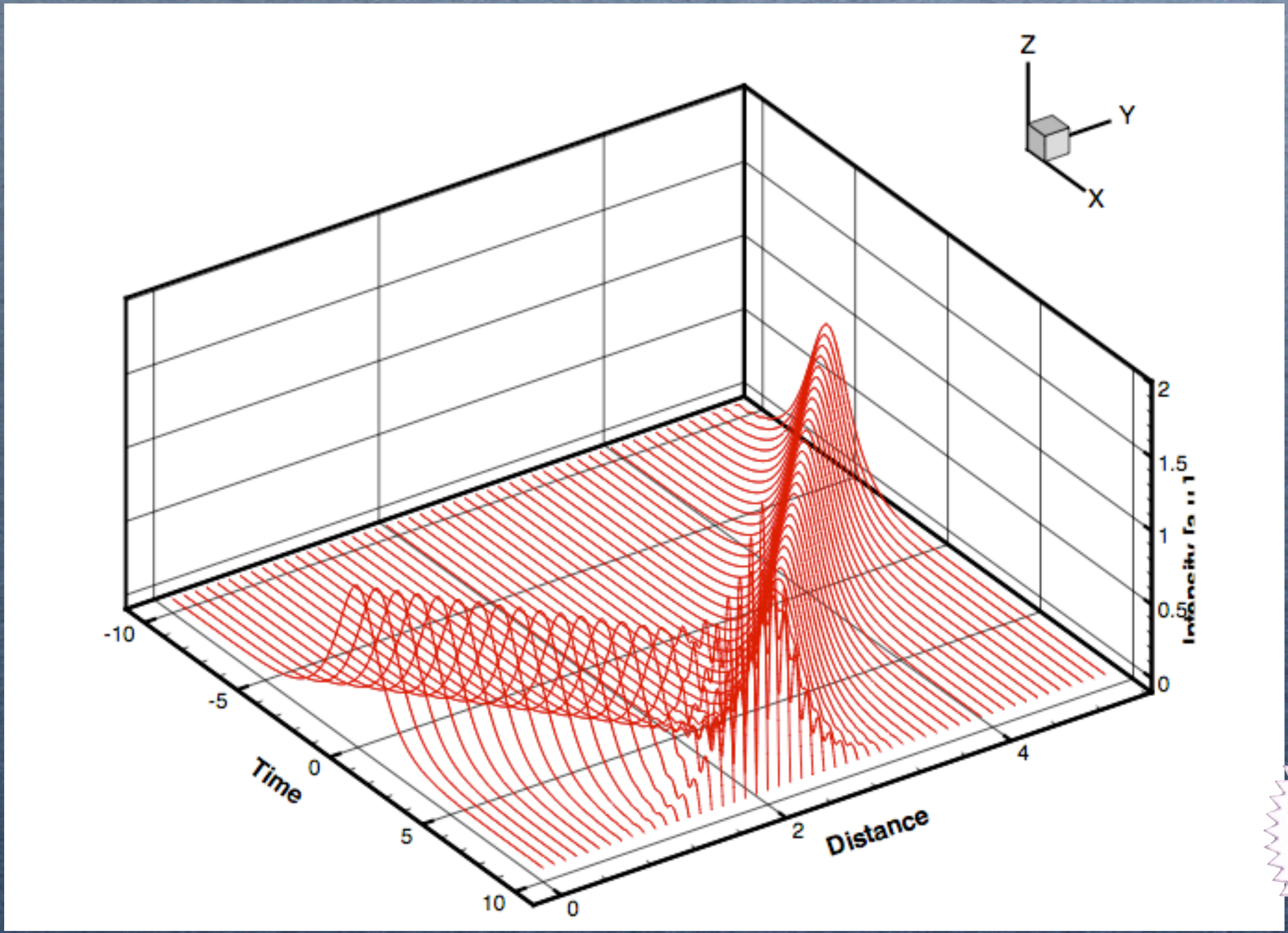
$$u(x, t = -dt) = \mathrm{Exp}(-100(x - \frac{1}{5} * dt - x_0)^2),$$

c(x): $c(x) = \dfrac{1}{5} + \mathrm{Sin}^2(x-1).$

Homework 7: Wave equation



PDEs: Wave Equation, without Periodic BC



PDEs: Wave Equation, Fourier method

For the equation

$$\frac{\partial U}{\partial z} = \hat{D}\,U,$$

where $\hat{D}$ is a differential operator, i.e.

$$\hat{D} \quad = \quad i\frac{D}{2}\frac{\partial^2}{\partial t^2}.$$

The Fourier method do the execution of the exponential operator $\exp(h\hat{D})$ in the Fourier domain,

$$\begin{aligned}\exp(h\hat{D})A(z,t) \quad &= \quad \{\mathbf{F}^{-1}\exp[h\hat{D}(i\omega)]\mathbf{F}\}A(z,t), \\ &= \quad \{\mathbf{F}^{-1}\exp[-i\frac{D}{2}\omega^2 h)]\mathbf{F}\}A(z,t),\end{aligned}$$

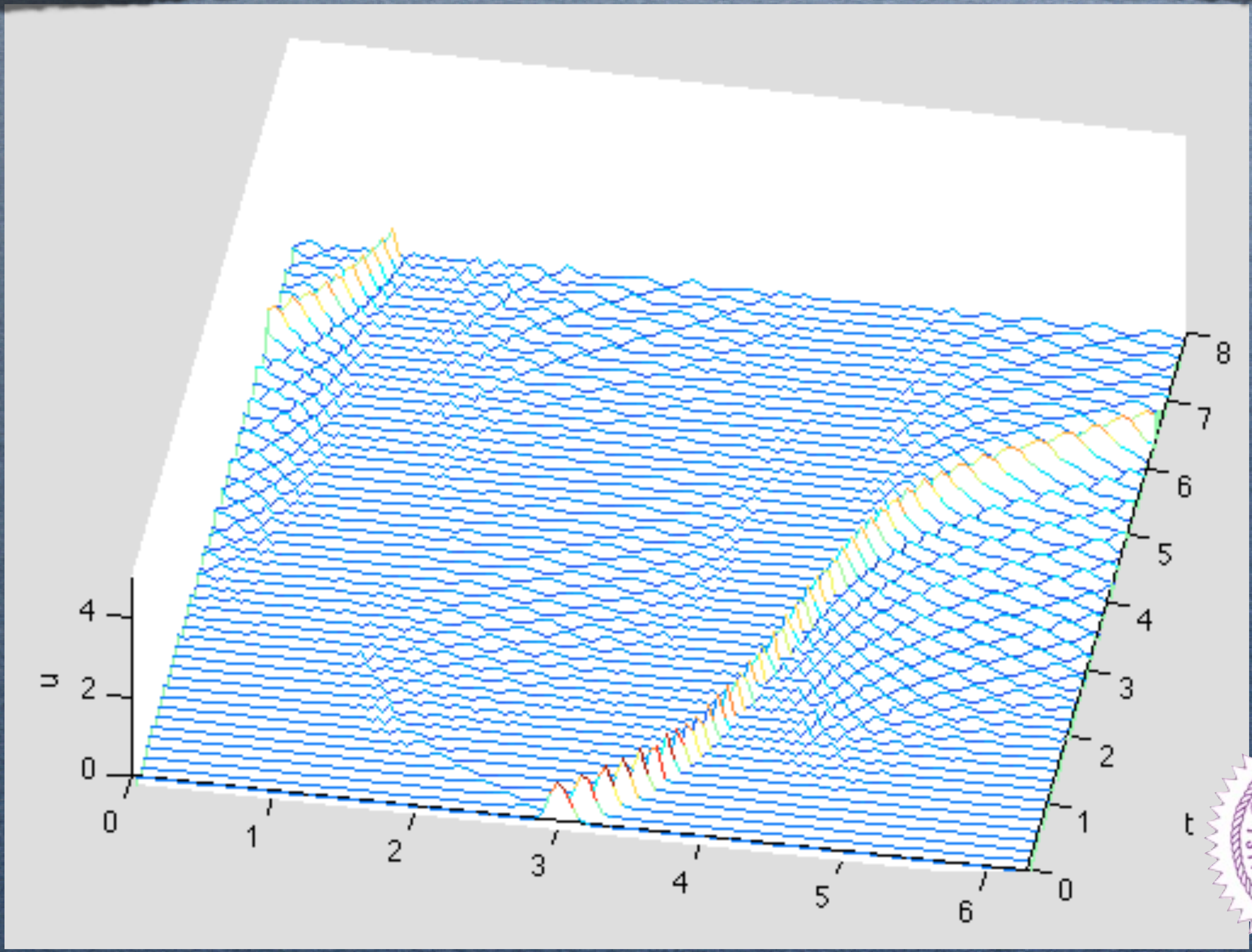
where $\mathbf{F}$ denotes the Fourier-transform operation. We replace the differential operator $\partial/\partial t$ by $i\omega$.

PDEs: Wave Equation, FFT method

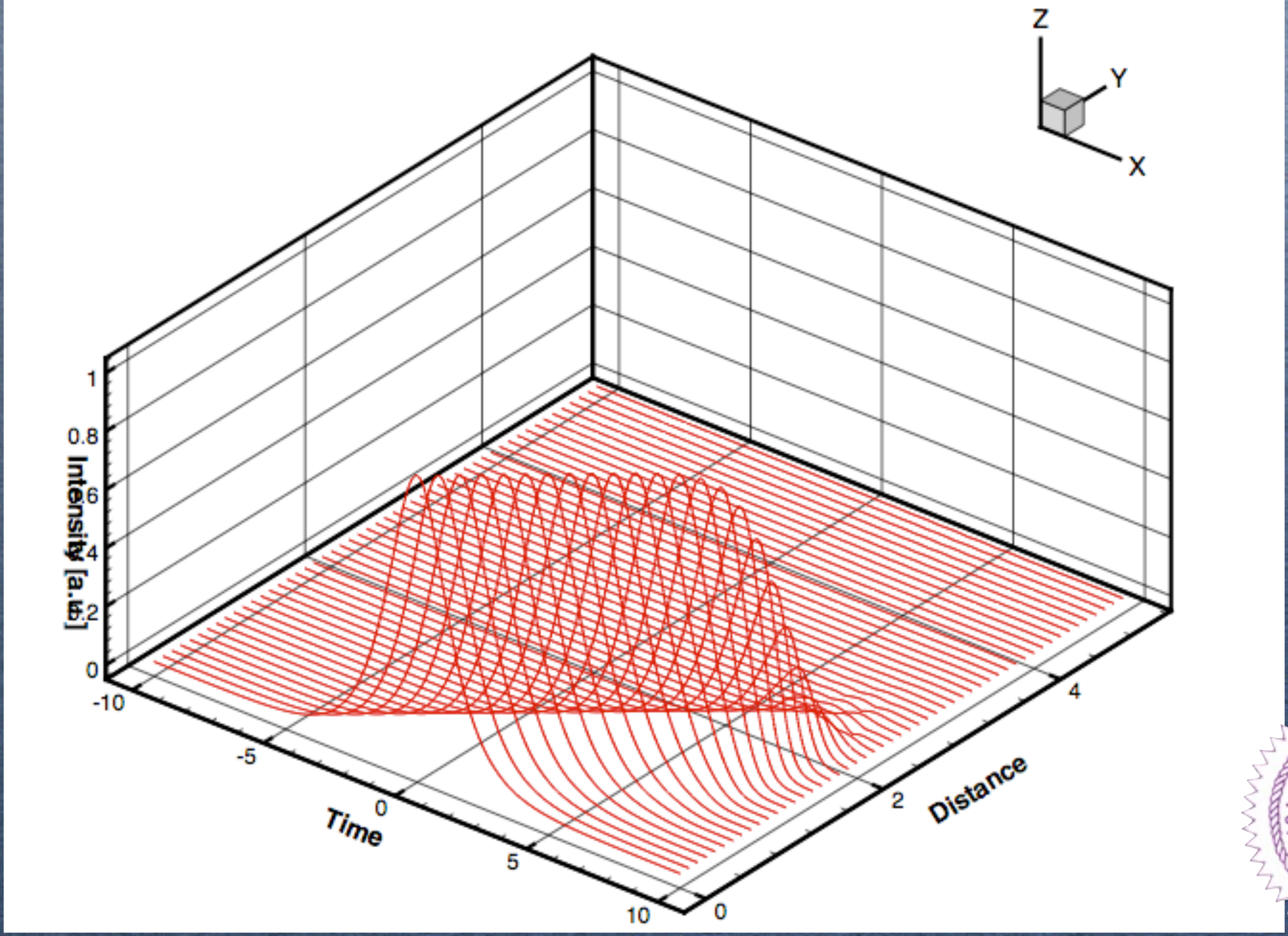
$$u_t + c(x)\, u_x = 0, \qquad c(x) = \frac{1}{5} + \sin^2(x-1),$$

- ☐ Given $u(x)$, compute $\tilde{U}(k)$,
- ☐ Define $\tilde{U}_k = (ik)^\mu \tilde{U}(k)$,
- ☐ Compute $\mathrm{D}_x u$ from $\tilde{U}_k$.

