THE UNIVERSITY of TENNESSEE at CHATTANOOGA

SIMCENTER

NATIONAL CENTER for COMPUTATIONAL ENGINEERING

Introduction to High-Order Continuous and Discontinuous Finite-Elements for CFD

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Purpose

- Motivation for exploring finite-element technology
- Provide detailed introduction to finite-element methods
- Thorough description of stabilized finite elements and discontinuous-Galerkin methods for fluid dynamics
- Implicit time-advancement for steady and unsteady flows
- Enabling technologies: mesh adaptation, overset meshes

Outline

- Preliminaries:
  - Assumptions on audience
  - Governing equations
  - Why finite elements
- Lecture 1: Introduction to finite elements
- Lecture 2: Stabilized finite elements / discontinuous Galerkin
- Lecture 3: Implicit schemes for turbulent flows
- Lecture 4: Adaptive, overset meshes

Outline

Lecture 1: Introduction to finite elements

- Weighted residual and weak statement
- Global basis functions
- Discretization for three-element example
- Element basis functions
- Element mapping
- Quadrature
- High-order basis functions
- Extension to multidimensions
- Example of equivalence between FE and FV
- Curved elements

Outline

Lecture 2: Stabilized finite elements / discontinuous Galerkin

- Stabilized finite elements
  - Inviscid flows
  - SUPG
  - Viscous flows and scaling of stabilization matrix
- Discontinuous-Galerkin
- Conservation
- Boundary conditions
- Method of manufactured solutions
- Accuracy and effort comparisons

Outline

Lecture 3: Implicit schemes, linearizations, and linear systems

- Implicit time stepping for steady flows
  - Newton's method
  - Residual linearization
  - GMRES
- Example calculations

Outline

Lecture 4: Adaptive, overset meshes for Petrov-Galerkin

- Overset meshes
- Adaptive meshing

Assumptions on Audience

- It is assumed that the audience has familiarity with finite-volume methods for solving compressible Navier-Stokes equations on unstructured meshes
- Minimal experience with stabilized finite elements or discontinuous Galerkin
- My own background includes extensive code development for finite-volume methods on structured and unstructured meshes
  - CFL3D – structured
  - FUN3D – unstructured (fun3d.larc.nasa.gov)
- Over the last five years developed high-order finite-element methods and believe they offer significant advantages over finite-volume method

Governing Equations

- Compressible Navier-Stokes with Spalart-Allmaras Turbulence Model

$$\frac{\partial \boldsymbol{Q}}{\partial t} + \nabla \cdot \left(\boldsymbol{F}_e\left(\boldsymbol{Q}\right) - \boldsymbol{F}_v\left(\boldsymbol{Q}, \nabla \boldsymbol{Q}\right)\right) = \boldsymbol{S}\left(\boldsymbol{Q}, \nabla \boldsymbol{Q}\right)$$

$$\boldsymbol{Q} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \\ \rho \tilde{\upsilon} \end{bmatrix} \quad \boldsymbol{F}_e^x = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u w \\ \left(\rho E + p\right) u \\ \rho u \tilde{\upsilon} \end{bmatrix} \quad \boldsymbol{F}_e^y = \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v w \\ \left(\rho E + p\right) v \\ \rho v \tilde{\upsilon} \end{bmatrix} \quad \boldsymbol{F}_e^z = \begin{bmatrix} \rho w \\ \rho u w \\ \rho v w \\ \rho w^2 + p \\ \left(\rho E + p\right) w \\ \rho w \tilde{\upsilon} \end{bmatrix}$$

Governing Equations

- Compressible Navier-Stokes with Spalart-Allmaras Turbulence Model

$$\boldsymbol{F}_v^x = \begin{bmatrix} 0 \\ \tau_{xx} \\ \tau_{xy} \\ \tau_{xz} \\ u\tau_{xx} + v\tau_{xy} + w\tau_{xz} + \kappa \frac{\partial T}{\partial x} \\ \frac{1}{\sigma}\mu\left(1+\psi\right)\frac{\partial \tilde{v}}{\partial x} \end{bmatrix} \quad \boldsymbol{F}_v^y = \begin{bmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \tau_{yz} \\ u\tau_{xy} + v\tau_{yy} + w\tau_{yz} + \kappa \frac{\partial T}{\partial y} \\ \frac{1}{\sigma}\mu\left(1+\psi\right)\frac{\partial \tilde{v}}{\partial y} \end{bmatrix} \quad \boldsymbol{F}_v^z = \begin{bmatrix} 0 \\ \tau_{xz} \\ \tau_{yz} \\ \tau_{zz} \\ u\tau_{xz} + v\tau_{yz} + w\tau_{zz} + \kappa \frac{\partial T}{\partial z} \\ \frac{1}{\sigma}\mu\left(1+\psi\right)\frac{\partial \tilde{v}}{\partial z} \end{bmatrix}$$

$$p = \left(\gamma - 1\right)\left(\rho E - \tfrac{1}{2}\rho\left(u^2 + v^2 + w^2\right)\right) \qquad \tau_{ij} = \left(\mu + \mu_T\right)\left(\frac{\partial \boldsymbol{u}_i}{\partial \boldsymbol{x}_j} + \frac{\partial \boldsymbol{u}_j}{\partial \boldsymbol{x}_i} - \frac{2}{3}\frac{\partial \boldsymbol{u}_k}{\partial \boldsymbol{x}_k}\delta_{ij}\right)$$

$$\boldsymbol{S} = \left[0, 0, 0, 0, 0, S_T\right]^T$$

Governing Equations

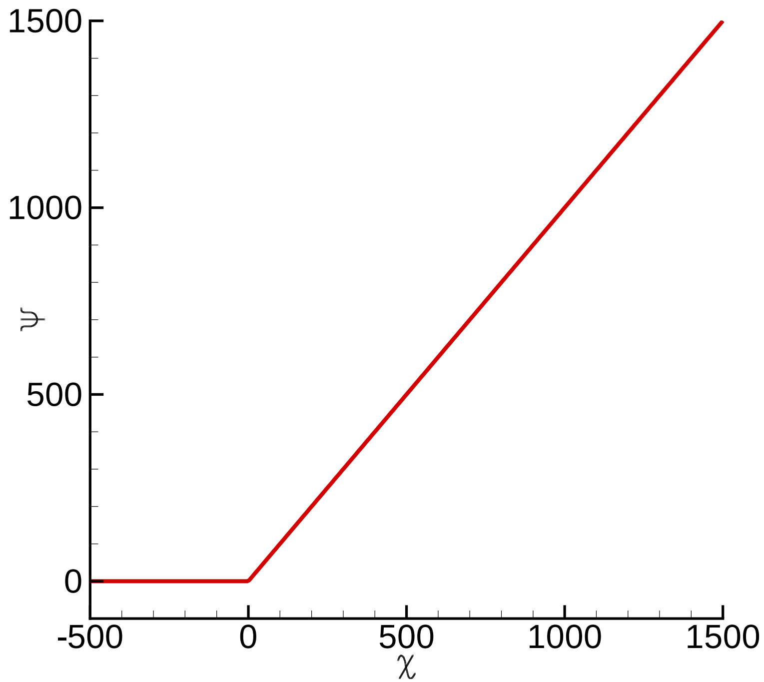
- Compressible Navier-Stokes with Spalart-Allmaras Turbulence Model

$$S_T = c_{b1}\tilde{S}\mu\psi - c_{w1}\rho f_w\left(\frac{\upsilon\psi}{d}\right)^2 + \frac{1}{\sigma}c_{b2}\rho\nabla\tilde{\upsilon}\cdot\nabla\tilde{\upsilon} - \frac{1}{\sigma}\upsilon\left(1+\psi\right)\nabla\rho\cdot\nabla\tilde{\upsilon}$$

ψ : auxiliary turbulence parameter

$\psi = f\left(\chi\right)$ and $\chi = \dfrac{\tilde{\upsilon}}{\upsilon}$

d : distance to nearest viscous wall



Governing Equations

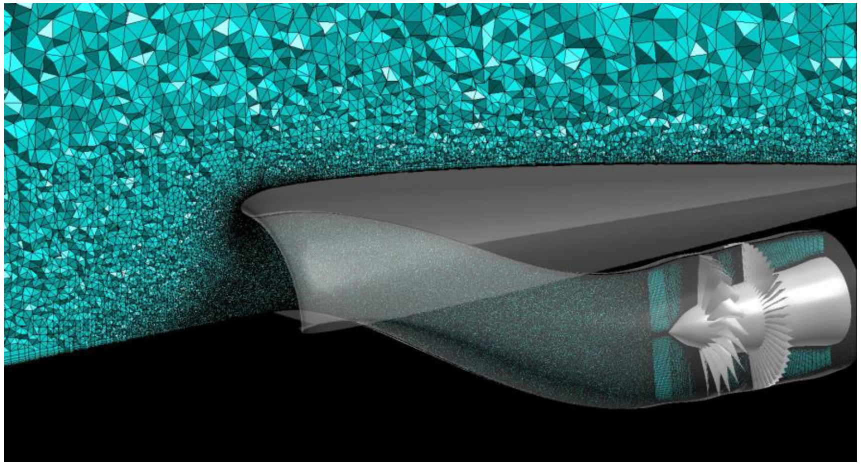
- Occasionally beneficial to examine performance of schemes using Maxwell's equations for electromagnetics
- Provides clean test without ambiguity from nonlinear variable choices

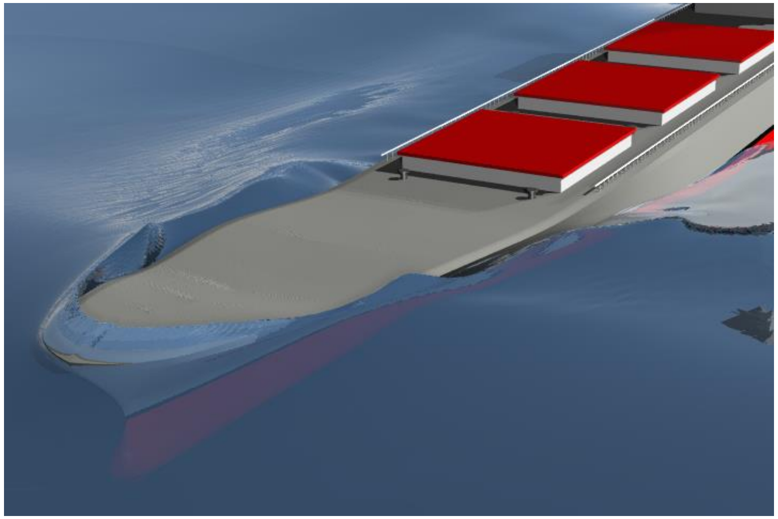
$$\frac{\partial \boldsymbol{Q}}{\partial t} + \nabla \cdot \left(\boldsymbol{F}_e \left(\boldsymbol{Q} \right) \right) = 0$$

$$\boldsymbol{Q} = \begin{bmatrix} D_x \\ D_y \\ D_z \\ B_x \\ B_y \\ B_z \end{bmatrix} \qquad \boldsymbol{F}_e^x = \begin{bmatrix} 0 \\ B_z / \mu \\ -B_y / \mu \\ 0 \\ -D_z / \varepsilon \\ D_y / \varepsilon \end{bmatrix} \qquad \boldsymbol{F}_e^y = \begin{bmatrix} -B_z / \mu \\ 0 \\ B_x / \mu \\ D_z / \varepsilon \\ 0 \\ -D_x / \varepsilon \end{bmatrix} \qquad \boldsymbol{F}_e^z = \begin{bmatrix} B_y / \mu \\ -B_x / \mu \\ 0 \\ -D_y / \varepsilon \\ D_x / \varepsilon \\ 0 \end{bmatrix}$$

Why Finite Elements

- Unstructured meshes have become very popular because of their ability to handle complex geometries and flow fields





- Finite-volume methods dominate modern CFD but have inherent limitations moving forward
- Review of finite-volume methodology to understand limitations

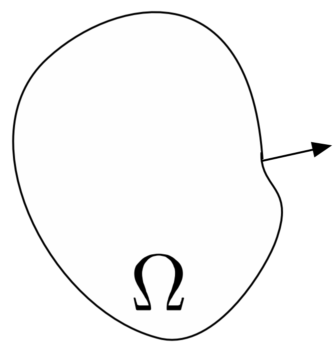
Finite-Volume Unstructured Grids

- Integrate equations over control volume, converting flux integrals into surface integrals using divergence theorem

$$\oiiint_{\Omega} \frac{\partial \boldsymbol{Q}}{\partial t} d\Omega + \oiiint_{\Omega} \nabla \cdot \left(\boldsymbol{F}_e\left(\boldsymbol{Q}\right) - \boldsymbol{F}_v\left(\boldsymbol{Q}, \nabla \boldsymbol{Q}\right)\right) d\Omega = 0$$

$$\Omega \frac{\partial \bar{\boldsymbol{Q}}}{\partial t} + \oiint_{\Gamma} \left(\boldsymbol{F}_e\left(\boldsymbol{Q}\right) - \boldsymbol{F}_v\left(\boldsymbol{Q}\right)\right) \cdot \hat{n} d\Gamma = 0$$

