Introduction to FEM

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- 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

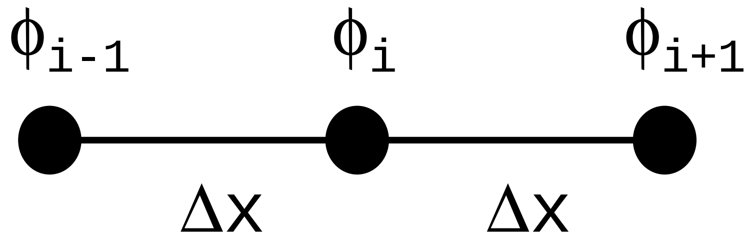
Kengo Nakajima (2/2)

- 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

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

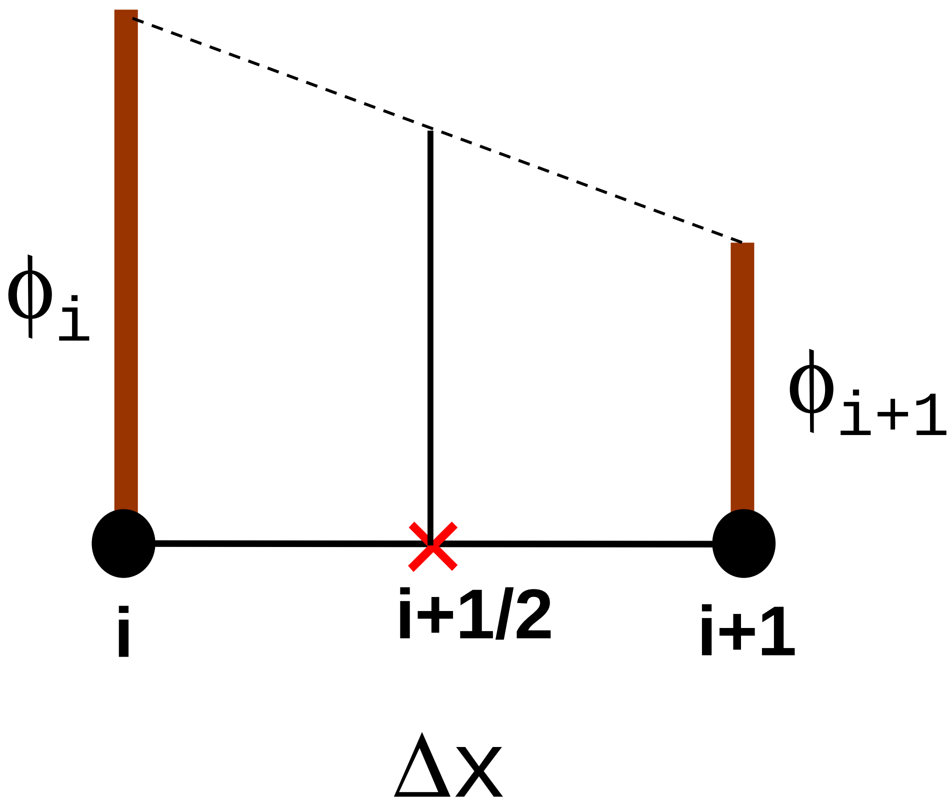
$$\phi_{i-1} = \phi_i - \Delta x \left(\frac{\partial \phi}{\partial x} \right)_i + \frac{(\Delta x)^2}{2!} \left(\frac{\partial^2 \phi}{\partial x^2} \right)_i - \frac{(\Delta x)^3}{3!} \left(\frac{\partial^3 \phi}{\partial x^3} \right)_i \cdots$$

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

Finite Difference Method (FDM)
(有限)差分法:巨視的微分
macroscopic differentiation

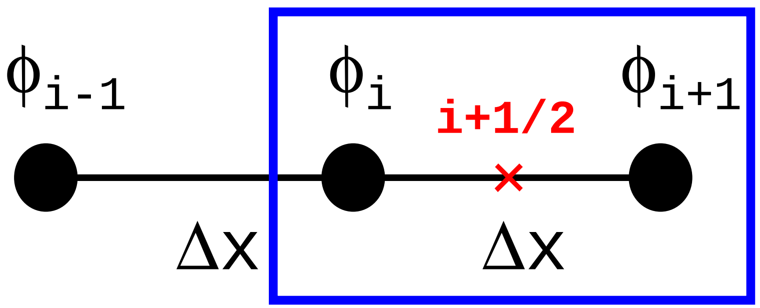
$$\left(\frac{d\phi}{dx}\right)_{i+1/2} \approx \frac{\phi_{i+1}-\phi_i}{\Delta x}$$