PDEs: Wave Equation, with Periodic BC



PDEs: Wave Equation, with Absorption BC



PDEs: Wave Equation, with Absorption BC

For the linear Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(x,t) = -\frac{1}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)$$

which can be written as

$$i\frac{\partial}{\partial t}\Psi(x,t) = -\frac{1}{2n}\frac{\partial}{\partial x}\frac{1}{n}\frac{\partial}{\partial x}\Psi(x,t)$$

where m, the mass, has been split into two spatially dependent functions n.

$$\Psi = \int_0^\infty A(\omega)\mathrm{exp}(\pm i\int k\mathrm{d}x - i\omega t)\mathrm{d}\omega,$$

where $k = \pm n\sqrt{2\omega}$ with their term inside the exponential is positive for waves moving to the left and negative for waves moving to the right.

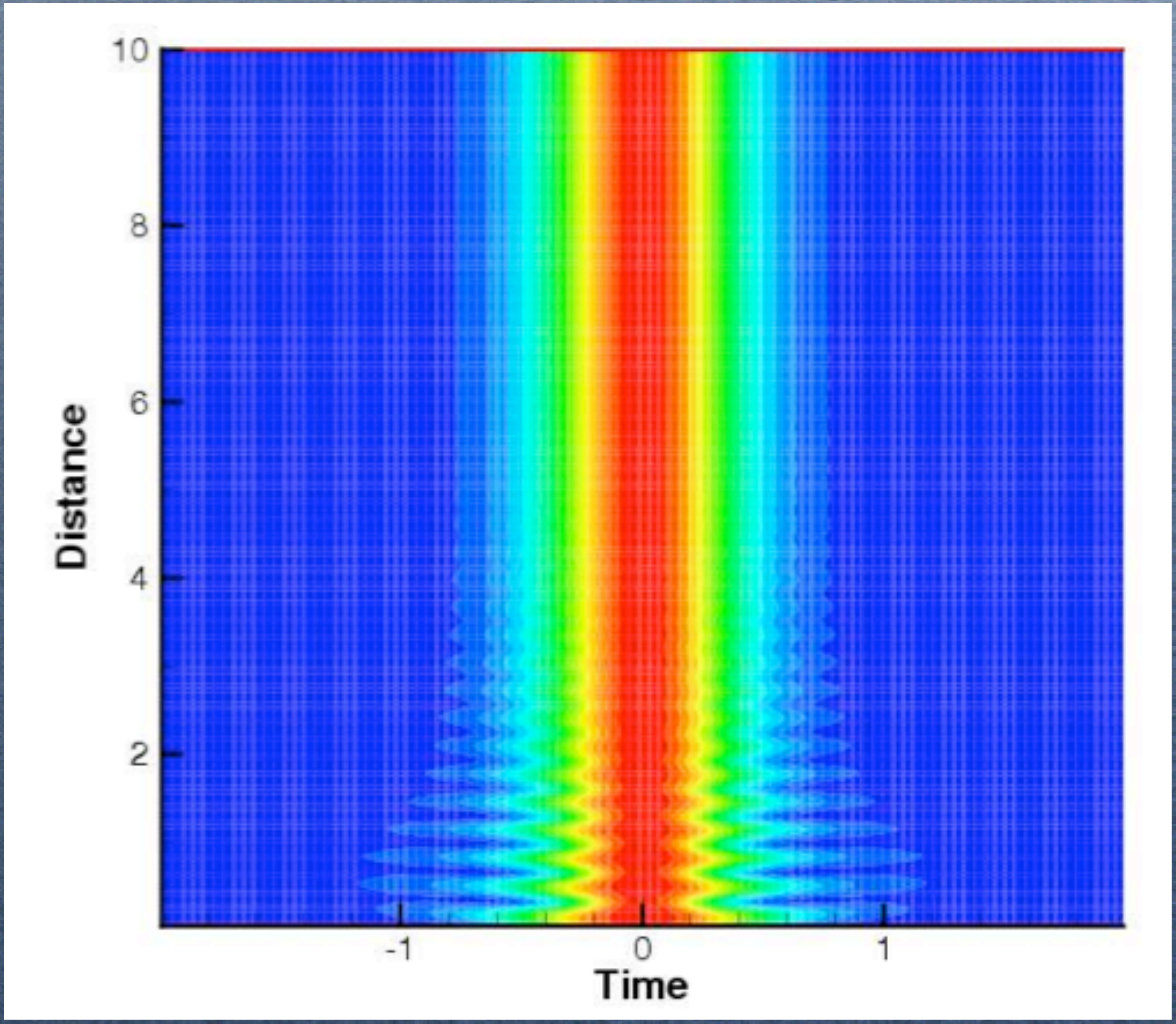
PDEs: Wave Equation, with Absorption BC

We can choose n to be, for example,

$$\boxed{n = \exp[\pm i \frac{\pi}{4}(1 - \tanh \frac{x - x_0}{a})],}$$

where x_0 is the position where the PML starts and a is a parameter which determines the sharpness of the transition between 1 and i.

PDEs: Wave Equation, PML



Wave equation: Helmholtz and Schrondinger eqs

- Helmholtz EM wave equation in free space:

$$\frac{\partial^2}{\partial t^2}E = \frac{1}{\mu_0 \epsilon_0}\nabla^2 E,$$

- Schrödinger matter wave equation in free space:

$$i\hbar\frac{\partial}{\partial t}\Psi = \frac{-1}{2m}\nabla^2\Psi,$$

Anything in common ?

What is in common for Waves ?

- Diffraction
- Superposition
- Interference
- Uncertainty Relation
- .....

Wave equation: Paraxial approximation

- Wave equation: In free space, the electric field, E, is defined as $E(r,t) = \vec{n}\psi(x,y,z)e^{j\omega t}$, which obeys the vector wave equation,

$$\nabla^2\psi + k^2\psi = 0.$$

- The paraxial wave equation: $\psi(x,y,z) = u(x,y,z)e^{-jkz}$, one obtains

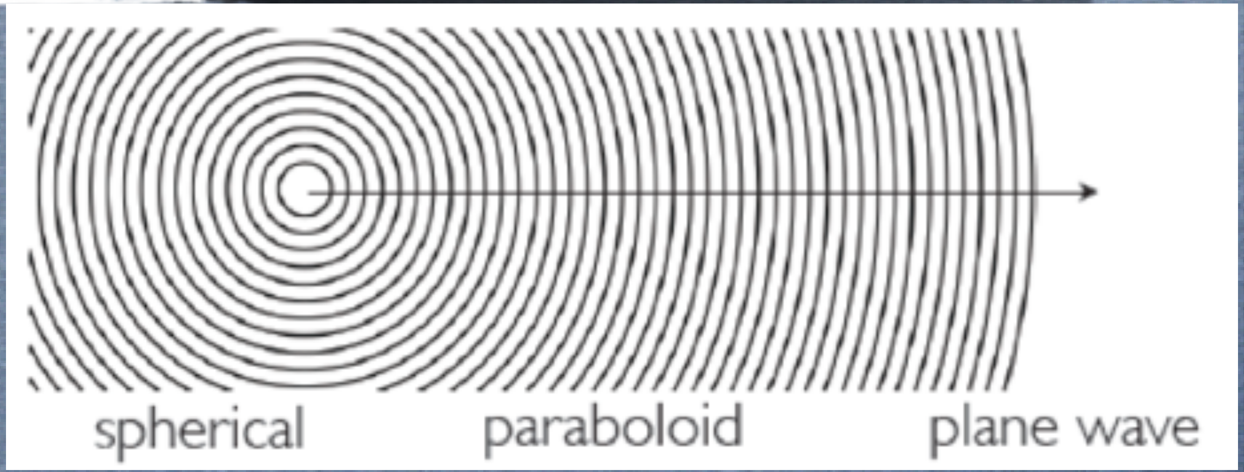
$$\boxed{\nabla_T^2 u - 2jk\frac{\partial u}{\partial z} = 0,}$$

where $\nabla_T \equiv \hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y}$.

- Compared to Schrödinger matter wave equation in free space:

$$i\hbar\frac{\partial}{\partial t}\Psi = \frac{-1}{2m}\nabla^2\Psi,$$

Paraxial wave equation: Fresnel kernel



$$\boxed{\nabla_T^2 u - 2jk\frac{\partial u}{\partial z} = 0,}$$

- This solution is proportional to the impulse response function (Fresnel kernel),

$$h(x, y, z) = \frac{j}{\lambda z} e^{-jk[(x^2+y^2)/2z]},$$

  i.e. $\nabla_T^2 h(x, y, z) - 2jk\frac{\partial h}{\partial z} = 0.$

- For paraxial waves, $\sqrt{x^2 + y^2} \ll z$,

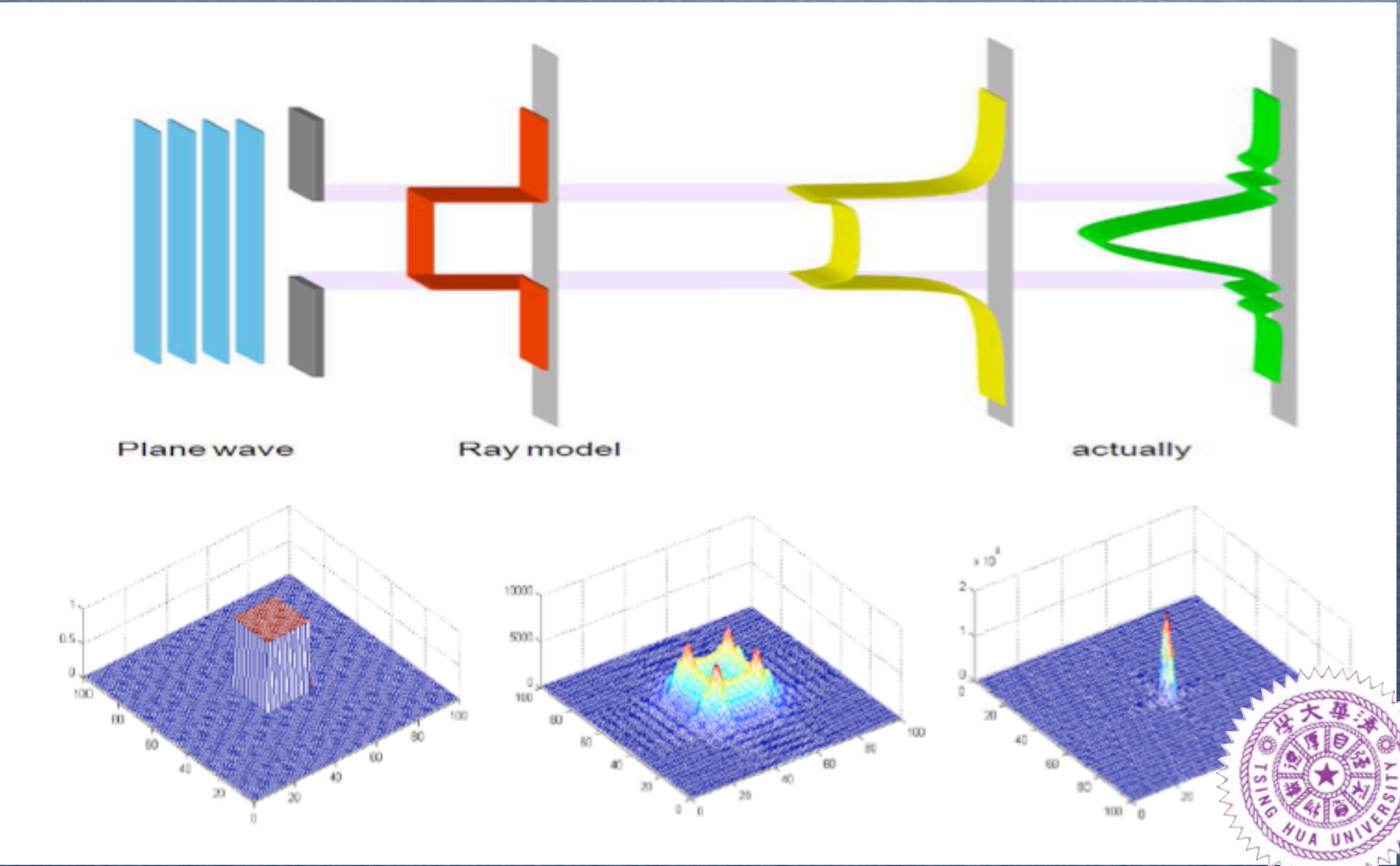
$$r = \sqrt{x^2 + y^2 + z^2} \approx z + \frac{x^2 + y^2}{2z},$$