$\bar{\boldsymbol{Q}}$: cell-average



$\hat{n}$: unit normal

- Can be cell-centered or node-centered implementation

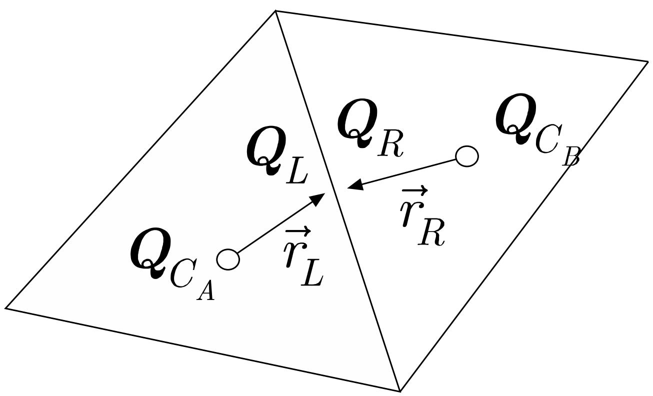
Finite-Volume Unstructured Grids

- In cell-centered scheme, control volume in 2D is defined by triangles and/or quadrilaterals
- Second-order scheme obtained by extrapolating variables from center of cell to the “left” and “right” sides of the interface

$$\boldsymbol{Q}_L = \boldsymbol{Q}_{C_A} + \nabla \boldsymbol{Q}_{C_A} \cdot \vec{r}_L \qquad \boldsymbol{Q}_R = \boldsymbol{Q}_{C_B} + \nabla \boldsymbol{Q}_{C_B} \cdot \vec{r}_R$$

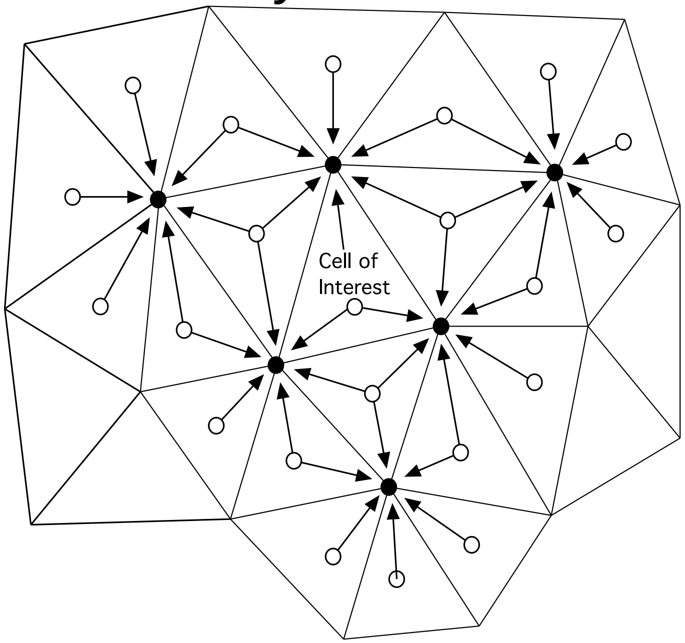
- Flux on cell boundary determined using Riemann solver

$$F\left(\boldsymbol{Q}_L, \boldsymbol{Q}_R\right) = \tfrac{1}{2}\left(F\left(\boldsymbol{Q}_L\right) + F\left(\boldsymbol{Q}_R\right) - \left|\tilde{A}\right|\left(\boldsymbol{Q}_R - \boldsymbol{Q}_L\right)\right)$$



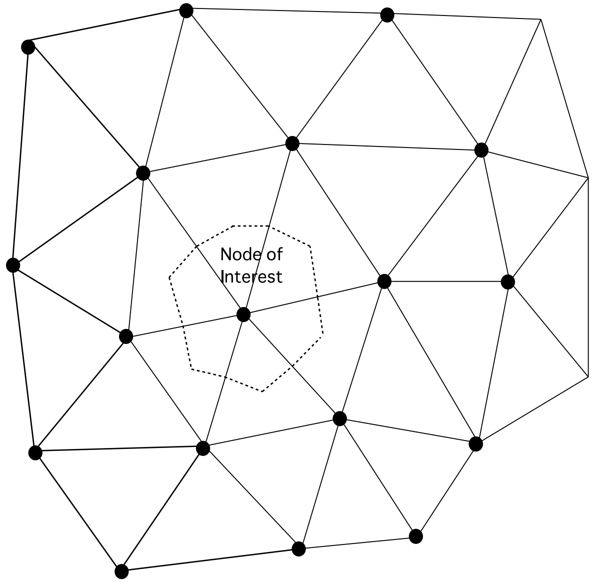
Finite-Volume Unstructured Grids

- Computing gradients in cell centers can be accomplished in many ways but usually involves averaging from cells
- A particularly bad example is when nodal quantities are obtained and then used to compute gradients
- Stencil is very large and data not easily accessed with typical data structures
- On highly stretched meshes, interpolation may also degrade to extrapolation



Finite-Volume Unstructured Grids

- First-order accuracy for node-centered scheme can be obtained using only nearest neighbors
- Second-order accuracy requires gradients at surrounding nodes, which significantly increases the stencil
- As with cell centered finite-volume scheme, stencil is very large and data not easily accessed with typical data structures



Finite-Volume Unstructured Grids

- Whether cell-centered or node-centered scheme, differencing stencil is large and not easily accessible with common data structures. This significantly impacts the ability to obtain an accurate linearization of the residual
  - Newton-type schemes
  - Sensitivity analysis
- Robust interpolation for overset meshes
- Extension to higher-order accuracy can be extremely tedious and error prone
  - Accurately reproducing higher-order polynomials requires even larger stencil
  - Recovering pointwise data from control volume averages

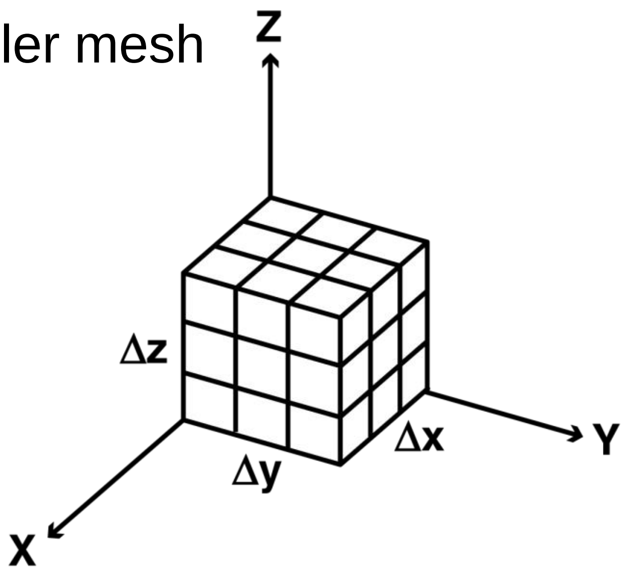
Why Finite Elements?

- Finite-element schemes allow for accurate discretization using a compact stencil that provides easy access to data with common data structures. This has several advantages
  - Newton-type schemes
  - Sensitivity analysis
  - Overset meshes
- Well-established methodologies exist for extending the order of accuracy beyond second-order

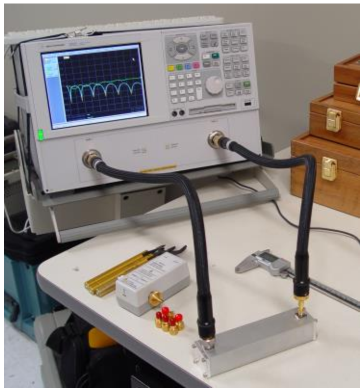
There are potentially very big advantages for developing high-order schemes

Why Higher Order (P > 1)?

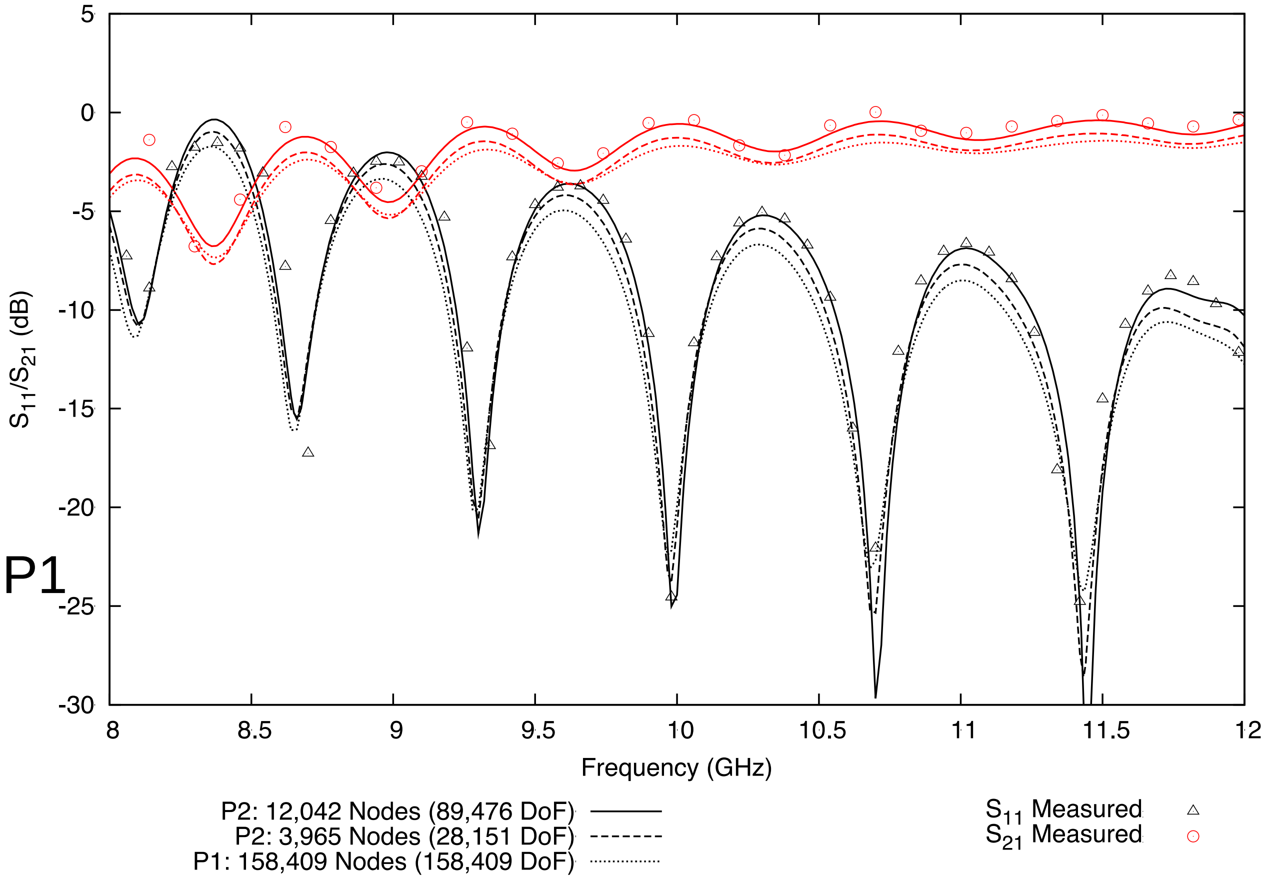
- Assuming cubic domain with equal mesh spacing
- 3D Mesh spacing $h \sim (N)^{-1/3}$ where N is the number of nodes
  - Equal truncation error => $N_{p+1} \sim (N_2)^{2/p+1}$
  - Example: One billion nodes for linear elements requires only one million nodes for equivalent accuracy with quadratic elements
- Very enabling for large-scale science and engineering applications
  - Current problems on smaller mesh
  - Larger problems



Why Higher Order (P > 1)?



P2 with 3,965 nodes more accurate than P1 with 158,409 nodes



- Despite generous assumptions, estimates are somewhat reasonable
- Very significant enabling technology for large-scale simulations !

Outline

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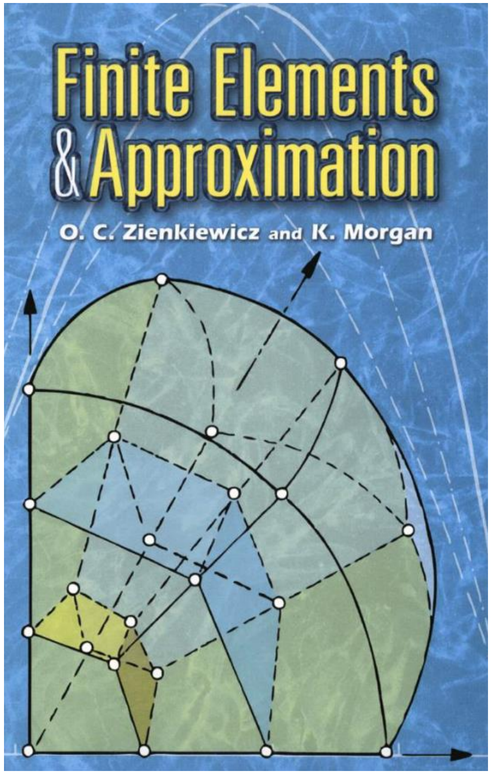
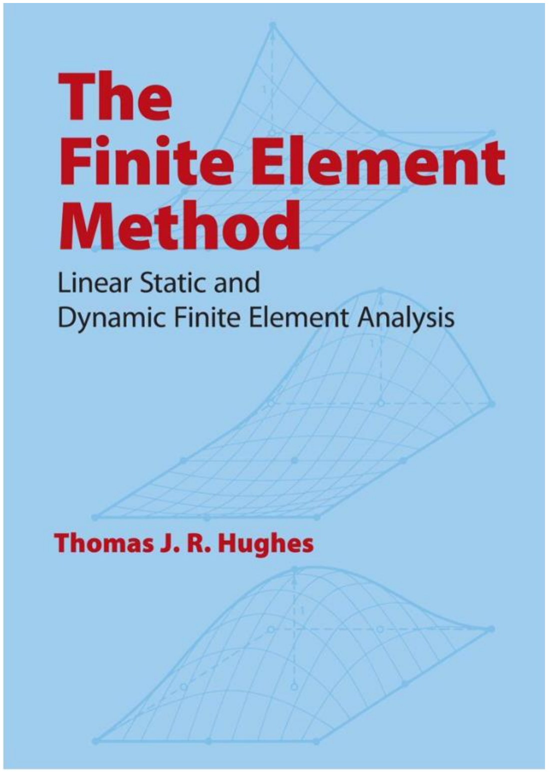
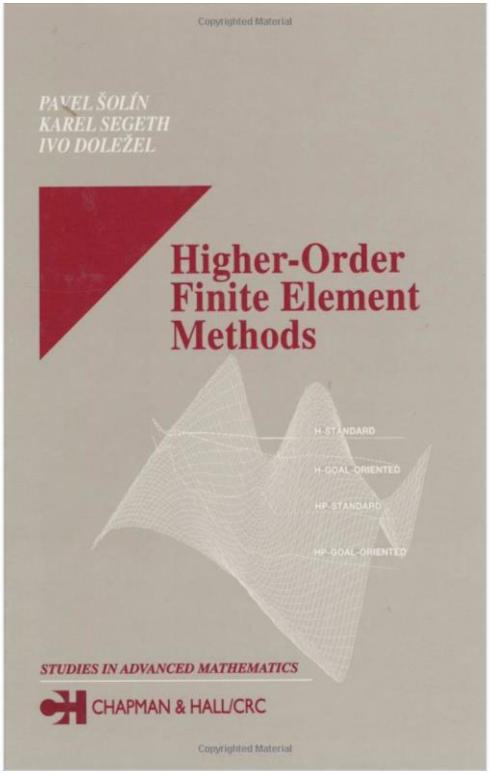
Introduction to Finite Elements