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



2nd Order Differentiation in FDM Taylor Series Expansion

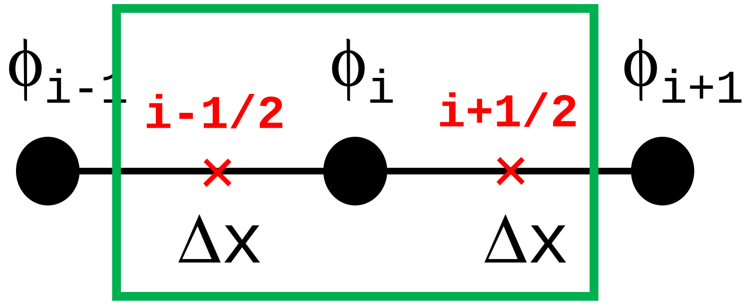
- **Approximate Derivative at × (center of *i* and *i+1*)**



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

Δx→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

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

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

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

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

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

FDM and FEM

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  - 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 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

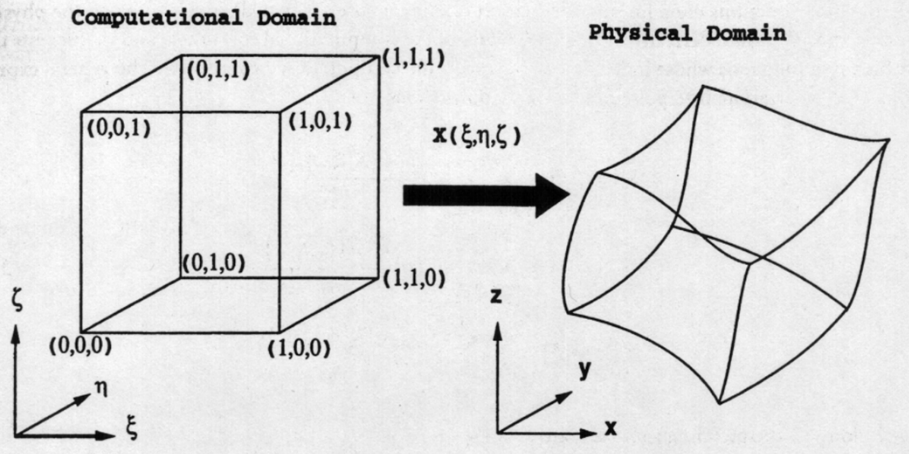


FIGURE 3.1 Transformation between computational and physical domains.

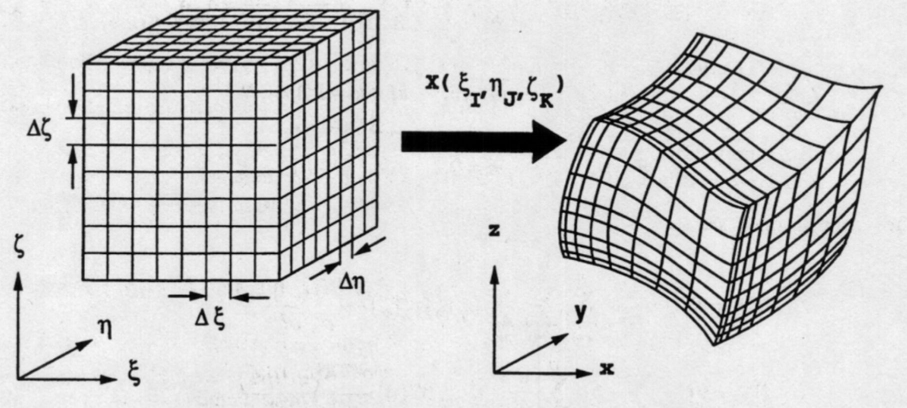
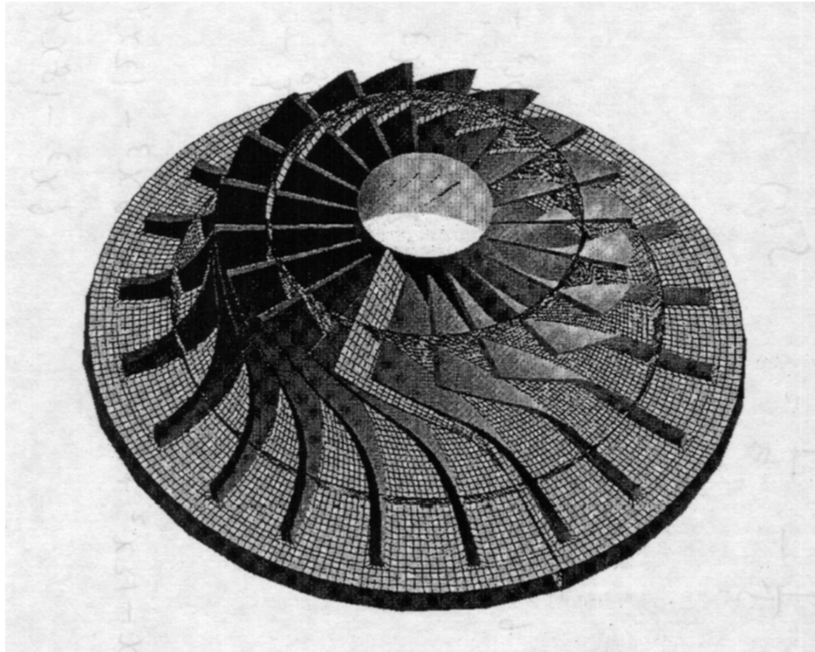


