

Introduction to FEM

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Kengo Nakajima (1/2) 中島研吾

- Current Position
 - Professor, Supercomputing Research Division, Information Technology Center 情報基盤センター
 - Professor, Department of Mathematical Informatics, Graduate School of Information Science & Engineering 数理情報学専攻
 - Professor, Department of Electrical Engineering & Information Systems, Graduate School of Engineering 電気系工学専攻
 - Deputy Director, RIKEN Center for Computational Science (R-CCS) (2018 April -)
- Research Interest
 - High-Performance Computing
 - Parallel Numerical Linear Algebra (Preconditioning)
 - Parallel Programming Model
 - Computational Mechanics, Computational Fluid Dynamics
 - Adaptive Mesh Refinement, Parallel Visualization



Kengo Nakajima (2/2)

- Education
 - B.Eng (Aeronautics, The University of Tokyo, 1985)
 - M.S. (Aerospace Engineering, University of Texas, 1993)
 - Ph.D. (Quantum Engineering & System Sciences, The University of Tokyo, 2003)
- Professional Background
 - Mitsubishi Research Institute, Inc. (1985-1999)
 - Research Organization for Information Science & Technology (1999-2004)
 - The University of Tokyo
 - Department Earth & Planetary Science (2004-2008)
 - Information Technology Center (2008-)
 - JAMSTEC (2008-2011), part-time
 - RIKEN (2009-), part-time

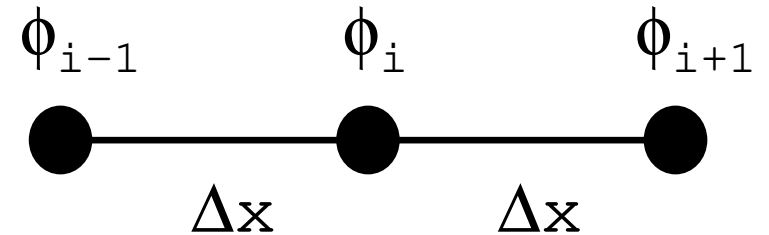
FDM and FEM

- Numerical Method for solving PDE's
 - Space is discretized into small pieces (elements, meshes)
 - PDE: Partial Differential Equation(s) 偏微分方程式
- Finite Difference Method (FDM) (有限) 差分法
 - Differential derivatives are directly approximated using Taylor Series Expansion.

Finite Difference Method (FDM)

Taylor Series Expansion

2nd-Order Central Difference



$$\phi_{i+1} = \phi_i + \Delta x \left(\frac{\partial \phi}{\partial x} \right)_i + \frac{(\Delta x)^2}{2!} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_i + \frac{(\Delta x)^3}{3!} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_i \dots$$

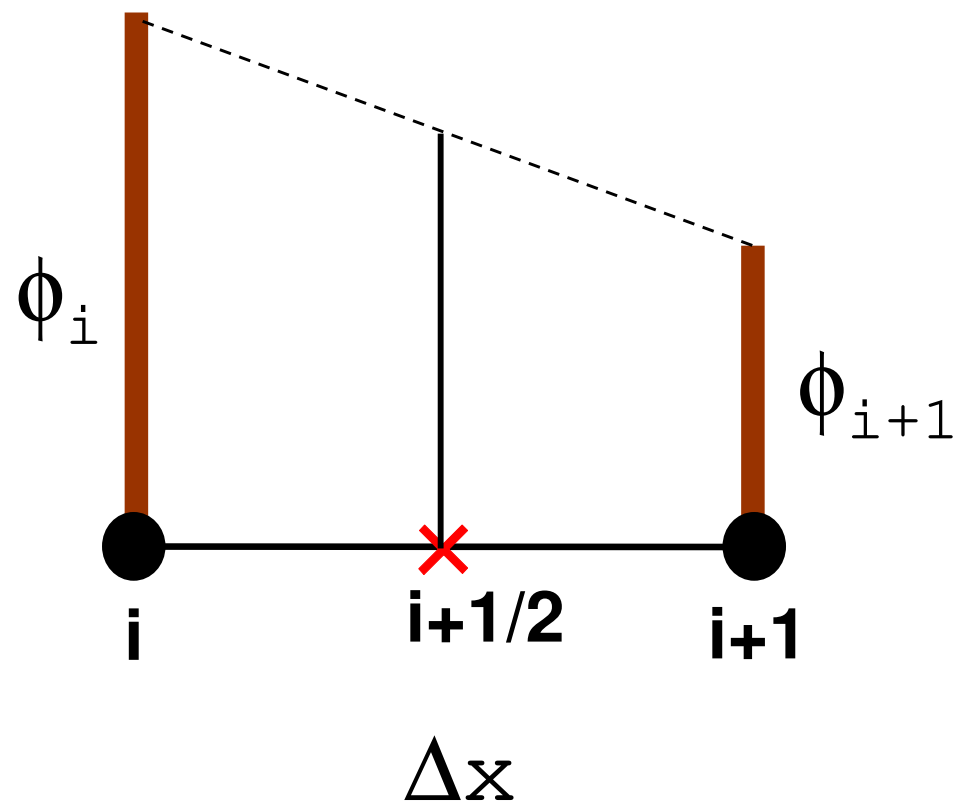
$$\phi_{i-1} = \phi_i - \Delta x \left(\frac{\partial \phi}{\partial x} \right)_i + \frac{(\Delta x)^2}{2!} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_i - \frac{(\Delta x)^3}{3!} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_i \dots$$

$$\frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x} = \left(\frac{\partial \phi}{\partial x} \right)_i + \frac{2 \times (\Delta x)^2}{3!} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_i \dots$$

Finite Difference Method (FDM)

(有限)差分法：巨視的微分
macroscopic differentiation

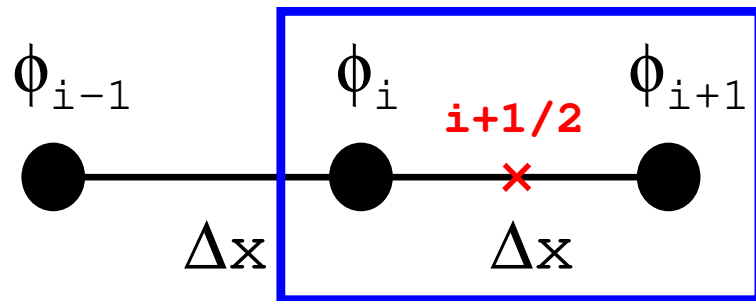
$$\left(\frac{d\phi}{dx}\right)_{i+1/2} \approx \frac{\phi_{i+1} - \phi_i}{\Delta x}$$
$$\left(\frac{d\phi}{dx}\right)_{i+1/2} = \lim_{\Delta x \rightarrow 0} \frac{\phi_{i+1} - \phi_i}{\Delta x}$$



2nd Order Differentiation in FDM

Taylor Series Expansion

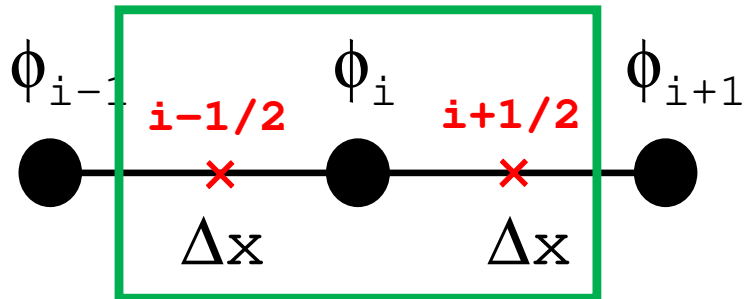
- Approximate Derivative at x (center of i and $i+1$)



$$\left(\frac{d\phi}{dx} \right)_{i+1/2} \approx \frac{\phi_{i+1} - \phi_i}{\Delta x}$$

$\Delta x \rightarrow 0$: Real Derivative

- 2nd-Order Differentiation at i



$$\left(\frac{d^2\phi}{dx^2} \right)_i \approx \frac{\left(\frac{d\phi}{dx} \right)_{i+1/2} - \left(\frac{d\phi}{dx} \right)_{i-1/2}}{\Delta x}$$

$$= \frac{\frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

1D Heat Conduction

- 2nd-Order Central Difference

$$\left(\frac{d^2\phi}{dx^2}\right)_i \approx \frac{\left(\frac{d\phi}{dx}\right)_{i+1/2} - \left(\frac{d\phi}{dx}\right)_{i-1/2}}{\Delta x} = \frac{\frac{\phi_{i+1} - \phi_i}{\Delta x} - \frac{\phi_i - \phi_{i-1}}{\Delta x}}{\Delta x} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

- Linear Equation at Each Grid Point

$$\lambda \frac{d^2\phi}{dx^2} + BF = 0$$



$$\lambda \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} + BF(i) = 0 \quad (1 \leq i \leq N)$$

$$\frac{\lambda}{\Delta x^2} \phi_{i+1} - \frac{2\lambda}{\Delta x^2} \phi_i + \frac{\lambda}{\Delta x^2} \phi_{i-1} + BF(i) = 0 \quad (1 \leq i \leq N)$$

$$A_L(i) \times \phi_{i-1} + A_D(i) \times \phi_i + A_R(i) \times \phi_{i+1} = BF(i) \quad (1 \leq i \leq N)$$

$$A_L(i) = \frac{\lambda}{\Delta x^2}, \quad A_D(i) = -\frac{2\lambda}{\Delta x^2}, \quad A_R(i) = \frac{\lambda}{\Delta x^2}$$

FDM and FEM

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 - PDE: Partial Differential Equation(s) 偏微分方程式
- Finite Difference Method (FDM) (有限) 差分法
 - Differential derivatives are directly approximated using Taylor Series Expansion.
- Finite Element Method (FEM) 有限要素法
 - Solving “weak form” derived from integral equations.
 - “Weak solutions” are obtained.
 - Method of Weighted Residual (MWR), Variational Method
 - Suitable for Complicated Geometries
 - Although FDM can handle complicated geometries ...