- the spherical waves can be approximated by,

$$U(r) = \frac{A}{r}\exp(-i\mathbf{k} \cdot r) \approx \frac{A}{z}\exp(-ikz)\exp(\frac{-ik(x^2 + y^2)}{2z}),$$

- for the wavefront, constant phase plane, $\frac{x^2+y^2}{2z}$ is paraboloid,

Diffraction: Fresnel and Fraunhofer



Paraxial wave equation: Gauss beams

- solution for $x, y \ll z$, is the paraboloidal wave, i.e. $U(r) = A(r)\exp(-ikz)$,

$$A(r) = \frac{A_0}{z}\exp[\frac{-ik(x^2+y^2)}{2z}] = \frac{A_0}{z}\exp(\frac{-ik\rho^2}{2z}),$$

- shifted paraboloidal wave,

$$A(r) = \frac{A_1}{q(z)}\exp(\frac{-ik\rho^2}{2q(z)}),$$

where

$$q(z) = z - z' - \zeta = z - z' + iz_0, \qquad z_0 \text{ is the Rayleigh range},$$

- complex amplitude (general solution),

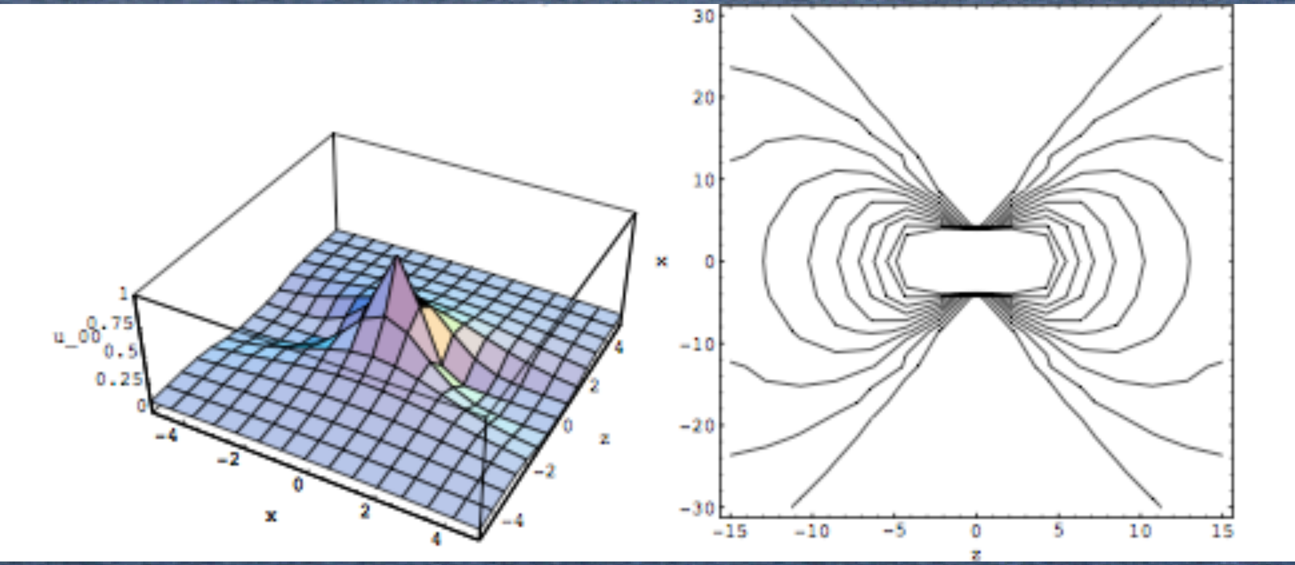
$$\frac{1}{q(z)} = \frac{1}{R(z)} - i\frac{\lambda}{\pi W^2(z)},$$

Paraxial Wave equation: Gaussian Optics

- The solution of the scalar paraxial wave equation is,

$$u_{00}(x,y,z) = \frac{\sqrt{2}}{\sqrt{\pi} w} exp(j\phi) exp(-\frac{x^2+y^2}{w^2}) exp[-\frac{jk}{2R}(x^2+y^2)],$$

- beam width: $w^2(z) = \frac{2b}{k}(1+\frac{z^2}{b^2}) = w_0^2[1+(\frac{\lambda z}{\pi w_0^2})^2],$
- radius of phase front: $\frac{1}{R(z)} = \frac{z}{z^2+b^2} = \frac{z}{z^2+(\pi w_0^2/\lambda)^2},$
- phase delay: $\tan\phi = \frac{z}{b} = \frac{z}{\pi w_0^2/\lambda},$
- with the minimum beam radius $w_0 = \sqrt{2bk}.$



Quantum mechanics: Free particle expansion

- the Hamiltonian for a free particle, $\hat{H} = \frac{\hat{p}^2}{2m}$, then

$$\hat{U} = \exp(-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t).$$

- the Schrödinger wavefunction,

$$\begin{aligned}\Psi(q,t) = \langle q|\hat{U}|\Psi(0)\rangle &= \int_{-\infty}^{\infty} \mathrm{d}p\langle|p\rangle\Psi(p,0)\exp(-\frac{i}{\hbar}\frac{p^2}{2m}t), \\ &= \frac{1}{(2\pi)^{1/4}(\Delta q + i\hbar t/2m\Delta q)^{1/2}}\exp[-\frac{q^2}{4(\Delta q)^2 + 2i\hbar t/m}],\end{aligned}$$

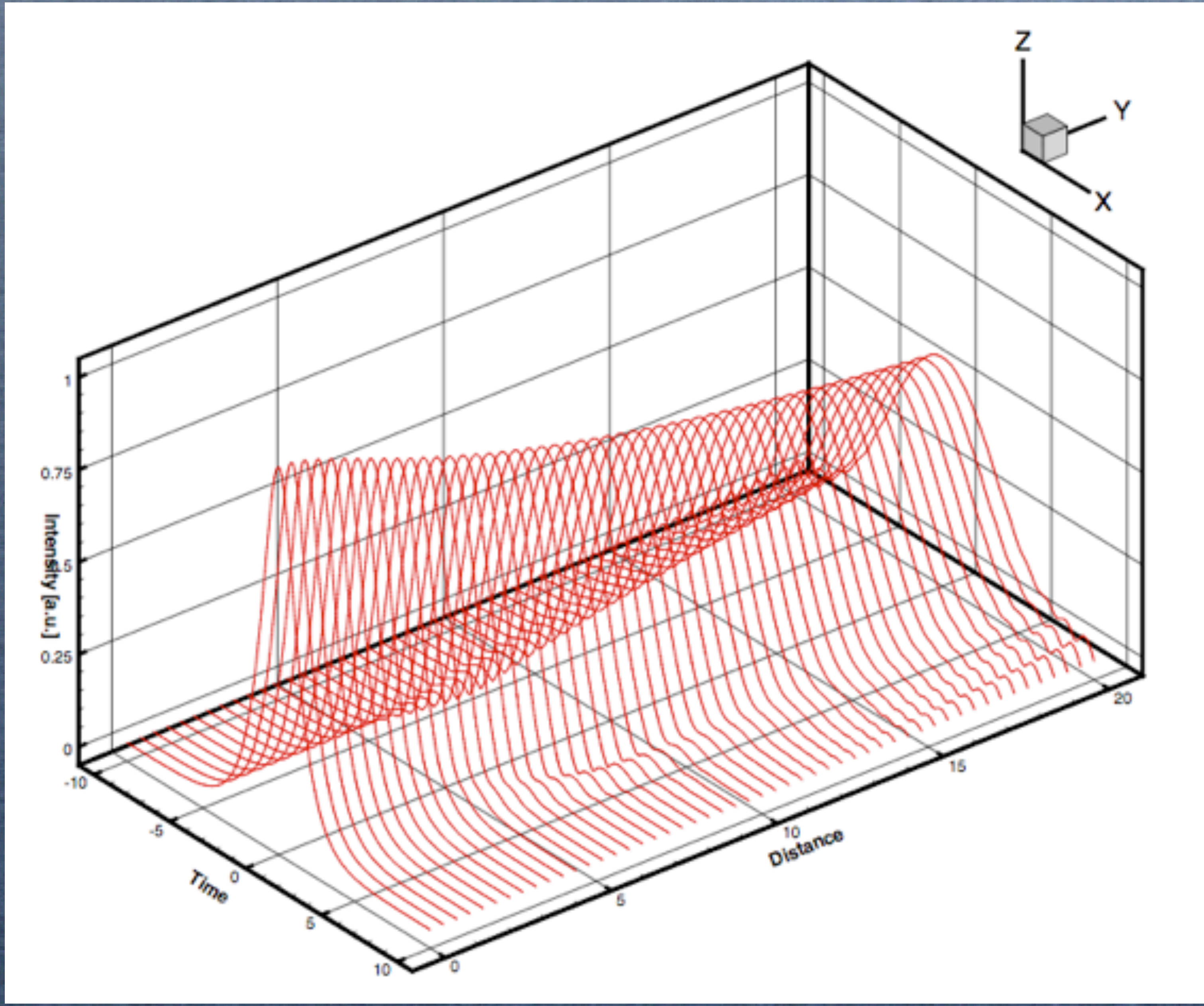
where $\Delta q = \hbar/2\langle\hat{p}^2\rangle^{1/2}$, and $\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(\frac{ipq}{\hbar})$.

- even though the momentum uncertainty $\langle\Delta\hat{p}^2\rangle$ is preserved,
- the position uncertainty increases as time develops,

$$\langle\Delta\hat{q}^2(t)\rangle = (\Delta\hat{q})^2 + \frac{\hbar^2 t^2}{4m^2(\Delta q)^2}$$

PDEs: Example, Wave propagation

$$\frac{\partial}{\partial z}U(z,t) = \frac{i}{2}\frac{\partial^2}{\partial t^2}U(z,t)$$



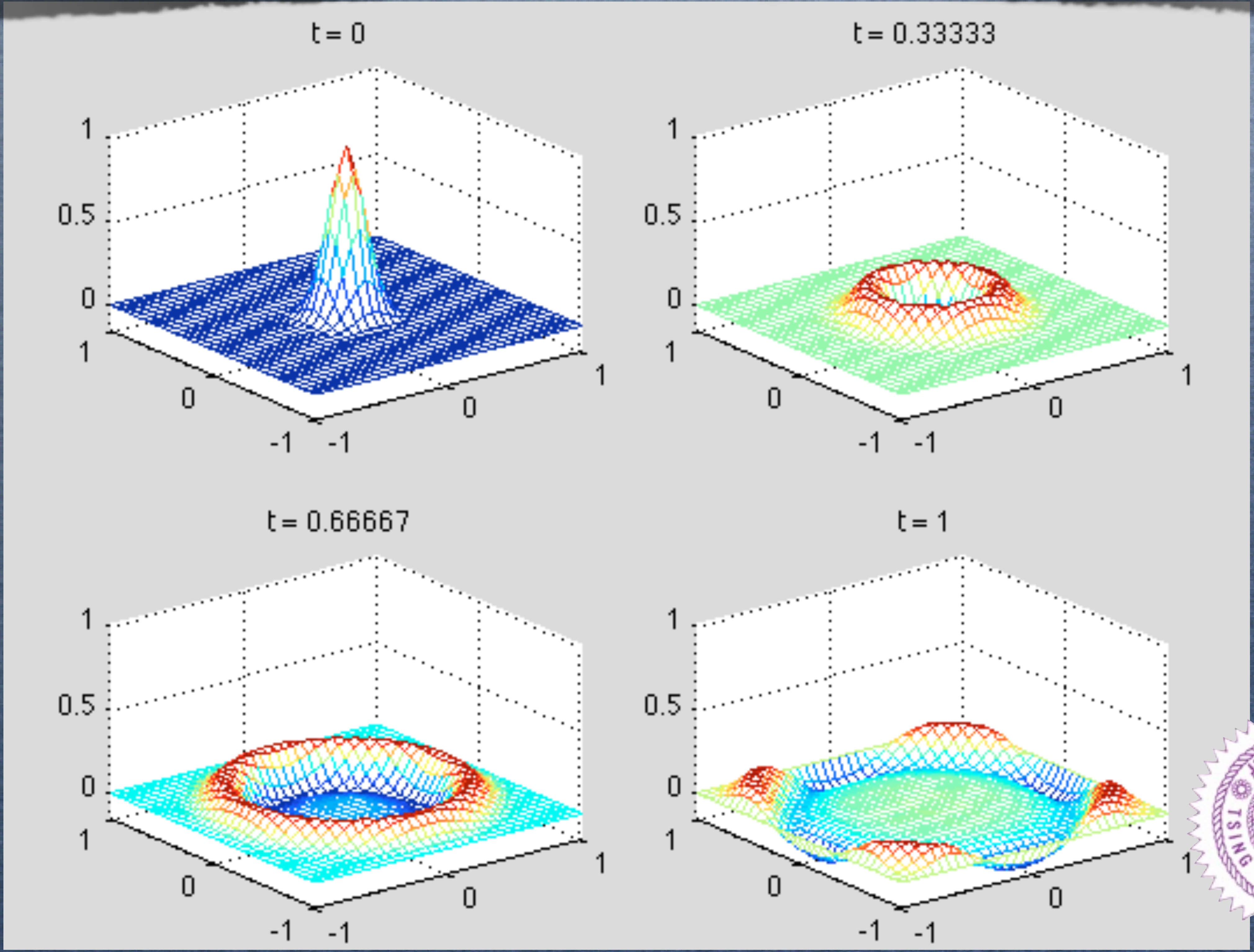
Homework 7: 2D Wave equation

PDE: $u_{tt} = \nabla_{\perp}^2 u = u_{xx} + u_{yy}, \qquad -1 < x, y < 1, \quad \text{and} \quad 0 < t < 1$