- There are many excellent references for finite elements
- References below extensively used in development of notes





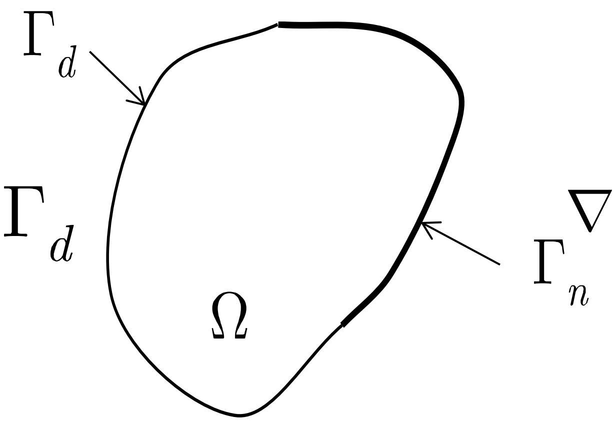


Introduction to Finite Elements

- Galerkin finite-element method for model problem

$$\nabla^2 \psi + p = 0 \;\; \text{in } \Omega$$

$$\psi = g \text{ on } \Gamma_d$$



$$\nabla \cdot \psi = h \text{ on } \Gamma \backslash \Gamma_n$$

- Will first consider one spatial dimension

$\frac{\partial \psi}{\partial x}$ Specified on left end

ψ Specified on right end

Introduction to Finite Elements

$$\nabla^2 \psi + p = 0 \quad \text{in } \Omega$$ Partial differential equation

$$\iiint_{\Omega} \phi \left(\nabla^2 \psi + p \right) d\Omega = 0$$ Weighted residual

- Weak statement obtained through integration by parts

$$\iiint_{\Omega} \phi \left(\nabla^2 \psi + p \right) d\Omega = -\iiint_{\Omega} \left(\nabla \phi \cdot \nabla \psi - \phi p \right) d\Omega + \iint_{\Gamma} \left(\phi \nabla \psi \cdot \hat{n} \right) d\Gamma$$

- Weak statement indicates admissible set of basis functions
  - Differentiable on element
  - To be convergent they must be complete

Basis Functions

- Weak statement after specialization to one spatial dimension

$$-\int_{\Omega}\left(\frac{\partial\phi}{\partial x}\cdot\frac{\partial\psi}{\partial x}\right)d\Omega+\int_{\Omega}\phi p\,d\Omega+\int_{\Gamma}\left(\phi\frac{\partial\psi}{\partial x}\cdot\hat{n}\right)d\Gamma=0$$

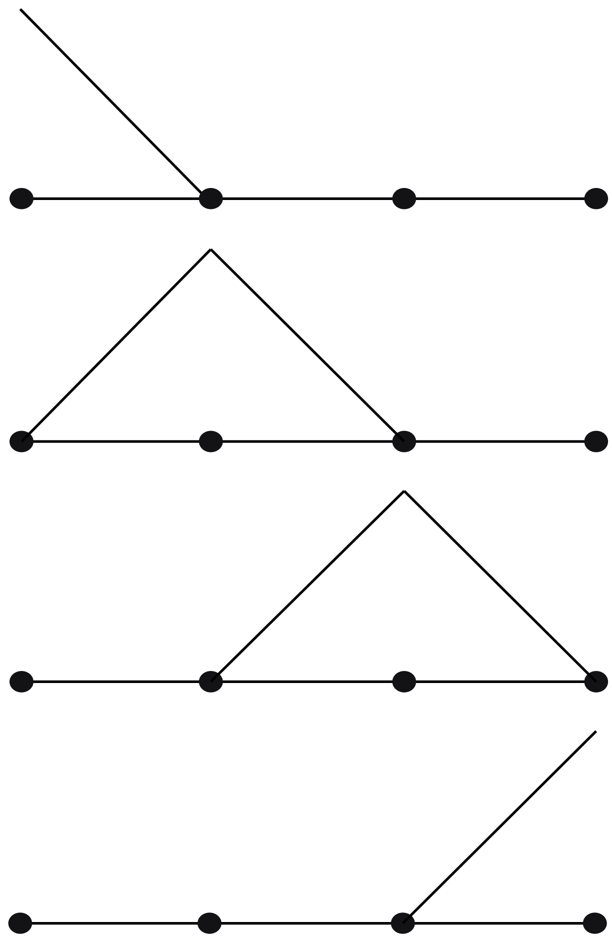
- Consider example with only four nodes in grid with ψ specified on right end, derivatives of ψ specified on left
- ϕ Weighting functions
  - Arbitrary constants c_i
  - Globally defined basis functions N_i

$$\phi=\sum_{i=1}^{3}c_iN_i \quad \frac{\partial\phi}{\partial x}=\sum_{i=1}^{3}c_i\frac{\partial N_i}{\partial x}$$

- ψ is expanded in terms of basis functions plus additional basis function at right end for enforcing boundary condition

Linear Basis Functions
Three-Element Example

N_1, N_2, N_3, N_4



$$N_1 = \begin{cases} 1-3x & 0 \le x \le 1/3 \\ 0 & 1/3 \le x \le 2/3 \\ 0 & 2/3 \le x \le 1 \end{cases}$$

$$N_2 = \begin{cases} 3x & 0 \le x \le 1/3 \\ 2-3x & 1/3 \le x \le 2/3 \\ 0 & 2/3 \le x \le 1 \end{cases}$$

$$N_3 = \begin{cases} 0 & 0 \le x \le 1/3 \\ -1+3x & 1/3 \le x \le 2/3 \\ 3-3x & 2/3 \le x \le 1 \end{cases}$$

$$N_4 = \begin{cases} 0 & 0 \le x \le 1/3 \\ 0 & 1/3 \le x \le 2/3 \\ -2+3x & 2/3 \le x \le 1 \end{cases}$$

Equations for Three-Element Example

- Substitution of discretized functions into weak statement

$$-\int_{\Omega}\left[\left(c_1\frac{\partial N_1}{\partial x}+c_2\frac{\partial N_2}{\partial x}+c_3\frac{\partial N_3}{\partial x}\right)\left(\psi_1\frac{\partial N_1}{\partial x}+\psi_2\frac{\partial N_2}{\partial x}+\psi_3\frac{\partial N_3}{\partial x}+g\frac{\partial N_4}{\partial x}\right)\right]d\Omega$$

$$+c_1h+\int_{\Omega}\left[\left(c_1N_1+c_2N_2+c_3N_3\right)p\right]d\Omega=0$$

- With c's arbitrary there are 3 equations and 3 unknowns

$$-\int_{\Omega}\left[\frac{\partial N_1}{\partial x}\left(\psi_1\frac{\partial N_1}{\partial x}+\psi_2\frac{\partial N_2}{\partial x}+\psi_3\frac{\partial N_3}{\partial x}+g\frac{\partial N_4}{\partial x}\right)\right]d\Omega+\int_{\Omega}\left(N_1p\right)d\Omega+h=0$$

$$-\int_{\Omega}\left[\frac{\partial N_2}{\partial x}\left(\psi_1\frac{\partial N_1}{\partial x}+\psi_2\frac{\partial N_2}{\partial x}+\psi_3\frac{\partial N_3}{\partial x}+g\frac{\partial N_4}{\partial x}\right)\right]d\Omega+\int_{\Omega}\left(N_2p\right)d\Omega=0$$

$$-\int_{\Omega}\left[\frac{\partial N_3}{\partial x}\left(\psi_1\frac{\partial N_1}{\partial x}+\psi_2\frac{\partial N_2}{\partial x}+\psi_3\frac{\partial N_3}{\partial x}+g\frac{\partial N_4}{\partial x}\right)\right]d\Omega+\int_{\Omega}\left(N_3p\right)d\Omega=0$$

Matrix Equations for Three Elements

- Equations arranged in matrix form

$$\begin{bmatrix} -\int \frac{\partial N_1}{\partial x}\frac{\partial N_1}{\partial x}d\Omega & -\int \frac{\partial N_1}{\partial x}\frac{\partial N_2}{\partial x}d\Omega & -\int \frac{\partial N_1}{\partial x}\frac{\partial N_3}{\partial x}d\Omega \\ -\int \frac{\partial N_2}{\partial x}\frac{\partial N_1}{\partial x}d\Omega & -\int \frac{\partial N_2}{\partial x}\frac{\partial N_2}{\partial x}d\Omega & -\int \frac{\partial N_2}{\partial x}\frac{\partial N3}{\partial x}d\Omega \\ -\int \frac{\partial N_3}{\partial x}\frac{\partial N_1}{\partial x}d\Omega & -\int \frac{\partial N_3}{\partial x}\frac{\partial N_2}{\partial x}d\Omega & -\int \frac{\partial N_3}{\partial x}\frac{\partial N_3}{\partial x}d\Omega \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{Bmatrix} = \begin{Bmatrix} RHS_1 \\ RHS_2 \\ RHS_3 \end{Bmatrix}$$

- Solve for $\left(\psi_1, \psi_2, \psi_3\right)$

$$\begin{Bmatrix} RHS_1 \\ RHS_2 \\ RHS_3 \end{Bmatrix} = \begin{Bmatrix} \int\left(\frac{\partial N_1}{\partial x}\frac{\partial N_4}{\partial x}g - N_1 p\right)d\Omega - h \\ \int\left(\frac{\partial N_2}{\partial x}\frac{\partial N_4}{\partial x}g - N_2 p\right)d\Omega \\ \int\left(\frac{\partial N_3}{\partial x}\frac{\partial N_4}{\partial x}g - N_3 p\right)d\Omega \end{Bmatrix}$$