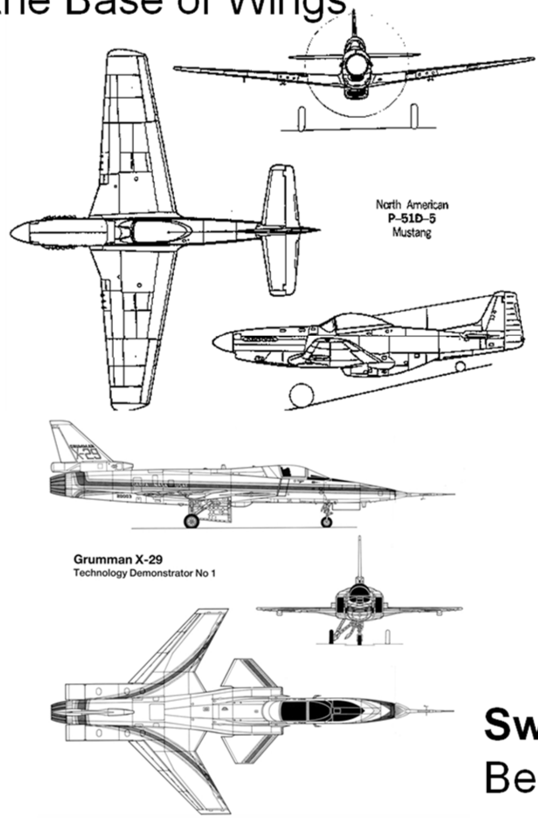
FIGURE 3.2 Grids in computational and physical domains.

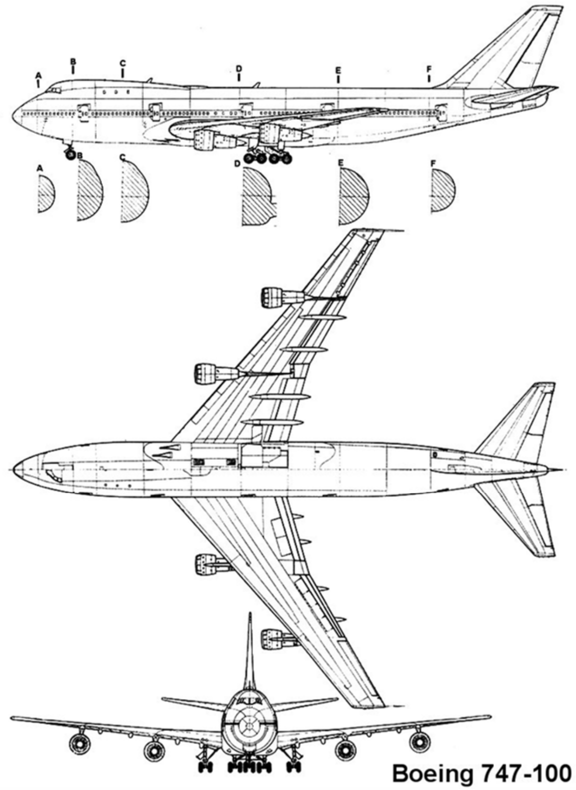


History of FEM

- 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

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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