IC: $u(x, y, 0) = \text{Exp}\{-40[(x - x_0)^2 + (y - y_0)^2]\},$

$u_t(x, y, 0) = 0.$

Homework 7: 2D Wave equation



Elliptical PDEs

Laplace equation in 2D:

$$\boxed{\nabla_\perp^2 u \equiv u_{xx} + u_{yy} = 0.}$$

Poisson equation in 2D:

$$\boxed{\nabla_\perp^2 u \equiv u_{xx} + u_{yy} = f(x, y).}$$

Power Series: Laplace's Equation, Chap. 12.10

Laplace's equation

$$\boxed{\nabla^2 u \equiv u_{xx} + u_{yy} + u_{zz} = 0.}$$

- Laplacian in Spherical Coordinates, i.e. $x = r\cos\theta\sin\phi$, $y = r\sin\theta\sin\phi$, and $z = r\cos\phi$,

$$\begin{aligned}\nabla^2 u &= \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \phi^2} + \frac{\cot\phi}{r^2}\frac{\partial u}{\partial \phi} + \frac{1}{r^2\sin^2\phi}\frac{\partial^2 u}{\partial \theta^2} \\ &= \frac{1}{r^2}\left[\frac{\partial}{\partial r}(r^2\frac{\partial u}{\partial r}) + \frac{1}{\sin\phi}\frac{\partial}{\partial \phi}(\sin\phi\frac{\partial u}{\partial \phi}) + \frac{1}{\sin^2\phi}(\frac{\partial^2 u}{\partial \theta^2})\right].\end{aligned}$$

- Dirichlet problem with the boundary conditions:

$$u(R,\phi) = f(\phi), \qquad \text{and} \qquad \lim_{r\to\infty} u(r,\phi) = 0.$$

Power Series: Laplace's Equation, Chap. 12.10

- Assume $u(r, \phi) = G(r)H(\phi)$, one has

$$r^2 \frac{\mathrm{d}^2 G}{\mathrm{d}r^2} + 2r\frac{\mathrm{d}G}{\mathrm{d}r} = n(n+1)G, \qquad \text{Euler-Cauchy equation,}$$
$$\frac{1}{\sin\phi}\frac{\mathrm{d}}{\mathrm{d}\phi}(\sin\phi\frac{\mathrm{d}}{\mathrm{d}\phi}H) + n(n+1)H = 0.$$

- By setting $\cos\phi \equiv w$, we have the Legendre's equation

$$(1-w^2)\frac{\mathrm{d}^2 H}{\mathrm{d}w^2} - 2w\frac{\mathrm{d}H}{\mathrm{d}w} + n(n+1)H = 0.$$

Power Series: Legendre's Function

Hint:

$$\boxed{(1-x^2)y'' - 2xy' + n(n+1)y = 0.}$$

- The coefficients $\frac{-2x}{(1-x^2)}$ and $\frac{n(n+1)}{(1-x^2)}$ are analytic at $x=0$, then Legendre's equation has power series solutions of the form

$$y(x) = \sum_{m=0}^{\infty} a_m x^m.$$

- Recursive relation:

Solution:

$$a_{s+2} = -\frac{(n-s)(n+s+1)}{(s+2)(s+1)} a_s, \qquad s = 0, 1, 2, \ldots$$

$$\begin{aligned} y_1(x) &= 1 - \frac{n(n+1)}{2!}x^2 + \frac{(n-2)n(n+1)(n+3)}{4!}x^4 - \ldots \\ y_2(x) &= x - \frac{(n-1)(n+2)}{3!}x^3 + \frac{(n-3)(n-1)(n+2)(n+4)}{5!}x^5 - \ldots \end{aligned}$$

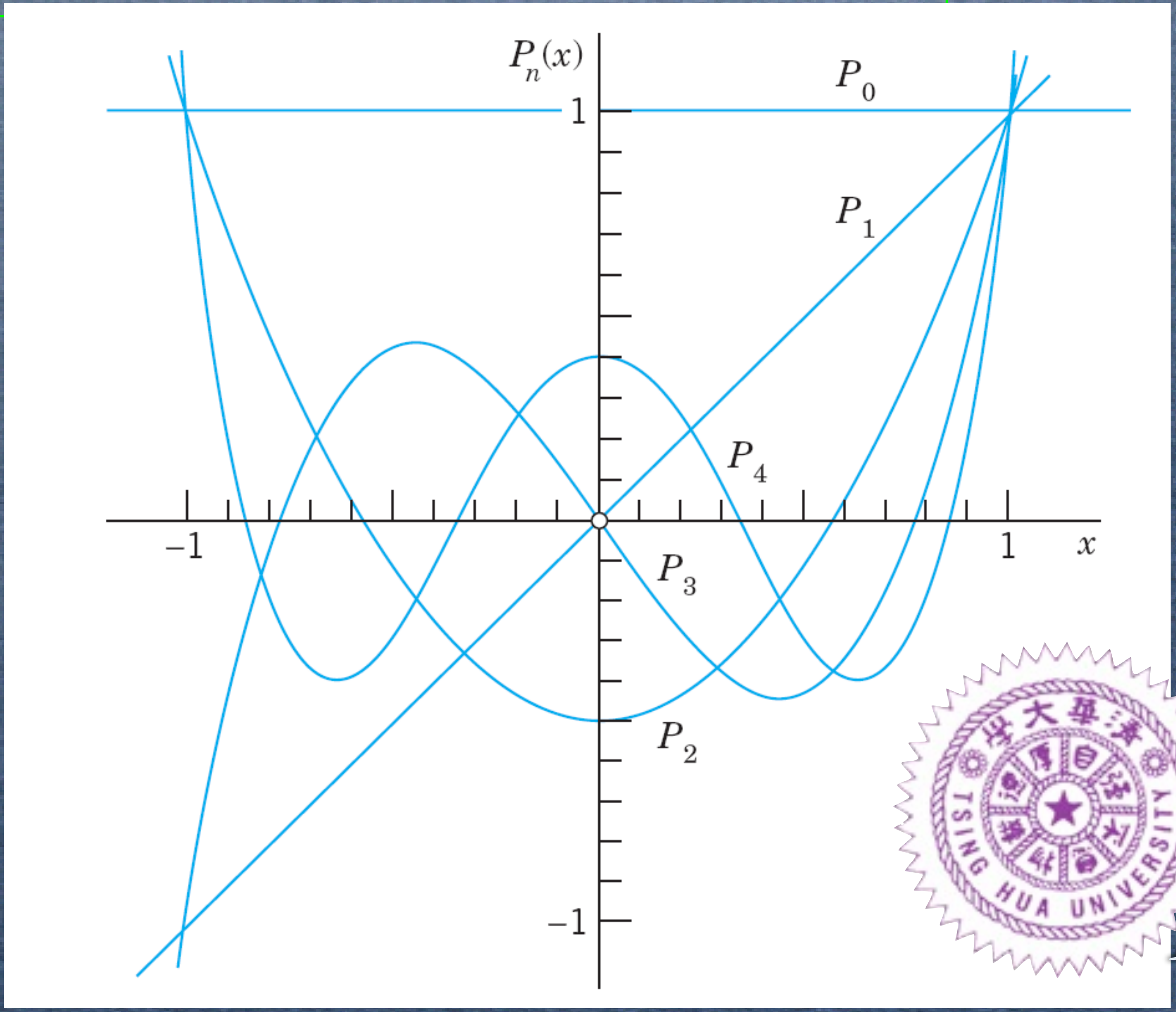
Power Series: Legendre's Polynomials, cont.

Legendre's polynomial of degree n :

$$
\begin{array}{lll}
P_0(x) = 1 & ; & P_1(x) = x \\
P_2(x) = \frac{1}{2}(3x^2 - 1) & ; & P_3(x) = \frac{1}{2}(5x^3 - 3x) \\
P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3) & ; & P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)
\end{array}
$$

to meet the boundary condition

$$P_n(x) = 1.$$



Laplace's Equation, Chap. 12.10

Laplace's equation in *spherical* coordinates:

$$\boxed{\nabla^2 u \equiv u_{xx} + u_{yy} + u_{zz} = 0.}$$

- Laplacian in Spherical Coordinates, i.e. $x = r\cos\theta\sin\phi$, $y = r\sin\theta\sin\phi$, and $z = r\cos\phi$,

$$\begin{aligned}
\nabla^2 u &= \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \phi^2} + \frac{\cot\phi}{r^2}\frac{\partial u}{\partial \phi} + \frac{1}{r^2\sin^2\phi}\frac{\partial^2 u}{\partial \theta^2} \\
&= \frac{1}{r^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right) + \frac{1}{\sin\phi}\frac{\partial}{\partial \phi}\left(\sin\phi\frac{\partial u}{\partial \phi}\right) + \frac{1}{\sin^2\phi}\left(\frac{\partial^2 u}{\partial \theta^2}\right)\right].
\end{aligned}$$

- Fundamental solutions:

$$\boxed{u(r,\phi) = \sum_n A_n r^n P_n(\cos\phi) + \frac{B_n}{r^{n+1}} P_n(\cos\phi).}$$

Elliptical PDEs

Laplace equation in 2D:

$$\boxed{\nabla_\perp^2 u \equiv u_{xx} + u_{yy} = 0.}$$

Poisson equation in 2D:

$$\boxed{\nabla_\perp^2 u \equiv u_{xx} + u_{yy} = f(x, y).}$$

Poisson equation: Finite difference approximation

Poisson equation in 2D:

$$\boxed{\nabla_{\perp}^2 u \equiv u_{xx} + u_{yy} = f(x,y).}$$

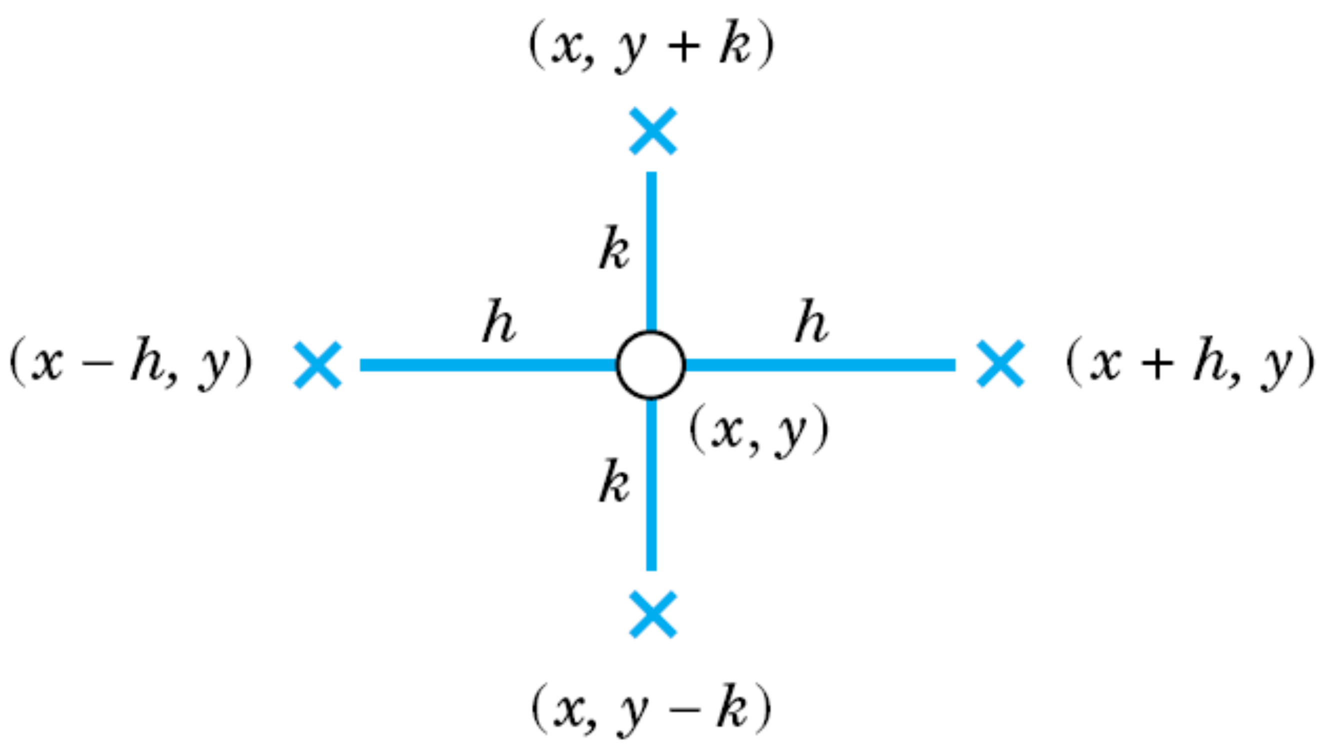
Finite-difference approximation:

$$u(x+h,y) + u(x,y+h) + u(x-h,y) + u(x,y-h) - 4\,u(x,y) = h^2\, f(x,y),$$

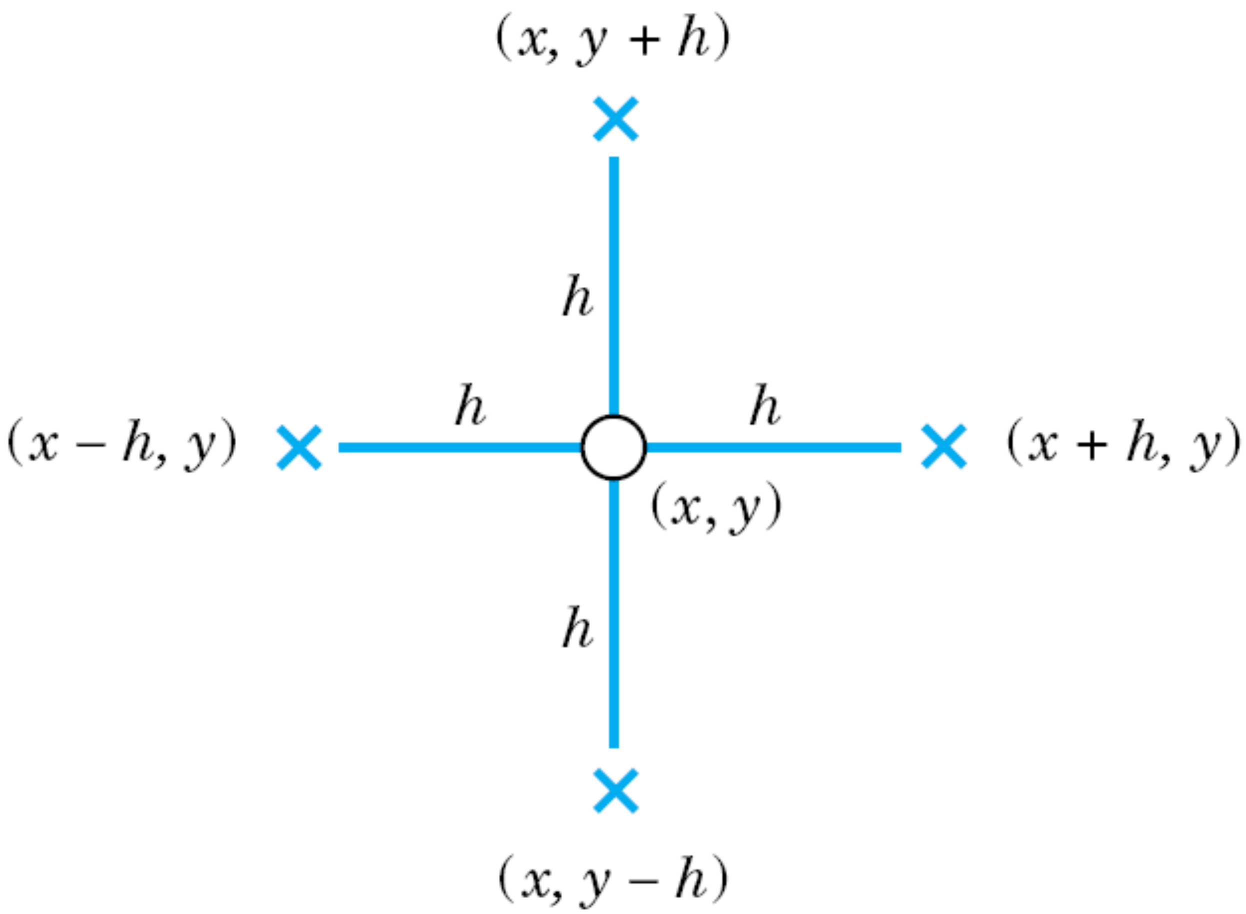
where h is called the mesh size.
Define neighbors as E, N, W, and S, then

$$u(E) + u(N) + u(W) + u(S) - 4\,u(x,y) = h^2\, f(x,y),$$

Poisson equation: Finite difference approximation

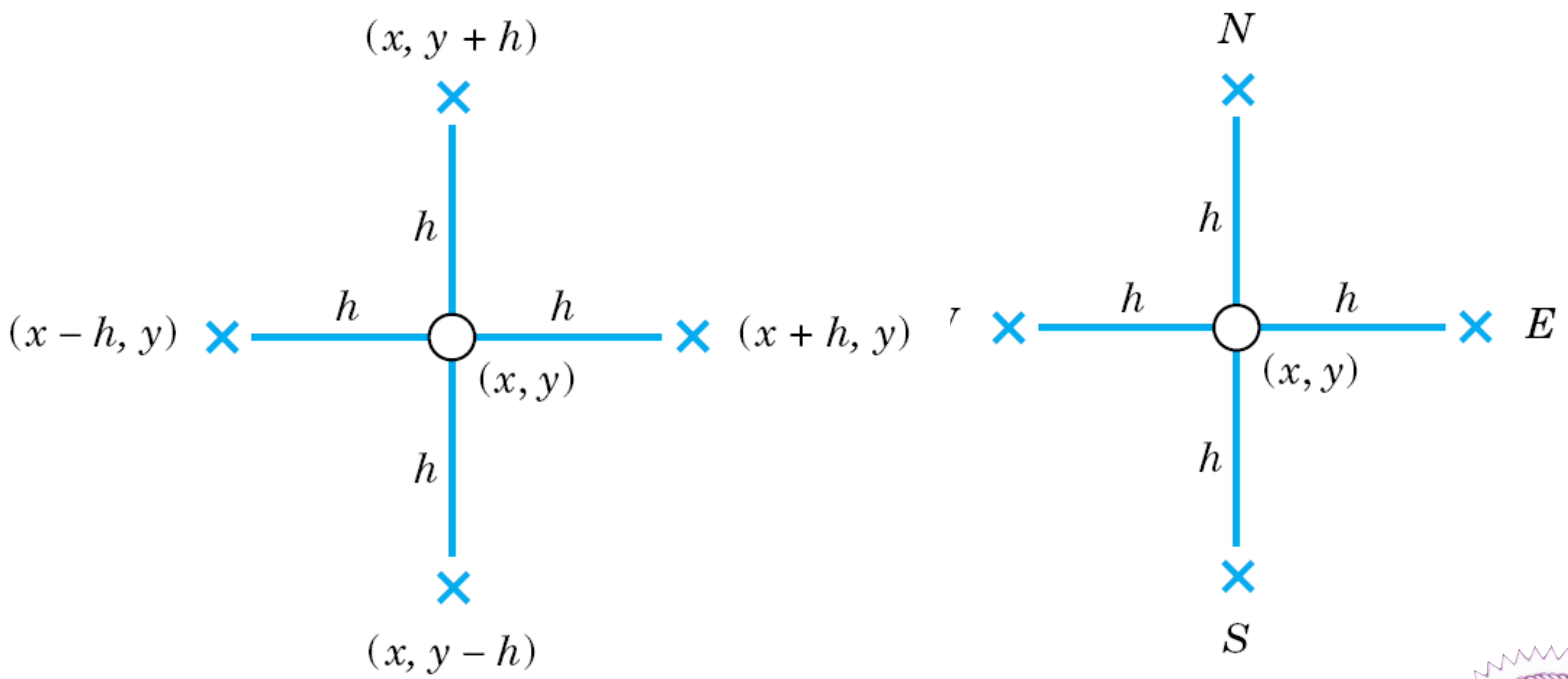


(a) Points in (5) and (6)



(b) Points in (7) and (8)

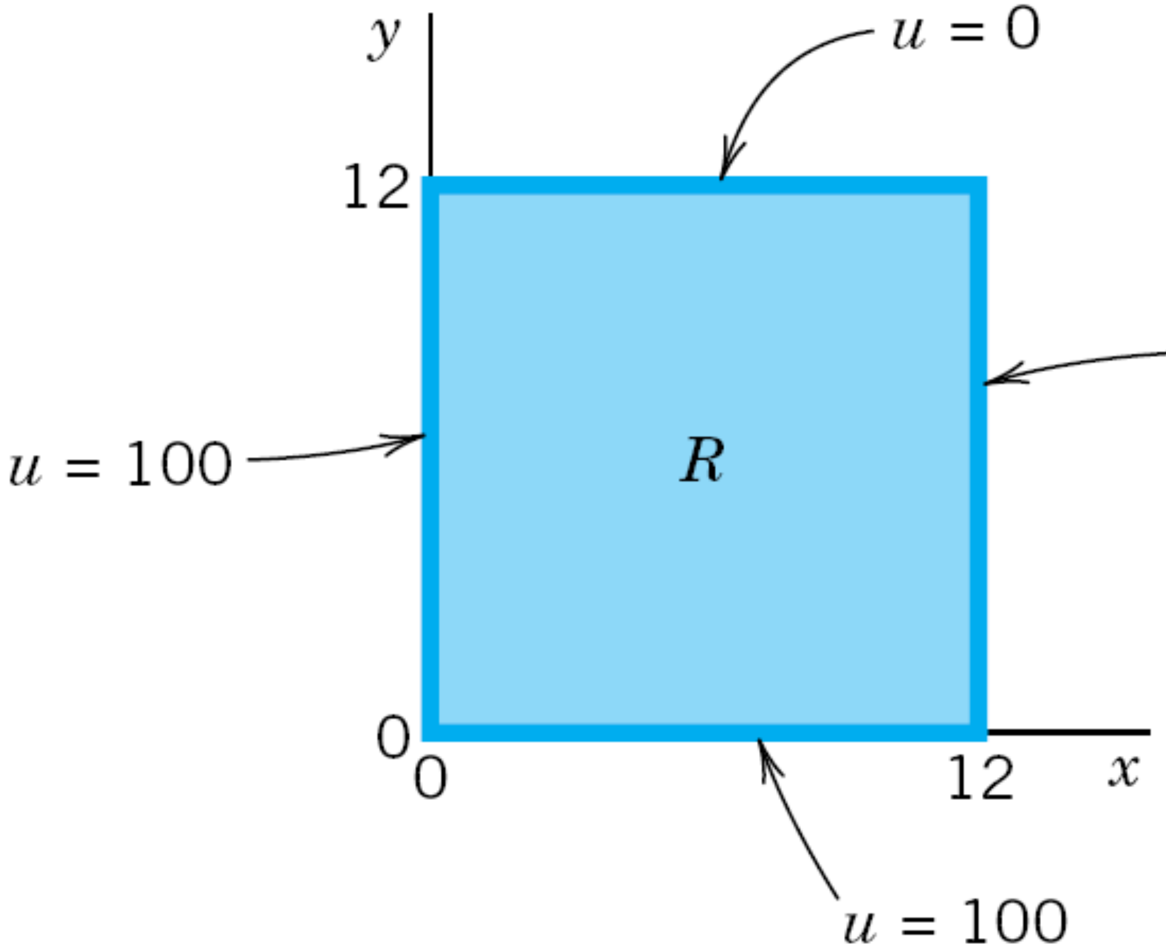
Poisson equation: Finite difference approximation



