9. Approximation Theory (Spectral Methods)

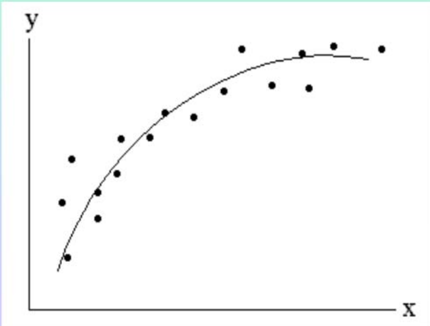
§ Curve fitting

GIVEN: $(x_i, y_i), \quad i = 1, 2, \cdots, N$

Find: a function which best approxomates

the unknown function $y = f(x)$

(not necessary passing the data points)



Approximation Theory :

STEP1: choose a proper funtion from $y = f(x; a, b, c, \cdots)$

with some adjustable parameters $a, b, c, \cdots$

STEP2: optimize the fitting in some way, i.e., minimize the error term

$$E \equiv \sum_{i=1}^{N} \left(y_i - f(x_i; a, b, c, \cdots) \right)^2 = E(a, b, c, \cdots)$$

i.e. looking for a set of $\{a, b, c, \cdots\}$ such that

$$\frac{\partial E}{\partial a} = 0$$

$$\frac{\partial E}{\partial b} = 0$$

$$\frac{\partial E}{\partial c} = 0$$

Example: Given (x_i, y_i) and find a linear curve fitting.

Assume $y = ax + b$.

Define the derivation as

$$E \equiv \sum_{i=1}^{N} (y_i - ax_i - b)^2 = E(a,b)$$

To minimize the error $E(a,b)$, we look for (a,b) such that

$$\frac{\partial E}{\partial a} = 0 = \sum_{i=1}^{N} 2(y_i - ax_i - b)(-x_i)$$

$$\frac{\partial E}{\partial b} = 0 = \sum_{i=1}^{N} 2(y_i - ax_i - b)(-1)$$

$$0 = -\sum_{i=1}^{N} x_i y_i + a\sum_{i=1}^{N} x_i^2 + b\sum_{i=1}^{N} x_i$$

$$0 = -\sum_{i=1}^{N} y_i + a\sum_{i=1}^{N} x_i + b\sum_{i=1}^{N} 1$$

$$a = \frac{N\left(\sum_{i=1}^{N} x_i y_i\right) - \left(\sum_{i=1}^{N} x_i\right)\left(\sum_{i=1}^{N} y_i\right)}{N\left(\sum_{i=1}^{N} x_i^2\right) - \left(\sum_{i=1}^{N} x_i\right)^2}$$

$$b = \frac{\left(\sum_{i=1}^{N} x_i^2\right)\left(\sum_{i=1}^{N} y_i\right) - \left(\sum_{i=1}^{N} x_i y_i\right)\left(\sum_{i=1}^{N} x_i\right)}{N\left(\sum_{i=1}^{N} x_i^2\right) - \left(\sum_{i=1}^{N} x_i\right)^2}$$

§ Approximation Theory

GIVEN: some function $f(x)$ and some domain $[a,b]$

STEP1: select a proper set of linearly independent funtions $\{\phi_i(x)\}$

STEP2: approximate the funtion from $y = f(x)$ of the form

$$f(x) \approx S(x) = \sum_{i=0}^{n} c_i \phi_i(x)$$

which is expected to be convergent to the exact function $f(x)$ as $n \to \infty$

STEP3: adjust the values of parameters $\{c_i\}$ so that the resulting approximation $S(x)$ is the best.

Definition (linearly Independence)

The set of funtions $\{\phi_0(x), \phi_1(x), \phi_2(x), \cdots, \phi_n(x)\}$ is said to be linearly independent on $[a,b]$ if whenever

$c_0\phi_0(x) + c_1\phi_1(x) + \cdots + c_n\phi_n(x) = 0$ for $c_i's \in R$ and all $x \in [a,b]$,

then $c_0 = c_1 = \cdots = c_n = 0$.

Definition (**Orthogonal**)

$\{\phi_0, \phi_1, \phi_2, \cdots, \phi_n\}$ is said to be an orthogonal set of functions on the interval $[a,b]$ with respect to the weight function $\omega(x)$ if

$$\int_a^b \omega(x)\,\phi_i(x)\,\phi_j(x)\,dx = \begin{Bmatrix} 0 & \text{if } i \neq j \\ \alpha_i \neq 0 & \text{if } i = j \end{Bmatrix} = \alpha_i \delta_{ij}$$

where $\omega(x) \geq 0$ for all $x \in [a,b]$
but $\omega(x) \neq 0$ on any subinterval of $[a,b]$.

Definition (Ortho-Normal):: orthogonal with α_i=1

$$f(x) \approx S(x) = \sum_{i=0}^{n} c_i\,\phi_i(x)$$

- Best approximation:
  define the ω-weighted error term as follows

$$E \equiv \int_a^b \omega(x)\big(f(x) - S(x)\big)^2\,dx$$
$$= \int_a^b \omega(x)\left(f(x) - \sum_{i=0}^{n} c_i\,\phi_i(x)\right)^2 dx$$

The best approximation has a set of $\{c_i\}$ which minimizes the error E.

$$\frac{\partial E}{\partial c_j} = 0 \text{ for all } j = 0,1,2,\cdots,n$$

~ (n+1) equations solve (n+1) unknowns $\{c_i\}$ ~

Solution:

$$0=\frac{\partial E}{\partial c_j}=\frac{\partial}{\partial c_j}\int_a^b \omega(x)\left(f(x)-\sum_{i=0}^{n} c_i\,\phi_i(x)\right)^2 dx$$

$$=\int_a^b \omega(x)2\left(f(x)-\sum_{i=0}^{n} c_i\,\phi_i(x)\right)\left(-\phi_j(x)\right)dx$$

$$=-2\left\{\int_a^b \omega(x)f(x)\phi_j(x)dx-\sum_{i=0}^{n} c_i\int_a^b \omega(x)\phi_i(x)\phi_j(x)dx\right\}$$

$$\sum_{i=0}^{n} c_i\int_a^b \omega(x)\phi_i(x)\phi_j(x)dx=\int_a^b \omega(x)f(x)\phi_j(x)dx$$

~ (n+1) equations (j=0,1,2,…,n) for (n+1) unknowns ~

(solutions exists as long as $\{\phi_i\}$ is L.I.)

With orthogonality (not necessary), we have

$$\int_a^b \omega(x)\phi_i(x)\phi_j(x)dx=\left\{\begin{matrix} 0 & \text{if } i\neq j \\ \alpha_i\neq 0 & \text{if } i=j\end{matrix}\right\}=\alpha_i\delta_{ij}$$

$$\sum_{i=0}^{n} c_i\alpha_i\delta_{ij}=\int_a^b \omega(x)f(x)\phi_j(x)dx$$

$$\alpha_j c_j=\int_a^b \omega(x)f(x)\phi_j(x)dx$$

$$c_j=\int_a^b \omega(x)f(x)\phi_j(x)dx\Big/\alpha_j$$

$$=\int_a^b \omega(x)f(x)\phi_j(x)dx\Big/\int_a^b \omega(x)\phi_j(x)\phi_j(x)dx$$

§ Commonly used functions $\{\phi_i\}$

(i) Fourier series (orthogonal)

choose $[a,b]=[-\pi,\pi]$ and $w(x)=1$ and

$\phi_0(x)=1$

$\phi_k(x)=\cos(kx)$ for $k=1,2,\cdots,n$

$\phi_{k+n}(x)=\sin(kx)$ for $k=1,2,\cdots,n$

$$\int_{-\pi}^{\pi}\sin^2(kx)dx=\int_{-\pi}^{\pi}\cos^2(kx)dx=\pi$$

$\phi_k(x)=\exp(\sqrt{-1}\,kx)$, for $k=0,1,2,\cdots,n$

(ii) Chebychev polynomials (orthogonal)

choose $[a,b]=[-1,1]$ and $w(x)=1/\sqrt{1-x^2}$ and

$\phi_k(x)=T_k(x)=\cos\left(k\cos^{-1}x\right)$ for $k=0,1,2,\cdots,n$

$$\int_{-1}^{1}T_k^2(x)/\sqrt{1-x^2}\,dx=\begin{cases}\pi/2 & \text{for } k\ge 1\\ \pi & \text{for } k=0\end{cases}$$