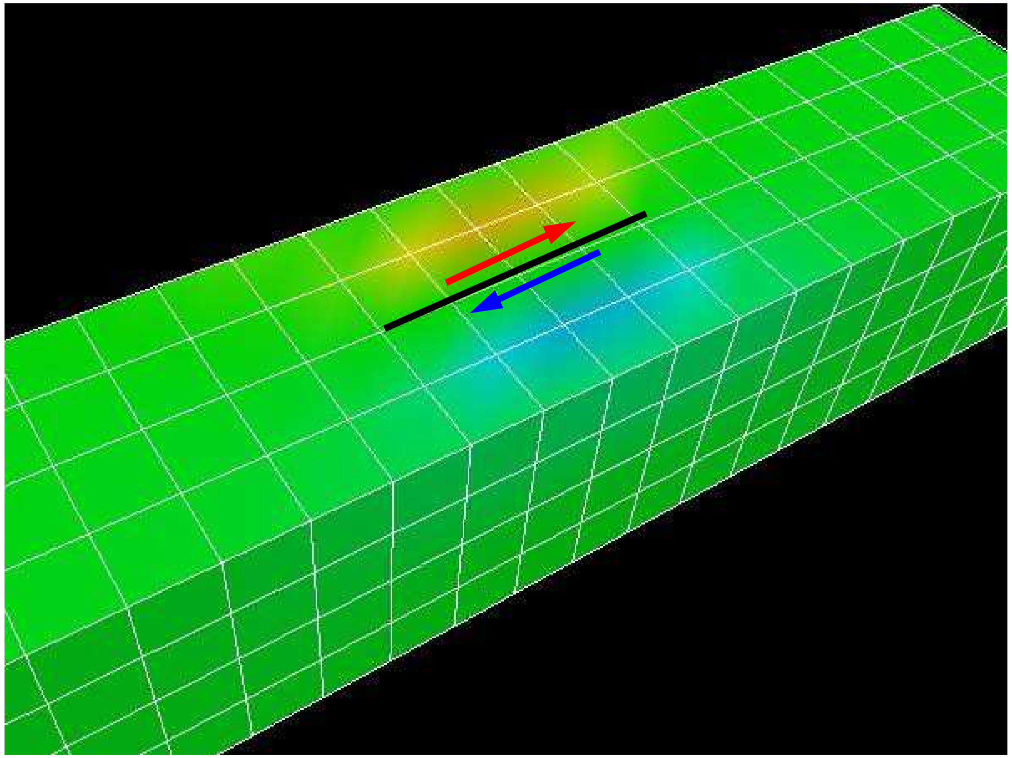
Recent Research Topics

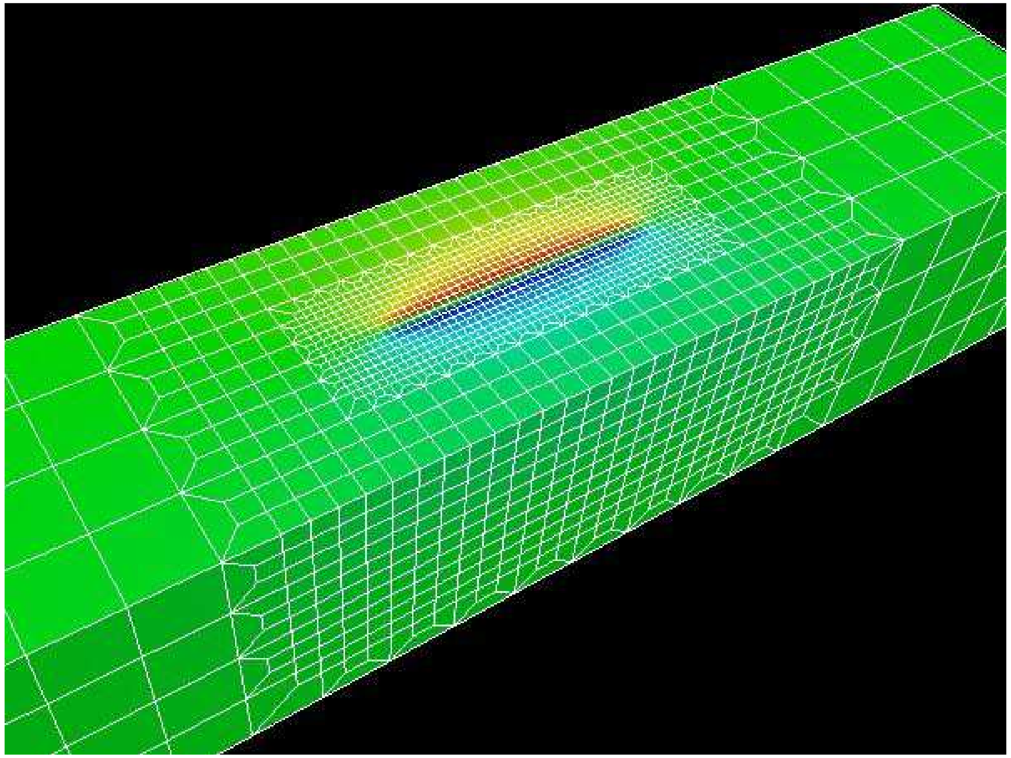
- Non-Linear Problems
  - Crash, Contact, Non-Linear Material
  - Discontinuous Approach
    - X-FEM
- Parallel Computing
  - also in commercial codes
- Adaptive Mesh Refinement (AMR)
  - Shock Wave, Separation
  - Stress Concentration
  - Dynamic Load Balancing (DLB) at Parallel Computing
- Mesh Generation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