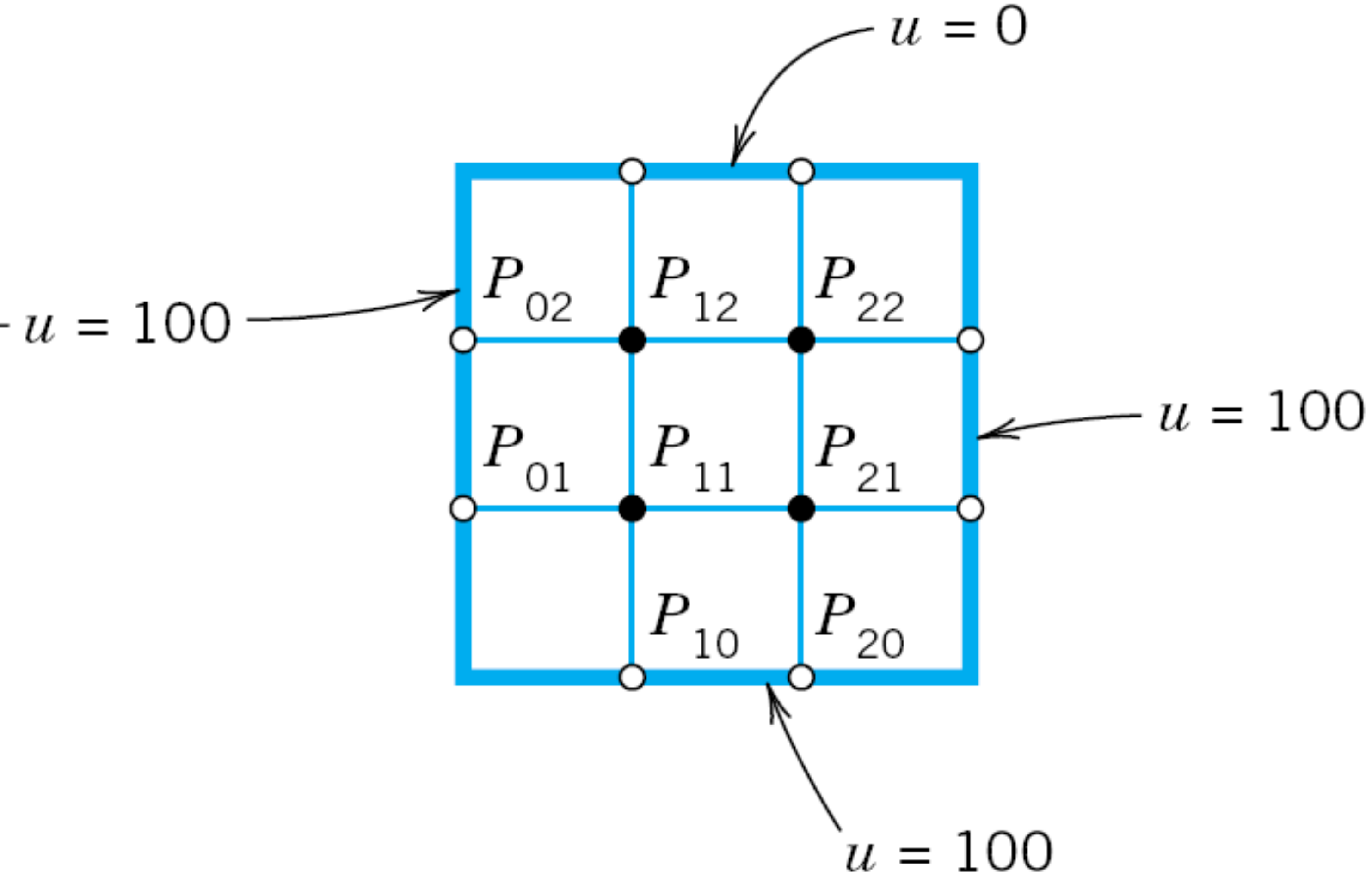
(b) Points in (7) and (8)

(c) Notation in (7*)

Elliptical PDEs



(a) Given problem



(b) Grid and mesh points

Iteration method

Consider

$$\boxed{3x + 1 = 0.}$$

- $2x = -x + 1, \to x_{k+1} = -\frac{1}{2}x_k - \frac{1}{2},$

$$\begin{aligned} x_k &= \frac{-1/2[1-(-1/2)^k]}{1-(-1/2)} + (-1/2)^k x_0, \\ &= \frac{-1}{3}, \quad \text{as} \quad k \to \infty \end{aligned}$$

- $x = -2x + 1, \to x_{k+1} = -2x_k - 1,$

$$\begin{aligned} x_k &= \frac{-[1-(-2)^k]}{1-(-2)} + (-2)^k x_0, \\ &= \infty, \quad \text{as} \quad k \to \infty \end{aligned}$$

Jacobi Iteration method

$$\mathbf{A}\cdot\mathbf{x}=\mathbf{b},\quad \begin{bmatrix} 3 & 2 \\ 1 & 2 \end{bmatrix}\cdot\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}=\begin{bmatrix} 1 \\ -1 \end{bmatrix},$$

Jacobi's method for iteration

$$\begin{bmatrix} x_{1,k+1} \\ x_{2,k+1} \end{bmatrix}=\begin{bmatrix} 0 & -2/3 \\ -1/2 & 0 \end{bmatrix}\cdot\begin{bmatrix} x_{1,k} \\ x_{2,k} \end{bmatrix}+\begin{bmatrix} 1/3 \\ -1/2 \end{bmatrix},$$

$$\mathbf{x}_{k+1}=\tilde{\mathbf{A}}\cdot\mathbf{x}_k+\tilde{\mathbf{b}},$$

Jacobi Iteration method, with Matlab

```
A = [3 2; 1 2]; b = [1 -1]';
x0 = [0 0]';

jacobi(A, b, x0, 20)

X =
    [0.3333 -0.5000]' %01 [0.6667 -0.6667]' %02
    [0.7778 -0.8333]' %03 [0.8889 -0.8889]' %04
    [0.9259 -0.9444]' %05 [0.9630 -0.9630]' %06
    [0.9753 -0.9815]' %07 [0.9877 -0.9877]' %08
    [0.9918 -0.9938]' %09 [0.9959 -0.9959]' %10
    [0.9973 -0.9979]' %11 [0.9986 -0.9986]' %12
    [0.9991 -0.9993]' %13 [0.9995 -0.9995]' %14
    [0.9997 -0.9998]' %15 [0.9998 -0.9998]' %16
    [0.9999 -0.9999]' %17 [0.9999 -0.9999]' %18
    [1.0000 -1.0000]' %19 [1.0000 -1.0000]' %20
```

Jacobi Iteration method

$$\mathbf{A} \cdot \mathbf{x} = \mathbf{b},$$

Jacobi's method for iteration

$$\mathbf{x}_{k+1} = \tilde{\mathbf{A}} \cdot \mathbf{x}_k + \tilde{\mathbf{b}},$$

where

$$\tilde{\mathbf{A}} = \begin{bmatrix} 0 & -a_{12}/a_{11} & \cdots & -a_{1N}a_{11} \\ -a_{21}/a_{22} & 0 & \cdots & -a_{2N}/a_{22} \\ & \cdots & & \\ -a_{N1}/a_{NN} & -a_{N2}/a_{NN} & \cdots & 0 \end{bmatrix}, \quad \tilde{\mathbf{b}} = \begin{bmatrix} b_1/a_{11} \\ b_2/a_{22} \\ \vdots \\ b_N/a_{NN} \end{bmatrix}.$$

$$x_m^{(k+1)} = -\sum_{n \neq m}^{N} \frac{a_{mn}}{a_{mm}} x_n^{(k)} + \frac{b_m}{a_{mm}}, \quad \text{for} \quad m = 1, 2, \ldots$$

Gauss-Seidel Iteration method

$$
\begin{aligned}
x_1 - 0.25x_2 - 0.25x_3 \qquad\qquad &= 50 \\
-0.25x_1 + x_2 \qquad\qquad - 0.25x_4 &= 50 \\
-0.25x_1 \qquad + x_3 - 0.25x_4 &= 25 \\
- 0.25x_2 - 0.25x_3 + x_4 &= 25.
\end{aligned}
$$

$$
\begin{aligned}
x_1 &= \qquad 0.25x_2 + 0.25x_3 \qquad + 50 \\
x_2 &= 0.25x_1 \qquad\qquad + 0.25x_4 + 50 \\
x_3 &= 0.25x_1 \qquad\qquad + 0.25x_4 + 25 \\
x_4 &= \qquad 0.25x_2 + 0.25x_3 \qquad + 25.
\end{aligned}
$$

Gauss-Seidel Iteration method

Use “old” values
(“New” values here not yet available)

$$
\begin{aligned}
x_1^{(1)} &= \phantom{0.25x_1^{(1)} + {}} 0.25x_2^{(0)} + 0.25x_3^{(0)} + 50.00 = 100.00 \\
x_2^{(1)} &= 0.25x_1^{(1)} \phantom{{}+ 0.25x_2^{(0)}} + 0.25x_4^{(0)} + 50.00 = 100.00 \\
x_3^{(1)} &= 0.25x_1^{(1)} \phantom{{}+ 0.25x_2^{(0)}} + 0.25x_4^{(0)} + 25.00 = 75.00 \\
x_4^{(1)} &= \phantom{0.25x_1^{(1)} + {}} 0.25x_2^{(1)} + 0.25x_3^{(1)} + 25.00 = 68.75
\end{aligned}
$$

Use “new” values

Gauss-Seidel Iteration method

$$
\begin{aligned}
x_1^{(2)} &= \phantom{0.25x_1^{(2)} +{}} 0.25x_2^{(1)} + 0.25x_3^{(1)} \phantom{+ 0.25x_4^{(1)}} + 50.00 = 93.750 \\
x_2^{(2)} &= 0.25x_1^{(2)} \phantom{+ 0.25x_2^{(1)} + 0.25x_3^{(1)}} + 0.25x_4^{(1)} + 50.00 = 90.625 \\
x_3^{(2)} &= 0.25x_1^{(2)} \phantom{+ 0.25x_2^{(1)} + 0.25x_3^{(1)}} + 0.25x_4^{(1)} + 25.00 = 65.625 \\
x_4^{(2)} &= \phantom{0.25x_1^{(2)} +{}} 0.25x_2^{(2)} + 0.25x_3^{(2)} \phantom{+ 0.25x_4^{(1)}} + 25.00 = 64.062
\end{aligned}
$$

$$
\mathbf{x}^{(m+1)} = \mathbf{b} - \underbrace{\mathbf{L}\mathbf{x}^{(m+1)}}_{\text{“New”}} - \underbrace{\mathbf{U}\mathbf{x}^{(m)}}_{\text{“Old”}} \qquad (a_{jj} = 1)
$$

Gauss-Seidel Iteration method

Gauss-seidel iteration:

$$
\begin{aligned}
x_{1,k+1} &= -\frac{2}{3}x_{2,k} + \frac{1}{3}, \\
x_{2,k+1} &= -\frac{1}{2}x_{1,k+1} - \frac{1}{2}.
\end{aligned}
$$

for $m = 1, 2, \ldots, N$,

$$
\begin{aligned}
x_m^{(k+1)} &= -\sum_{n=1}^{m-1} \frac{a_{mn}}{a_{mm}} x_n^{(k+1)} - \sum_{n=m+1}^{N} \frac{a_{mn}}{a_{mm}} x_n^{(k)} + \frac{b_m}{a_{mm}}, \\
&= \frac{b_m - \sum_{n=1}^{m-1} a_{mn} x_n^{(k+1)} - \sum_{n=m+1}^{N} a_{mn} x_n^{(k)}}{a_{mm}}
\end{aligned}
$$

converge more fast!