FDM can handle complicated geometries: BFC

Handbook of Grid Generation

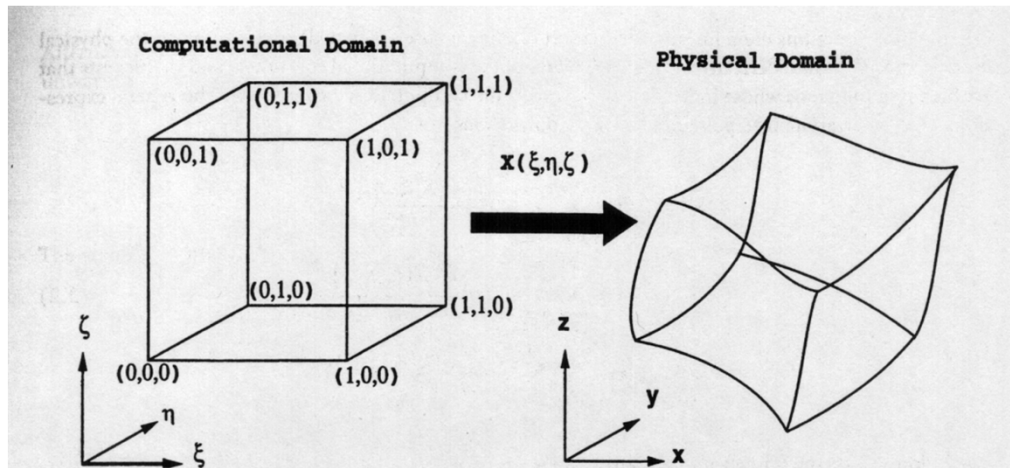


FIGURE 3.1 Transformation between computational and physical domains.

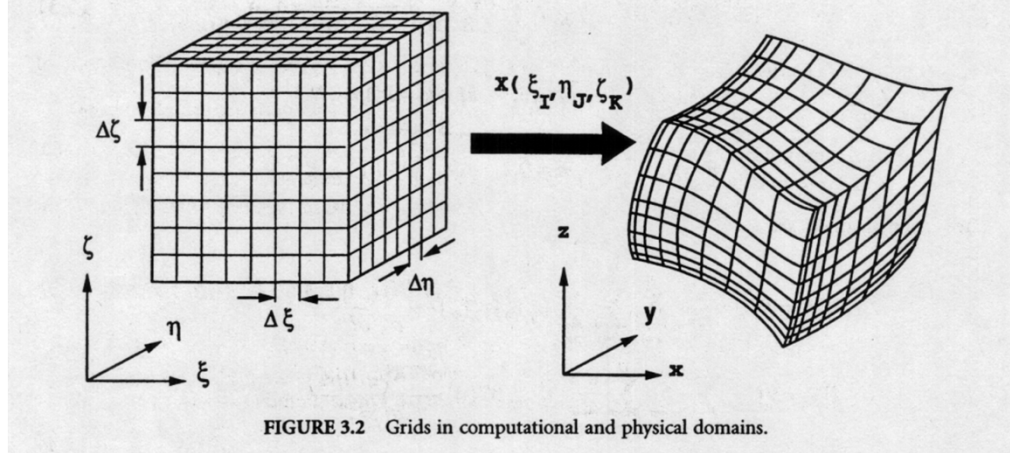
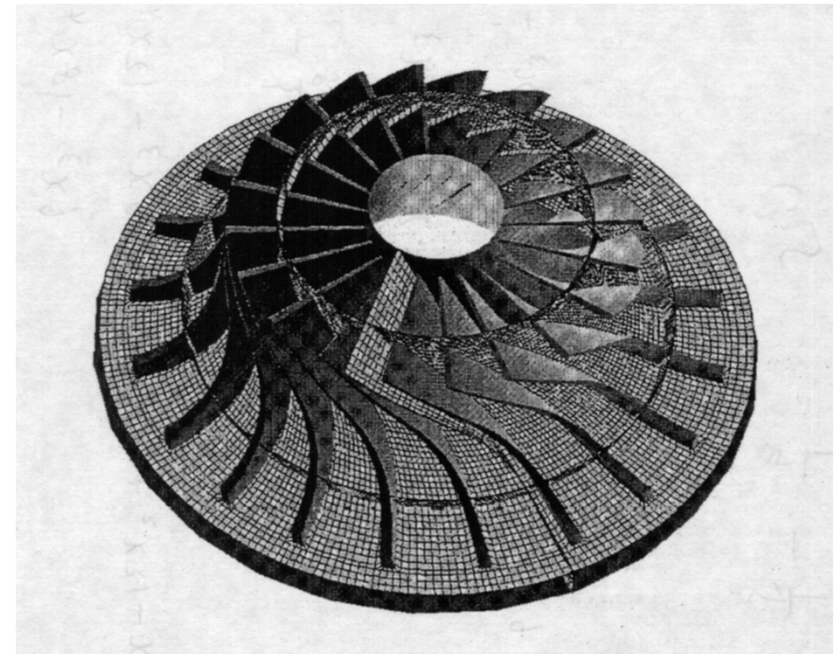


FIGURE 3.2 Grids in computational and physical domains.

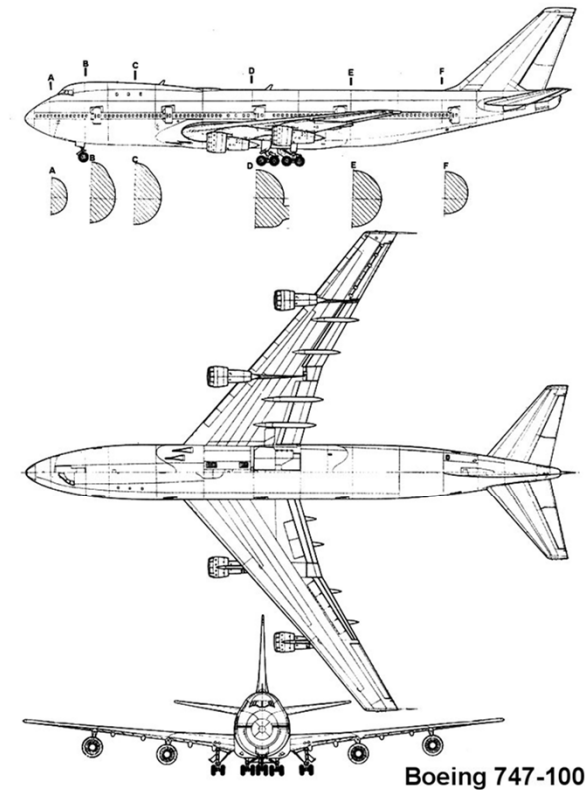
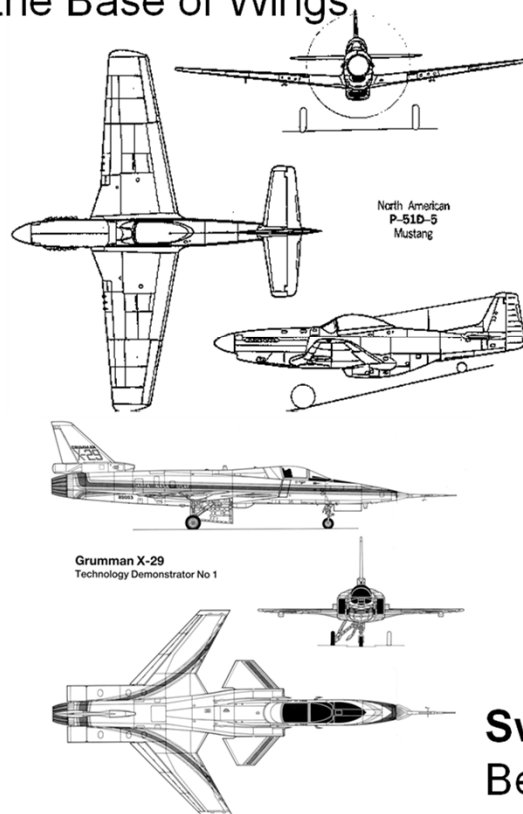


History of FEM

- In 1950's, FEM was originally developed as a method for structure analysis of wings of airplanes under collaboration between Boeing and University of Washington (M.J. Turner, H.C. Martin etc.).

- “Beam Theory” cannot be applied to sweptback wings for airplanes with jet engines.