3D Simulations for Earthquake Generation Cycle
San Andreas Faults, CA, USA

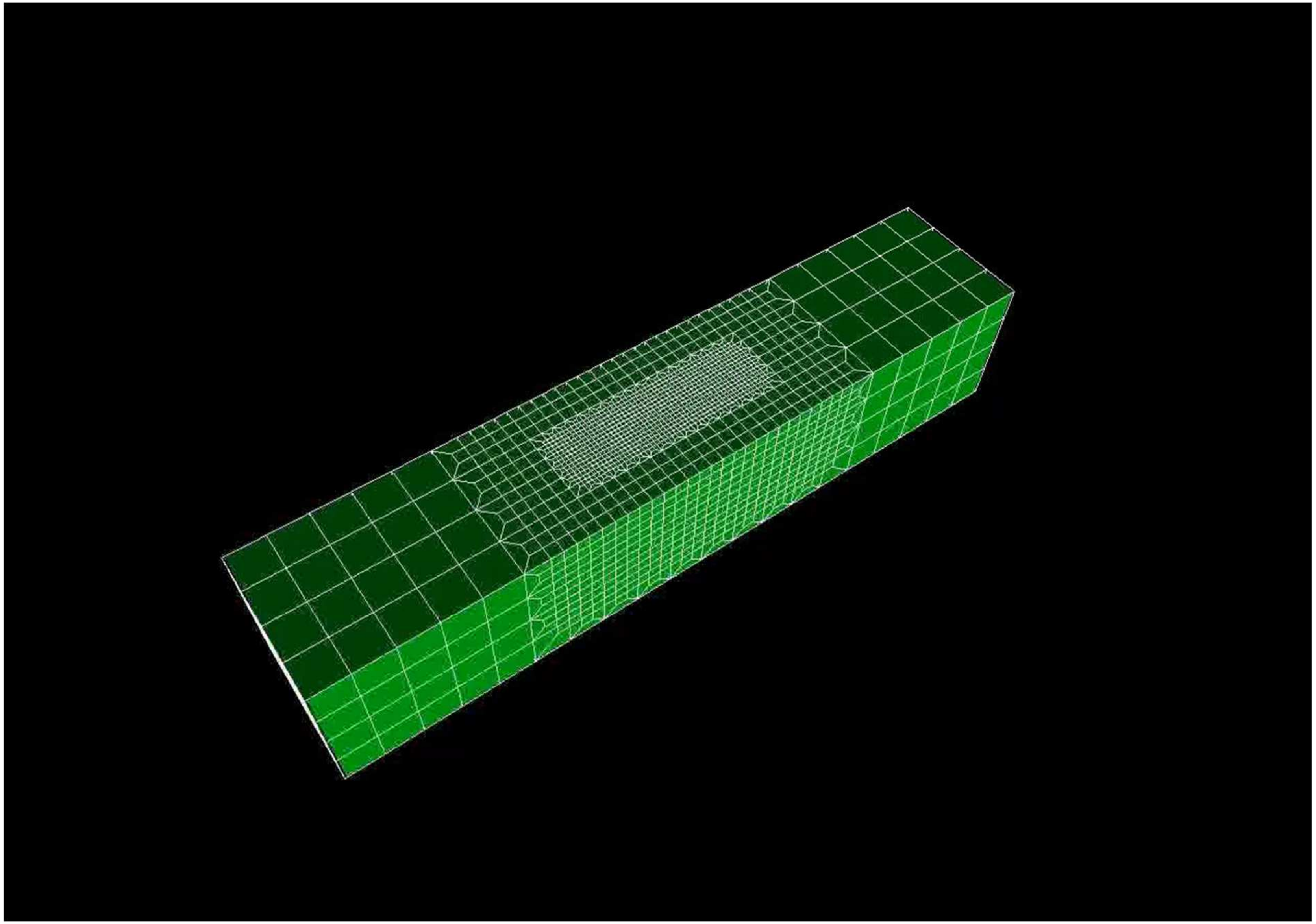
Stress Accumulation at Transcurrent Plate Boundaries

Adaptive Mesh Refinement (AMR)





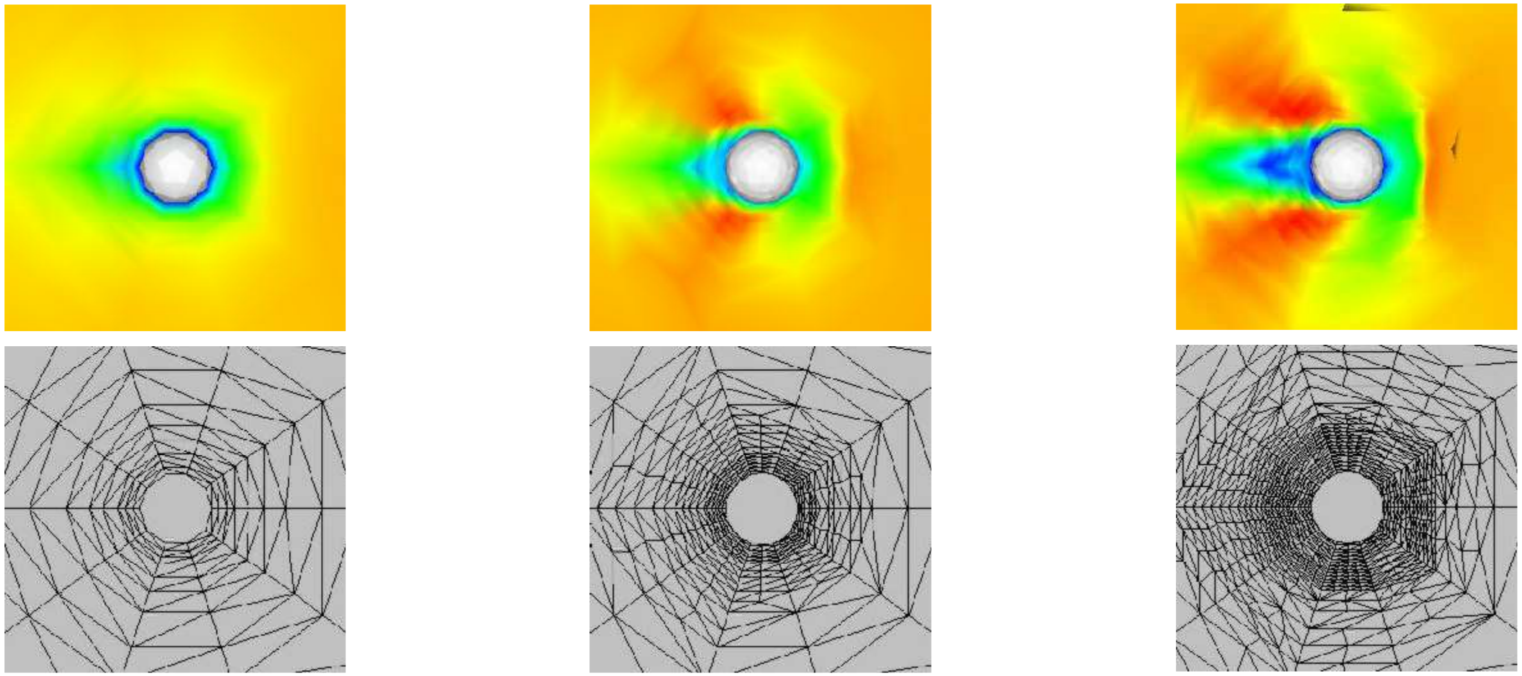
Adaptive FEM: High-resolution needed at meshes with large deformation (large accumulation)