Gauss-Seidel Iteration method, with Matlab

```
A = [3 2; 1 2]; b = [1 -1]';
x0 = [0 0]';

gauseid(A, b, x0, 10)

X =
    [0.3333 -0.6667]' %01 [0.7778 -0.8889]' %02
    [0.9259 -0.9630]' %03 [0.9753 -0.9877]' %04
    [0.9918 -0.9986]' %05 [0.9973 -0.9986]' %06
    [0.9991 -0.9995]' %07 [0.9997 -0.9998]' %08
    [0.9999 -0.9999]' %09 [1.0000 -1.0000]' %10
```

convergence condition:

$$|a_{mm}| > \sum_{n \neq m}^{N} |a_{mn}|, \quad \text{for} \quad m = 1, 2, \ldots, N$$

Gauss-Seidel Iteration method, Nonlinear eq.

nonlinear equations:

$$\begin{aligned} x_1^2 + 10x_1 + 2x_2^2 - 13 &= 0, \\ 2x_1^3 - x_2^2 + 5x_2 - 6 &= 0, \end{aligned}$$

with the Gauss-Seidel scheme,

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} (13 - x_1^2 - 2x_2^2)/10 \\ (6 - 2x_1^3 + x_2^2)/5 \end{bmatrix}.$$

with the conditions

$$|\mathbf{x}_{k+1} - \mathbf{x}_k| < \epsilon, \quad \text{or} \quad \frac{|\mathbf{x}_{k+1} - \mathbf{x}_k|}{|\mathbf{x}_k + \text{eps}|} < \epsilon$$

SOR Iteration method

Relaxation technique:

$$x_m^{(k+1)} = (1-\omega)x_m^{(k)} + \omega \frac{b_m - \sum_{n=1}^{m-1} a_{mn} x_n^{(k+1)} - \sum_{n=m+1}^{N} a_{mn} x_n^{(k)}}{a_{mm}}$$

with $0 < \omega < 2$

- $1 < \omega < 2$: SOR, Successive Over-Relaxation,
- $0 < \omega < 1$: successive under-relaxation.

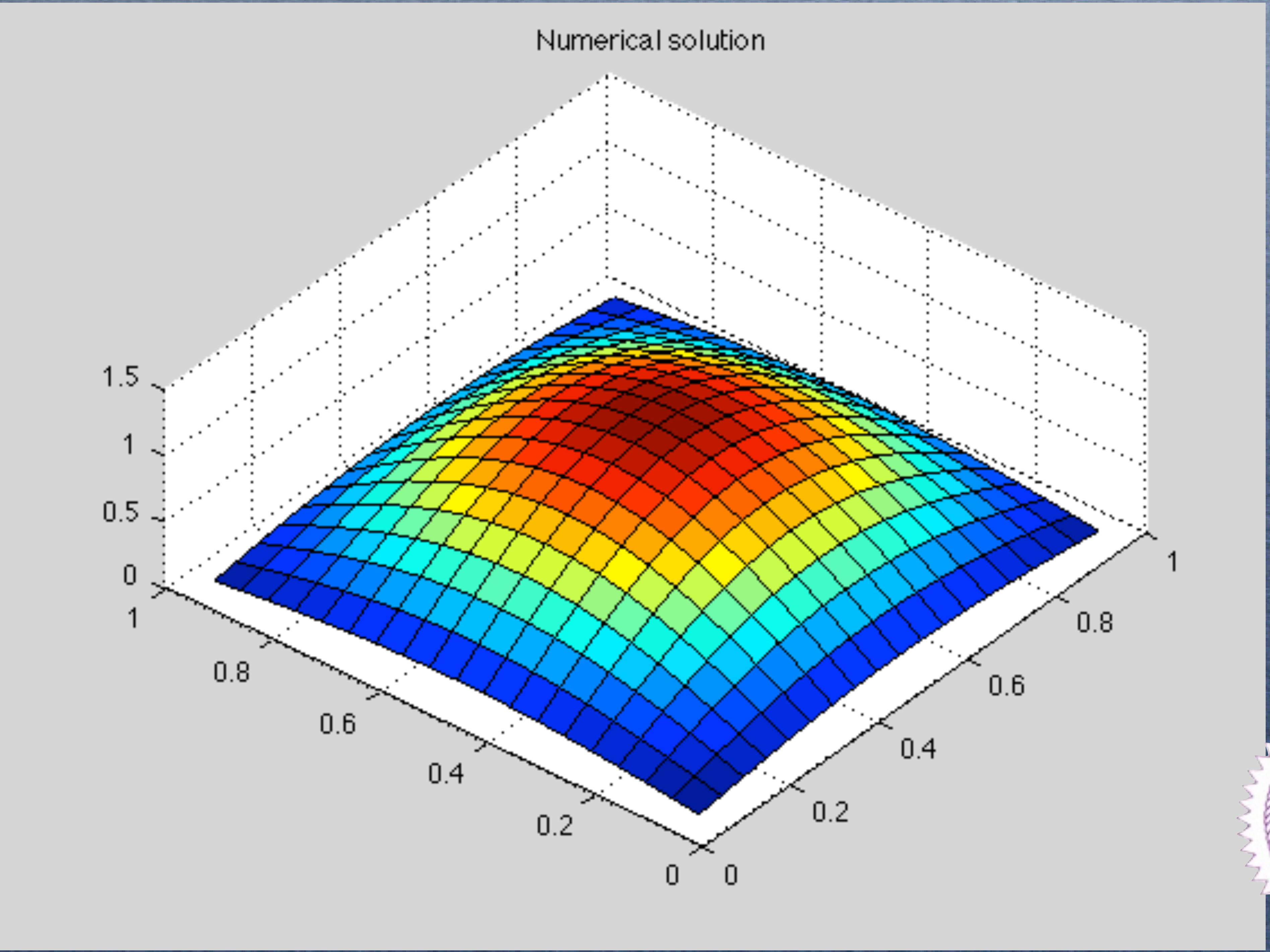
Homework 8: 2D Poisson equation

Poisson equation in 2D:

$$\boxed{\nabla_{\perp}^2 u \equiv u_{xx} + u_{yy} = -2\pi^2 \sin(\pi x)\, \sin(\pi y),}$$

with the Dirichlet boundary condition, i.e.,
u(0,y) = u(1,y)=u(x,0)=u(x,1) = 0, for x:[0,1], y:[0,1].

Homework 8: 2D Poisson equation

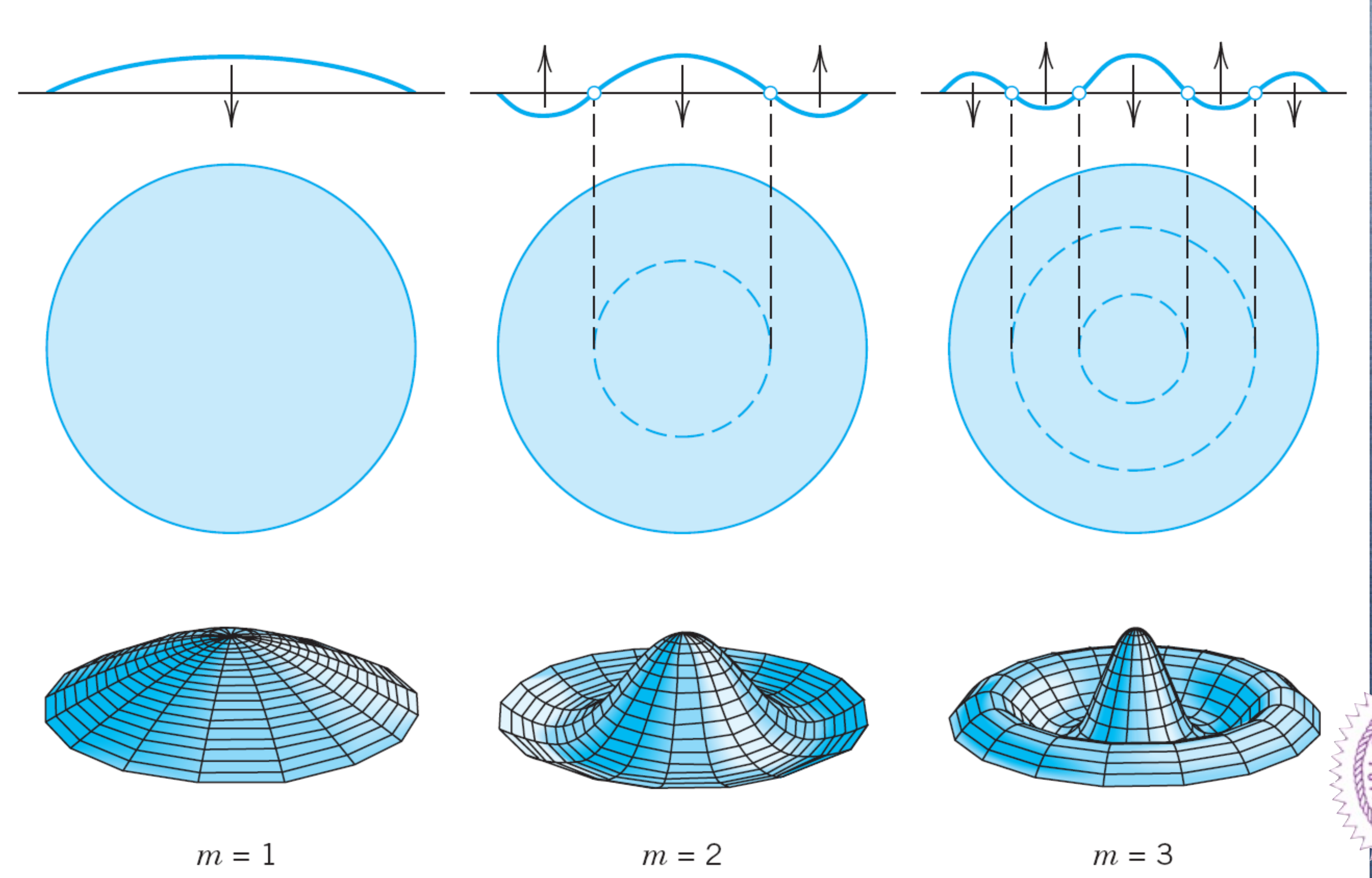


Elliptical PDEs, ADI method

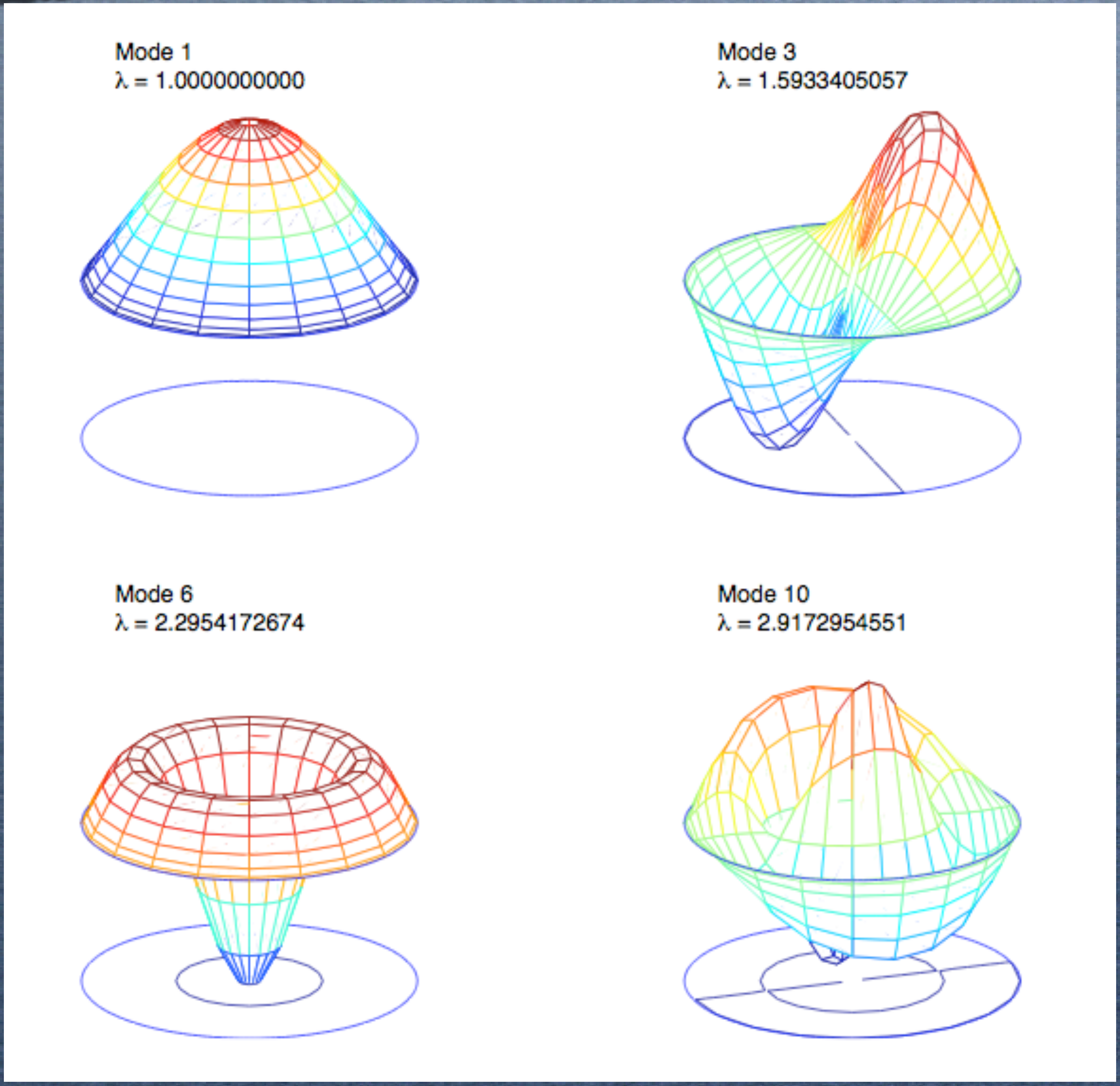
$$
\begin{aligned}
&(j=1) \qquad u_{10} - 4u_{11}^{(2)} + u_{12}^{(2)} &&= -u_{01} - u_{21}^{(1)} \\
&(j=2) \qquad u_{11}^{(2)} - 4u_{12}^{(2)} + u_{13} &&= -u_{02} - u_{22}^{(1)}.
\end{aligned}
$$

$$
\begin{aligned}
&(j=1) \qquad u_{20} - 4u_{21}^{(2)} + u_{22}^{(2)} &&= -u_{11}^{(1)} - u_{31} \\
&(j=2) \qquad u_{21}^{(2)} - 4u_{22}^{(2)} + u_{23} &&= -u_{12}^{(1)} - u_{32}.
\end{aligned}
$$