Matrix Equations for Three Element Example

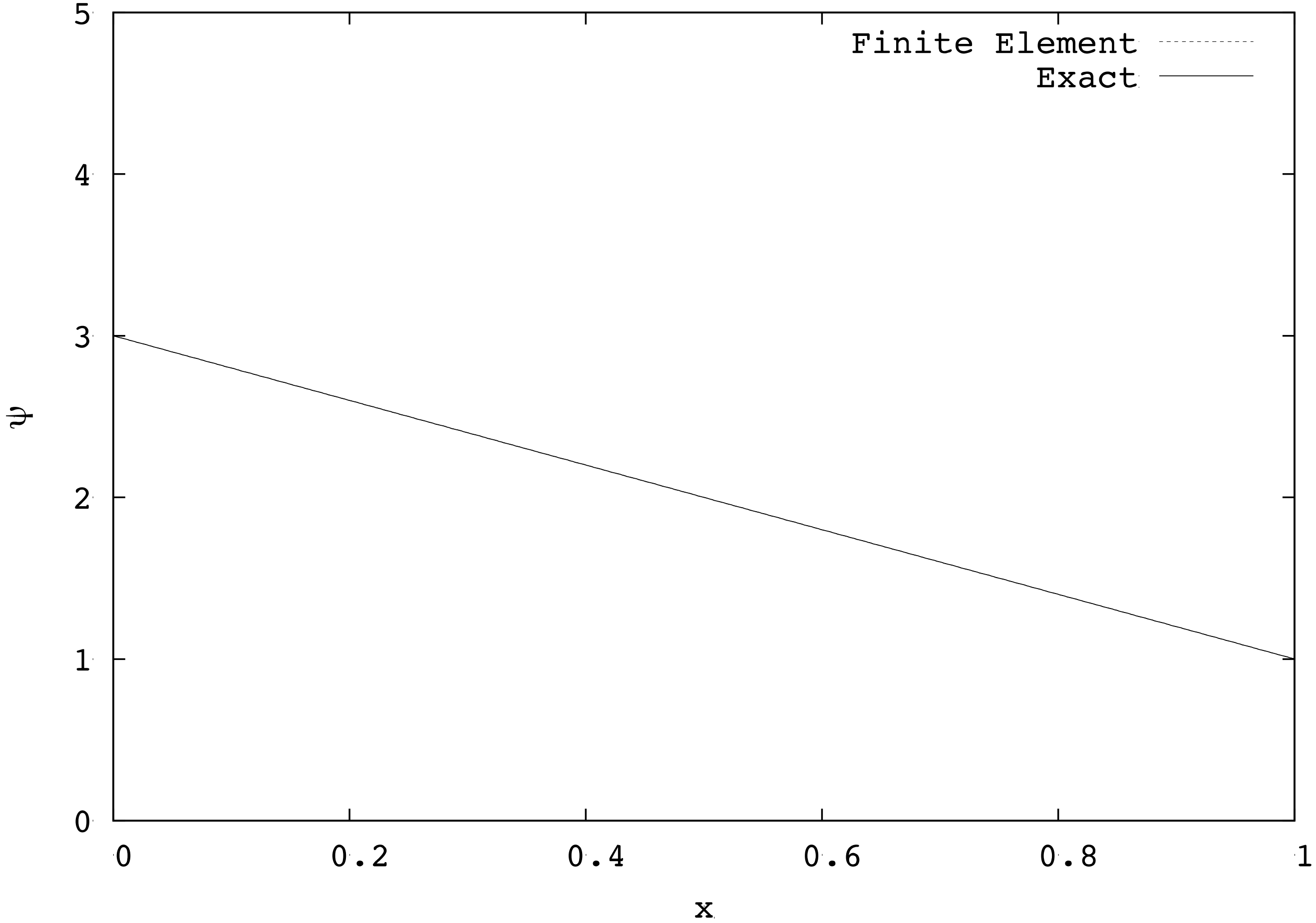
- Equations arranged in matrix form

$$\begin{bmatrix} -3 & 3 & 0 \\ 3 & -6 & 3 \\ 0 & 3 & -6 \end{bmatrix} \begin{Bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{Bmatrix} = \begin{Bmatrix} -h - \frac{p}{6} \\ -\frac{p}{3} \\ -3g - \frac{p}{3} \end{Bmatrix}$$

- Solve for $\left(\psi_1, \psi_2, \psi_3\right)$

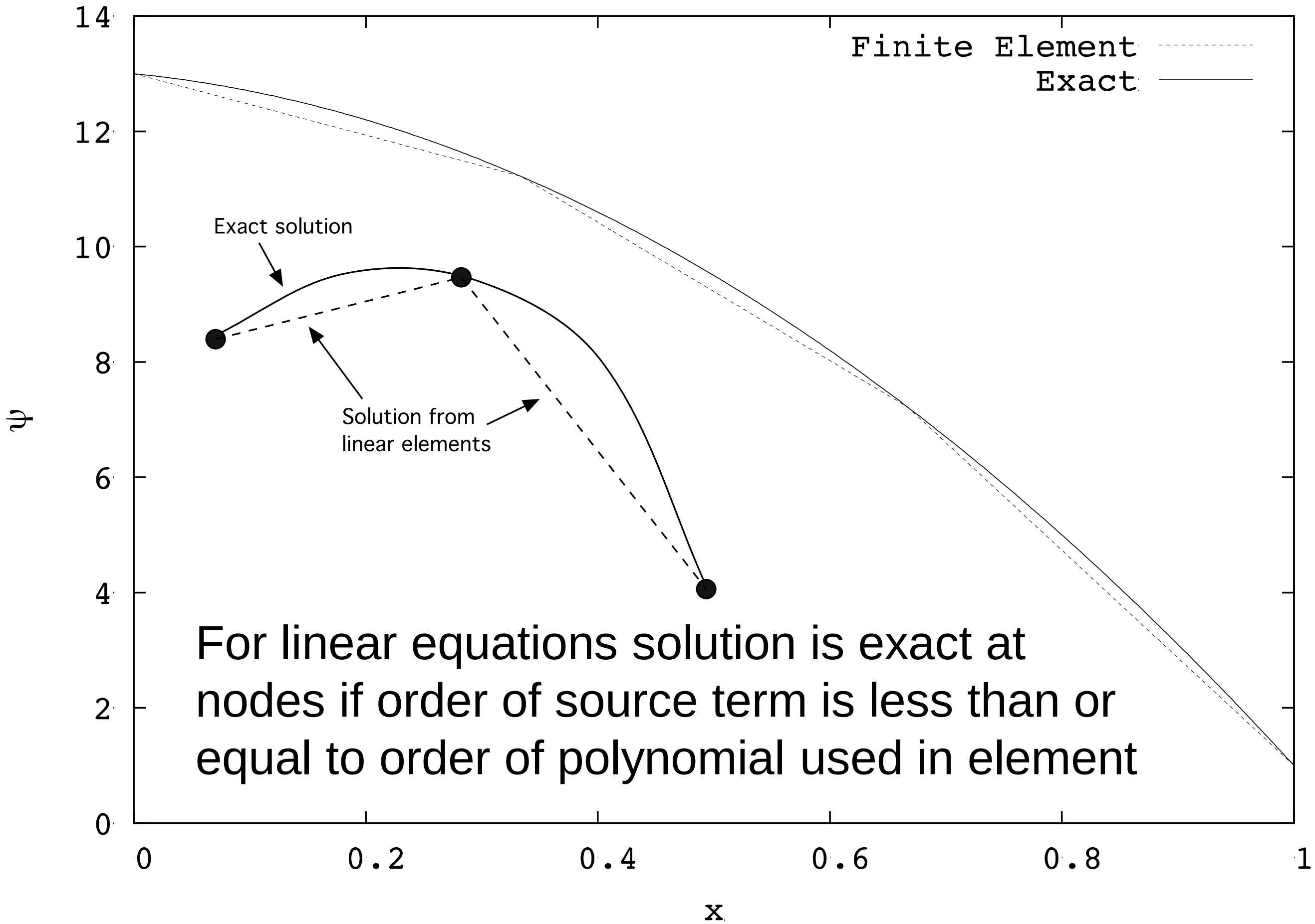
Results for Linear Basis Functions

$$\nabla^2 \psi = 0 \quad \text{in } \Omega$$



Results for Linear Basis Functions

$$\nabla^2\psi + 20 = 0 \quad \text{in } \Omega$$



For linear equations solution is exact at nodes if order of source term is less than or equal to order of polynomial used in element

Element Basis Functions

- Note that in the example there are 3 "residual" equations

$$-\int_{\Omega}\left[\frac{\partial N_1}{\partial x}\left(\psi_1\frac{\partial N_1}{\partial x}+\psi_2\frac{\partial N_2}{\partial x}+\psi_3\frac{\partial N_3}{\partial x}+g\frac{\partial N_4}{\partial x}\right)\right]d\Omega+\int_{\Omega}\left(N_1 p\right)d\Omega+h=0$$

$$-\int_{\Omega}\left[\frac{\partial N_2}{\partial x}\left(\psi_1\frac{\partial N_1}{\partial x}+\psi_2\frac{\partial N_2}{\partial x}+\psi_3\frac{\partial N_3}{\partial x}+g\frac{\partial N_4}{\partial x}\right)\right]d\Omega+\int_{\Omega}\left(N_2 p\right)d\Omega=0$$

$$-\int_{\Omega}\left[\frac{\partial N_3}{\partial x}\left(\psi_1\frac{\partial N_1}{\partial x}+\psi_2\frac{\partial N_2}{\partial x}+\psi_3\frac{\partial N_3}{\partial x}+g\frac{\partial N_4}{\partial x}\right)\right]d\Omega+\int_{\Omega}\left(N_3 p\right)d\Omega=0$$

- Each residual equation has similar terms and only differs by the multiplication factor from weighting function or by presence of boundary term
- Also note that each integral is non-zero only when both multiplied terms from the basis functions are non-zero

Element Basis Functions

- Residual associated with node 1

$$-\int_{\Omega}\left[\frac{\partial N_1}{\partial x}\frac{\partial N_1}{\partial x}\psi_1+\frac{\partial N_1}{\partial x}\frac{\partial N_2}{\partial x}\psi_2+\underbrace{\frac{\partial N_1}{\partial x}\frac{\partial N_3}{\partial x}}_{0}\psi_3+\underbrace{\frac{\partial N_1}{\partial x}\frac{\partial N_4}{\partial x}}_{0}g\right]d\Omega+\int_{\Omega}\left(N_1 p\right)d\Omega+h=0$$

- Residual associated with node 2

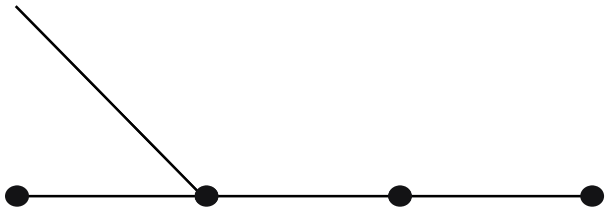
$$-\int_{\Omega}\left[\frac{\partial N_2}{\partial x}\frac{\partial N_1}{\partial x}\psi_1+\frac{\partial N_2}{\partial x}\frac{\partial N_2}{\partial x}\psi_2+\frac{\partial N_2}{\partial x}\frac{\partial N_3}{\partial x}\psi_3+\underbrace{\frac{\partial N_2}{\partial x}\frac{\partial N_4}{\partial x}}_{0}g\right]d\Omega+\int_{\Omega}\left(N_2 p\right)d\Omega=0$$

- Residual associated with node 3

$$-\int_{\Omega}\left[\underbrace{\frac{\partial N_3}{\partial x}\frac{\partial N_1}{\partial x}}_{0}\psi_1+\frac{\partial N_3}{\partial x}\frac{\partial N_2}{\partial x}\psi_2+\frac{\partial N_3}{\partial x}\frac{\partial N_3}{\partial x}\psi_3+\frac{\partial N_3}{\partial x}\frac{\partial N_4}{\partial x}g\right]d\Omega+\int_{\Omega}\left(N_3 p\right)d\Omega=0$$

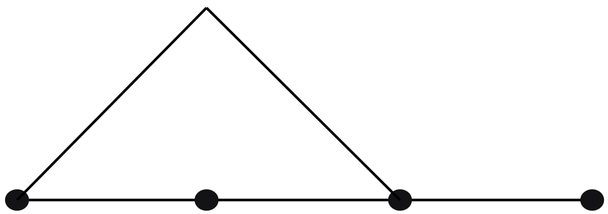
Linear Basis Functions
Three Element Example

N_1



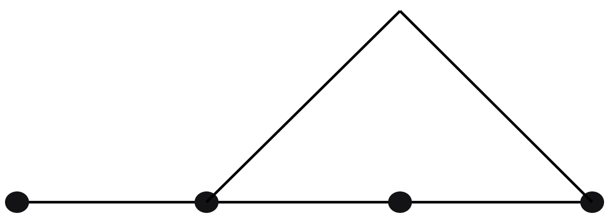
$$N_1 = \begin{cases} 1-3x & 0 \le x \le 1/3 \\ 0 & 1/3 \le x \le 2/3 \\ 0 & 2/3 \le x \le 1 \end{cases}$$

N_2



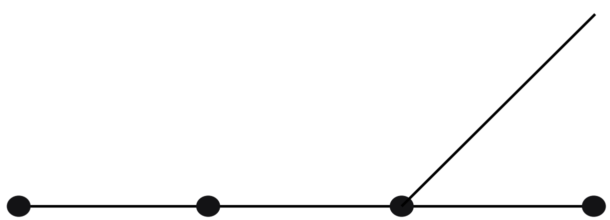
$$N_2 = \begin{cases} 3x & 0 \le x \le 1/3 \\ 2-3x & 1/3 \le x \le 2/3 \\ 0 & 2/3 \le x \le 1 \end{cases}$$

N_3



$$N_3 = \begin{cases} 0 & 0 \le x \le 1/3 \\ -1+3x & 1/3 \le x \le 2/3 \\ 3-3x & 2/3 \le x \le 1 \end{cases}$$

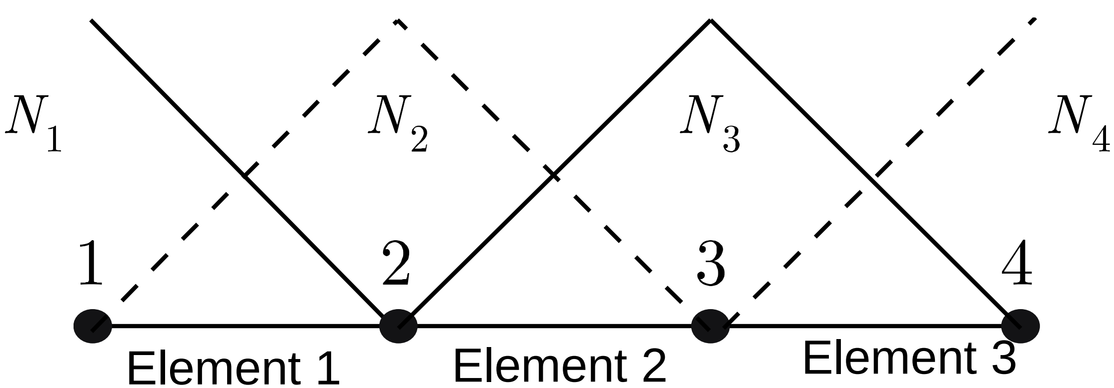
N_4



$$N_4 = \begin{cases} 0 & 0 \le x \le 1/3 \\ 0 & 1/3 \le x \le 2/3 \\ -2+3x & 2/3 \le x \le 1 \end{cases}$$