Straight Wing: Subsonic
Beam Theory for Calc. of Load at the Base of Wings



Swept Wing: Transonic-Supersonic
Beam Theory cannot be applied

History of FEM

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 - “Beam Theory” cannot be applied to sweptback wings for airplanes with jet engines.
- **Extended to Various Applications**
 - Non-Linear: T.J.Oden
 - Non-Structure Mechanics: O.C.Zienkiewicz
- **Commercial Package**
 - **NASTRAN**
 - Originally developed by NASA
 - Commercial Version by MSC
 - PC version is widely used in industries

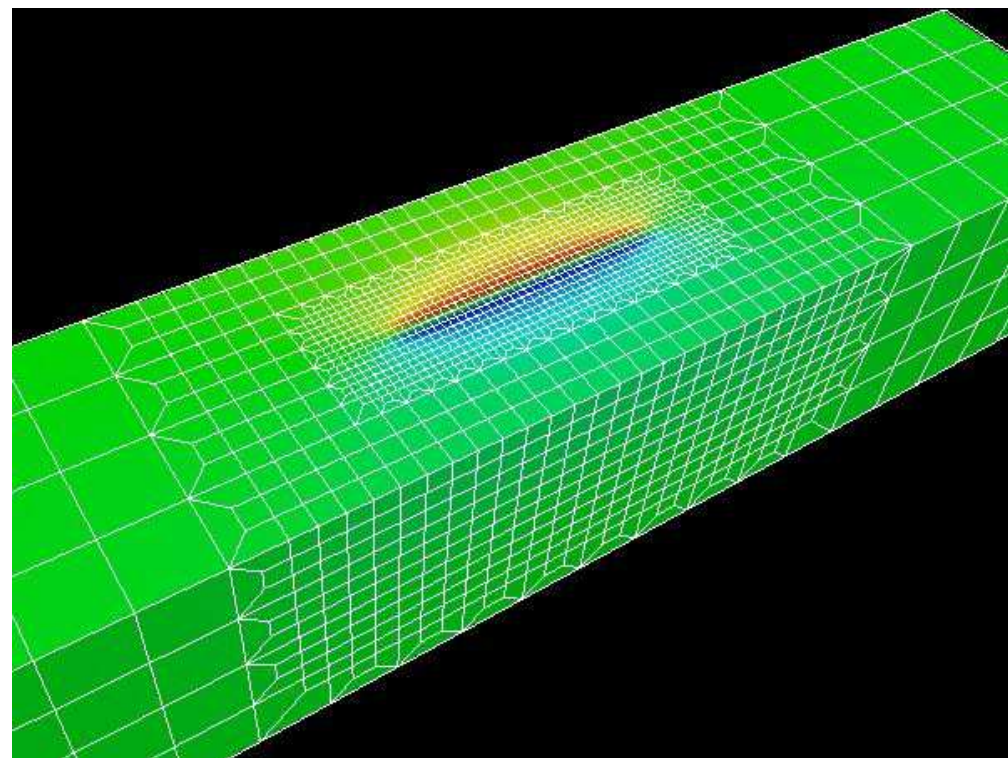
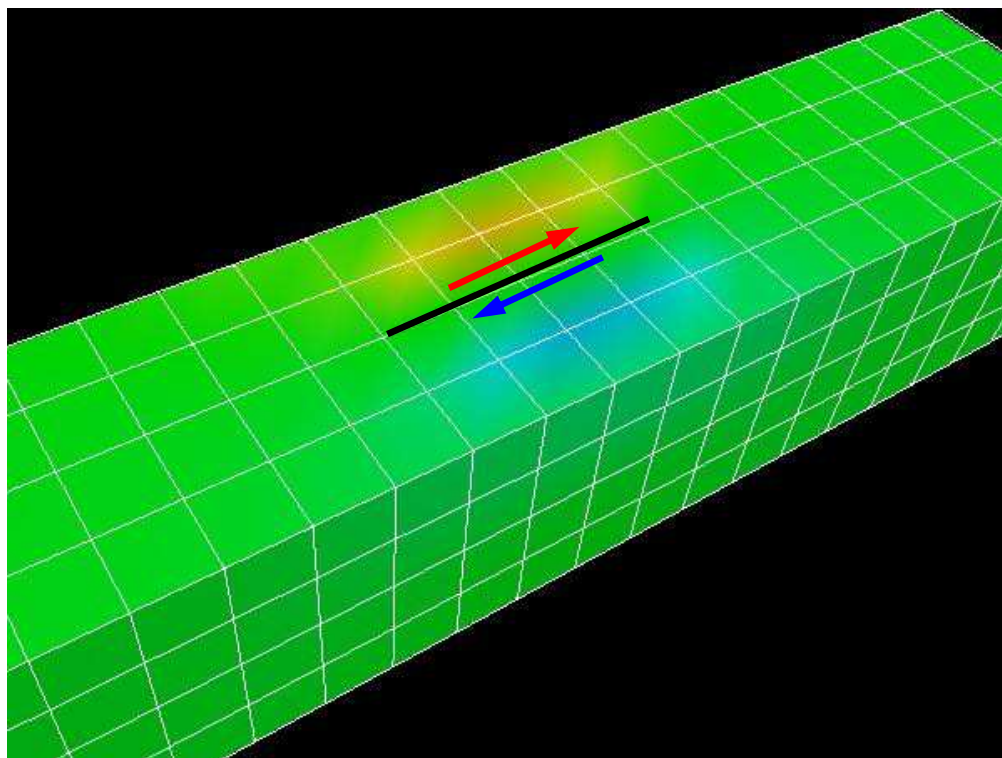
Recent Research Topics

- Non-Linear Problems
 - Crash, Contact, Non-Linear Material
 - Discontinuous Approach
 - X-FEM
- Parallel Computing
 - also in commercial codes
- Adaptive Mesh Refinement (AMR)
 - Shock Wave, Separation
 - Stress Concentration
 - Dynamic Load Balancing (DLB) at Parallel Computing
- Mesh Generation
 - Large-Scale Parallel Mesh Generation

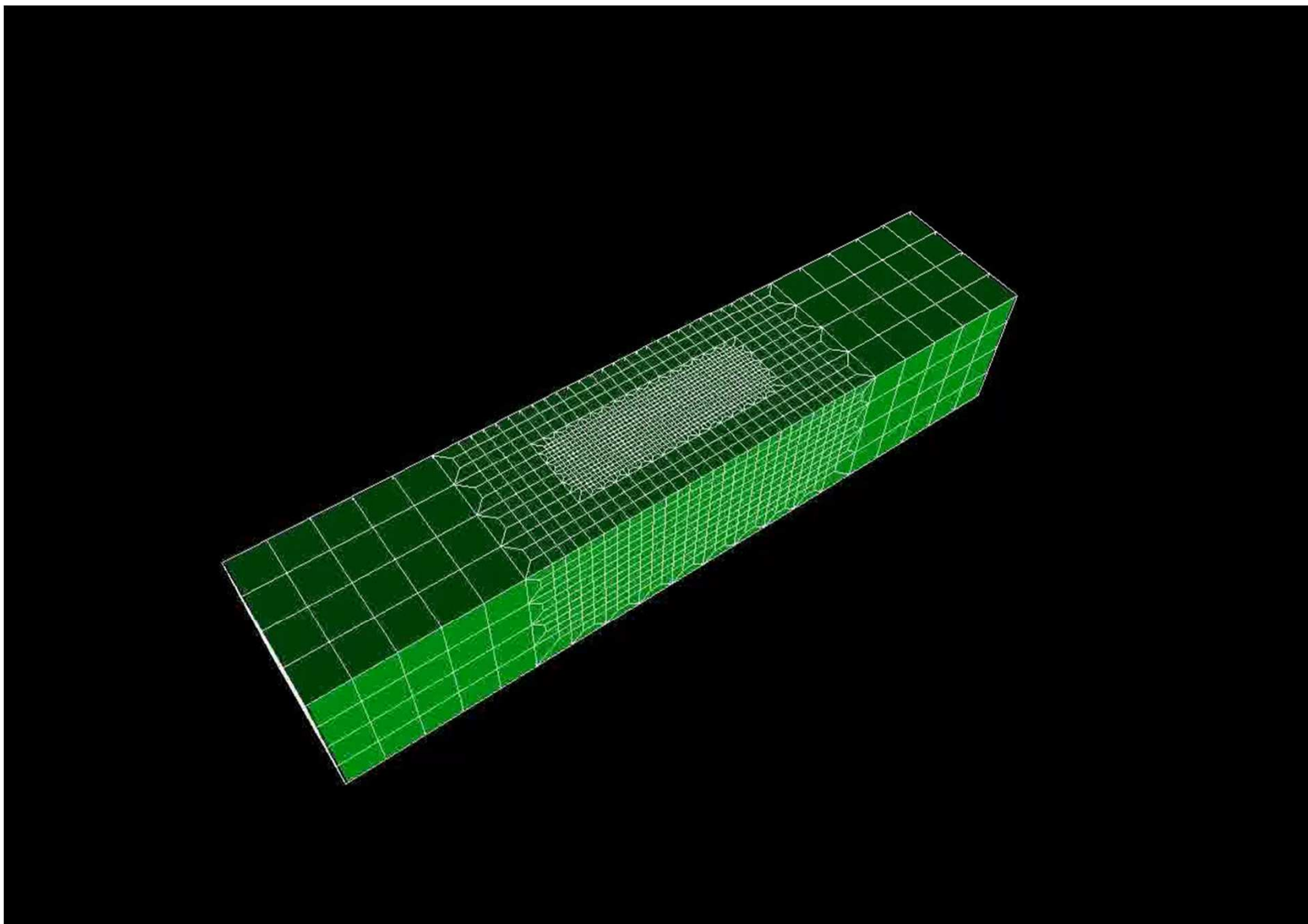
3D Simulations for Earthquake Generation Cycle

San Andreas Faults, CA, USA

Stress Accumulation at Transcurrent Plate Boundaries
Adaptive Mesh Refinement (AMR)

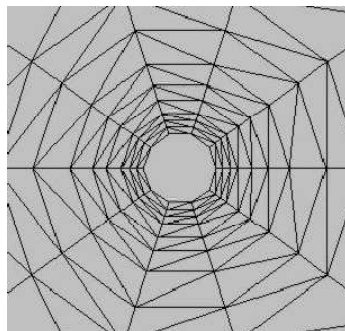
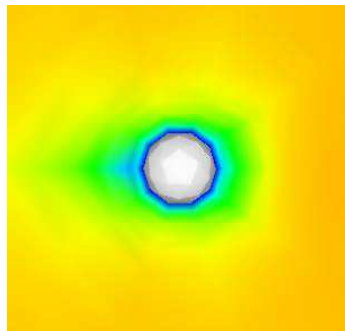


