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		Discretizing differential equations	Discretize differential equations using forward,
04/07	Class 1		backward, and central difference, with high order,
			and evaluate the discretization error
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04/14	Class 3		test functions, isoparametric elements, and
			use it to solve elasticity equations.
04/18	Class 4	Spectral methods	Explain the advantages of orthogonal
			basis functions such as Fourier, Chebyshev,
			Legendre, and Bessel.
04/21	Class 5	Boundary element methods	Understand the relation between inverse
			matrices, $\delta$ functions and Green's functions,
ļ			and solve boundary integral equations.
04/25	Class 6	Molecular dynamics	Understand the significance of symplectic
	Ciabb 0		time integrators and thermostats, and solve
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05/02	Class 8		interpolations schemes when both particle and
			mesh-based discretizations are used.

### Weighted residual method



$$\int_{0}^{2} \left( -\frac{\partial}{\partial x} \left( c \frac{\partial \tilde{u}}{\partial x} \right) - f \right) w dx = 0$$

$$\int_{0}^{2} -\frac{\partial}{\partial x} \left( c \frac{\partial \tilde{u}}{\partial x} \right) w dx = \int_{0}^{2} f w dx$$
$$\int_{\Omega} (\nabla^{2} u) W d\Omega = \int_{\Omega} f W d\Omega$$

## Weighted residual method

$$\int_{\Omega} (\nabla^2 u) W d\Omega = \int_{\Omega} f W d\Omega$$

$W_i = \delta( \mathbf{x} - \mathbf{x}_i )$	Collocation Method	
$W_i = \frac{\partial R}{\partial u_i}$	Least Squares Method	
$W_i = \mathbf{x}^i$	Method of Moments	
$W_i = \phi_i$	Galerkin Method	FEM
$W_i = G( \mathbf{x} - \mathbf{x}_i )$	Green's Function Solution	BEM

## Weak form

$$\begin{split} \int_{\Omega} (\nabla^2 u) W d\Omega &= \int_{\Omega} f W d\Omega \\ & \downarrow \quad \text{integration by parts} \\ \int_{\Omega} \nabla \cdot (\nabla u W) d\Omega - \int_{\Omega} (\nabla u) \cdot \nabla W d\Omega &= \int_{\Omega} f W d\Omega \\ & \downarrow \quad \text{Gauss' divergence theorem} \quad \int_{\Omega} \nabla \cdot \mathbf{u} d\Omega = \int_{\Gamma} \mathbf{n} \cdot \mathbf{u} d\Gamma \\ \int_{\Gamma} \mathbf{n} \cdot (\nabla u W) d\Gamma - \int_{\Omega} (\nabla u) \cdot \nabla W d\Omega &= \int_{\Omega} f W d\Omega \\ & \downarrow \quad \mathbf{n} \cdot \nabla = \partial / \partial n \\ \int_{\Gamma} \frac{\partial u}{\partial n} W d\Gamma - \int_{\Omega} (\nabla u) \cdot \nabla W d\Omega = \int_{\Omega} f W d\Omega \end{split}$$

# Integration by parts

$$\int_{0}^{2} -\frac{\partial}{\partial x} \left( c \frac{\partial \tilde{u}}{\partial x} \right) w dx = \int_{0}^{2} f w dx$$

$$\int_{0}^{2} -\frac{\partial}{\partial x} \left( c \frac{\partial \tilde{u}}{\partial x} \right) w dx = \int_{0}^{2} c \frac{\partial \tilde{u}}{\partial x} \frac{\partial w}{\partial x} dx - \left[ c \frac{\partial \tilde{u}}{\partial x} w \right]_{0}^{2}$$

### Boundary conditions

$$w(0) = 0 \qquad u_3 \qquad k_2 \\ \frac{\partial \tilde{u}(2)}{\partial x} = 0 \qquad \text{fixed} \qquad 0$$

Inverse form  

$$\int_{\Gamma} \frac{\partial u}{\partial n} W d\Gamma - \int_{\Omega} (\nabla u) \cdot \nabla W d\Omega = \int_{\Omega} f W d\Omega$$

$$\downarrow \quad \text{integration by parts}$$

$$\int_{\Gamma} \frac{\partial u}{\partial n} W d\Gamma - \int_{\Omega} \nabla \cdot (u \nabla W) d\Omega + \int_{\Omega} u (\nabla^2 W) d\Omega = \int_{\Omega} f W d\Omega$$

$$\downarrow \quad \text{Gauss' divergence theorem}$$

$$\int_{\Gamma} \frac{\partial u}{\partial n} W d\Gamma - \int_{\Gamma} u \frac{\partial W}{\partial n} d\Gamma + \int_{\Omega} u (\nabla^2 W) d\Omega = \int_{\Omega} f W d\Omega$$

$$\downarrow \quad W = G$$

$$\int_{\Gamma} \frac{\partial u}{\partial n} G d\Gamma - \int_{\Gamma} u \frac{\partial G}{\partial n} d\Gamma + \int_{\Omega} u (\nabla^2 G) d\Omega = \int_{\Omega} f G d\Omega$$

### Green's function

$$\int_{\Gamma} \frac{\partial u}{\partial n} G d\Gamma - \int_{\Gamma} u \frac{\partial G}{\partial n} d\Gamma + \int_{\Omega} u (\nabla^2 G) d\Omega = \int_{\Omega} f G d\Omega \qquad \nabla^2 G = -\delta$$

$$\int_{\Omega} u (\nabla^2 G) d\Omega = -\int_{\Omega} u \delta d\Omega$$

$$\int_{\Gamma} \frac{\partial u}{\partial n} G d\Gamma - \int_{\Gamma} u \left( \frac{1}{2} \delta + \frac{\partial G}{\partial n} \right) d\Gamma = \int_{\Omega} f G d\Omega \qquad -\int_{\Omega} u \delta d\Omega = -u \\ -\int_{\Gamma} u \delta d\Gamma = -1/2u$$



#### Boundary condition



### Discretization





#### High order elements $= \int_{-1}^{1} u_{j1}\phi_1(\xi) \frac{\partial G}{\partial n} |J_j| d\xi + \int_{-1}^{1} u_{j2}\phi_2(\xi) \frac{\partial G}{\partial n} |J_j| d\xi$ Order Function Continous $\int_{\Gamma_j} u \frac{\partial G}{\partial n} d\Gamma_j = |J_j| \sum_k u_{jk} \int_{-1}^1 \phi_k(\xi) \frac{\partial G}{\partial n} d\xi$ $\phi_1 = 1$ 0 no 1 yes $\int_{-1}^{1} \phi_k(\xi) \frac{\partial G}{\partial n} d\xi = \sum_{l} \phi_k(\xi_l) \frac{\partial G_{jkl}}{\partial n} w_l$ 1 no $\int_{\Gamma} u \frac{\partial G}{\partial n} d\Gamma = \sum_{i} |J_{j}| \sum_{k} u_{jk} \sum_{l} \phi_{k}(\xi_{l}) \frac{\partial G_{jkl}}{\partial n} w_{l}$ $= \xi(\xi - 1)/2$ yes 2

## **Triple loop**



### Final matrix form



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