Element Basis Functions

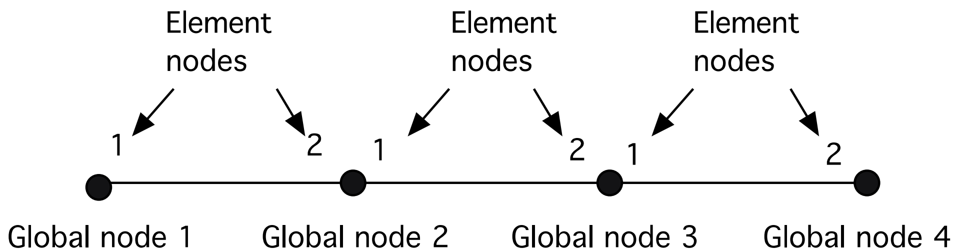
- Each global basis function is nonzero only on elements associated with node i
- The non-zero global basis functions within each element can be used to define local basis functions



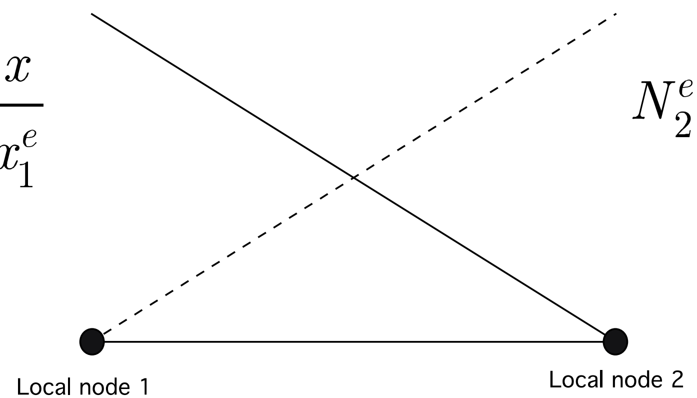
Element 1	Element 2	Element 3
$N_1^e = 1 - 3x$	$N_1^e = 2 - 3x$	$N_1^e = -2 + 3x$
$N_2^e = 3x$	$N_2^e = -1 + 3x$	$N_2^e = 3 - 3x$

Element Basis Functions

- Within each element, local basis functions can be defined that have identical form for all elements



$$N_1^e = \frac{x_2^e - x}{x_2^e - x_1^e}$$



$$N_2^e = \frac{x - x_1^e}{x_2^e - x_1^e}$$

Element Basis Functions

- Residual at node i can be computed by considering one element at a time

$$R_i^e = R_i^e - \int_{\Omega_e} \frac{\partial N_i^e}{\partial x}\left[\sum_{j=1}^{2}\frac{\partial N_j^e}{\partial x}\psi_j^e\right]d\Omega_e + \int_{\Omega_e}\left(N_i^e p\right)d\Omega_e$$

$$i = 1,2$$

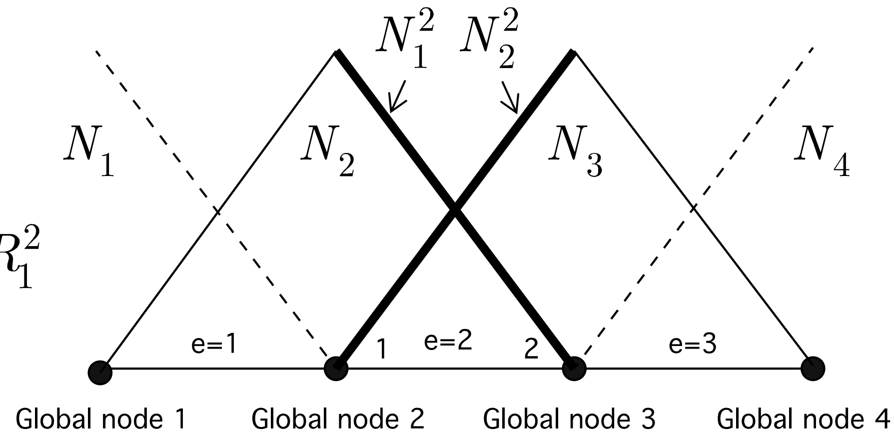
- After interior elements are accounted for an additional loop is required to include contributions from boundary conditions

$$R_i^e = R_i^e + \int_{\Gamma} N_i^e \nabla\psi \cdot \hat{n}\, d\Gamma \quad \text{Boundary term added at ends}$$

Element Basis Functions

- For example, updating global node 2 from within element 2

$$R_2 = R_2^1 + R_1^2$$



$$R_1^2 = \int_{\Omega_2} \frac{\partial N_1^2}{\partial x} \left(\frac{\partial N_1^2}{\partial x} \psi_1^2 + \frac{\partial N_2^2}{\partial x} \psi_2^2 \right) d\Omega_e + \int_{\Omega_2} N_1^2 p \, d\Omega_e$$

Global node 2

$$R_1^2 = \int_{\Omega_2} \frac{\partial N_2}{\partial x} \left(\frac{\partial N_2}{\partial x} \psi_2 + \frac{\partial N_3}{\partial x} \psi_3 \right) d\Omega_e + \int_{\Omega_2} N_2 p \, d\Omega_e$$

Element Mapping

- Motivation
  - In general, PDE may preclude exact integration
  - Without mapping, basis functions need to be defined element-by-element
  - When extending to multidimensions, closed form integration over element topology does not exist except in special cases
  - A unified formulation for defining basis function and performing integration is desirable (automation)
- Mapping from physical element to a “parent” element mitigates many of these problems

Element Mapping

- Define "parent" element that all elements get mapped to

x_1^e ——— x_2^e $\Rightarrow$ $\xi_1^e = 0$ ——— $\xi_2^e = 1$

$$x = x(\xi)$$

$$N_1^e(x) = (x_2^e - x)/(x_2^e - x_1^e) \qquad x = \sum N_i^e(\xi) x_i^e \qquad N_1^e(\xi) = 1 - \xi$$

$$N_2^e(x) = (x - x_1^e)/(x_2^e - x_1^e) \qquad N_2^e(\xi) = \xi$$

- Functions, derivatives, and integrals must be transformed

$$\psi = \sum N_i^e(\xi) \psi_i^e \qquad \frac{d(\bullet)}{dx} = \left(\frac{dx}{d\xi}\right)^{-1} \frac{d(\bullet)}{d\xi}$$

$$\int_{\Omega} f(x) d\Omega = \int_{\hat{\Omega}} f(x(\xi)) \left|\frac{dx}{d\xi}\right| d\hat{\Omega}$$

Quadrature

- General numerical formulas for integrating over common element types

$$\int_{\hat{\Omega}} f\left(x\left(\xi\right)\right)\left|\frac{\partial x}{d\xi}\right| d\hat{\Omega} \approx \sum_{i=1}^{NQ} f\left(x\left(\xi_i\right)\right)\left|\frac{\partial x}{d\xi}\right| w_i$$

where NQ is the number of quadrature points, each located within the element at location ξ_i and w_i is an associated weight

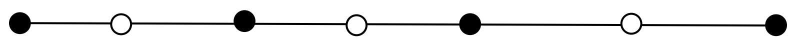
- Familiar quadrature rule in one dimension is Simpson's rules

$$\int_{\hat{\Omega}} f\left(x\left(\xi\right)\right)\left|\frac{\partial x}{d\xi}\right| d\hat{\Omega} \approx \frac{h^e}{6}\left(f\left(x\left(0\right)\right) + 4f\left(x\left(\tfrac{1}{2}\right)\right) + f\left(x\left(1\right)\right)\right)$$

$$\left|\frac{dx}{d\xi}\right| = \left(x_2^e - x_1^e\right) = h^e$$

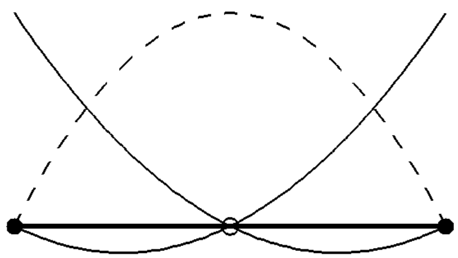
High-Order Basis Functions

- High-order solutions obtained by increasing polynomial order of the basis functions



Element e

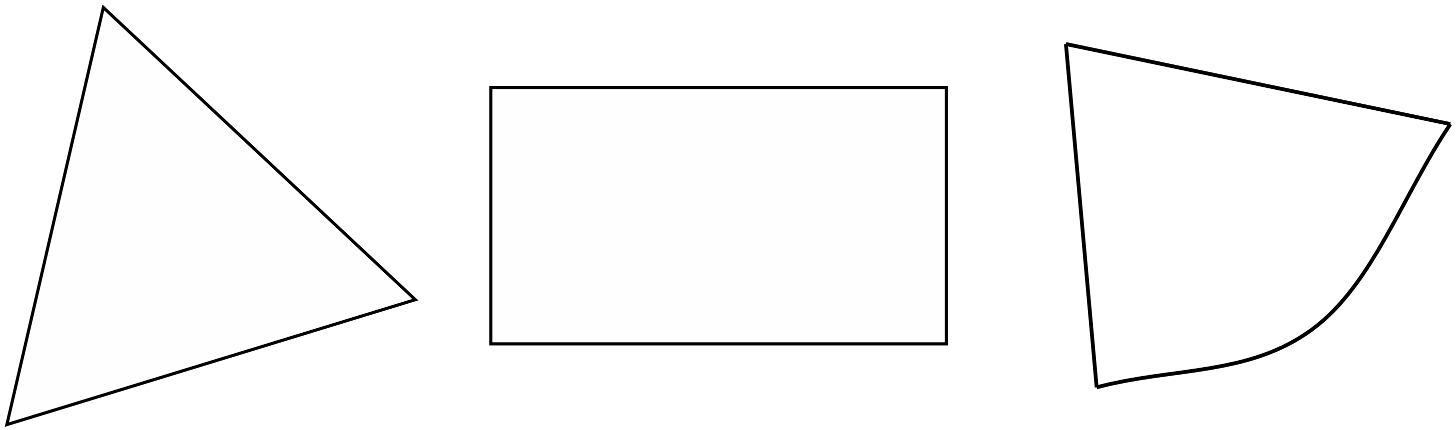
$$N_1^e = (1-\xi)(1-2\xi) \qquad N_3^e = 4\xi(1-\xi) \qquad N_2^e = -\xi(1-2\xi)$$



- Requires higher-order quadrature as well

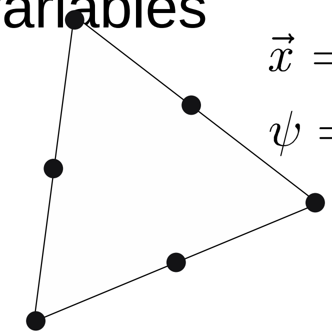
Extension to Multidimensions

- General procedure identical to one-dimension
- Basis functions and quadrature rules defined on parent element
- Elements can be different sizes and shapes but may also be curved



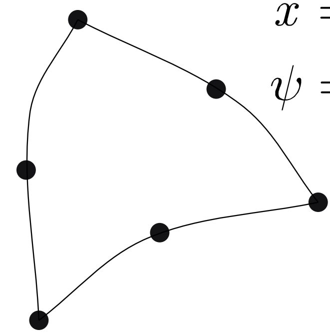
Basis Functions

- Usually defined in mapped space over parent element
- Polynomial orders may be different for geometry and variables



$$\vec{x} = \vec{x}\left(\vec{\xi}\right) \quad \text{Linear}$$

$$\psi = \psi\left(\vec{\xi}\right) \quad \text{Quadratic}$$



$$\vec{x} = \vec{x}\left(\vec{\xi}\right) \quad \text{Quadratic}$$

$$\psi = \psi\left(\vec{\xi}\right) \quad \text{Quadratic}$$

$$\vec{x} = \sum_{i=1}^{m} N_i^e\left(\vec{\xi}\right)\vec{x}_i$$

$$\psi = \sum_{i=1}^{n} N_i^e\left(\vec{\xi}\right)\psi_i$$

$m > n$ Superparametric

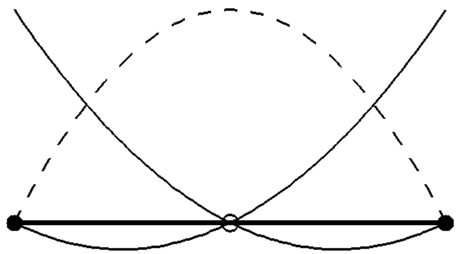
$m = n$ Isoparametric

$m < n$ Subparametric

Types of Basis Functions

- Lagrangian – unknowns within element represent actual data and shape functions are high-order polynomials

$$N_1^e = \left(1-\xi\right)\left(1-2\xi\right) \qquad N_3^e = 4\xi\left(1-\xi\right) \qquad N_2^e = -\xi\left(1-2\xi\right)$$

