| 04/07 |  | Course schedule | Required learning |
| :---: | :---: | :---: | :---: |
|  | Class 1 | Discretizing differential equations | Discretize differential equations using forward, backward, and central difference, with high order, and evaluate the discretization error |
| 04/ \| | Class 2 | Finite difference methods | Understand stability of low and high order time integration, and use it to solve convection, diffusion, and wave equations |
| 04/14 | Class 3 | Finite element methods | Understand the concepts of Galerkin methods, 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. |
| 04/2 1 | Class 5 | Boundary element methods | Understand the relation between inverse matrices, $\delta$ functions and Green's functions, and solve boundary integral equations. |
| 04/25 | Class 6 | Molecular dynamics | Understand the significance of symplectic time integrators and thermostats, and solve the dynamics of interacting molecules. |
| 04/28 | Class 7 | Smooth particle hydrodynamics (SPH) | Evaluate the conservation and dissipation properties of differential operators formed from radial basis functions. |
| 05/02 | Class 8 | Particle mesh methods | How to conserve higher order moments for interpolations schemes when both particle and mesh-based discretizations are used. |

## Weighted residual method

$$
\begin{aligned}
& \int_{0}^{2} r w=0 \\
& \text { Weighted residual } \\
& \int_{0}^{2}\left(-\frac{\partial}{\partial x}\left(c \frac{\partial \tilde{u}}{\partial x}\right)-f\right) w d x=0 \\
& \int_{0}^{2}-\frac{\partial}{\partial x}\left(c \frac{\partial \tilde{u}}{\partial x}\right) w d x=\int_{0}^{2} f w d x \\
& \int_{\Omega}^{2}\left(\nabla^{2} u\right) W d \Omega=0 \quad \text { Weast squares } \\
& \int_{0}^{2} f W h d \Omega
\end{aligned}
$$

## Weighted residual method

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

| $W_{i}=\delta\left(\left\|\mathbf{x}-\mathbf{x}_{i}\right\|\right)$ | 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 |
| $W_{i}=G\left(\left\|\mathbf{x}-\mathbf{x}_{i}\right\|\right)$ | Green's Function Solution |

FEM
BEM

## Weak form

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

## Integration by parts

$$
\begin{aligned}
& \int_{0}^{2}-\frac{\partial}{\partial x}\left(c \frac{\partial \tilde{u}}{\partial x}\right) w d x=\int_{0}^{2} f w d x \\
& \int_{0}^{2}-\frac{\partial}{\partial x}\left(c \frac{\partial \tilde{u}}{\partial x}\right) w d x=\int_{0}^{2} c \frac{\partial \tilde{u}}{\partial x} \frac{\partial w}{\partial x} d x-\left[c \frac{\partial \tilde{u}}{\partial x} w\right]_{0}^{2}
\end{aligned}
$$

## Boundary conditions

$$
\begin{gathered}
w(0)=0 \\
\frac{\partial \tilde{u}(2)}{\partial x}=0
\end{gathered}
$$



## Inverse form

$$
\left.\begin{array}{rl}
\int_{\Gamma} \frac{\partial u}{\partial n} W d \Gamma- & \int_{\Omega}(\nabla u) \cdot \nabla W d \Omega=\int_{\Omega} f W d \Omega \\
& \quad \text { integration by parts } \\
\int_{\Gamma} \frac{\partial u}{\partial n} W d \Gamma- & \int_{\Omega} \nabla \cdot(u \nabla W) d \Omega+\int_{\Omega} u\left(\nabla^{2} W\right) d \Omega=\int_{\Omega} f W d \Omega \\
& \quad \text { Gauss' divergence theorem }
\end{array}\right\} \begin{aligned}
\int_{\Gamma} \frac{\partial u}{\partial n} W d \Gamma- & \int_{\Gamma} u \frac{\partial W}{\partial n} d \Gamma+\int_{\Omega} u\left(\nabla^{2} W\right) d \Omega=\int_{\Omega} f W d \Omega \\
& \|_{\Gamma} W=G \\
\int_{\Gamma} \frac{\partial u}{\partial n} G d \Gamma- & \int_{\Gamma} u \frac{\partial G}{\partial n} d \Gamma+\int_{\Omega} u\left(\nabla^{2} G\right) d \Omega=\int_{\Omega} f G d \Omega
\end{aligned}
$$

## Green's function

$$
\begin{aligned}
& \int_{\Gamma} \frac{\partial u}{\partial n} G d \Gamma-\int_{\Gamma} u \frac{\partial G}{\partial n} d \Gamma+\int_{\Omega} u\left(\nabla^{2} G\right) d \Omega=\int_{\Omega} f G d \Omega \\
& \nabla^{2} G=-\delta \\
& 1 \\
& \int_{\Gamma} \frac{\partial u}{\partial n} G d \Gamma-\int_{\Gamma} u\left(\frac{1}{2} \delta+\frac{\partial G}{\partial n}\right) d \Gamma=\int_{\Omega} f G d \Omega \\
& \begin{array}{l}
-\int_{\Omega} u \delta d \Omega=-u \\
-\int_{\Gamma} u \delta d \Gamma=-1 / 2 u
\end{array} \\
& N_{\Gamma} \overbrace{\left[\begin{array}{lll}
\ddots & & \\
& G\left(r_{i j}\right) & \\
& & \ddots
\end{array}\right] \underbrace{N_{\Gamma}}_{\text {unknown }}\left[\begin{array}{c}
\vdots \\
\frac{\partial u_{j}}{\partial n} \\
\vdots
\end{array}\right]}=\overbrace{\left[\begin{array}{ll}
\ddots & \\
\frac{1}{2} \delta_{i j}+\frac{\partial G\left(r_{i j}\right)}{\partial n} \\
& \ddots
\end{array}\right]}^{N_{\Gamma}}\left[\begin{array}{c}
\vdots \\
u_{j} \\
\vdots
\end{array}\right]+\overbrace{\left[\begin{array}{lll}
\ddots & & \\
& G\left(r_{i j}\right) & \\
& & \ddots
\end{array}\right]}^{N_{2}}\left[\begin{array}{c}
\vdots \\
f_{j} \\
\vdots
\end{array}\right]
\end{aligned}
$$