(iii) Legendre polynomials (orthogonal)

choose $[a,b]=[-1,1]$ and $w(x)=1$ and

$\phi_k(x)=L_k(x)$ for $k=0,1,2,\cdots,n$

$$\int_{-1}^{1}L_k^2(x)\,dx=\frac{2}{2k+1}$$

§ Application to ODEs ~ Rayleigh-Ritz method

Consider a linear 2nd-order ODE : $y = y(x)$

$$-\frac{d}{dx}\left(p(x)\frac{dy}{dx}\right)+q(x)y=f(x)$$

for $0 \le x \le 1$ and $y(0)=y(1)=0$

where $p(x) \in C^1[0,1]$, $q, f \in C^0[0,1]$

and $\exists \delta > 0 \ni p(x) \ge \delta \ge 0$ and $q(x) \ge 0$ for $0 \le x \le 1$

(sufficient conditions for a unique solution)

PRINCIPLE OF VARIATION

The unique solution is the function which

- $\in C^2[0,1]$
- satisfies BCs
- minimizes the integral

$$I(u(x)) \equiv \int_0^1 \left\{ p(x)\left(\frac{du}{dx}\right)^2 + q(x)u(x)^2 - 2f(x)u(x) \right\} dx$$

§ Approximation Theory ~ ONE IDEA

- select a set of $LI \left\{\phi_k(x)\right\}_{k=0}^{n}$

  each of which satisfies the given BCs:

  $\phi_k(0) = \phi_k(1) = 0$

Define $\Phi_n \equiv$ the set of functions spaned by $\left\{\phi_k(x)\right\}_{k=0}^{n}$

$$= \left\{ y_n(x) \,\middle|\, y_n(x) = \sum_{k=0}^{n} c_k \phi_k(x) \right\}$$

- select a function from Φ_n

  to approximate the exact soultuion $y(\mathrm{x})$

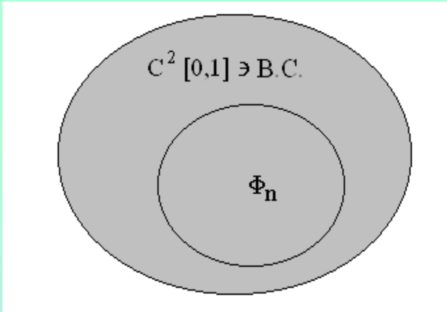
$$y(x) \approx y_n(x) = \sum_{k=0}^{n} c_k \phi_k(x) \in \Phi_n$$

The approximation $y_n(x) \in \Phi_n \subseteq C^2[0,1]$ and $\ni$ B.C.s

$$y_n(0) = \sum_{k=0}^{n} c_k \phi_k(0) = 0$$

$$y_n(1) = \sum_{k=0}^{n} c_k \phi_k(1) = 0$$

The exact solution $y(x) \in C^2[0,1]$ and $\ni$ B.C.s



$$\Phi_n \to C^2[0,1] \quad \text{as } n \to \infty$$

- Which y_n is the best? The one having a minimum value of I

Convergence : $y_n \to y(x)$ as $n \to \infty$

SOLUTION::

$$I(u(x)) \equiv \int_0^1 \left\{ p(x)\left(\frac{du}{dx}\right)^2 + q(x)u(x)^2 - 2f(x)u(x) \right\} dx$$

$$I\left(y_n(x) \in \Phi_n\right) = I\left(\sum_{k=0}^{n} c_k \phi_k(x)\right)$$

$$= \int_0^1 \left\{ p(x)\left(\sum_{k=0}^{n} c_k \phi_k'(x)\right)^2 + q(x)\left(\sum_{k=0}^{n} c_k \phi_k(x)\right)^2 - 2f(x)\sum_{k=0}^{n} c_k \phi_k(x) \right\} dx$$

MINIMIAZATION: $\dfrac{\partial I(\Phi)}{\partial c_j} = 0, \quad \text{for } j = 0,1,2,\cdots,n$

$$0=\frac{\partial I(\Phi)}{\partial c_j}$$

$$=\frac{\partial}{\partial c_j}\int_0^1\left\{p(x)\left(\sum_{k=0}^{n}c_k\phi_k'(x)\right)^2+q(x)\left(\sum_{k=0}^{n}c_k\phi_k(x)\right)^2-2f(x)\sum_{k=0}^{n}c_k\phi_k(x)\right\}dx$$

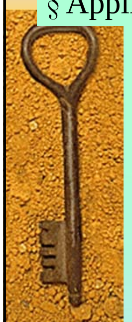
$$=\int_0^1\left\{2p(x)\phi_j'(x)\left(\sum_{k=0}^{n}c_k\phi_k'(x)\right)+2q(x)\phi_j(x)\left(\sum_{k=0}^{n}c_k\phi_k(x)\right)-2f(x)\phi_j(x)\right\}dx$$

$$=2\sum_{k=0}^{n}\left\{c_k\underbrace{\int_0^1\left[p(x)\phi_j'(x)\phi_k'(x)+q(x)\phi_j(x)\phi_k(x)\right]dx}_{a_{kj}=a_{jk}}\right\}-2\underbrace{\int_0^1 f(x)\phi_j(x)dx}_{b_j}$$

Thus we obtain $\sum_{k=0}^{n}a_{jk}c_k=b_j$, for $j=0,1,2,\cdots,n$

~ Solving ODE becomes solving matrix (algebraic) equations ~

§ Application to PDE ~ spectral methods, finite element methods, etc.



Given: $\frac{\partial u}{\partial t}=L(u)+f(x,t)$

where L is some spartial operatior, e.g. Laplacian $L=\nabla^2$

$f(x,t)$ is a known external source term.

I.C.: $u(x,0)=g(x),\ a\le x\le b$

FIND: $u(x,t)$ for $t\ge 0$

§ Global approximation theory:

STEP1: find a set of LI $\{\phi_j(x)\}$ and

the associated weight function $w(x)$

$$u(x,t) \approx u_n(x,t) = \sum_{j=0}^{n} c_j(t)\phi_j(x)$$

P.S. The coefficients $\{c_j\}$ is a function of t now.

for all $x \in \Omega$

STEP2 : Substitute the above formula into PDE : $\frac{\partial u}{\partial t} = L(u) + f$

$$\sum_{j=0}^{n} \frac{dc_j}{dt}\phi_j(x) \overset{?}{=} L\left(\sum_{j=0}^{n} c_j\phi_j(x)\right) + f(x,t)$$

§ Global approximation theory:

$$\sum_{j=0}^{n} \frac{dc_j}{dt}\phi_j(x) \overset{?}{=} L\left(\sum_{j=0}^{n} c_j\phi_j(x)\right) + f(x,t)$$

Let $\Phi_n \equiv$ the space spaned by $\{\phi_j^k(x)\}_{j=0}^{n}$.

$$LHS \in \Phi_n$$

$$RHS \overset{?}{\in} \Phi_n$$

not necessary!