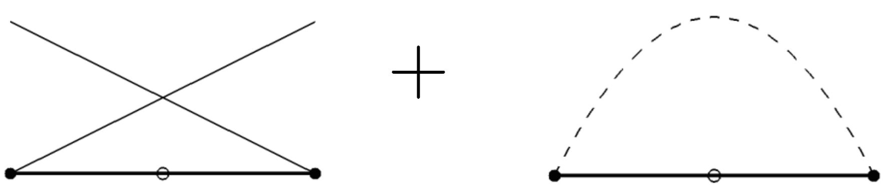


- Hierarchical – unknowns represented as linear contribution with additional modes that represent perturbations

$$N_1^e\left(\vec{\xi}\right) = \text{Linear}$$

$$N_2^e\left(\vec{\xi}\right) = \text{Linear}$$

$$N_3^e\left(\vec{\xi}\right) = \text{Quadratic}$$



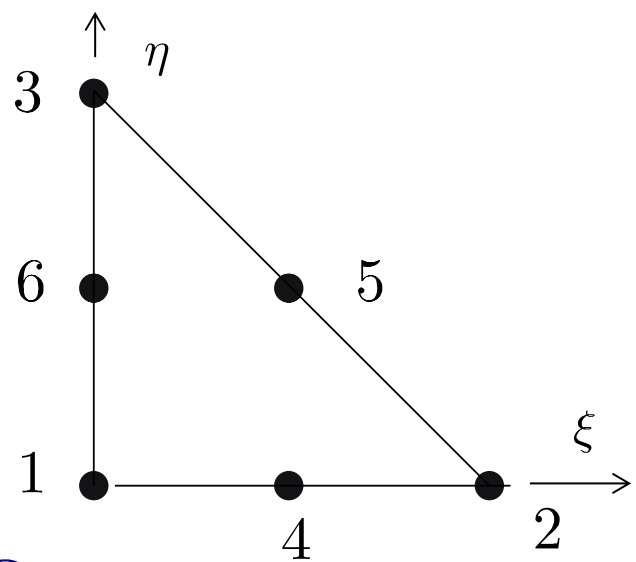
Lagrangian Basis Functions

- Can be determined algebraically

$$N_i^e\left(\xi_j,\eta_j\right) = a + b\xi_j + c\eta_j + d\xi_j^2 + e\eta_j^2 + f\xi_j\eta_j$$

$$N_i^e\left(\xi_j,\eta_j\right) = 1 \quad \text{if} \quad i = j$$

$$N_i^e\left(\xi_j,\eta_j\right) = 0 \quad \text{if} \quad i \neq j$$



$$N_1^e = 1 - 3\left(\xi + \eta\right) + 2\left(\xi^2 + \eta^2\right) + 4\xi\eta$$

$$N_2^e = 2\xi\left(\xi - \tfrac{1}{2}\right)$$

$$N_3^e = 2\eta\left(\eta - \tfrac{1}{2}\right)$$

$$N_4^e = 4\xi\left(1 - \xi - \eta\right)$$

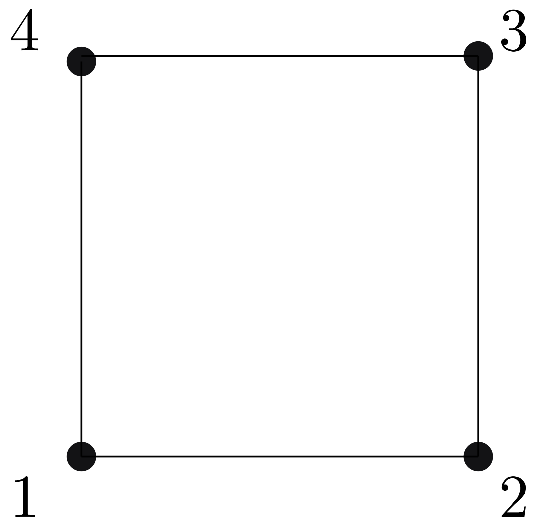
$$N_5^e = 4\xi\eta$$

$$N_6^e = 4\eta\left(1 - \xi - \eta\right)$$

Lagrangian Basis Functions

- For triangles and tetrahedrons, number of nodes in element matches number of unknown coefficients in polynomial
- For other elements this may not be the case

$$N_i^e\left(\xi_j,\eta_j\right)=a+b\xi_j+c\eta_j+d\xi_j^2+e\eta_j^2+f\xi_j\eta_j$$



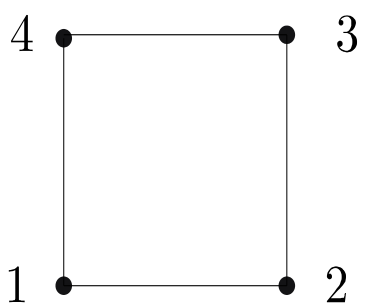
- 4 Nodes in Element but 6 unknown coefficients required for complete quadratic polynomial
- 4 nodes gives complete linear polynomial but incomplete quadratic polynomial
- Pascal's triangle to determine terms to keep

Pascal's Triangle

- Higher-order quadrilateral, hexahedral, pyramidal, and pentahedral elements have more degrees of freedom than required for complete polynomial

$$
\begin{array}{ccccccc}
 & & & 1 & & & \\
 & & \xi & & \eta & & \\
 & \xi^2 & & \xi\eta & & \eta^2 & \\
\xi^3 & & \xi^2\eta & & \xi\eta^2 & & \eta^3
\end{array}
$$

- Usually choose terms to maintain symmetry of element



$$N_i^e\left(\xi_j, \eta_j\right) = a + b\xi_j + c\eta_j + d\xi_j\eta_j$$

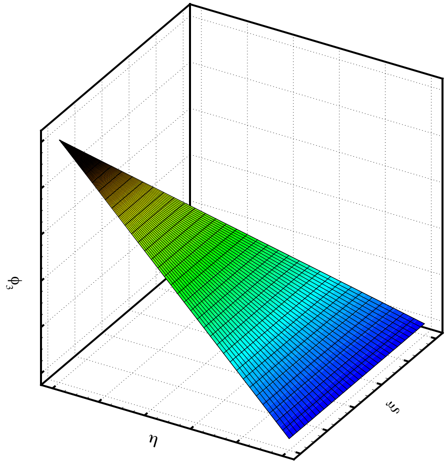
Hierarchical Basis Functions

- Basis functions are combination of linear basis functions plus basis functions that represent perturbations
- Consider cubic basis functions

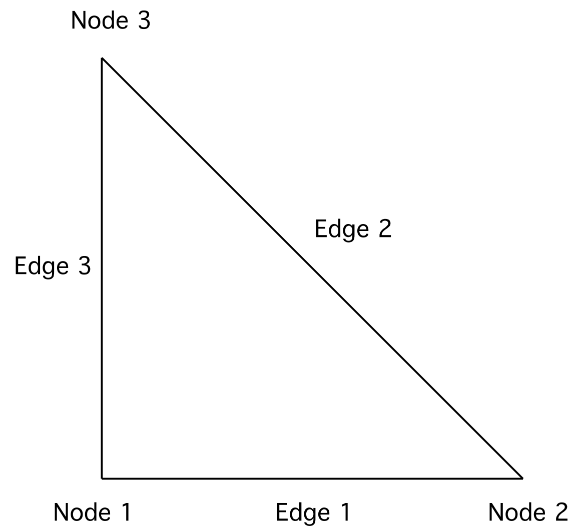
$$\psi^e\left(\xi,\eta\right) = \sum_{i=1}^{3} \text{linear vertex functions} + \sum_{i=1}^{3} \text{quadratic edge functions} + \sum_{i=1}^{3} \text{cubic edge functions} + \text{ bubble function}$$

  - Linear basis functions correspond to nodal basis functions
  - Edge functions are zero on two edges, Lobatto polynomial on third edge
  - Hierarchical basis functions better conditioned
  - Solution variables represent modal coefficients

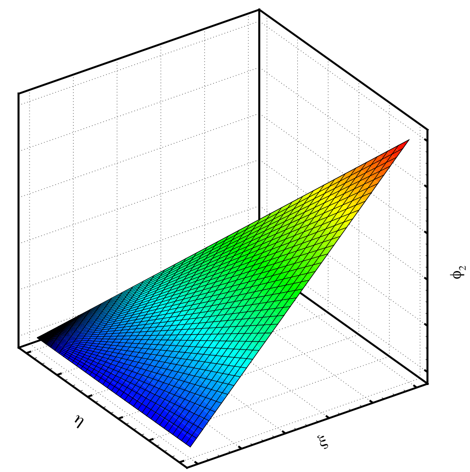
Hierarchical Basis Functions
Linear Contributions

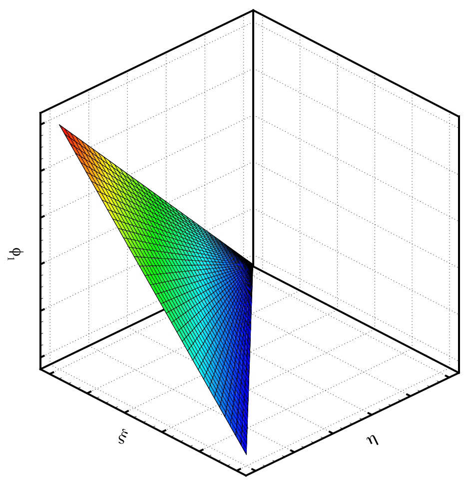


$$N_3^v = \eta$$



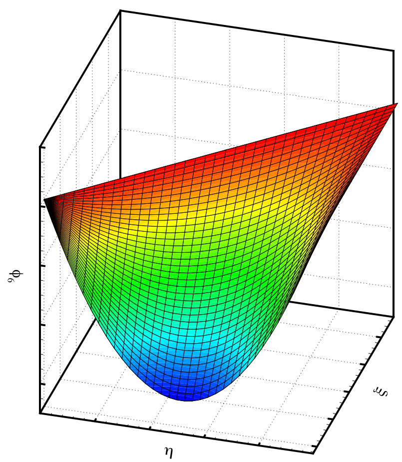
$$N_2^v = \xi$$

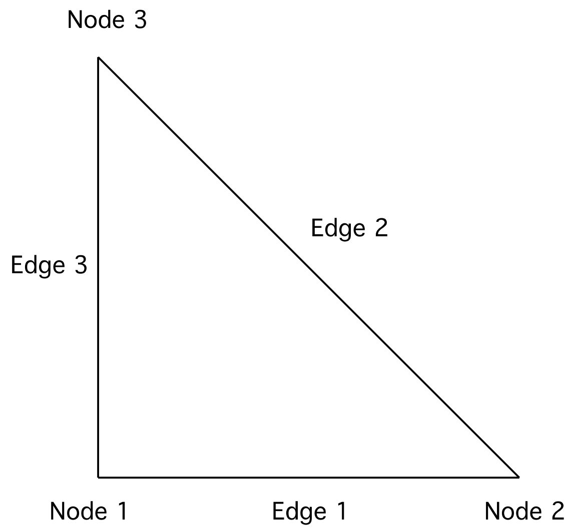


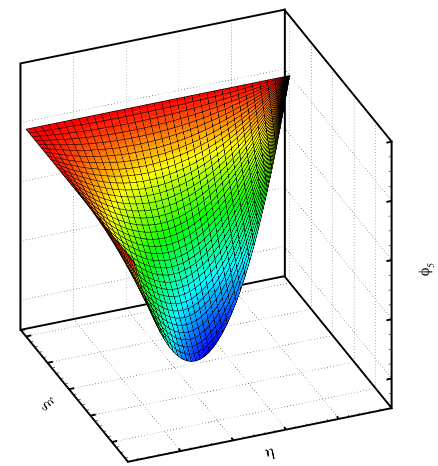


$$N_1^v = 1 - \xi - \eta$$

Hierarchical Basis Functions
Quadratic Edge Functions

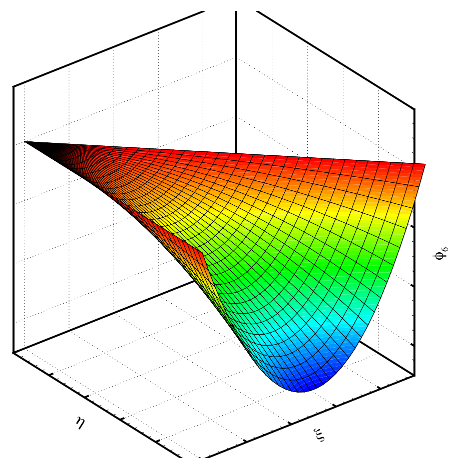






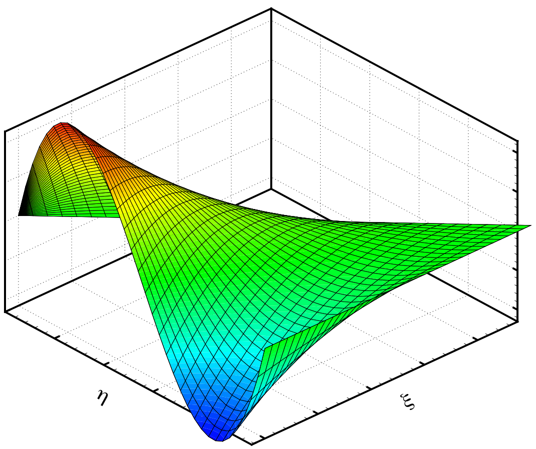
$$^{2}N_3^e = -2\sqrt{\frac{3}{2}}\left(1-\xi-\eta\right)\eta$$

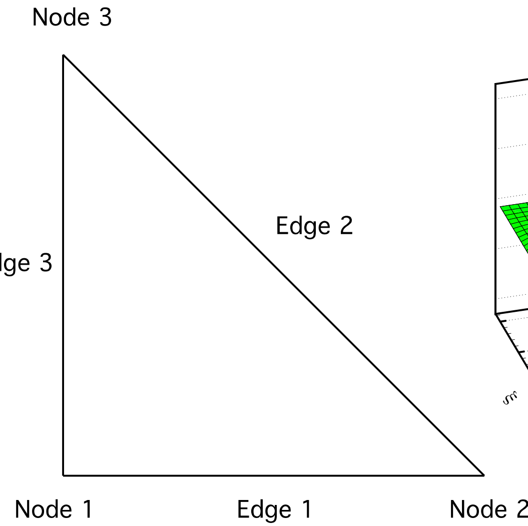
$$^{2}N_2^e = -2\sqrt{\frac{3}{2}}\xi\eta$$