Adaptive FEM: High-resolution needed at meshes with large deformation (large accumulation)

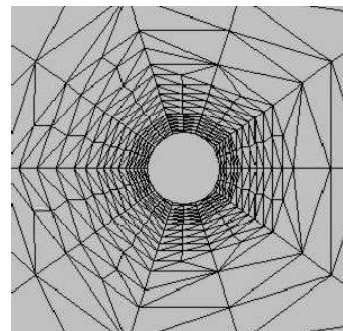
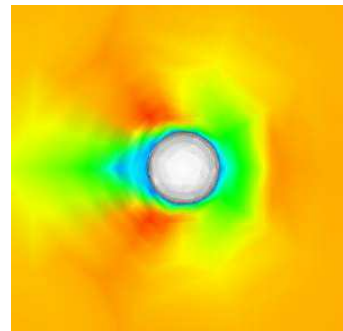


Supersonic Flow around a Sphere

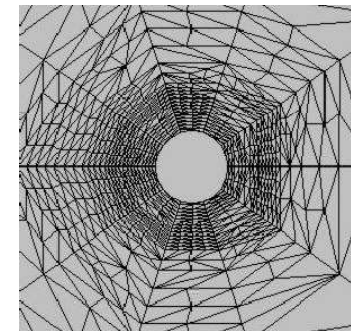
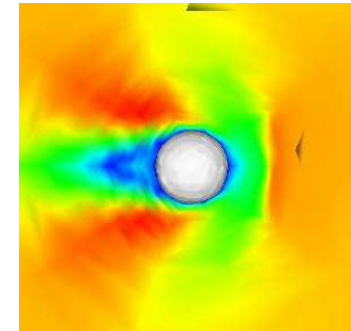
Ideal Gas, $M=1.40$, Uniform Flow, $Re=10^6$
before/after Dynamic Load Balancing



Initial Grid



1-Lev. Adapted



2-Lev. Adapted

			<u>before</u>	<u>after</u>	<u>before</u>	<u>after</u>
PE0	137	-	793	652	3834	2527
PE1	137	-	696	650	2769	2526
PE2	136	-	668	652	2703	2522
PE3	136	-	448	651	1390	2524

- Numerical Method for PDE (Method of Weighted Residual)
- Gauss-Green's Theorem
- Numerical Method for PDE (Variational Method)

Approximation Method for PDE

Partial Differential Equations: 偏微分方程式

- Consider solving the following differential equation (boundary value problem), domain V , boundary S :

$$L(u) = f$$

- u (solution of the equation) can be approximated by function u_M (linear combination)

$$u_M = \sum_{i=1}^M a_i \Psi_i$$

Ψ_i **Trial/Test Function (試行関数)** (known function of position, defined in domain and at boundary. “Basis” in linear algebra.

a_i Coefficients (unknown)

Method of Weighted Residual

MWR: 重み付き残差法

- u_M is exact solution of u if R (residual : 残差) = 0:

$$R = L(u_M) - f$$

- In MWR, consider the condition where the following integration of R multiplied by w (weight/weighting function : 重み関数) over entire domain is 0

$$\int_V w R(u_M) dV = 0$$

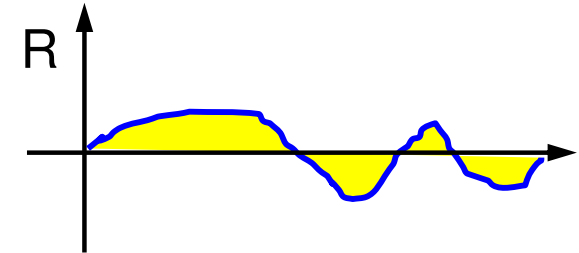
- MWR provides “smoothed” approximate solution, which satisfies $R=0$ in the domain V

Method of Weighted Residual

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- MWR provides “smoothed” approximate solution, which satisfies $R=0$ in the domain V

Variational Method (Ritz) (1/2)

変分法

- It is widely known that exact solution u provides extreme values (max/min) of “functional : 汎関数” $I(u)$
 - Euler equation: differential equation satisfied by u , if functional has extreme values (極値)
 - Euler equation is satisfied, if u provides extreme values of $I(u)$.
 - *provide extreme values* : 停留させる (or *stationarize*)
- For example, functional, which corresponds to governing equations of linear elasticity (principle of virtual work, equilibrium equations), is “principle of minimum potential energy (principle of minimum strain energy) (エネルギー最小, 歪みエネルギー最小)” .

Variational Method (Ritz) (2/2)

変分法

- Substitute the following approx. solution into $I(u)$, and calculate coefficients a_i under the condition where $I_M = I(u_M)$ provides extreme values, then u_M is obtained:

$$u_M = \sum_{i=1}^M a_i \Psi_i$$

- Variational method is theoretical method, and can be only applied to differential equations, which has equivalent variational problem.
 - In this class, we mainly use MWR
 - Brief overview of Ritz method will be given later in this material.

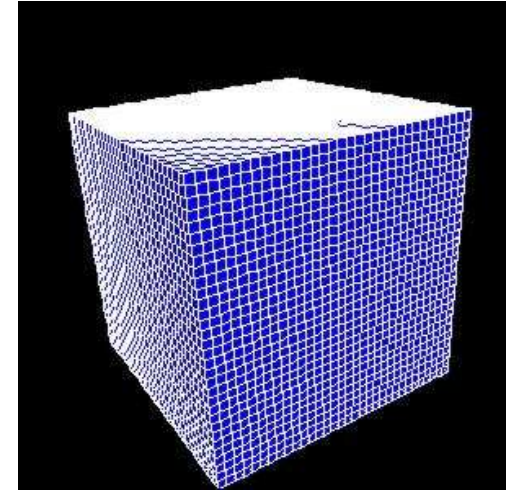
Finite Element Method (FEM)

有限要素法

- Entire region is discretized into fine elements (要素), and the following approximation is applied to each element:

$$u_M = \sum_{i=1}^M a_i \Psi_i$$

- MWR or Variational Method is applied to each element
- Each element matrix is accumulated to global matrix, and solution of obtained linear equations provides approx. solution of PDE.
- **Details of FEM will be provided in the next material.**



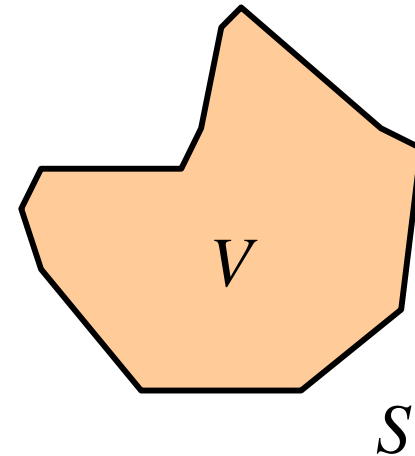
Example of MWR (1/3)

- Thermal Equation

$$\lambda \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + Q = 0 \quad \text{in } V$$

λ : Conductivity, Q : Heat Gen./Volume

$T = 0$ at boundary S



- Approximate Solution

$$T = \sum_{j=1}^n a_j \Psi_j$$

- Residual

$$R(a_j, x, y) = \lambda \sum_{j=1}^n a_j \left(\frac{\partial^2 \Psi_j}{\partial x^2} + \frac{\partial^2 \Psi_j}{\partial y^2} \right) + Q$$

Example of MWR (2/3)

- Multiply weighting function w_i , and apply integration over V :

$$\int_V w_i R dV = 0$$

- If a set of weighting function w_i is a set of n different functions, the above integration provides a set of n linear equations:
 - # trial/test functions = # weighting functions

$$\sum_{j=1}^n a_j \int_V w_i \lambda \left(\frac{\partial^2 \Psi_j}{\partial x^2} + \frac{\partial^2 \Psi_j}{\partial y^2} \right) dV = - \int_V w_i Q dV \quad (i = 1, \dots, n)$$

Example of MWR (3/3)

- Matrix form of the equations is described as follows:

$$[B]\{a\} = \{Q\}$$

$$B_{ij} = \int_V w_i \lambda \left(\frac{\partial^2 \Psi_j}{\partial x^2} + \frac{\partial^2 \Psi_j}{\partial y^2} \right) dV, \quad Q_i = - \int_V w_i Q dV$$

Actual approach is slightly different from this
(more detailed discussions in the next material)

Various types of MWR's

- Various types of weighting functions
- Collocation Method 選点法
- Least Square Method 最小自乗法
- Galerkin Method ガラーキン法

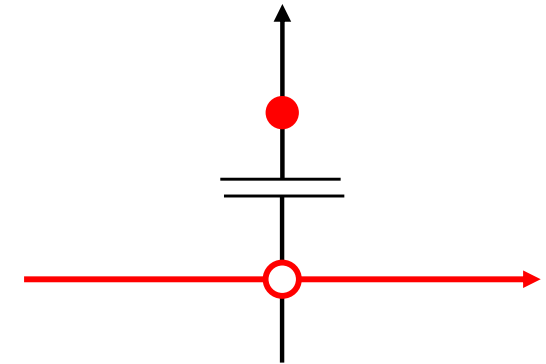
Collocation Method

- Weighting function: Dirac's Delta Function δ

$$\delta(z) = \infty \quad \text{if} \quad z = 0$$

$$\delta(z) = 0 \quad \text{if} \quad z \neq 0, \quad \int_{-\infty}^{+\infty} \delta(z) dz = 1$$

$$w_i = \delta(\mathbf{x} - \mathbf{x}_i) \quad \mathbf{x}: \text{location}$$



- In collocation method, R (residual) is set to 0 at n collocation points by feature of Dirac's Delta Fn. δ :

$$\int_V R \delta(\mathbf{x} - \mathbf{x}_i) dV = R \Big|_{\mathbf{x}=\mathbf{x}_i} \quad \begin{array}{l} \delta(\mathbf{x} - \mathbf{x}_i) = \infty \text{ at } \mathbf{x} = \mathbf{x}_i \\ \delta(\mathbf{x} - \mathbf{x}_i) = 0 \text{ at } \mathbf{x} \neq \mathbf{x}_i \end{array}$$

- If n increases, R approaches to 0 over entire domain.