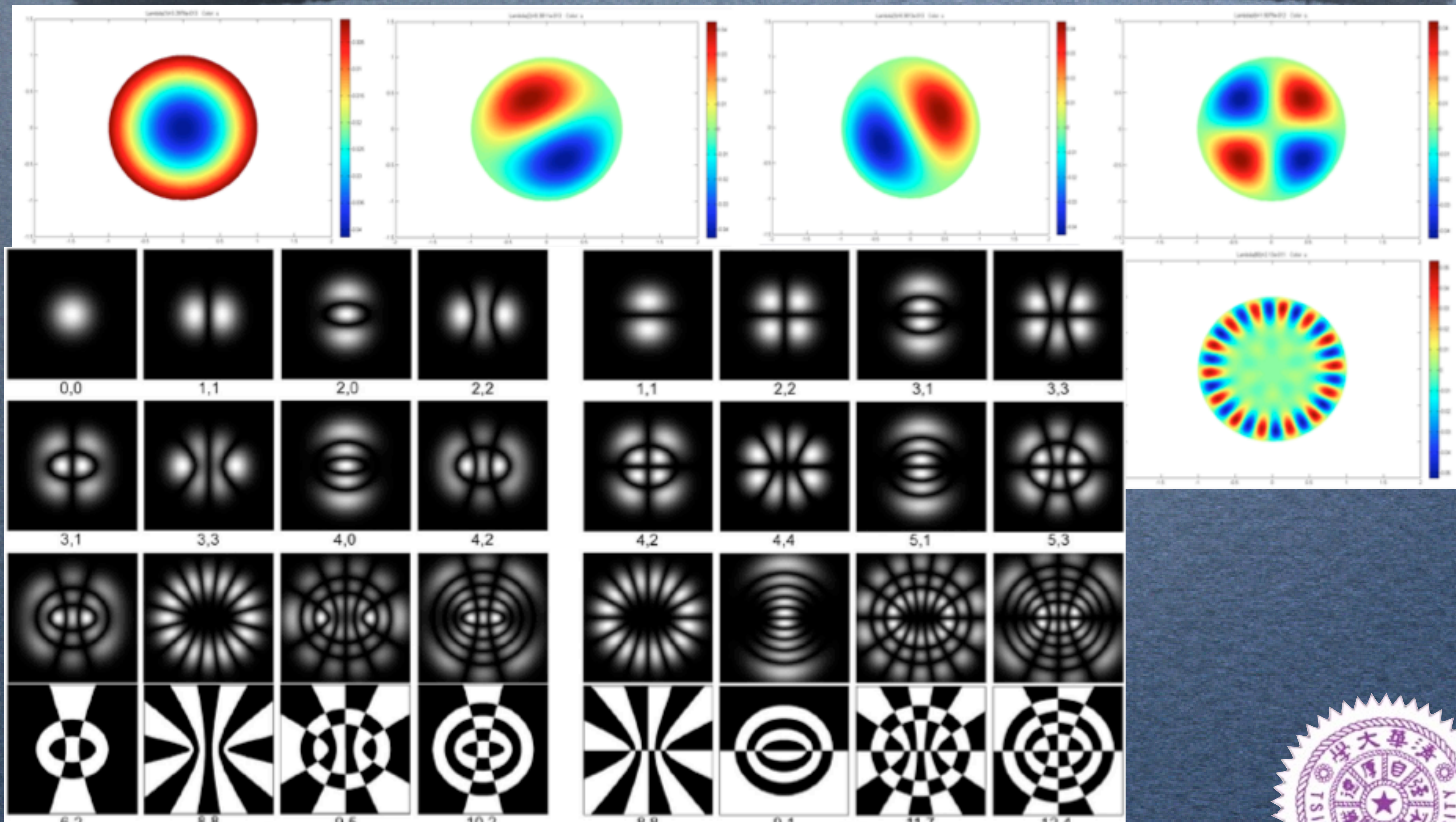
Laplace's Equation, Chap. 12.9



Laplace's equation in a Disk

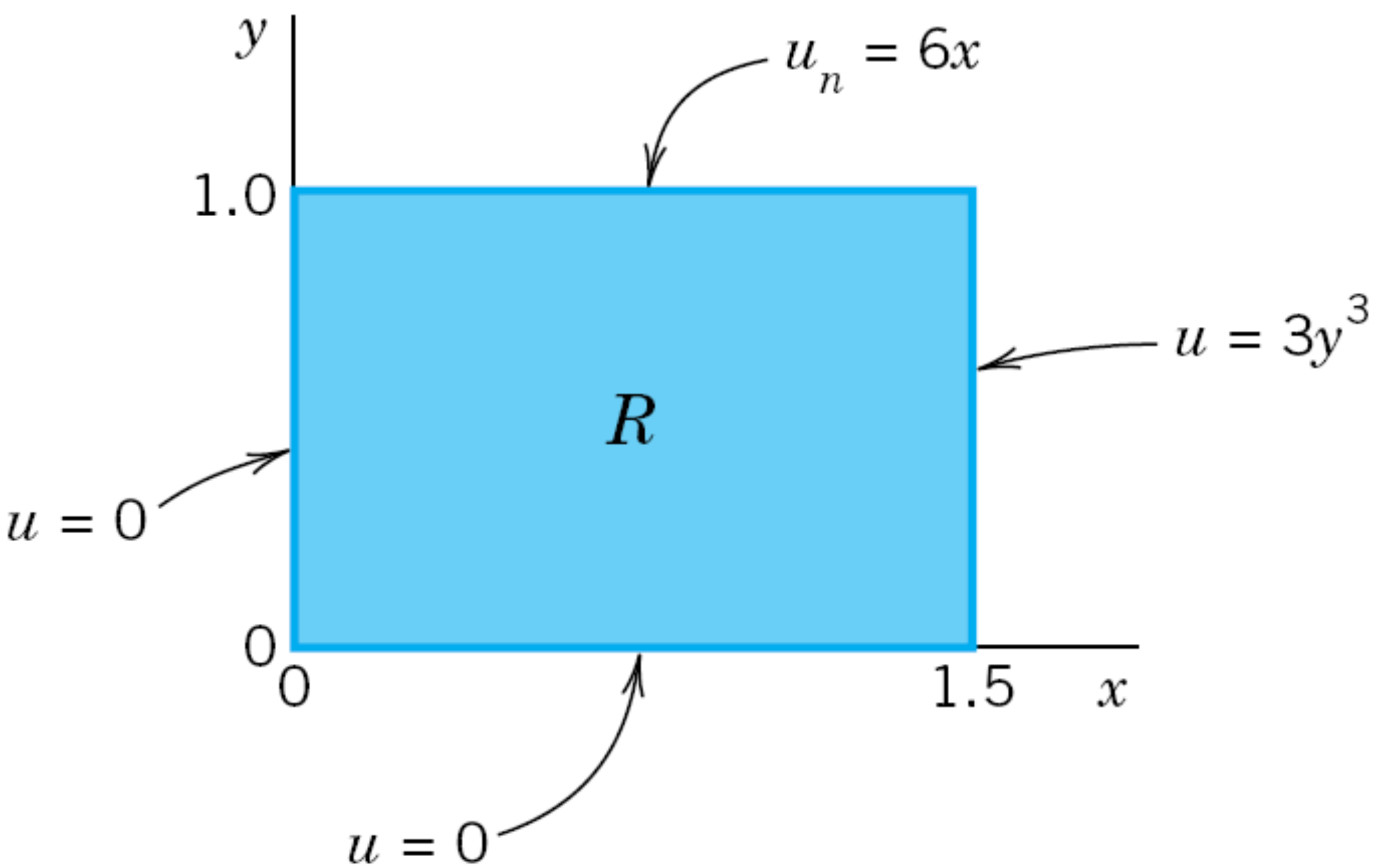


Cavity modes

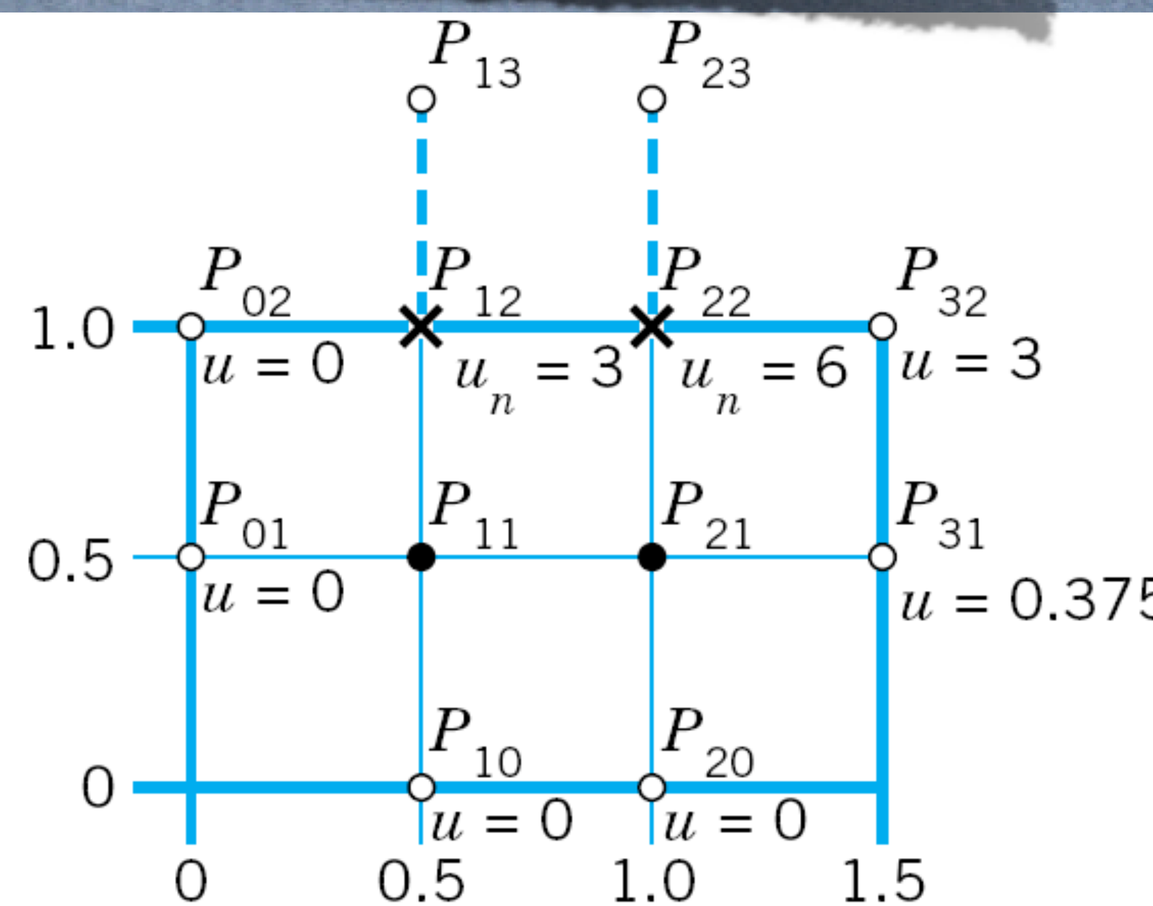


M. A. Bandres, J. Opt. Soc. Am. A, 21, 873880, (2004).

Elliptical PDEs, Mixed BCs



(a) Region R and boundary values



(b) Grid ($h = 0.5$)

Elliptical PDEs, Irregular BCs