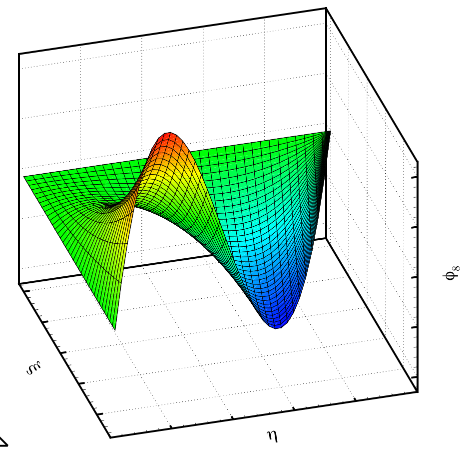


$$^{2}N_1^e = -2\sqrt{\frac{3}{2}}\left(1-\xi-\eta\right)\xi$$

Hierarchical Basis Functions
Cubic Edge Functions



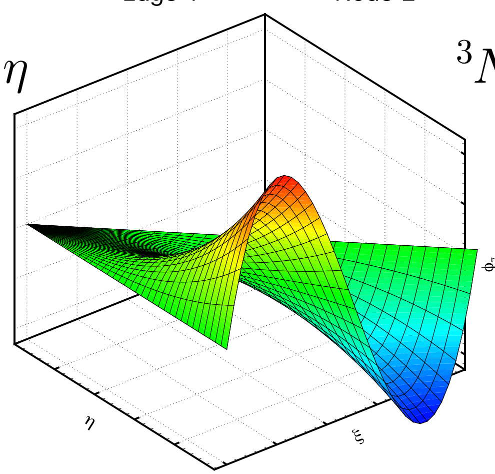




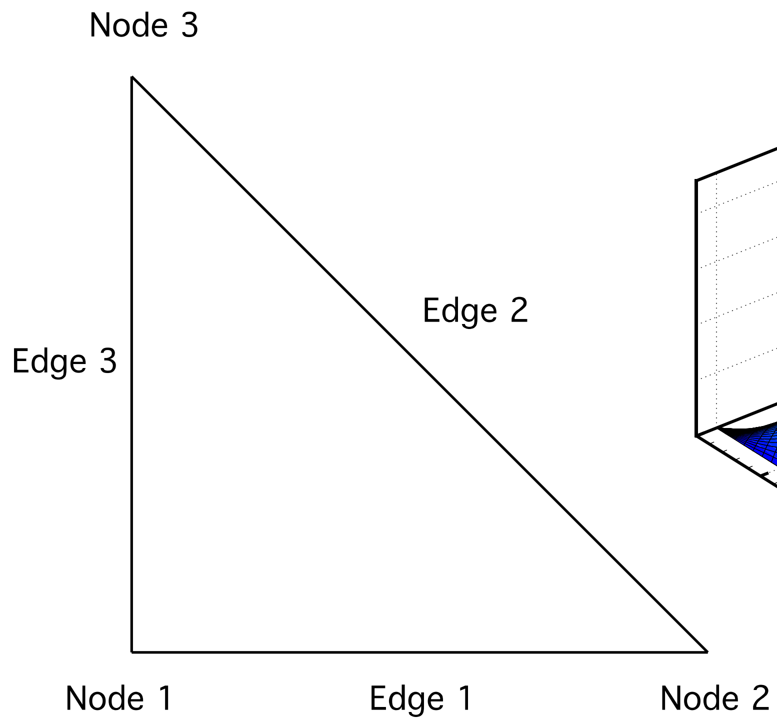
$$ {}^{3}N_3^e = -2\sqrt{\tfrac{5}{2}}\big(1-\xi-\eta\big)\big(1-2\eta-\xi\big)\eta $$

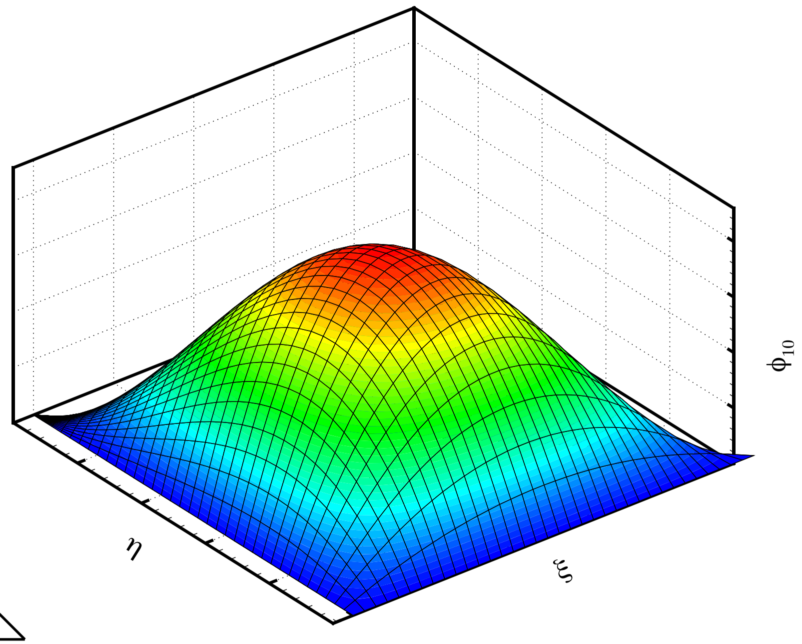
$$ {}^{3}N_2^e = -2\sqrt{\tfrac{5}{2}}\big(\xi-\eta\big)\xi\eta $$

$$ {}^{3}N_1^e = 2\sqrt{\tfrac{5}{2}}\big(1-\xi-\eta\big)\big(1-2\xi-\eta\big)\xi $$



Hierarchical Basis Functions
Bubble Function for Cubic Element





$$N_1^b = \left(1-\xi-\eta\right)\xi\eta$$

FE / FV Equivalence

- Examine special case where finite-element and finite-volume schemes are identical
- Consider Laplace's equation as model problem

$$\nabla^2 \psi = 0 \quad \text{in } \Omega$$

Partial differential equation

$$\iiint_{\Omega} \phi \left(\nabla^2 \psi \right) d\Omega = 0$$

Weighted residual

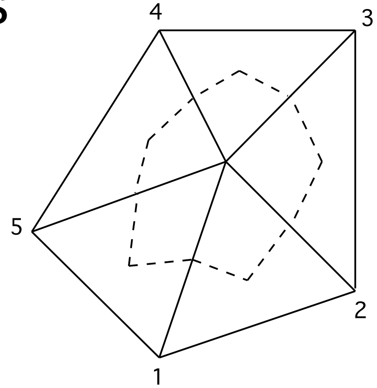
- For finite-volume scheme weighting function is simply unity so integration by parts yields the following

$$\iiint_{\Omega} \nabla^2 \psi \, d\Omega = \iint_{\Gamma} \left(\nabla \psi \cdot \hat{n} \right) d\Gamma$$

- To compute residual at a node the surface integral for the control volume surrounding the node needs to be evaluated

FE / FV Equivalence

- For finite-volume scheme with linear elements use “median dual” formed by connecting centroid of the triangle with the midpoints of the edges

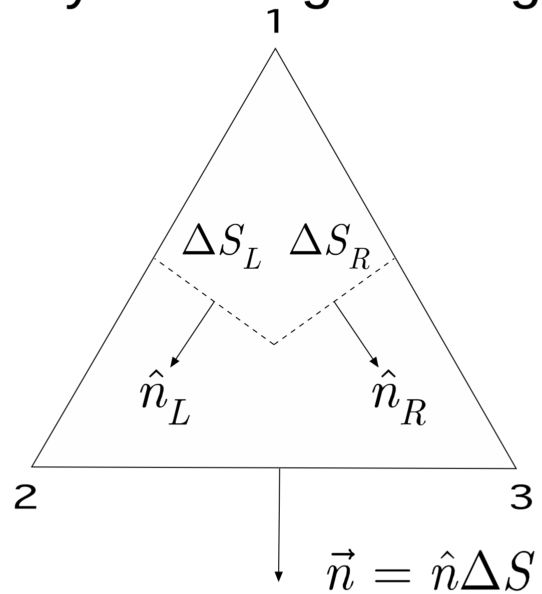


- Integral is approximated by summing over all segments that comprise the boundaries of the median dual

$$\iint_{\Gamma} \left(\nabla \psi \cdot \hat{n} \right) d\Gamma \approx \sum \left(\frac{\partial \psi}{\partial x} \hat{n}_{x_i} + \frac{\partial \psi}{\partial y} \hat{n}_{y_i} \right) \Delta S_i$$

FE / FV Equivalence

- Consider the geometry of a single triangle



- Sum of normal components from median dual is half the normal of the opposite edge

$$\hat{n}_{x_L}\Delta S_L + \hat{n}_{x_R}\Delta S_R = \frac{n_x}{2} \qquad \hat{n}_{y_L}\Delta S_L + \hat{n}_{y_R}\Delta S_R = \frac{n_y}{2}$$

FE / FV Equivalence

- With linear elements the gradients within the cell are constant over the entire cell
- Contribution to integral from single element is given by summing over dual edges and relating the normal components in the dual edge to that of the triangle

$$\sum_{i=1}^{2}\left(\frac{\partial\psi}{\partial x}\hat{n}_{x_i}+\frac{\partial\psi}{\partial y}\hat{n}_{y_i}\right)\Delta S_i=\left(\frac{\partial\psi}{\partial x}\frac{n_x}{2}+\frac{\partial\psi}{\partial y}\frac{n_y}{2}\right)$$

Finite-volume

FE / FV Equivalence

- Consider Laplace's equation as model problem

$$\nabla^2 \psi = 0 \ \text{ in } \Omega$$ Partial differential equation

$$\iiint_{\Omega} \phi \left(\nabla^2 \psi \right) d\Omega = 0$$ Weighted residual

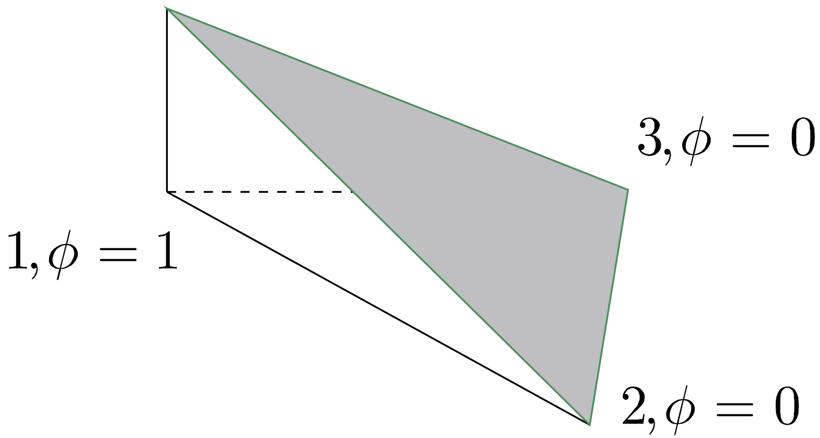
- The weak statement is given as

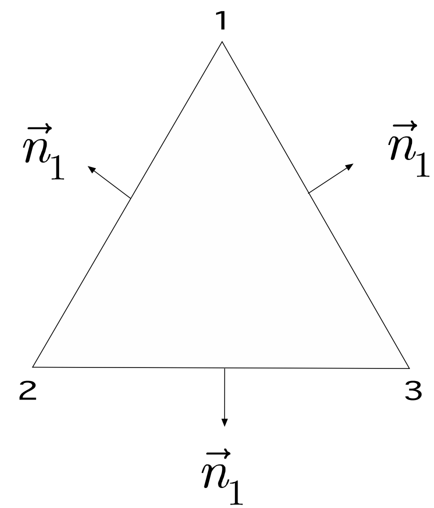
$$\iiint_{\Omega} \phi \nabla^2 \psi d\Omega = -\iiint_{\Omega} \nabla \phi \cdot \nabla \psi \, d\Omega + \iint_{\Gamma} \phi \left(\nabla \psi \cdot \hat{n} \right) d\Gamma$$

- Consider only volume integral (surface integral is over boundaries of domain)

FEM / FV Equivalence

- Weighting function is zero except at node under consideration





- Therefore

$$\frac{\partial \phi}{\partial x} = -\frac{1}{2V}\left(\phi_1 n_{x_1} + \phi_2 n_{x_2} + \phi_3 n_{x_3}\right) \qquad \frac{\partial \phi}{\partial y} = -\frac{1}{2V}\left(\phi_1 n_{y_1} + \phi_2 n_{y_2} + \phi_3 n_{y_3}\right)$$

$$\frac{\partial \phi}{\partial x} = -\frac{1}{2V} n_{x_1} \qquad V = \text{Area} \qquad \frac{\partial \phi}{\partial y} = -\frac{1}{2V} n_{y_1}$$

FE / FV Equivalence

- Because gradient of basis function and weighting function are both constant over the element the volume integral can be approximated as

$$-\iiint_{\Omega} \nabla\phi \cdot \nabla\psi \, d\Omega \approx -\left(\frac{\partial\phi}{\partial x}\frac{\partial\psi}{\partial x} + \frac{\partial\phi}{\partial y}\frac{\partial\psi}{\partial y}\right)V = \left(\frac{n_x}{2}\frac{\partial\psi}{\partial x} + \frac{n_y}{2}\frac{\partial\psi}{\partial y}\right)$$