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 before	1-Lev. Adapted after	2-Lev. Adapted before	2-Lev. Adapted after
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

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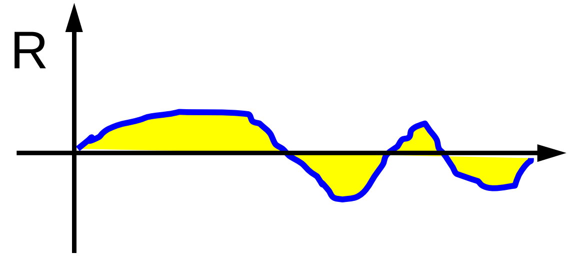

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Variational Method (Ritz) (1/2) 変分法

- 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）”.

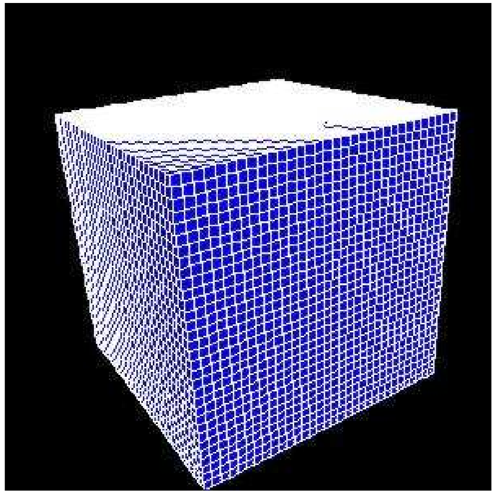
Variational Method (Ritz) (2/2) 変分法

- 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.

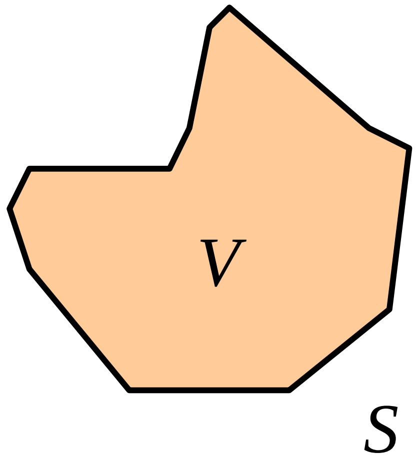
Example of MWR (1/3)

- 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

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

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

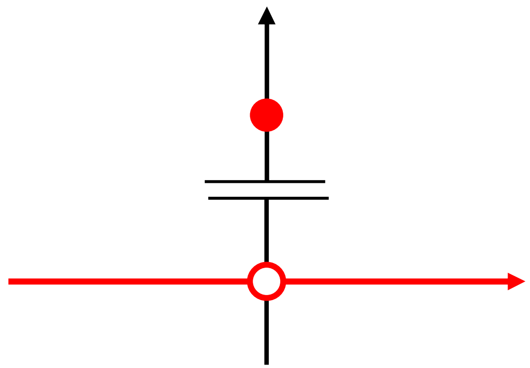
Collocation Method

- Weighting function: Dirac's Delta Function δ

$$\delta(z)=\infty \quad if \quad z=0$$

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

$$w_i=\delta(\mathbf{x}-\mathbf{x_i}) \qquad \mathbf{x}: \text{location}$$



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

$$\int_V R\,\delta(\mathbf{x}-\mathbf{x_i})\,dV = R\,|_{\mathbf{x}=\mathbf{x_i}} \qquad \begin{array}{l}\delta(\mathbf{x}-\mathbf{x_i})=\infty \; at \; \mathbf{x}=\mathbf{x_i}\\ \delta(\mathbf{x}-\mathbf{x_i})=0 \; at \; \mathbf{x}\neq\mathbf{x_i}\end{array}$$