Least Square Method

- Weighting function:

$$w_i = \frac{\partial R}{\partial a_i}$$

- Minimize the following integration according to a_i (unknowns):

$$I(a_i) = \int_V [R(a_i, \mathbf{x})]^2 dV$$
$$\frac{\partial}{\partial a_i} [I(a_i)] = 2 \int_V \left[R(a_i, \mathbf{x}) \frac{\partial R(a_i, \mathbf{x})}{\partial a_i} \right] dV = 0$$



$$\int_V \left[R(a_i, \mathbf{x}) \frac{\partial R(a_i, \mathbf{x})}{\partial a_i} \right] dV = 0$$

Galerkin Method

- Weighting Function = Test/Trial Function:

$$w_i = \Psi_i$$

- Galerkin, Boris Grigorievich
 - 1871-1945
 - Engineer and Mathematician of Russia
 - He got a hint for Galerkin Method while he was imprisoned because of anti-czarism (1906-1907).



Example (1/2)

- Governing Equation

$$\frac{d^2 u}{dx^2} + u + x = 0 \quad (0 \leq x \leq 1)$$

- Boundary Conditions: Dirichlet

$$u = 0 @ x = 0$$

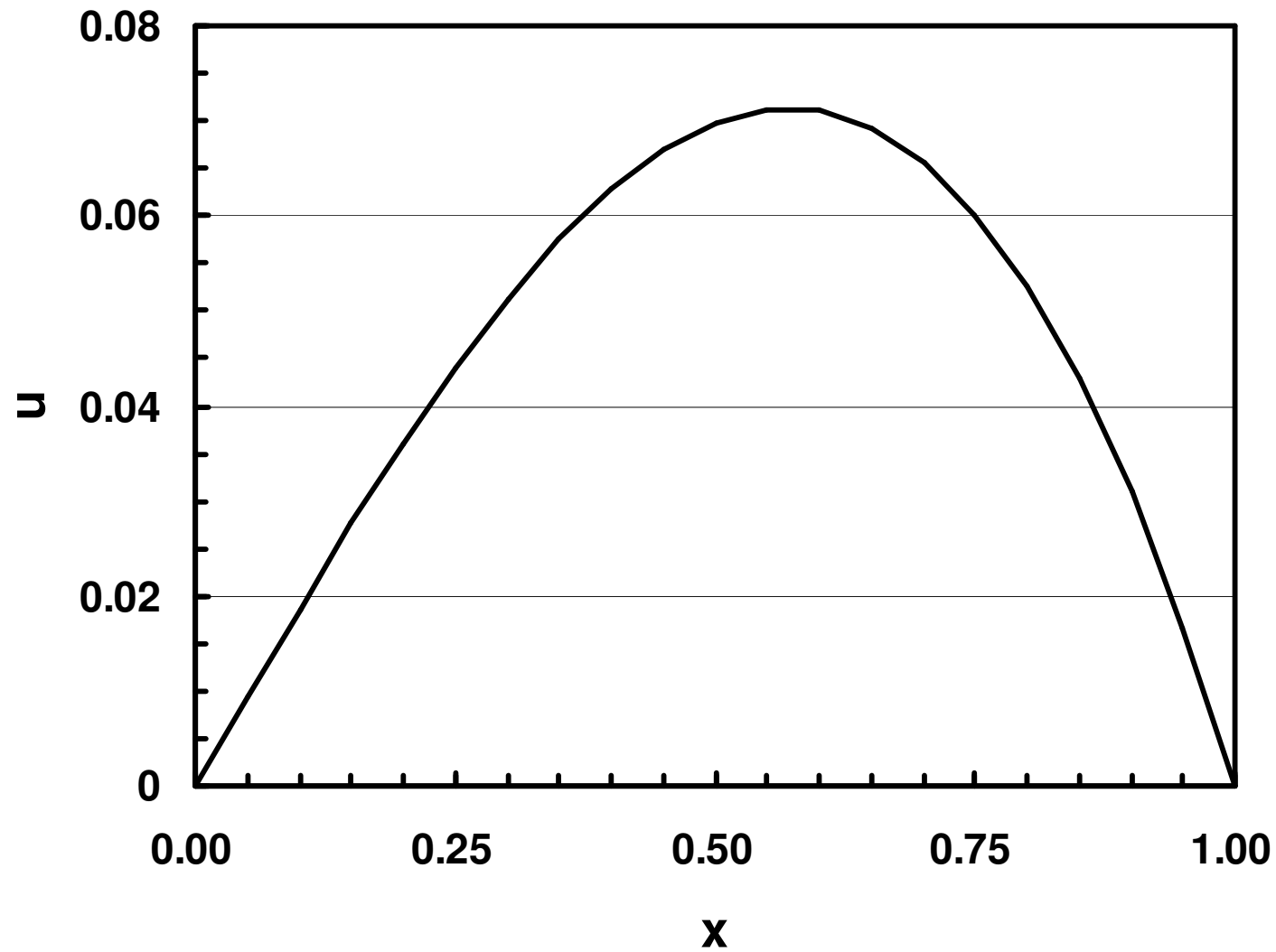
$$u = 0 @ x = 1$$

- Exact Solution

$$u = \frac{\sin x}{\sin 1} - x$$

Exact Solution

$$u = \frac{\sin x}{\sin 1} - x$$



Example (2/2)

- Assume the following approx. solution:

$$u = x(1-x)(a_1 + a_2x) = x(1-x)a_1 + x^2(1-x)a_2 = a_1\Psi_1 + a_2\Psi_2$$

$$\Psi_1 = x(1-x), \quad \Psi_2 = x^2(1-x)$$

Test/trial function satisfies $u=0@x=0,1$

- Residual is as follows:

$$R(a_1, a_2, x) = x + (-2 + x - x^2)a_1 + (2 - 6x + x^2 - x^3)a_2$$

- Let's apply various types of MWR to this equation
 - We have two unknowns (a_1, a_2), therefore we need two independent weighting functions.

Collocation Method

- $n=2$, $x=1/4$, $x=1/2$ for collocation points:

$$R(a_1, a_2, \frac{1}{4}) = 0, \quad R(a_1, a_2, \frac{1}{2}) = 0$$

$$R(a_1, a_2, x) = x + (-2 + x - x^2)a_1 + (2 - 6x + x^2 - x^3)a_2$$

- Solution:

$$\begin{bmatrix} 29/16 & -35/64 \\ 7/4 & 7/8 \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 1/4 \\ 1/2 \end{Bmatrix} \quad \longrightarrow \quad a_1 = \frac{6}{31}, \quad a_2 = \frac{40}{217}$$

$$u = \frac{x(1-x)}{217} (42 + 40x)$$

Least Square Method

- Weighting functions, Residual:

$$w_1 = \frac{\partial R}{\partial a_1} = -2 + x - x^2, \quad w_2 = \frac{\partial R}{\partial a_2} = 2 - 6x + x^2 - x^3$$

$$R(a_1, a_2, x) = x + (-2 + x - x^2)a_1 + (2 - 6x + x^2 - x^3)a_2$$

- Solution:

$$\int_0^1 R(a_1, a_2, x) \frac{\partial R}{\partial a_1} dx = \int_0^1 R(a_1, a_2, x) (-2 + x - x^2) dx = 0$$

$$\int_0^1 R(a_1, a_2, x) \frac{\partial R}{\partial a_2} dx = \int_0^1 R(a_1, a_2, x) (2 - 6x + x^2 - x^3) dx = 0$$

$$\begin{bmatrix} 202 & 101 \\ 707 & 1572 \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 55 \\ 399 \end{Bmatrix} \quad \longrightarrow \quad a_1 = \frac{46161}{246137}, \quad a_2 = \frac{41713}{246137}$$

$$u = \frac{x(1-x)}{246137} (46161 + 41713x)$$

Galerkin Method

- Weighting functions, Residual:

$$w_1 = \Psi_1 = x(1-x), \quad w_2 = \Psi_2 = x^2(1-x)$$

$$R(a_1, a_2, x) = x + (-2 + x - x^2)a_1 + (2 - 6x + x^2 - x^3)a_2$$

- Results:

$$\int_0^1 R(a_1, a_2, x) \Psi_1 dx = \int_0^1 R(a_1, a_2, x) (x - x^2) dx = 0$$

$$\int_0^1 R(a_1, a_2, x) \Psi_2 dx = \int_0^1 R(a_1, a_2, x) (x^2 - x^3) dx = 0$$

$$\begin{bmatrix} 3/10 & 3/20 \\ 3/20 & 13/105 \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 1/12 \\ 1/20 \end{Bmatrix} \quad \longrightarrow \quad a_1 = \frac{71}{369}, \quad a_2 = \frac{7}{41}$$

$$u = \frac{x(1-x)}{369} (71 + 63x)$$

Results

X	Analytical	Collocation 0.25-0.50	Collocation 0.33-0.67	Least- Square	Galerkin
0.25	0.04401	0.04493	0.04462	0.04311	0.04408
0.50	0.06975	0.07143	0.07031	0.06807	0.06944
0.75	0.06006	0.06221	0.06084	0.05900	0.06009

- Galerkin Method provides the most accurate solution
 - If functional exists, solutions of variational method and Galerkin method agree.
 - A kind of analytical solution (later of this material)
- Many commercial FEM codes use Galerkin method.
- In this class, Galerkin method is used.
- Least-square may provide robust solution in Navier-Stokes solvers for high Re.