• Several ways to obtain an approximation:

(i) best approximation: look for a set of $\{c_j(t)\}$ which minimizes

$$\left\| \sum_{j=0}^{n} \frac{dc_j}{dt} \phi_j(x) - L\left(\sum_{j=0}^{n} c_j \phi_j(x) \right) - f(x,t) \right\|$$

(ii) Collocation methods : choose a set of nodes $\{x_i\}_{i=0}^{n}$ at which

$$\sum_{j=0}^{n} \frac{dc_j}{dt} \phi_j(x_i) = L\left(\sum_{j=0}^{n} c_j \phi_j(x_i) \right) + f(x_i,t)$$

(iii) Galerkin approximation

$$\int_a^b \omega(x)\phi_i(x) \cdot \sum_{j=0}^{n} \frac{dc_j}{dt} \phi_j(x) dx$$

$$= \int_a^b \omega(x)\phi_i(x) L\left(\sum_{j=0}^{n} c_j \phi_j(x) \right) dx + \int_a^b \omega(x)\phi_i(x) f(x,t) dx$$

§ Galerkin approximation – linear L

$$\sum_{j=0}^{n} \frac{dc_j}{dt} \cdot \int_a^b \omega(x)\phi_i(x)\phi_j(x) dx$$

$$= \sum_{j=0}^{n} c_j \int_a^b \omega(x)\phi_i(x) L\phi_j(x) dx + \int_a^b \omega(x)\phi_i(x) f(x,t) dx$$

define $a_{ij} = \int_a^b \omega(x)\phi_i(x)\phi_j(x)\, dx = \delta_{ij}$ if $\omega-$ orthonormal

$$b_{ij} = \int_a^b \omega(x)\phi_i(x) L\phi_j(x) dx$$

$$r_i(t) = \int_a^b \omega(x)\phi_i(x) f(x,t) dx$$

$$\sum_{j=0}^{n} a_{ij} \frac{dc_j}{dt} = \sum_{j=0}^{n} b_{ij} c_j(t) + r_i(t)$$

~ PDE is reduced to a system of coupled ODEs ~

~ go time-marching ~

• special case: ω-orthonormal $\{\phi_j(x)\}: a_{ij} = \delta_{ij}$

$$\frac{dc_j}{dt} = \sum_{j=0}^{n} b_{ij} c_j(t) + r_i(t) \quad \text{~ decoupled on LHS ~}$$

§ Initial Conditions, i.e. $c_j(0)$

$$u(x,0) = g(x) \approx u_n(x,0) = \sum_{j=0}^{n} c_j(0)\phi_j(x)$$

• best approximation : minimize $\left\| g(x) - \sum_{j=0}^{n} c_j(0)\phi_j(x) \right\|$

•Collocation: $g(x_i) = \sum_{j=0}^{n} c_j(0)\phi_j(x_i)$

• Galerkin : $\int_a^b \omega(x)\phi_i(x)g(x)dx = \sum_{j=0}^{n} c_j(0)\int_a^b \omega(x)\phi_i(x)\phi_j(x)dx$

§ Boundary Conditions:

e.g. $Bu(x,t) = 0$ for some linear spatial operator B

(a) select $\{\phi_j(x)\}$ with the addional restriction

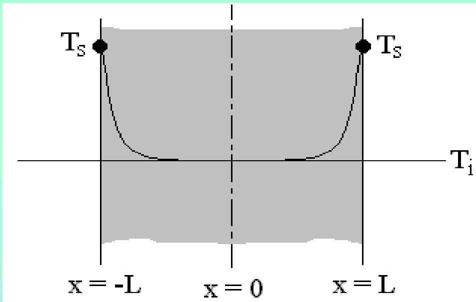
that each $\phi_j(x) \ni BCs.$ i.e. $B\phi_j(x) = 0$

$$\Rightarrow Bu_n(x,t) = B\sum_{j=0}^{n} c_j(t)\phi_j(x) = \sum_{j=0}^{n} c_j(t)B\phi_j(x) = 0$$

(b) (Tau method) Discard as may ODEs as the number of BCs and impose

$$Bu_n(x,t) = \sum_{j=0}^{n} c_j(t)B\phi_j(x) = 0$$

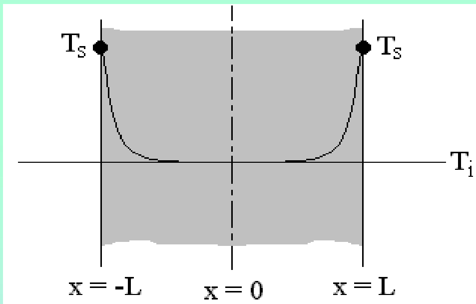
§ Example: thermal boundary layer



Governing equation : $\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2}$

I.C.: $T(x, t=0) = T_i$

B.C.s: $T(x = \pm 1, t \geq 0^+) = T_s$



Governing equation : $\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2}$

I.C.: $T(x, t=0) = T_i$

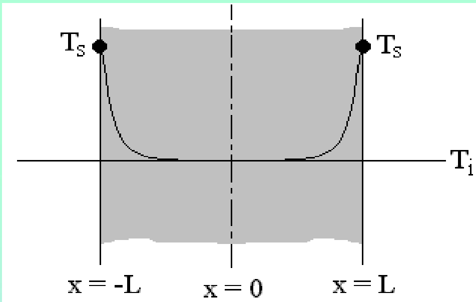
B.C.s: $T(x = \pm 1, t \geq 0^+) = T_s$

define $\Theta(x,t) = \frac{T - T_i}{T_s - T_i}$

$$\frac{\partial \Theta}{\partial t} = D \frac{\partial^2 \Theta}{\partial x^2}$$

$$\Theta(x, 0) = 0$$

$$\Theta(1, t) = 1$$



- A thermal bounday layer is expected to develop near $x = \pm 1$

  $\Rightarrow$ better denser grid points near $x = \pm 1$

- Expect the solution is symmetric.

  $\Rightarrow$ choose Chebychev polynomials of even degrees

  $$\left\{ T_{2j}(x) = \cos\left(2j\cos^{-1}x\right) \right\}$$

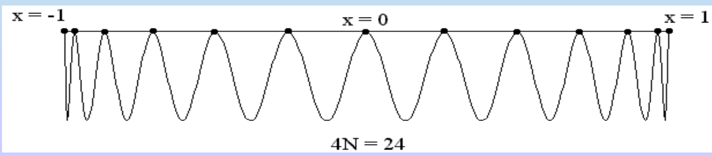
§ collocation + τ methods

- choose $\phi_j(x) = T_{2j}(x)$

  $$\Theta(x,t) \approx \Theta_n(x,t) \equiv \sum_{j=0}^{n} c_j(t)\, T_{2j}(x)$$

- collocation grid points: choose the locations of peaks of Chebychev,

$$x_i \equiv \text{locations of peak of } T_{4n}(x) = \cos\left(\frac{2(n-i)\pi}{4n}\right) \quad i = 0,1,2\cdots,n$$



§ collocation + τ methods

$$\frac{\partial \Theta}{\partial t} = D \frac{\partial^2 \Theta}{\partial x^2}$$

$$\Theta(x,t) \approx \Theta_n(x,t) \equiv \sum_{j=0}^{n} c_j(t) T_{2j}(x)$$

$$\sum_{j=0}^{n} \frac{dc_j}{dt} T_{2j}(x) \overset{?}{=} D \sum_{j=0}^{n} c_j \frac{d^2 T_{2j}(x)}{dx^2}$$

$$\sum_{j=0}^{n} \frac{dc_j}{dt} T_{2j}(x_i) = D \sum_{j=0}^{n} c_j(t) \frac{d^2 T_{2j}(x)}{dx^2}(x_i)$$

for $\quad i = 0,1,2\cdots,n-1 \quad (i = n \text{ discareded})$

B.C.: $\Theta(1,t) = \sum_{j=0}^{n} c_j(t) T_{2j}(1) = \sum_{j=0}^{n} c_j(t) = 1$

• Initial Conditions

$$\Theta(x,t) \approx \Theta_n(x,t) \equiv \sum_{j=0}^{n} c_j(t) T_{2j}(x)$$

$$\Theta(x_i,0) = 0 = \sum_{j=0}^{n} c_j(0) T_{2j}(x_i)$$

for $i = 0,1,2,\cdots,n-1$

$$\Theta(\pm 1,0) = 1 = \sum_{j=0}^{n} c_j(0)$$

~ (*n*+1) equations for (*n*+1) unknowns ~

§ Galerkin method+$\{\phi_j(x)\}$ ⇒ B.C.s

- Since $T_0(x)=1$ and $T_{2j}(\pm 1)=1$

Let $\phi_j(x)\equiv T_{2j}(x)-T_0(x)$. Thus $\phi_j(\pm 1)=0$

$$\Theta(x,t)\approx\Theta_n(x,t)\equiv 1+\sum_{j=1}^{n}c_j(t)\phi_j(x)$$

$$=1+\sum_{j=1}^{n}c_j(t)\left(T_{2j}(x)-T_0(x)\right)$$

$$\Theta_n(\pm 1,t)=1+\sum_{j=1}^{n}c_j(t)\phi_j(\pm 1)=1+\sum_{j=1}^{n}c_j(t)\cdot 0=1 \quad \Rightarrow \textbf{B.C.s}$$