- 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):

$$I(a_i) = \int_V [R(a_i, \mathbf{x})]^2 \, dV$$

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

$$\Downarrow$$

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

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

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

- Boundary Conditions: Dirichlet

$$u = 0 @ x = 0$$

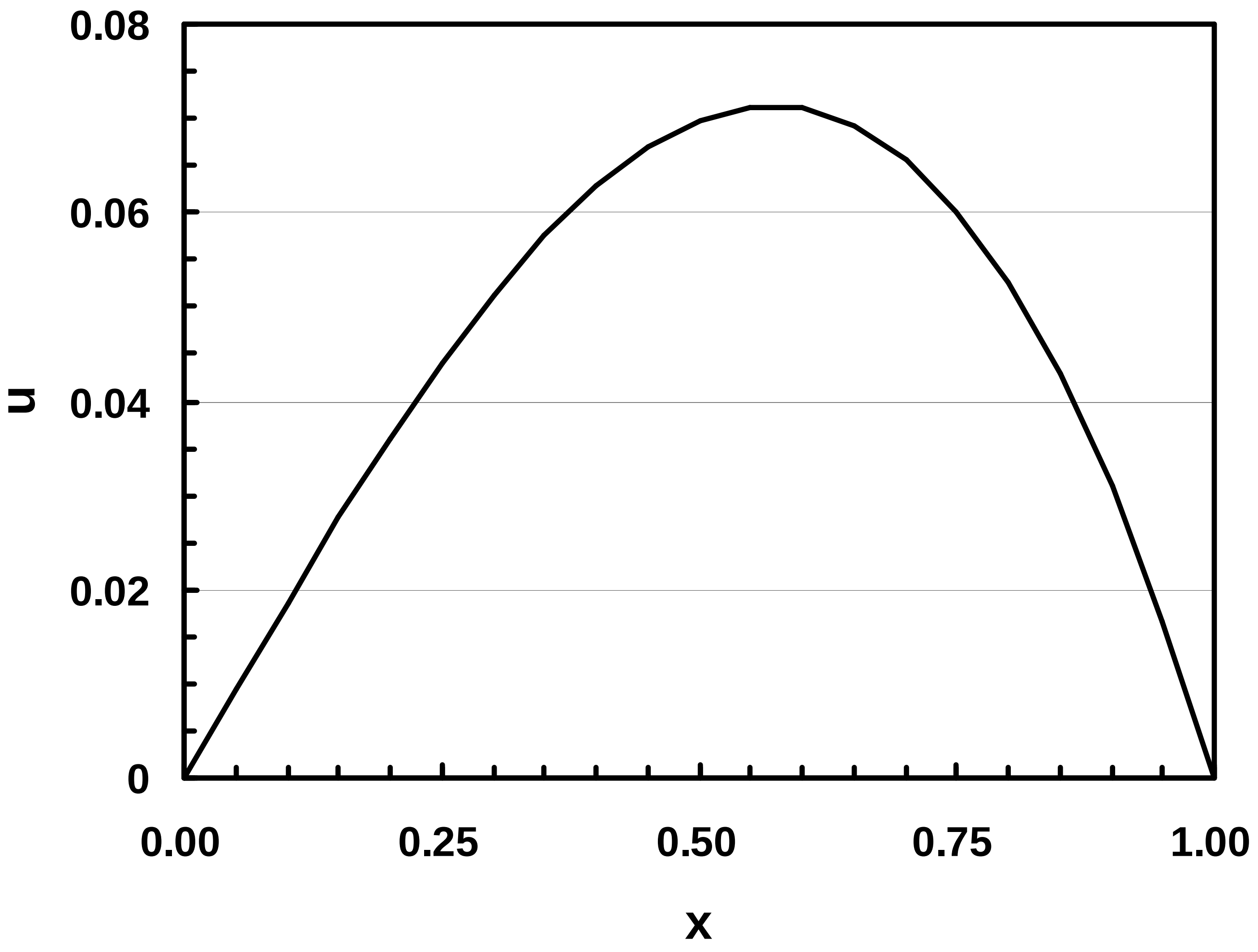
$$u = 0 @ x = 1$$

- 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:

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

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

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:

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

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

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:

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

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

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

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

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:

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

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

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

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

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 method 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-collocaion points” with exact solution
  - Explain the behavior
  - Try different collocation points

Homework (2/2)