Boundary condition

(a) Dirichlet

(b) Neumann

(c) Mixed



## Discretization



$$
\begin{aligned}
& \int_{\Gamma_{j}} u \frac{\partial G}{\partial n} d \Gamma_{j}=\int_{\Gamma_{j}} u_{j 1} \phi_{1}(x) \frac{\partial G}{\partial n} d \Gamma_{j}+\int_{\Gamma_{j}} u_{j 2} \phi_{2}(x) \frac{\partial G}{\partial n} d \Gamma_{j} \\
& =\int_{-1}^{1} u_{j 1} \phi_{1}(\xi) \frac{\partial G}{\partial n}\left|J_{j}\right| d \xi+\int_{-1}^{1} u_{j 2} \phi_{2}(\xi) \frac{\partial G}{\partial n}\left|J_{j}\right| d \xi \\
& \phi_{1}(\xi)=(1-\xi) / 2 \\
& \phi_{2}(\xi)=(1+\xi) / 2 \\
& J_{j}=\partial \mathbf{x}_{j} / \partial \boldsymbol{\xi}
\end{aligned}
$$

## High order elements

$$
\begin{gathered}
=\int_{-1}^{1} u_{j 1} \phi_{1}(\xi) \frac{\partial G}{\partial n}\left|J_{j}\right| d \xi+\int_{-1}^{1} u_{j 2} \phi_{2}(\xi) \frac{\partial G}{\partial n}\left|J_{j}\right| d \xi \\
\int_{\Gamma_{j}} u \frac{\partial G}{\partial n} d \Gamma_{j}=\left|J_{j}\right| \sum_{k} u_{j k} \int_{-1}^{1} \phi_{k}(\xi) \frac{\partial G}{\partial n} d \xi \\
\int_{-1}^{1} \phi_{k}(\xi) \frac{\partial G}{\partial n} d \xi=\sum_{l} \phi_{k}\left(\xi_{l}\right) \frac{\partial G_{j k l}}{\partial n} w_{l} \\
\int_{\Gamma} u \frac{\partial G}{\partial n} d \Gamma=\sum_{j}\left|J_{j}\right| \sum_{k} u_{j k} \sum_{l} \phi_{k}\left(\xi_{l}\right) \frac{\partial G_{j k l}}{\partial n} w_{l}
\end{gathered}
$$

|  | Order | Continous | Function |
| :--- | :---: | :---: | :---: |

## Triple loop


(a) Element centric

(b) Node centeric

$$
\int_{\Gamma} u \frac{\partial G}{\partial n} d \Gamma=\sum_{j}\left|J_{j}\right| \sum_{k} u_{j k} \sum_{l} \phi_{k}\left(\xi_{l}\right) \frac{\partial G_{j k l}}{\partial n} w_{l}
$$

$$
\int_{\Gamma} u \frac{\partial G}{\partial n} d \Gamma=\sum_{j} u_{j} \sum_{k}\left|J_{j k}\right| \sum_{l} \phi_{j k}\left(\xi_{l}\right) \frac{\partial G_{j k l}}{\partial n} w_{l}
$$

Final matrix form

$$
\begin{aligned}
& \int_{\Gamma} u \frac{\partial G}{\partial n} d \Gamma=N_{\Gamma} \overbrace{\left(\begin{array}{ll}
\ddots & \\
\sum_{k}\left|J_{j k}\right| \sum_{l} \phi_{j k}\left(\xi_{l}\right) \frac{\partial G_{j k l}}{\partial n} w_{l} \\
& \ddots
\end{array}\right]}^{N_{\Gamma}}\left[\begin{array}{c}
\vdots \\
u_{j} \\
\vdots
\end{array}\right] \\
& N_{\Gamma} \overbrace{\left[\begin{array}{lll}
\ddots & & \\
& G\left(r_{i j}\right) & \\
& & \ddots
\end{array}\right] \underbrace{N_{\Gamma}}_{\text {unknown }}{ }_{\left[\begin{array}{c}
\vdots \\
\frac{\partial u_{j}}{\partial n} \\
\vdots
\end{array}\right]}=\overbrace{\left[\begin{array}{ll}
\ddots & \\
\frac{1}{2} \delta_{i j}+\frac{\partial G\left(r_{i j}\right)}{\partial n} \\
& \ddots
\end{array}\right]}^{N_{\Gamma}}\left[\begin{array}{c}
\vdots \\
u_{j} \\
\vdots
\end{array}\right]+\overbrace{\left[\begin{array}{lll}
\ddots & & \\
& G\left(r_{i j}\right) & \\
& & \ddots
\end{array}\right]}^{N_{2}}\left[\begin{array}{c}
\vdots \\
f_{j} \\
\vdots
\end{array}\right],\left[\begin{array}{c} 
\\
\\
\\
\end{array}\right]}
\end{aligned}
$$

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