- Substitute into governing equation: $\dfrac{\partial\Theta}{\partial t}=D\dfrac{\partial^2\Theta}{\partial x^2}$

$$\Theta_n(x,t)=1+\sum_{j=1}^{n}c_j(t)\phi_j(x)$$

$$\sum_{j=1}^{n}\frac{dc_j}{dt}\phi_j(x)\overset{?}{=}D\sum_{j=1}^{n}c_j(t)\frac{d^2\phi_j(x)}{dx^2}$$

- Use orthogonal property:

$$\sum_{j=1}^{n}\frac{dc_j}{dt}\cdot\int_{-1}^{1}\frac{\phi_i(x)\phi_j(x)}{\sqrt{1-x^2}}dx=D\sum_{j=1}^{n}c_j(t)\int_{-1}^{1}\frac{\phi_i(x)\left(d^2\phi_j(x)/dx^2\right)}{\sqrt{1-x^2}}dx$$

$$\sum_{j=1}^{n}a_{ij}\frac{dc_j}{dt}=D\sum_{j=1}^{n}b_{ij}c_j(t) \quad \text{for } i=1,2,\cdots,n$$

$$a_{ij} = \int_{-1}^{1} \frac{\phi_i(x)\phi_j(x)}{\sqrt{1-x^2}} dx \quad , \quad i,j = 1,2,\cdots,n$$

$$= \int_{-1}^{1} (T_{2i}(x) - T_0(x))(T_{2j}(x) - T_0(x)) \Big/ \sqrt{1-x^2}\, dx$$

$$= \int_{-1}^{1} \left(T_{2i}T_{2j} - T_0 T_{2i} - T_0 T_{2j} + T_0^2\right) \Big/ \sqrt{1-x^2}\, dx$$

$$= \int_{-1}^{1} \left(T_{2i}T_{2j} + T_0^2\right) \Big/ \sqrt{1-x^2}\, dx$$

$$= \begin{cases} \pi & \text{if } i \neq j \\ \dfrac{3\pi}{2} & \text{if } i = j \geq 1 \end{cases}$$

$$b_{ij} \equiv \int_{-1}^{1} \phi_i(x) \frac{d^2\phi_j(x)}{dx^2} \Big/ \sqrt{1-x^2}\, dx$$

$$= \int_{-1}^{1} \left\{ (T_{2i}(x) - T_0(x)) \cdot \frac{d^2}{dx^2} (T_{2j}(x) - T_0(x)) \right\} \Big/ \sqrt{1-x^2}\, dx$$

$$= \int_{-1}^{1} \left\{ (T_{2i} - T_0) \cdot \frac{d^2 T_{2j}}{dx^2} \right\} \Big/ \sqrt{1-x^2}\, dx$$

$$\frac{d^2 T_{2j}(x)}{dx^2} = P_{2j-2}(x) = \sum_{k=0}^{j-1} \gamma_k T_{2k}(x)$$

$$b_{ij} = \sum_{k=0}^{j-1} \gamma_k \cdot \int_{-1}^{1} \left(T_{2i}T_{2k} - T_0 T_{2k}\right) \Big/ \sqrt{1-x^2}\, dx$$

- Initial Conditions: $\Theta(x,0)=0$

$$\Theta_n(x,t)=1+\sum_{j=1}^{n}c_j(t)\phi_j(x)$$

$$\Theta_n(x,0)=1+\sum_{j=1}^{n}c_j(0)\phi_j(x)$$

$$\int_{-1}^{1}\frac{(\Theta(x,0)-1)\phi_i(x)}{\sqrt{1-x^2}}dx=\sum_{j=1}^{n}c_j(0)\int_{-1}^{1}\frac{\phi_i(x)\phi_j(x)}{\sqrt{1-x^2}}dx$$

$$\pi=\int_{-1}^{1}\frac{(1-T_{2i}(x))}{\sqrt{1-x^2}}dx=\sum_{j=1}^{n}a_{ij}c_j(0)\quad \text{for } i=1,2,\cdots,n$$

♣ **Local approximation theory**

- divide the interested domain $\Omega\equiv[a,b]$

into several subdomins $\Omega=\bigcup_{k=1}^{K}\Omega_k$

$$u(x,t)\approx u_n^k(x,t)\equiv\sum_{j=0}^{n}c_j^k(t)\phi_j^k(x)\quad \text{for all } x\in\Omega_k$$

P.S. $\{\phi_j^k(x)\}_{j=0}^{n}$ is different from one subdomain to another.

i.e. require K sets of L.I. functions $\{\phi_j^k(x)\}_{j=0}^{n}$

and will have K sets of corresponding coefficients $\{c_j^k(t)\}_{j=0}^{n}$

§ Finite Element Methods ~ piecewise approximation

Test problem : (domain Ω with boundary $\partial\Omega$)

$$\frac{\partial}{\partial x}\left(p(x,y)\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial y}\left(q(x,y)\frac{\partial u}{\partial y}\right)+r(x,y)u(x,y)=f(x,y)$$

$$u(x,y)=g(x,y) \quad on\ \partial\Omega$$

PRINCIPLE OF VARIATION ::

The exact solution (if exists and unique) is the function $\in C^2(\Omega)$ which satisfies BCs and minimizes the value of

$$I(u)=\int_{\Omega}\left\{\frac{1}{2}\left[p(x,y)\left(\frac{\partial u}{\partial x}\right)^2+q(x,y)\left(\frac{\partial u}{\partial y}\right)^2-r(x,y)u^2\right]+f(x,y)u(x,y)\right\}dxdy$$

STEP1: Divide the interested domain into several parts, i.e. $\Omega=\bigcup_{k=1}^{K}\Omega_k$

Each subdomain Ω_k is called an "element".

STEP2: within each subdomain Ω_k, choose a proper set of $\left\{\phi_j^k(x,y)\right\}_{j=0}^{n}$

$$u(x,y)\approx u_n^k(x,y)\equiv\sum_{j=0}^{n}c_j^k\phi_j^k(x,y) \quad \text{for } (x,y)\in\Omega_k$$

P.S. $\left\{\phi_j^k(x,y)\right\}_{j=0}^{n}$ are different from one element to another in general.

Put $u(x,y) \approx \bigcup_{k=1}^{K} u_n^k(x,y) = \bigcup_{k=1}^{K} \sum_{j=0}^{n} c_j^k \phi_j^k(x,y)$

STEP3: Look for the values of $\{ c_j^k \}, j = 0,1,\cdots,n$ and $k = 0,1,\cdots,K$

such that $\{ u_n^k(x,y) \}$ minizes $I(u)$

$$I(u) = \int_\Omega \left\{ \frac{1}{2} \left[p(x,y)\left(\frac{\partial u}{\partial x}\right)^2 + q(x,y)\left(\frac{\partial u}{\partial y}\right)^2 - r(x,y)u^2 \right] + f(x,y)u(x,y) \right\} dxdy$$

Thus $I(u) = \int_\Omega \cdots = \sum_{k=1}^{K} \int_{\Omega_k} \cdots = I(c_j^k)$