Homework (1/2)

- Apply the following two methods in the next page to the same equations:
 - Method of Moment
 - Sub-Domain Method
 - Results at $x=0.25, 0.50, 0.75$
- Compare the results of “collocation method” on “non-collocation points” with exact solution
 - Explain the behavior
 - Try different collocation points

Homework (2/2)

- Method of Moment (モーメント法)

$$w_i = \mathbf{x}^{i-1} \quad (i \geq 1)$$

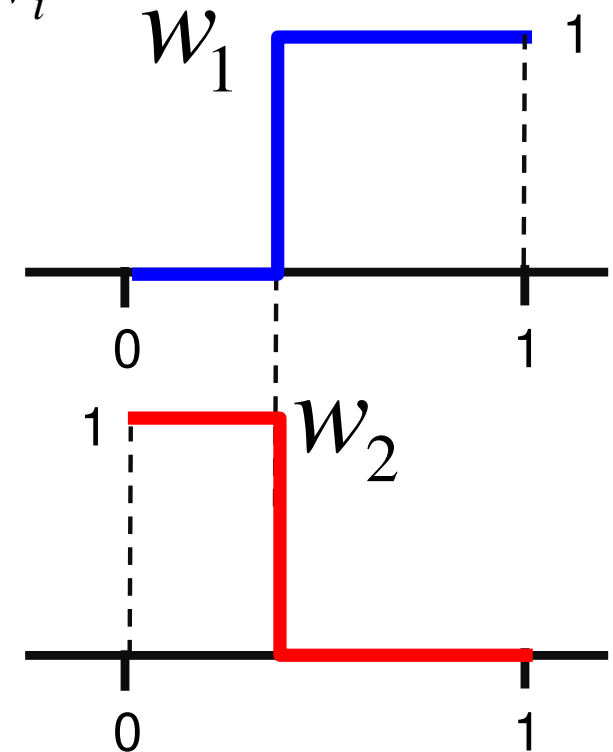
- Weighting functions ?

- Sub-Domain Method (部分領域法)

- Domain V is divided into sub-domains V_i ($i=1-n$), and weighting functions w_i are given as follows:

$$w_i = \begin{cases} 1 & \text{for points in } V_i \\ 0 & \text{for points out of } V_i \end{cases}$$

- Two unknowns, two sub domains
- Two sub-domains do not share any overlaps

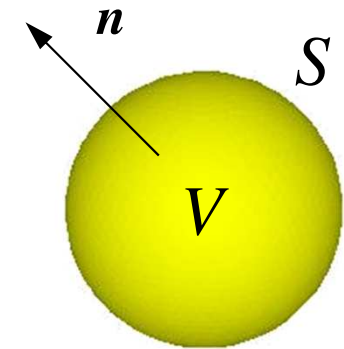


- Numerical Method for PDE (Method of Weighted Residual)
- Gauss-Green's Theorem
- Numerical Method for PDE (Variational Method)

Gauss's Theorem

$$\int_V \left(\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} \right) dV = \int_S (Un_x + Vn_y + Wn_z) dS$$

- 3D (x, y, z)
- Domain V surrounded by smooth closed surface S
- 3 continuous functions defined in V :
 - $U(x, y, z), V(x, y, z), W(x, y, z)$
- Outward normal vector \mathbf{n} on surface S :
 - n_x, n_y, n_z : direction cosine



Green's Theorem (1/2)

- Assume the following functions:

$$U = A \frac{\partial B}{\partial x}, \quad V = A \frac{\partial B}{\partial y}, \quad W = A \frac{\partial B}{\partial z}$$

- Thus :

$$\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} = A \left(\frac{\partial^2 B}{\partial x^2} + \frac{\partial^2 B}{\partial y^2} + \frac{\partial^2 B}{\partial z^2} \right) + \left(\frac{\partial A}{\partial x} \frac{\partial B}{\partial x} + \frac{\partial A}{\partial y} \frac{\partial B}{\partial y} + \frac{\partial A}{\partial z} \frac{\partial B}{\partial z} \right)$$

- Apply Gauss's theorem:

$$\begin{aligned} & \int_V A \left(\frac{\partial^2 B}{\partial x^2} + \frac{\partial^2 B}{\partial y^2} + \frac{\partial^2 B}{\partial z^2} \right) dV + \int_V \left(\frac{\partial A}{\partial x} \frac{\partial B}{\partial x} + \frac{\partial A}{\partial y} \frac{\partial B}{\partial y} + \frac{\partial A}{\partial z} \frac{\partial B}{\partial z} \right) dV \\ &= \int_S (Un_x + Vn_y + Wn_z) dS = \int_S A \left(\frac{\partial B}{\partial x} n_x + \frac{\partial B}{\partial y} n_y + \frac{\partial B}{\partial z} n_z \right) dS \end{aligned}$$

Green's Theorem (2/2)

- (cont.)

$$\int_S A \left(\frac{\partial B}{\partial x} n_x + \frac{\partial B}{\partial y} n_y + \frac{\partial B}{\partial z} n_z \right) dS = \int_S A \left(\frac{\partial B}{\partial x} \frac{\partial x}{\partial n} + \frac{\partial B}{\partial y} \frac{\partial y}{\partial n} + \frac{\partial B}{\partial z} \frac{\partial z}{\partial n} \right) dS$$

$$= \int_S A \frac{\partial B}{\partial n} dS \quad \frac{\partial B}{\partial n} \text{ Gradient of } B \text{ to the direction of normal vector}$$

- Finally:

$$\int_V A \left(\frac{\partial^2 B}{\partial x^2} + \frac{\partial^2 B}{\partial y^2} + \frac{\partial^2 B}{\partial z^2} \right) dV = \int_S A \frac{\partial B}{\partial n} dS - \int_V \left(\frac{\partial A}{\partial x} \frac{\partial B}{\partial x} + \frac{\partial A}{\partial y} \frac{\partial B}{\partial y} + \frac{\partial A}{\partial z} \frac{\partial B}{\partial z} \right) dV$$

- Appears often after next class
 - From 2nd order differentiation to 1st order differentiation.

In Vector Form

- Gauss's Theorem

$$\int_V \nabla \cdot \mathbf{w} \, dV = \int_S \mathbf{w}^T \mathbf{n} \, dS$$

- Green's Theorem

$$\int_V v \Delta u \, dV = \int_S (v \nabla u)^T \mathbf{n} \, dS - \int_V (\nabla^T v)(\nabla u) \, dV$$

- Numerical Method for PDE (Method of Weighted Residual)
- Gauss-Green's Theorem
- Numerical Method for PDE (Variational Method)

Variational Method (Ritz) (1/2)

変分法

- It is widely known that exact solution u provides extreme values (max/min) of “functional : 汎関数” $I(u)$
 - Euler equation: differential equation satisfied by u , if functional has extreme values (極値)
 - Euler equation is satisfied, if u provides extreme values of $I(u)$.
 - *provide extreme values* : 停留させる (or *stationarize*)
- For example, functional, which corresponds to governing equations of linear elasticity (principle of virtual work, equilibrium equations), is “principle of minimum potential energy (principle of minimum strain energy) (エネルギー最小, 歪みエネルギー最小)” .

Variational Method (Ritz) (2/2)

変分法

- Substitute the following approx. solution into $I(u)$, and calculate coefficients a_i under the condition where $I_M = I(u_M)$ provides extreme values, then u_M is obtained:

$$u_M = \sum_{i=1}^M a_i \Psi_i$$

- Variational method is theoretical method, and can be only applied to differential equations, which has equivalent variational problem.
 - In this class, we mainly use MWR
 - Brief overview of Ritz method will be given.