- Method of Moment（モーメント法）

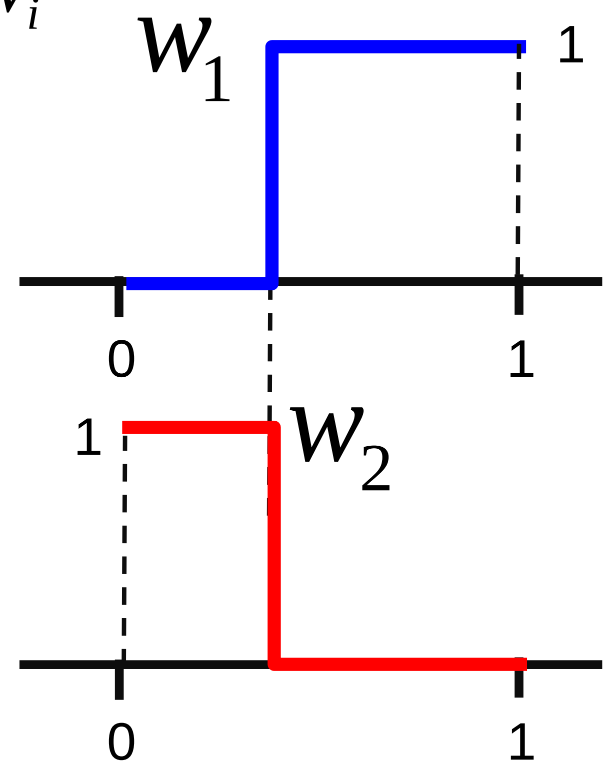
$$w_i = \mathbf{x}^{i-1} \quad (i \geq 1)$$

  - Weighting functions ?

- Sub-Domain Method（部分領域法）
  - Domain V is divided into sub-domains V_i $(i=1\text{-}n)$, and weighting functions w_i are given as follows:

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

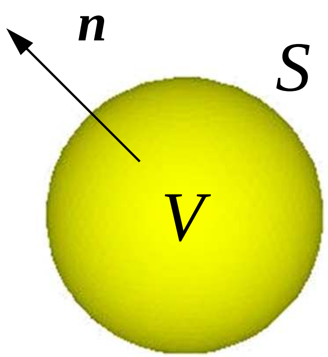
  - Two unknowns, two sub domains
  - Two sub-domains do not share any overlaps



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

Gauss's Theorem

$$\int_V \left(\frac{\partial U}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial W}{\partial z} \right) dV = \int_S \left(U n_x + V n_y + W n_z \right) dS$$



- 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 $\boldsymbol{n}$ 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:

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

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

Green's Theorem (2/2)

- (cont.)

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

$$= \int_S A\frac{\partial B}{\partial n}\, dS$$

$\frac{\partial B}{\partial n}$ Gradient of B 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:

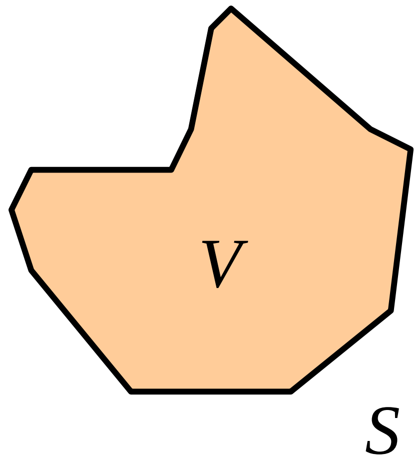
$$u_M = \sum_{i=1}^{M} a_i \Psi_i$$

- 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 (<u>next page</u>)

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

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

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

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

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

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

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

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

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) ：

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

$$where \quad \frac{\partial u^*}{\partial n} = \frac{\partial u^*}{\partial x} n_x + \frac{\partial u^*}{\partial y} n_y$$

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（十分条件）
  - Assume that u^* is solution of the Euler equation and $\alpha\eta = \delta u^*$

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

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

$\delta I = 0$
First Variation
第一変分

$\delta I^2 \geqq 0$
Second Variation
第二変分

Application of Variational Method (5/5)

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

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

- 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 !

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

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**):

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

(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:

$$u_n = x \cdot (1 - x) \cdot \left(a_1 + a_2 x + a_3 x^2 + \cdots + a_n x^{n-1}\right) \quad \text{(B-2)}$$

- 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 stationalizes $I(u)$ 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

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

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

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

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

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

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)

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

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

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

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

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

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

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

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

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

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

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

Approx. by Variational Method (4/4)

- Final linear equations are as follows:

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

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

- 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:

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

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

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

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

Ritz Method & Galerkin Method (1/4)

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

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

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

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

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

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

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

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

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

Ritz Method & Galerkin Method (2/4)

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

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

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

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

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

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

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

Ritz Method & Galerkin Method (3/4)

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

$$u=a_1w_1+a_2w_2$$

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

$$-\int_0^1 w_1\left\{\left(\frac{d^2w_1}{dx^2}a_1+\frac{d^2w_2}{dx^2}a_2\right)+\left(w_1a_1+w_2a_2\right)+x\right\}dx=0$$

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

Galerkin Method !!

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

$$-\int_0^1 w_2\left\{\left(\frac{d^2w_1}{dx^2}a_1+\frac{d^2w_2}{dx^2}a_2\right)+\left(w_1a_1+w_2a_2\right)+x\right\}dx=0$$

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

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.