Therefore for all $i \in \{0,1,\cdots,n\}$ and all $m \in \{0,1,\cdots,K\}$

$$0 = \frac{\partial I(u)}{\partial c_i^m} \quad \text{required (minimized)}$$

$$= \frac{\partial}{\partial c_i^m} \sum_{k=1}^{K} \int_{\Omega_k} \frac{1}{2} p(x,y) \left(\sum_{j=0}^{n} c_j^k \frac{\partial \phi_j^k}{\partial x} \right)^2 + \cdots$$

$$= \frac{\partial}{\partial c_i^m} \int_{\Omega_m} \frac{1}{2} p(x,y) \left(\sum_{j=0}^{n} c_j^m \frac{\partial \phi_j^m}{\partial x} \right)^2 + \cdots$$

$$= \int_{\Omega_m} \frac{\partial}{\partial c_i^m} \left\{ \frac{1}{2} p(x,y) \left(\sum_{j=0}^{n} c_j^m \frac{\partial \phi_j^m}{\partial x} \right)^2 + \cdots \right\} dxdy \qquad \sum_{j=0}^{n} \frac{\partial \phi_j^m}{\partial x} \delta_{ij} = \frac{\partial \phi_i^m}{\partial x}$$

$$= \int_{\Omega_m} \left\{ p(x,y) \left(\sum_{j=0}^{n} c_j^m \frac{\partial \phi_j^m}{\partial x} \right) \frac{\partial}{\partial c_i^m} \left(\sum_{j=0}^{n} c_j^m \frac{\partial \phi_j^m}{\partial x} \right) + \cdots \right\} dxdy$$

$$0 = \frac{\partial I(u)}{\partial c_i^m} \quad \text{required (minimized)}$$

$$= \int_{\Omega_m} \left\{ p(x,y) \sum_{j=0}^{n} c_j^m \frac{\partial \phi_j^m}{\partial x} \frac{\partial \phi_i^m}{\partial x} + q(x,y) \sum_{j=0}^{n} c_j^m \frac{\partial \phi_j^m}{\partial y} \frac{\partial \phi_i^m}{\partial y} - r(x,y) \sum_{j=0}^{n} c_j^m \phi_j^m \phi_i^m + f(x,y) \phi_i^m \right\} dxdy$$

After rearangement : (change variable $m \to k$)

$$0 = \sum_{j=0}^{n} c_j^k \cdot \int_{\Omega_k} \left\{ p(x,y) \frac{\partial \phi_j^k}{\partial x} \frac{\partial \phi_i^k}{\partial x} + q(x,y) \frac{\partial \phi_j^k}{\partial y} \frac{\partial \phi_i^k}{\partial y} - r(x,y) \phi_j^k \phi_i^k \right\} dxdy$$

$$- \int_{\Omega_k} f(x,y) \phi_i^k(x,y) dxdy$$

$$a_{ij}^k = \int_{\Omega_k} \left\{ p(x,y) \frac{\partial \phi_j^k}{\partial x} \frac{\partial \phi_i^k}{\partial x} + q(x,y) \frac{\partial \phi_j^k}{\partial y} \frac{\partial \phi_i^k}{\partial y} - r(x,y) \phi_i^k \phi_j^k \right\} dxdy$$

$$= a_{ji}^k$$

$$b_i^k = -\int_{\Omega_k} f(x,y) \phi_i^k(x,y) dxdy$$

$$\sum_{j=0}^{n} a_{ij}^k c_j^k = b_i^k \quad \text{or} \quad A^k c^k = b^k \sim \text{elemental matrix equation}$$

$$\text{for } k = 1, 2, \cdots, K$$

- A^k is singular! i.e. Each element matrix equation is underminate.
- ▸ too many degrees of freedom!

- Continuity requirement : if $(x, y) \in \Omega_{k_1}$, and also $\in \Omega_{k_2}$, then

$$u(x,y) \approx u_n^{k_1} = \sum_{j=0}^{n} c_j^{k_1} \phi_j^{k_1}(x,y)$$

$$u(x,y) \approx u_n^{k_2} = \sum_{j=0}^{n} c_j^{k_2} \phi_j^{k_2}(x,y)$$

Thus C^0-requirement needs

$$\sum_{j=0}^{n} c_j^{k_1} \phi_j^{k_1}(x,y) = \sum_{j=0}^{n} c_j^{k_2} \phi_j^{k_2}(x,y)$$

$\Rightarrow$ The minimization problem should be redone with the C^0-requirements

§ Example: use collocation points

STEP1: within element Ω_k, choose $(n+1)$ points denoted by (x_i^k, y_i^k) for $i = 0, 1, 2, \cdots, n$

STEP2 : within each element, choose an interpoint function, say two - dimentional Lagrangian polynomials, $\phi_i^k(x,y)$

$$\phi_i^k(x,y) \equiv \prod_{\substack{l=0 \\ l \neq i}}^{n} \frac{\sqrt{(x - x_l^k)^2 + (y - y_l^k)^2}}{\sqrt{(x_i^k - x_l^k)^2 + (y_i^k - y_l^k)^2}} \qquad \ni \phi_i^k(x_j^k, y_j^k) = \delta_{ij}$$

and approximate the desired function as

$$u(x,y) \approx u_n^k \equiv \sum_{i=0}^{n} c_i^k \phi_i^k(x,y), \qquad \text{whenever } (x,y) \in \Omega_k$$

$$u(x,y) \approx u_n^k \equiv \sum_{i=0}^{n} c_i^k \phi_i^k(x,y), \qquad \text{whenever } (x,y) \in \Omega_k$$

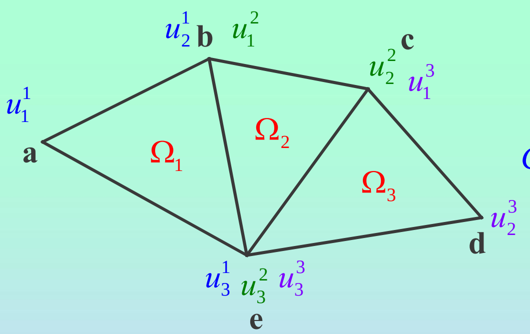
Notice:

$$u_n^k(x_i, y_i) \equiv u_i^k = \sum_{j=0}^{n} c_j^k \phi_j^k(x_i, y_i)$$

$$u_i^k = \sum_{j=0}^{n} c_j^k \delta_{ij} = c_i^k$$

$$u_n^k(x,y) = \sum_{j=0}^{n} u_j^k \phi_j^k(x,y)$$

§ example – triangular elements (linear interpolation)

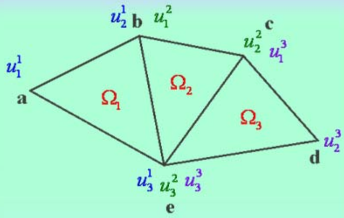


$$C^0: \begin{cases} u_1^1 = u_a \\ u_2^1 = u_1^2 = u_b \\ u_2^2 = u_1^3 = u_c \\ u_2^3 = u_d \\ u_3^1 = u_3^2 = u_3^3 = u_e \end{cases}$$

If no C^0 constraint: d.o.f.s $= u_1^1, u_2^1, u_3^1, u_1^2, u_2^2, u_3^2, u_1^3, u_2^3, u_3^3$

with C^0 - constraint: d.o.f.s $= u_a, u_b, u_c, u_d, u_e$

$*$ d.o.f. $u_a \left(=u_1^1\right)$:



$$0 = \frac{\partial I(u)}{\partial u_a}$$

$$= \frac{\partial}{\partial u_a} \sum_{k=1}^{K} \int_{\Omega_k} \cdots\cdots \sum_{j=0}^{n} u_j^k \phi_j^k (x, y) \cdots\cdots$$

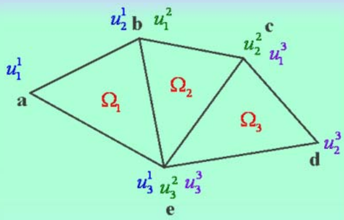
$$= \frac{\partial}{\partial u_a} \int_{\Omega_1} \cdots\cdots \sum_{j=0}^{n} u_j^1 \phi_j^1 (x, y) \cdots\cdots$$

$$= \frac{\partial}{\partial u_1^1} \int_{\Omega_1} \cdots\cdots \sum_{j=0}^{n} u_j^1 \phi_j^1 (x, y) \cdots\cdots$$

$$0 = \left\{ a_{11}^1 u_1^1 + a_{12}^1 u_2^1 + a_{13}^1 u_3^1 - b_1^1 \right\}$$

$*$d.o.f. $u_d \left(=u_2^3\right)$: $\quad 0 = \left\{ a_{21}^3 u_1^3 + a_{22}^3 u_2^3 + a_{23}^3 u_3^3 - b_2^3 \right\}$

$*$ d.o.f. $u_b \left(=u_2^1 = u_1^2\right)$:

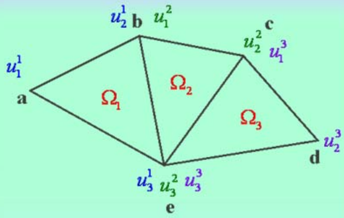


$$0 = \frac{\partial I(u)}{\partial u_b}$$

$$= \frac{\partial}{\partial u_b} \left(\int_{\Omega_1} \cdots \sum_{j=0}^{n} u_j^1 \phi_j^1 (x, y) \cdots + \int_{\Omega_2} \cdots \sum_{j=0}^{n} u_j^2 \phi_j^2 (x, y) \cdots \right)$$

$$= \frac{\partial}{\partial u_2^1} \int_{\Omega_1} \cdots \sum_{j=0}^{n} u_j^1 \phi_j^1 (x, y) \cdots \quad + \quad \frac{\partial}{\partial u_1^2} \int_{\Omega_2} \cdots \sum_{j=0}^{n} u_j^2 \phi_j^2 (x, y) \cdots$$

$$0 = \left\{ a_{21}^1 u_1^1 + a_{22}^1 u_2^1 + a_{23}^1 u_3^1 - b_2^1 \right\} + \left\{ a_{11}^2 u_1^2 + a_{12}^2 u_2^2 + a_{13}^2 u_3^2 - b_1^2 \right\}$$



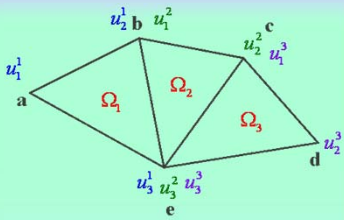
$*$ d.o.f. $u_c\left(=u_2^2=u_1^3\right)$:

$$0=\frac{\partial I(u)}{\partial u_c}$$

$$=\frac{\partial}{\partial u_c}\left(\int_{\Omega_2}\cdots\sum_{j=0}^{n}u_j^2\phi_j^2(x,y)\cdots+\int_{\Omega_3}\cdots\sum_{j=0}^{n}u_j^3\phi_j^3(x,y)\cdots\right)$$

$$=\frac{\partial}{\partial u_2^2}\int_{\Omega_2}\cdots\sum_{j=0}^{n}u_j^2\phi_j^2(x,y)\cdots\quad+\quad\frac{\partial}{\partial u_1^3}\int_{\Omega_3}\cdots\sum_{j=0}^{n}u_j^3\phi_j^3(x,y)\cdots$$

$$0=\left\{a_{21}^2u_1^2+a_{22}^2u_2^2+a_{23}^2u_3^2-b_2^2\right\}+\left\{a_{11}^3u_1^3+a_{12}^3u_2^3+a_{13}^3u_3^3-b_1^3\right\}$$



$*$d.o.f. $u_e\left(=u_3^1=u_3^2=u_3^3\right)$:

$$0=\frac{\partial I(u)}{\partial u_e}$$

$$=\frac{\partial}{\partial u_c}\left(\int_{\Omega_1+\Omega_2+\Omega_3}\cdots\cdots\right)$$

$$=\frac{\partial}{\partial u_3^1}\int_{\Omega_1}\cdots\sum_{j=0}^{n}u_j^1\phi_j^1(x,y)\cdots+\frac{\partial}{\partial u_3^2}\int_{\Omega_2}\cdots\sum_{j=0}^{n}u_j^2\phi_j^2(x,y)\cdots$$

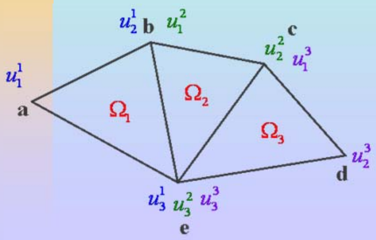
$$+\frac{\partial}{\partial u_3^3}\int_{\Omega_3}\cdots\sum_{j=0}^{n}u_j^3\phi_j^3(x,y)\cdots$$

$$0=\left\{a_{31}^1u_1^1+a_{32}^1u_2^1+a_{33}^1u_3^1-b_3^1\right\}+\left\{a_{31}^2u_1^2+a_{32}^2u_2^2+a_{33}^2u_3^2-b_3^2\right\}$$
$$+\left\{a_{31}^3u_1^3+a_{32}^3u_2^3+a_{33}^3u_3^3-b_3^3\right\}$$

- Global matrix equation $Au=b$

$$\begin{array}{ccccc} a & b & c & d & e \\ \end{array}$$

$$\begin{pmatrix} a_{11}^1 & a_{12}^1 & 0 & 0 & a_{13}^1 \\ a_{21}^1 & a_{22}^1+a_{11}^2 & a_{12}^2 & 0 & a_{23}^1+a_{13}^2 \\ 0 & a_{21}^2 & a_{22}^2+a_{11}^3 & a_{12}^3 & a_{23}^2+a_{13}^3 \\ 0 & 0 & a_{21}^3 & a_{22}^3 & a_{23}^3 \\ a_{31}^1 & a_{32}^1+a_{31}^2 & a_{32}^2+a_{31}^3 & a_{32}^3 & a_{33}^1+a_{33}^2+a_{33}^3 \end{pmatrix} \begin{pmatrix} u_a = u_1^1 \\ u_b = u_2^1 = u_1^2 \\ u_c = u_2^2 = u_1^3 \\ u_d = u_2^3 \\ u_e = u_3^1 = u_3^2 = u_3^3 \end{pmatrix} = \begin{pmatrix} b_1^1 \\ b_2^1+b_1^2 \\ b_2^2+b_1^3 \\ b_2^3 \\ b_3^1+b_3^2+b_3^3 \end{pmatrix}$$



$$\begin{pmatrix} a_{11}^1 & a_{12}^1 & 0 & 0 & a_{13}^1 \\ a_{21}^1 & a_{22}^1 & 0 & 0 & a_{23}^1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ a_{31}^1 & a_{32}^1 & 0 & 0 & a_{33}^1 \end{pmatrix} \begin{pmatrix} u_1^1 \\ u_2^1 \\ 0 \\ 0 \\ u_3^1 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & a_{11}^2 & a_{12}^2 & 0 & a_{13}^2 \\ 0 & a_{21}^2 & a_{22}^2 & 0 & a_{23}^2 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & a_{31}^2 & a_{32}^2 & 0 & a_{33}^2 \end{pmatrix} \begin{pmatrix} 0 \\ u_1^2 \\ u_2^2 \\ 0 \\ u_3^2 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_{11}^3 & a_{12}^3 & a_{13}^3 \\ 0 & 0 & a_{21}^3 & a_{22}^3 & a_{23}^3 \\ 0 & 0 & a_{31}^3 & a_{32}^3 & a_{33}^3 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ u_1^3 \\ u_2^3 \\ u_3^3 \end{pmatrix} = \begin{pmatrix} b_1^1 \\ b_2^1 \\ 0 \\ 0 \\ b_3^1 \end{pmatrix} + \begin{pmatrix} 0 \\ b_1^2 \\ b_2^2 \\ 0 \\ b_3^2 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ b_1^3 \\ b_2^3 \\ b_3^3 \end{pmatrix}$$

stiffness summation

- local matrix equation

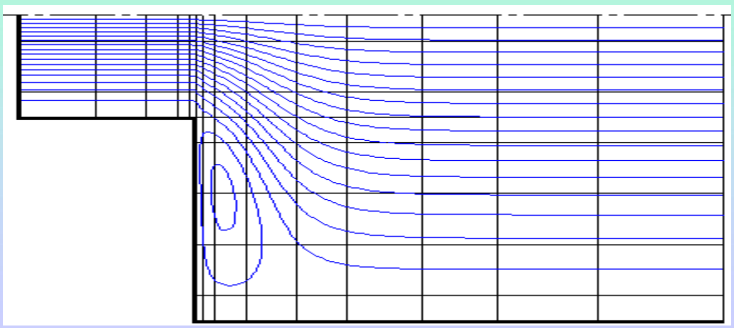
$$k=1:\quad \begin{pmatrix} a_{11}^1 & a_{12}^1 & a_{13}^1 \\ a_{21}^1 & a_{22}^1 & a_{23}^1 \\ a_{31}^1 & a_{32}^1 & a_{32}^1 \end{pmatrix}\begin{pmatrix} u_1^1 \\ u_2^1 \\ u_3^1 \end{pmatrix} = \begin{pmatrix} a_{11}^1 & a_{12}^1 & a_{13}^1 \\ a_{21}^1 & a_{22}^1 & a_{23}^1 \\ a_{31}^1 & a_{32}^1 & a_{32}^1 \end{pmatrix}\begin{pmatrix} u_a \\ u_b \\ u_e \end{pmatrix} = \begin{pmatrix} b_1^1 \\ b_2^1 \\ b_3^1 \end{pmatrix}$$