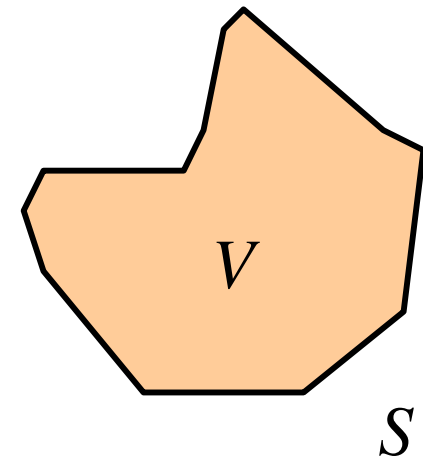
Application of Variational Method (1/5)

- Consider the following integration $I(u)$ in 2D-domain V , where $u(x,y)$ is unknown function of x and y :

$$I(u) = \int_V \frac{1}{2} \left\{ \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 - 2Qu \right\} dV$$

Q : known value

$u = 0$ at boundary S



- $I(u)$ is “functional (汎関数)” of function u
- u^* is a twice continuously differentiable function and minimizes $I(u)$. η is an arbitrary function which satisfies $\eta=0$ at boundary S , and α is a parameter. Consider the following equation:

$$u(x, y) = u^*(x, y) + \alpha \cdot \eta(x, y)$$

Application of Variational Method (2/5)

- At this stage, the following condition is necessary (必要条件) :

$$I(u) \geq I(u^*)$$

- Assume that functional $I(u^* + \alpha\eta)$ is a function of α . Functional I provides minimum value, if $\alpha=0$. Therefore, the following equation is obtained:

$$\left. \frac{\partial}{\partial \alpha} I(u^* + \alpha \cdot \eta) \right|_{\alpha=0} = 0$$

- According to the definition of functional $I(u)$, following equation is obtained (next page)

$$\int_V \left(\frac{\partial u^*}{\partial x} \frac{\partial \eta}{\partial x} + \frac{\partial u^*}{\partial y} \frac{\partial \eta}{\partial y} - Q\eta \right) dV = 0$$

$$I(u) = \int_V \frac{1}{2} \left\{ \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 - 2Qu \right\} dV$$

$$u(x, y) = u^*(x, y) + \alpha \cdot \eta(x, y)$$

$$\left. \frac{\partial}{\partial \alpha} I(u^* + \alpha \cdot \eta) \right|_{\alpha=0} = 0$$

$$\frac{\partial}{\partial \alpha} \left\{ \frac{1}{2} \left(\frac{\partial u}{\partial x} \right)^2 \right\} = \frac{\partial u}{\partial x} \cdot \frac{\partial}{\partial \alpha} \left(\frac{\partial u}{\partial x} \right), \quad \frac{\partial u}{\partial x} = \frac{\partial(u^* + \alpha \cdot \eta)}{\partial x} = \frac{\partial u^*}{\partial x} + \alpha \frac{\partial \eta}{\partial x}$$

$$\frac{\partial}{\partial \alpha} \left(\frac{\partial u}{\partial x} \right) = \frac{\partial \eta}{\partial x}, \quad \alpha = 0 \Rightarrow \frac{\partial}{\partial \alpha} \left\{ \frac{1}{2} \left(\frac{\partial u}{\partial x} \right)^2 \right\} = \frac{\partial u^*}{\partial x} \frac{\partial \eta}{\partial x}, \quad \frac{\partial}{\partial \alpha} \left\{ \frac{1}{2} \left(\frac{\partial u}{\partial y} \right)^2 \right\} = \frac{\partial u^*}{\partial y} \frac{\partial \eta}{\partial y}$$

$$\frac{\partial}{\partial \alpha} (Qu) = Q \frac{\partial(u^* + \alpha \cdot \eta)}{\partial \alpha} = Q\eta$$

$$\int_V \left(\frac{\partial u^*}{\partial x} \frac{\partial \eta}{\partial x} + \frac{\partial u^*}{\partial y} \frac{\partial \eta}{\partial y} - Q\eta \right) dV = 0$$

Application of Variational Method (3/5)

- Apply Green's theorem on 1st and 2nd term of LHS, and apply integration by parts, then following equation is obtained: ($A=\eta$, $B=u^*$) (next page) :

$$-\int_V \left(\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} + Q \right) \eta \, dV + \int_S \eta \frac{\partial u^*}{\partial n} \, dS = 0$$

where $\frac{\partial u^*}{\partial n} = \frac{\partial u^*}{\partial x} n_x + \frac{\partial u^*}{\partial y} n_y$ Gradient of u^* in the direction of normal vector

- At boundary S , $\eta=0$:

$$-\int_V \left(\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} + Q \right) \eta \, dV = 0$$

- (A) is required, if the above is true for arbitrary η

$$\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} + Q = 0 \quad (\text{A})$$

Green's Theorem

$$\int_V \left(\frac{\partial u^*}{\partial x} \frac{\partial \eta}{\partial x} + \frac{\partial u^*}{\partial y} \frac{\partial \eta}{\partial y} - Q\eta \right) dV = 0$$

- $(A = \eta, B = u^*)$:

$$\int_V A \left(\frac{\partial^2 B}{\partial x^2} + \frac{\partial^2 B}{\partial y^2} \right) dV = \int_S A \frac{\partial B}{\partial n} dS - \int_V \left(\frac{\partial A}{\partial x} \frac{\partial B}{\partial x} + \frac{\partial A}{\partial y} \frac{\partial B}{\partial y} \right) dV$$

$$\int_V \eta \left(\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} \right) dV = \int_S \eta \frac{\partial u^*}{\partial n} dS - \int_V \left(\frac{\partial \eta}{\partial x} \frac{\partial u^*}{\partial x} + \frac{\partial \eta}{\partial y} \frac{\partial u^*}{\partial y} \right) dV$$

$$\int_V \left(\frac{\partial \eta}{\partial x} \frac{\partial u^*}{\partial x} + \frac{\partial \eta}{\partial y} \frac{\partial u^*}{\partial y} \right) dV = - \int_V \eta \left(\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} \right) dV + \int_S \eta \frac{\partial u^*}{\partial n} dS$$

Application of Variational Method (4/5)

- Equation (A) is called “Euler equation”
 - Necessary condition (必要条件) of u^* , which minimizes functional $I(u)$, is that u^* satisfies the Euler equation.
- Sufficient condition (充分条件)
 - Assume that u^* is solution of the Euler equation and $\alpha\eta = \delta u^*$

$$I(u^* + \delta u^*) - I(u^*) =$$

$$-\int_V \left(\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} + Q \right) \delta u^* dV + \int_V \frac{1}{2} \left\{ \left(\frac{\partial(\delta u^*)}{\partial x} \right)^2 + \left(\frac{\partial(\delta u^*)}{\partial y} \right)^2 \right\} dV$$

$$\delta I = 0$$

First Variation

第一变分

$$\delta I^2 \geq 0$$

Second Variation

第二变分

Application of Variational Method (5/5)

- It has been proved that u^* (solution of Euler equation) minimizes functional $I(u)$.

$$I(u^* + \delta u^*) \geq I(u^*)$$

- Therefore, boundary value problem by Euler equation (A) with B.C. ($u=0@S$) is equivalent to variational problem.
 - Solving equivalent variational problem provides solution of Euler equation (Poisson's equation/Heat Conduction Equation in this case)
 - Functional must exist !

$$\frac{\partial^2 u^*}{\partial x^2} + \frac{\partial^2 u^*}{\partial y^2} + Q = 0 \quad (A)$$

Approx. by Variational Method (1/4)

- Functional

$$I(u) = \int_0^1 \left\{ \frac{1}{2} \left(\frac{du}{dx} \right)^2 - \frac{1}{2} u^2 - xu \right\} dx$$

- Boundary Condition

$$u = 0 @ x = 0$$

$$u = 0 @ x = 1$$

- Obtain u , which “stationalizes” functional $I(u)$ under this B.C.

– Corresponding Euler equation is as follows (same as equation in **p.29**):

$$\frac{d^2 u}{dx^2} + u + x = 0 \quad (0 \leq x \leq 1)$$

(B-1)

Approx. by Variational Method (2/4)

- Assume the following test function with n -th order for function u , which is twice continuously differentiable:

$$u_n = x \cdot (1-x) \cdot (a_1 + a_2x + a_3x^2 + \cdots + a_nx^{n-1}) \quad (\text{B-2})$$

- If we increase the order of test function, u_n is closer to exact solution u . Therefore, functional $I(u)$ can be approximated by $I(u_n)$:
 - If $I(u_n)$ stationarizes, $I(u)$ also stationarizes.
- We need to obtain set of unknown coefficients a_k , which satisfies the following stationary condition:

$$\frac{\partial I(u_n)}{\partial a_k} = 0 \quad (k = 1 \sim n) \quad (\text{B-3})$$

Ritz Method

- Equation (B-3) is linear equations for a_1-a_n .
- If this solutions is applied to equation (B-2), approximate solution, which satisfies Euler equation (B-1), is obtained.
 - Approximate solution, but stationarizes $I(u)$ strictly
- This type of method using a set of coefficients a_1-a_n is called “Ritz Method”.

Approx. by Variational Method (3/4)

- Ritz Method, $n=2$

$$u_2 = x \cdot (1-x) \cdot (a_1 + a_2 x) = x \cdot (1-x) \cdot a_1 + x^2 \cdot (1-x) \cdot a_2$$

$$\begin{aligned} \frac{\partial I(u_2)}{\partial a_1} = 0 \Rightarrow & \left[\int_0^1 (1-x-x^2)(1-3x+x^2) dx \right] a_1 \\ & + \left[\int_0^1 \left\{ (1-2x)(2x-3x^2) - x^3(1-x)^2 \right\} dx \right] a_2 + \int_0^1 x^2(1-x) dx = 0 \end{aligned}$$

$$\begin{aligned} \frac{\partial I(u_2)}{\partial a_2} = 0 \Rightarrow & \left[\int_0^1 \left\{ (1-2x)(2x-3x^2) - x^3(1-x)^2 \right\} dx \right] a_1 \\ & + \left[\int_0^1 (2x-3x^2+x^3)(2x-2x^2-x^3) dx \right] a_2 + \int_0^1 x^3(1-x) dx = 0 \end{aligned}$$

Supplementation for (3/4) (1/3)

- Ritz Method, $n=2$

$$u_2 = x \cdot (1-x) \cdot (a_1 + a_2 x) = x \cdot (1-x) \cdot a_1 + x^2 \cdot (1-x) \cdot a_2$$

$$I(u) = \int_0^1 \left\{ \frac{1}{2} \left(\frac{du}{dx} \right)^2 - \frac{1}{2} u^2 - xu \right\} dx$$

$$\frac{1}{2} \left(\frac{du}{dx} \right)^2 - \frac{1}{2} u^2 - xu =$$

$$\frac{1}{2} \left[(1-2x)a_1 + (2x-3x^2)a_2 \right]^2 - \frac{1}{2} \left[x \cdot (1-x) \cdot a_1 + x^2 \cdot (1-x) \cdot a_2 \right]^2 - \left[x^2 \cdot (1-x) \cdot a_1 + x^3 \cdot (1-x) \cdot a_2 \right]$$