$$k=2:\quad \begin{pmatrix} a_{11}^2 & a_{12}^2 & a_{13}^2 \\ a_{21}^2 & a_{22}^2 & a_{23}^2 \\ a_{31}^2 & a_{32}^2 & a_{32}^2 \end{pmatrix}\begin{pmatrix} u_1^2 \\ u_2^2 \\ u_3^2 \end{pmatrix} = \begin{pmatrix} a_{11}^2 & a_{12}^2 & a_{13}^2 \\ a_{21}^2 & a_{22}^2 & a_{23}^2 \\ a_{31}^2 & a_{32}^2 & a_{32}^2 \end{pmatrix}\begin{pmatrix} u_b \\ u_c \\ u_e \end{pmatrix} = \begin{pmatrix} b_1^2 \\ b_2^2 \\ b_3^2 \end{pmatrix}$$

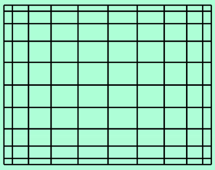
$$k=3:\quad \begin{pmatrix} a_{11}^3 & a_{12}^3 & a_{13}^3 \\ a_{21}^3 & a_{22}^3 & a_{23}^3 \\ a_{31}^3 & a_{32}^3 & a_{32}^3 \end{pmatrix}\begin{pmatrix} u_1^3 \\ u_2^3 \\ u_3^3 \end{pmatrix} = \begin{pmatrix} a_{11}^3 & a_{12}^3 & a_{13}^3 \\ a_{21}^3 & a_{22}^3 & a_{23}^3 \\ a_{31}^3 & a_{32}^3 & a_{32}^3 \end{pmatrix}\begin{pmatrix} u_c \\ u_d \\ u_e \end{pmatrix} = \begin{pmatrix} b_1^3 \\ b_2^3 \\ b_3^3 \end{pmatrix}$$

§ Example – 2D Poisson Solver

$$\nabla^2 P = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = f(x,y,t)$$



- Let



$$h_i^k(x) \equiv \prod_{\substack{m=0 \\ m \neq i}}^{N} \frac{(x - x_i^k)}{(x_m^k - x_i^k)}$$

$$h_j^k(y) \equiv \prod_{\substack{m=0 \\ m \neq j}}^{N} \frac{(y - y_j^k)}{(y_m^k - y_j^k)}$$

where $\{x_i^k\}_{i=0}^N$ and $\{y_j^k\}_{j=0}^N$ are Gauss Quadrature Intergration nodes

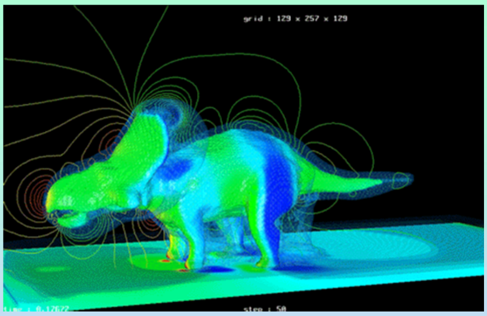
$$P(x,y,t) = \sum_{k=1}^{K}{}' \sum_{i=0}^{N} \sum_{j=0}^{N} P_{ij}^k h_i^k(x) h_j^k(y)$$

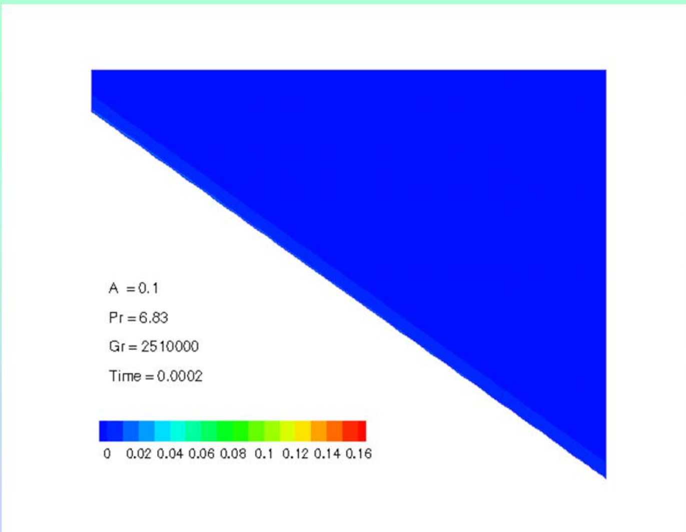
$$f(x,y,t) = \sum_{k=1}^{K}{}' \sum_{i=0}^{N} \sum_{j=0}^{N} f_{ij}^k h_i^k(x) h_j^k(y)$$

Numerical Analysis

- 挑戰人類結合數學及物理知識能力
- 激發人類的創造力與邏輯思考
- 數位化儀器的秘密武器
- 提供經濟的設計分析工具

- 數值誤差 – **truncation error & rounding error**
- 數值現象 – **numerical diffusion & dispersion**
- 穩定性、準確性、效率

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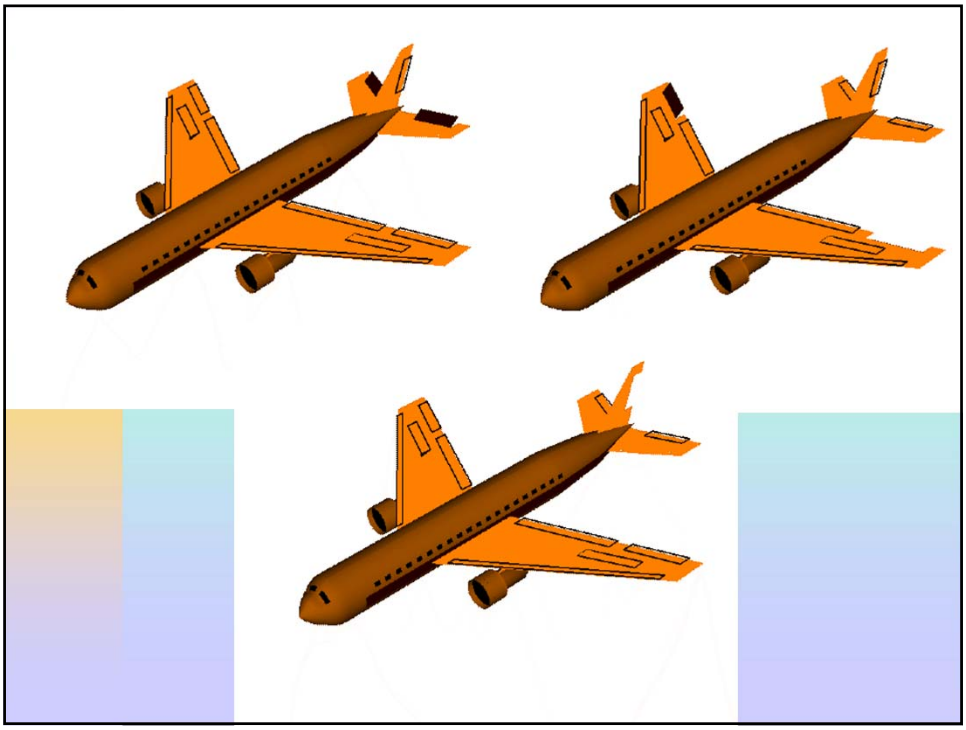
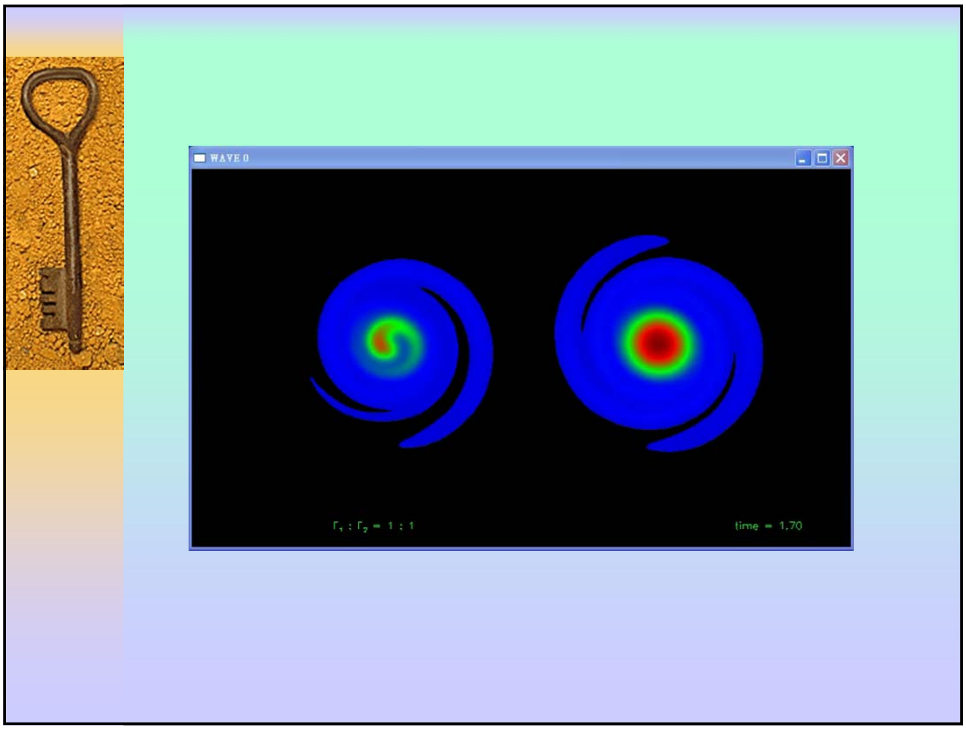
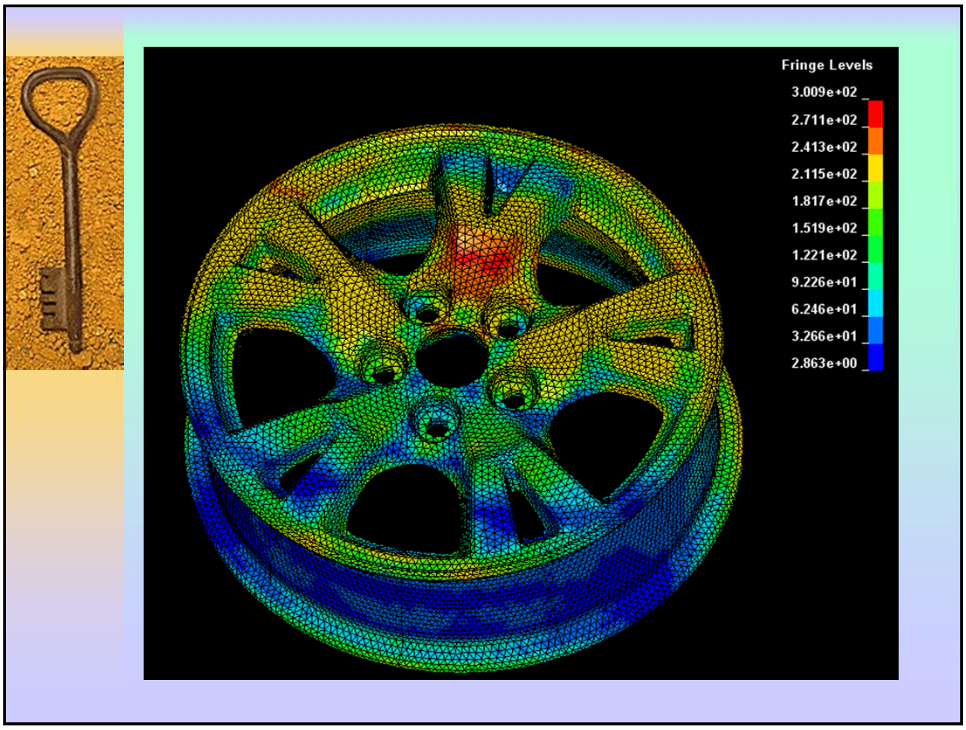
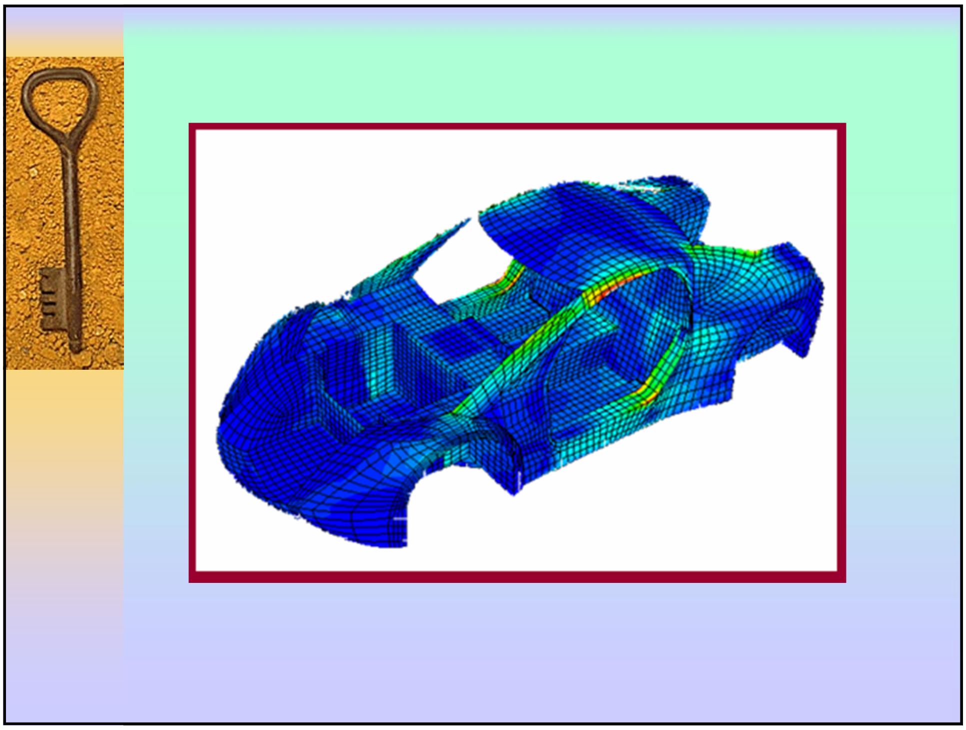
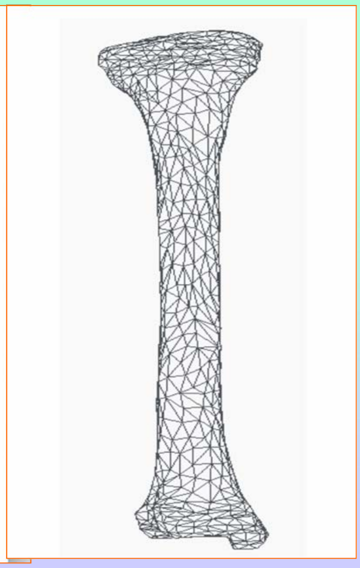
Pr = 6.83
Gr = 2510000
Time = 0.0002
0 0.02 0.04 0.06 0.08 0.1 0.12 0.14 0.16




WAVE 0
$\Gamma_1 : \Gamma_2 = 1 : 1$
time = 1.70


Fringe Levels
3.009e+02
2.711e+02
2.413e+02
2.115e+02
1.817e+02
1.519e+02
1.221e+02
9.226e+01
6.246e+01
3.266e+01
2.863e+00





Happy Summer Vacation!