Supplementation for (3/4) (2/3)

$$\frac{1}{2} \left(\frac{du}{dx} \right)^2 - \frac{1}{2} u^2 - xu =$$

$$\frac{1}{2} \left[(1-2x)a_1 + (2x-3x^2)a_2 \right]^2 - \frac{1}{2} \left[x \cdot (1-x) \cdot a_1 + x^2 \cdot (1-x) \cdot a_2 \right]^2 - \left[x^2 \cdot (1-x) \cdot a_1 + x^3 \cdot (1-x) \cdot a_2 \right]$$

$$\frac{\partial I(u_2)}{\partial a_1} = 0 \Rightarrow$$

$$\left[\int_0^1 \left\{ (1-2x)^2 - x^2 \cdot (1-x)^2 \right\} dx \right] a_1 + \left[\int_0^1 \left\{ (1-2x)(2x-3x^2) - x^3 \cdot (1-x)^2 \right\} dx \right] a_2 - \int_0^1 x^2 \cdot (1-x) dx = 0$$

Supplementation for (3/4) (3/3)

$$\frac{1}{2} \left(\frac{du}{dx} \right)^2 - \frac{1}{2} u^2 - xu =$$

$$\frac{1}{2} \left[(1-2x)a_1 + (2x-3x^2)a_2 \right]^2 - \frac{1}{2} \left[x \cdot (1-x) \cdot a_1 + x^2 \cdot (1-x) \cdot a_2 \right]^2 - \left[x^2 \cdot (1-x) \cdot a_1 + x^3 \cdot (1-x) \cdot a_2 \right]$$

$$\frac{\partial I(u_2)}{\partial a_2} = 0 \Rightarrow$$

$$\left[\int_0^1 \left\{ (1-2x)(2x-3x^2) - x^3 \cdot (1-x)^2 \right\} dx \right] a_1 + \left[\int_0^1 \left\{ (2-3x^2)^2 - x^4 \cdot (1-x)^2 \right\} dx \right] a_2 - \int_0^1 x^3 \cdot (1-x) dx = 0$$

Approx. by Variational Method (4/4)

- Final linear equations are as follows:

$$\begin{bmatrix} 3/10 & 3/20 \\ 3/20 & 13/105 \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 1/12 \\ 1/20 \end{Bmatrix} \quad \longrightarrow \quad a_1 = \frac{71}{369}, \quad a_2 = \frac{7}{41}$$

$$u = \frac{x(1-x)}{369} (71 + 63x)$$

- This result is identical with that of Galerkin Method
– NOT a coincidence !!

Galerkin Method

- Weighting functions (which satisfy $u=0$ @ $x=0,1$),
Residual:

$$w_1 = \Psi_1 = x(1-x), \quad w_2 = \Psi_2 = x^2(1-x)$$

$$R(a_1, a_2, x) = x + (-2 + x - x^2)a_1 + (2 - 6x + x^2 - x^3)a_2$$

- Results:

$$\int_0^1 R(a_1, a_2, x) \Psi_1 dx = \int_0^1 R(a_1, a_2, x) (x - x^2) dx = 0$$

$$\int_0^1 R(a_1, a_2, x) \Psi_2 dx = \int_0^1 R(a_1, a_2, x) (x^2 - x^3) dx = 0$$

$$\begin{bmatrix} 3/10 & 3/20 \\ 3/20 & 13/105 \end{bmatrix} \begin{Bmatrix} a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} 1/12 \\ 1/20 \end{Bmatrix} \quad \longrightarrow \quad a_1 = \frac{71}{369}, \quad a_2 = \frac{7}{41}$$

$$u = \frac{x(1-x)}{369} (71 + 63x)$$

Ritz Method & Galerkin Method (1/4)

$$u_2 = x \cdot (1-x) \cdot (a_1 + a_2 x) = a_1 w_1 + a_2 w_2$$

$$I(u) = \int_0^1 \left\{ \frac{1}{2} \left(\frac{du}{dx} \right)^2 - \frac{1}{2} u^2 - xu \right\} dx$$

$$\frac{\partial}{\partial a_1} \left[\frac{1}{2} \left(\frac{du_2}{dx} \right)^2 \right] = \frac{du_2}{dx} \cdot \frac{\partial}{\partial a_1} \left(\frac{du_2}{dx} \right) = \left(a_1 \frac{dw_1}{dx} + a_2 \frac{dw_2}{dx} \right) \frac{dw_1}{dx}$$

$$\frac{\partial}{\partial a_1} \left[\frac{1}{2} u_2^2 \right] = u_2 \cdot \frac{\partial u_2}{\partial a_1} = (a_1 w_1 + a_2 w_2) \cdot w_1$$

$$\frac{\partial}{\partial a_1} [xu_2] = x \cdot \frac{\partial u_2}{\partial a_1} = x \cdot w_1$$

$$\frac{\partial I(u_2)}{\partial a_1} = 0 \Rightarrow$$

$$\left[\int_0^1 \left\{ \left(\frac{dw_1}{dx} \right)^2 a_1 + \frac{dw_1}{dx} \frac{dw_2}{dx} a_2 \right\} dx \right] - \left[\int_0^1 w_1 \{ (w_1 a_1 + w_2 a_2) + x \} dx \right] = 0$$

$$\frac{\partial I(u_2)}{\partial a_2} = 0 \Rightarrow$$

$$\left[\int_0^1 \left\{ \frac{dw_1}{dx} \frac{dw_2}{dx} a_1 + \left(\frac{dw_2}{dx} \right)^2 a_2 \right\} dx \right] - \left[\int_0^1 w_2 \{ (w_1 a_1 + w_2 a_2) + x \} dx \right] = 0$$

Ritz Method & Galerkin Method (2/4)

$$\frac{\partial I(u_2)}{\partial a_1} = 0 \Rightarrow$$

$$\left[\int_0^1 \left\{ \left(\frac{dw_1}{dx} \right)^2 a_1 + \frac{dw_1}{dx} \frac{dw_2}{dx} a_2 \right\} dx \right] - \left[\int_0^1 w_1 \{ (w_1 a_1 + w_2 a_2) + x \} dx \right] = 0$$

$$w_1 = \Psi_1 = x(1-x),$$

$$w_2 = \Psi_2 = x^2(1-x)$$

$$\frac{\partial}{\partial x} \left(w_1 \frac{dw_1}{dx} \right) = \frac{dw_1}{dx} \frac{dw_1}{dx} + w_1 \frac{d^2 w_1}{dx^2}$$

$$\frac{\partial}{\partial x} \left(w_1 \frac{dw_2}{dx} \right) = \frac{dw_1}{dx} \frac{dw_2}{dx} + w_1 \frac{d^2 w_2}{dx^2}$$

$$\int_0^1 \left\{ \left(\frac{dw_1}{dx} \right)^2 a_1 \right\} dx = \left(a_1 w_1 \frac{dw_1}{dx} \right) \Big|_0^1 - \int_0^1 w_1 \left\{ \frac{d^2 w_1}{dx^2} a_1 \right\} dx = - \int_0^1 w_1 \left\{ \frac{d^2 w_1}{dx^2} a_1 \right\} dx$$

$$\int_0^1 \left\{ \left(\frac{dw_1}{dx} \frac{dw_2}{dx} \right) a_2 \right\} dx = \left(a_2 w_1 \frac{dw_2}{dx} \right) \Big|_0^1 - \int_0^1 w_1 \left\{ \frac{d^2 w_2}{dx^2} a_2 \right\} dx = - \int_0^1 w_1 \left\{ \frac{d^2 w_2}{dx^2} a_2 \right\} dx$$

Ritz Method & Galerkin Method (3/4)

$$\frac{\partial I(u_2)}{\partial a_1} = 0 \Rightarrow$$

$$\frac{d^2 u}{dx^2} + u + x = 0$$

$$u = a_1 w_1 + a_2 w_2$$

$$-\int_0^1 w_1 \left\{ \left(\frac{d^2 w_1}{dx^2} a_1 + \frac{d^2 w_2}{dx^2} a_2 \right) + (w_1 a_1 + w_2 a_2) + x \right\} dx = 0$$

$$-\int_0^1 w_1 \left(\frac{d^2 u_2}{dx^2} + u_2 + x \right) dx = 0$$

Galerkin Method !!

$$\frac{\partial I(u_2)}{\partial a_2} = 0 \Rightarrow$$

$$-\int_0^1 w_2 \left\{ \left(\frac{d^2 w_1}{dx^2} a_1 + \frac{d^2 w_2}{dx^2} a_2 \right) + (w_1 a_1 + w_2 a_2) + x \right\} dx = 0$$

$$-\int_0^1 w_2 \left(\frac{d^2 u_2}{dx^2} + u_2 + x \right) dx = 0$$

Ritz Method & Galerkin Method (4/4)

- This example is a very special case. But, generally speaking, results of Galerkin method and Ritz method agree, if functional exists.
- Although Ritz method provides approx. solution, that satisfies Euler equation in strict sense. Therefore, solution of Ritz method is closer to exact solution.
 - This is the main reason that Galerkin method is accurate.
 - Please just remember this.
- This relationship between Ritz and Galerkin is not correct if functional does not exist.
 - In these cases, Galerkin method is not necessarily the best method from the viewpoint of accuracy and robustness.