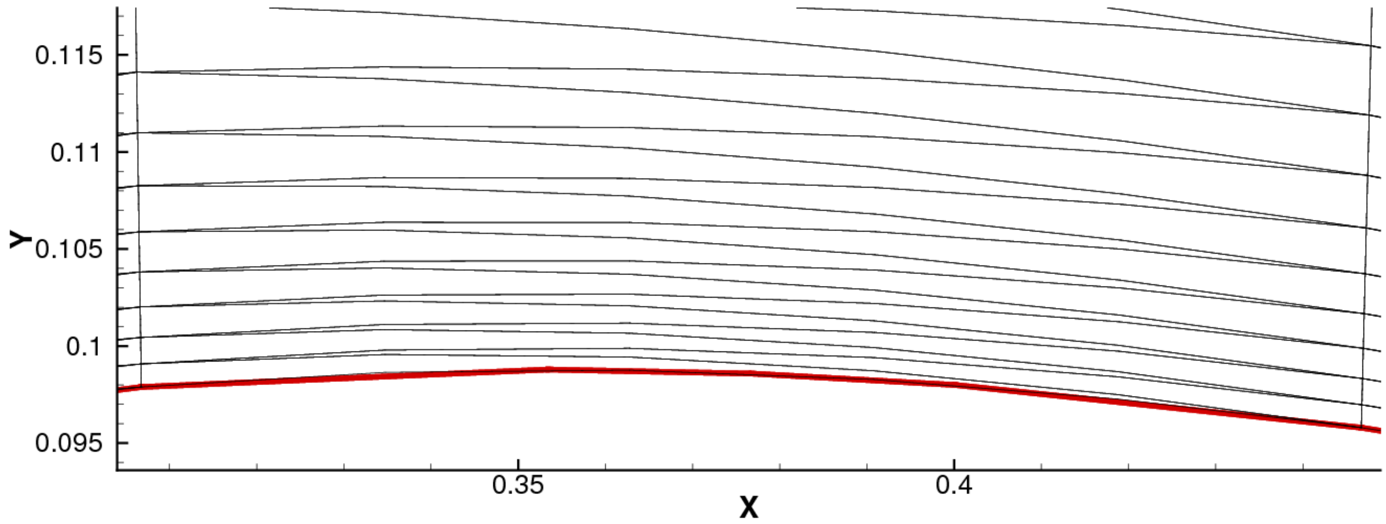
- Recall result from finite-volume

$$\iint_{\Gamma} \nabla\psi \cdot \hat{n} \, d\Gamma \approx \left(\frac{\partial\psi}{\partial x}\frac{n_x}{2} + \frac{\partial\psi}{\partial y}\frac{n_y}{2}\right)$$

- The contribution to the residual is equivalent between linear finite element and linear finite volume for this problem
- Higher-order scheme favors finite-element method

Curved Elements

- Solution of turbulent Navier-Stokes equations requires highly-stretched elements near surface to resolve boundary layer
- Recall that to retain high-order accuracy surfaces must be faithfully reproduced
- Surface curvature propagates into interior elements
- Effects of curved elements on accuracy need to be examined



Curved Elements

- Desired accuracy for quadratic triangle in physical space

$$\psi^e = a + bx + cy + dx^2 + ey^2 + fxy$$

- When element is curved, substitute $\vec{x} = \vec{x}\left(\vec{\xi}\right)$ into above
  - If linear

$$\psi^e = \gamma_1 + \gamma_2\xi + \gamma_3\eta + \gamma_4\xi^2 + \gamma_5\eta^2 + \gamma_6\xi\eta$$

  - If quadratic

$$\psi^e = \gamma_1 + \gamma_2\xi + \gamma_3\eta + \gamma_4\xi^2 + \gamma_5\eta^2 + \gamma_6\xi\eta + \Phi\left(\xi,\eta\right)$$

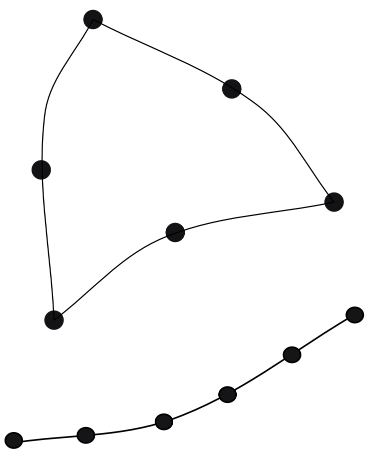
$$\Phi\left(\xi,\eta\right) = \gamma_7\xi^3 + \gamma_8\xi^2\eta + \gamma_9\xi\eta^2 + \gamma_{10}\eta^3 + \gamma_{11}\xi^4 + \gamma_{12}\xi^3\eta + \gamma_{13}\xi^2\eta^2 + \gamma_{14}\xi\eta^3 + \gamma_{15}\eta^4$$

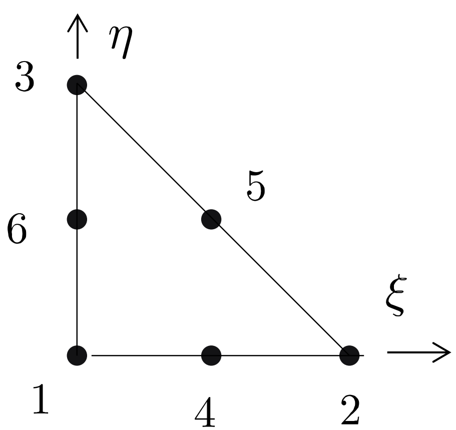
Curved Elements

- Nonlinear transformation requires more terms in mapped space to include all quadratic terms in physical space and be conforming between elements
- Mapping provides conformity but accuracy can be degraded if neglected terms are not below truncation error

$$\psi^e = a + bx + cy + dx^2 + ey^2 + fxy$$

Element-by-element

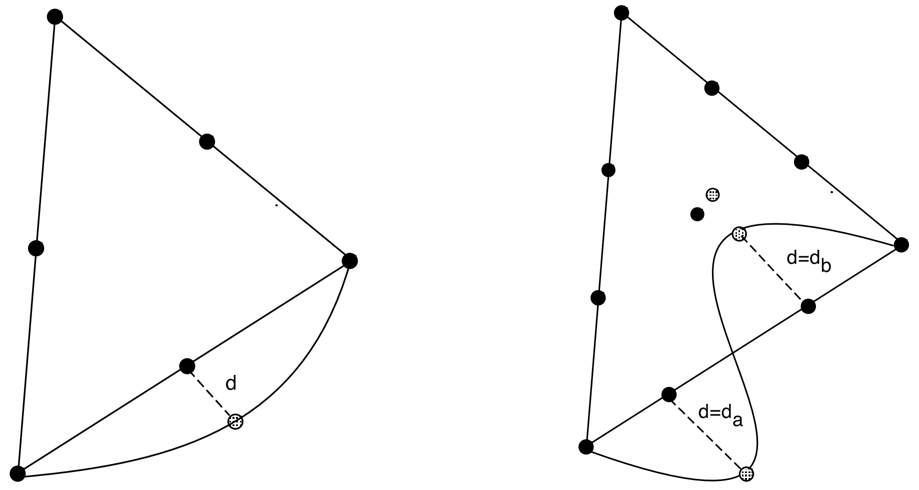




$$N_1^e = 1 - 3\left(\xi + \eta\right) + 2\left(\xi^2 + \eta^2\right) + 4\xi\eta$$
$$N_2^e = 2\xi\left(\xi - \tfrac{1}{2}\right)$$
$$N_3^e = 2\eta\left(\eta - \tfrac{1}{2}\right)$$
$$N_4^e = 4\xi\left(1 - \xi - \eta\right)$$
$$N_5^e = 4\xi\eta$$
$$N_6^e = 4\eta\left(1 - \xi - \eta\right)$$

Curved Elements

- Ciarlet derived conditions for accuracy to be maintained
- For quadratic elements, distance between straight-line segment and location of node must be reduced as h**2
- Cubic elements requires distances to reduce as h**3



- Can verify using "downscaling"

Curved Elements

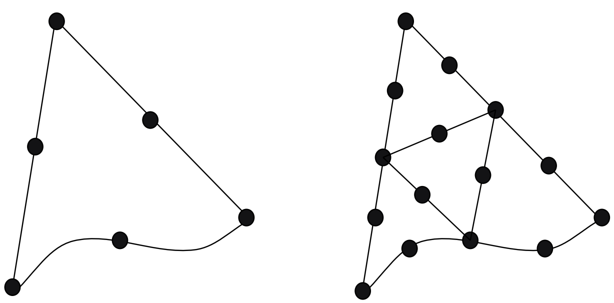
- Downscaling for curved elements verifies Ciarlet's theorem

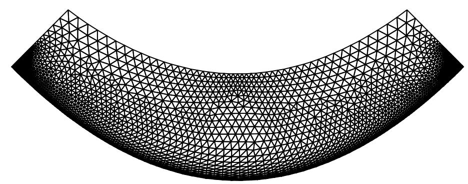
!	!	Polynomial!for!Curving!Edges!		
P4!	Mesh! Reduction! Order!	Quartic!(4)!	Cubic!(3)!	Quadratic!(2)!
	h**2!	3!	4!	5!
	h**3!	4!	5!	5!
	h**4!	5!	5!	5!
P3!	h**2!	!	3!	4!
	h**3!	!	4!	4!
P2!	h**2!	!	!	3!

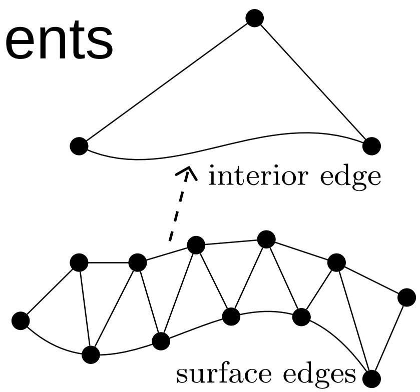
- Ciarlet also points out that on boundaries (e.g. cylinder), distances are reduced quadratically implying loss of accuracy
- Results improve as edges become less curved. Fortunately, this behavior corresponds to what happens in practice

Curved Elements

- Ciarlet's theorems assume element shape remains the same as the mesh is refined
- Uniform refinement changes shapes of elements







- Experiments indicate uniform refinement usually gives correct order property but mesh movement can cause problem
- For manufactured solution on parabolic domain, algebraic mesh movement failed to recover proper order of accuracy while linear elastic approach was successful

Summary of Lecture 1

- Motivated reason for considering high-order finite elements
- Weighted residual and weak statement
- Global basis functions
- Discretization for three-element example
- Element basis functions
- Element mapping
- Quadrature
- High-order basis functions
- Extension to multidimensions
- Curved elements

Suggested Reading

- Zienkiewicz, O.C., and Morgan, K., Finite Elements & Approximation, Dover Publications, 2006.
- Hughes, T.J.R., The Finite Element Method, Dover Publications, 2000.
- Solin, P., Segeth, K., and Dolezel, I., Higher-Order Finite Element Methods, Chapman & Hall/CRC, 2004.
- Ciarlet, P.G., The Finite Element Method for Elliptic Problems, SIAM, 2002.
- McLeod, R., "Node Requirements for High-Order Approximation over Curved Finite Elements," J. Inst. Maths Applics, Vol. 17, No. 2, 1976, pp. 249-254.

Suggested Reading

- Spalart, P. R., and Allmaras, S. R., “A One-Equation Turbulence Model for Aerodynamic Flows,” AIAA Paper No.92-0439, 1991.
- Moro, D., Nguyen, N.C., and Peraire, J., “Navier-Stokes Solution Using Hybridizable Discontinuous Galerkin Methods,” AIAA Paper 2011-3407.

Time-Dependent Problems

$$\frac{\partial \psi}{\partial t} - \nabla^2 \psi + p = 0 \quad \text{in } \Omega$$

$$\iiint_{\Omega} \phi \frac{\partial \psi}{\partial t} d\Omega - \iiint_{\Omega} \left(\nabla \phi \cdot \nabla \psi - p \right) d\Omega + \iint_{\Gamma} \left(\phi \nabla \psi \cdot \hat{n} \right) d\Gamma$$

$$\psi^e = \sum_{i=1}^{n} N(\xi) \psi_i(t) \quad \text{Semi-Discrete} \qquad \psi^e = \sum_{i=1}^{n} N(\xi, t) \psi_i \quad \text{Space-time}$$

- Semi-discrete Ω is spatial volume; time discretized independent
- Space-time Ω includes both space and time

Spalart-Allmaras Turbulence Model

$$\mu_T = \begin{cases} \rho\tilde{\upsilon} f_{v1} & \text{if } \tilde{\upsilon} \geq 0 \\ 0 & \text{if } \tilde{\upsilon} < 0 \end{cases} \qquad \tilde{S} = \begin{cases} S + \widehat{S} & \text{if } \widehat{S} \geq -c_{v2} S \\ S + \frac{S\left(c_{v2}^2 + c_{v3}\widehat{S}\right)}{\left(c_{v3} - 2c_{v2}\right)S - \widehat{S}} & \text{if } \widehat{S} < -c_{v2} S \end{cases}$$

$$S_T = c_{b1}\tilde{S}\mu\psi - c_{w1}\rho f_w \left(\frac{\upsilon\psi}{d}\right)^2 + \frac{1}{\sigma} c_{b2}\rho\nabla\tilde{\upsilon}\cdot\nabla\tilde{\upsilon} - \frac{1}{\sigma}\upsilon\left(1+\psi\right)\nabla\rho\cdot\nabla\tilde{\upsilon}$$

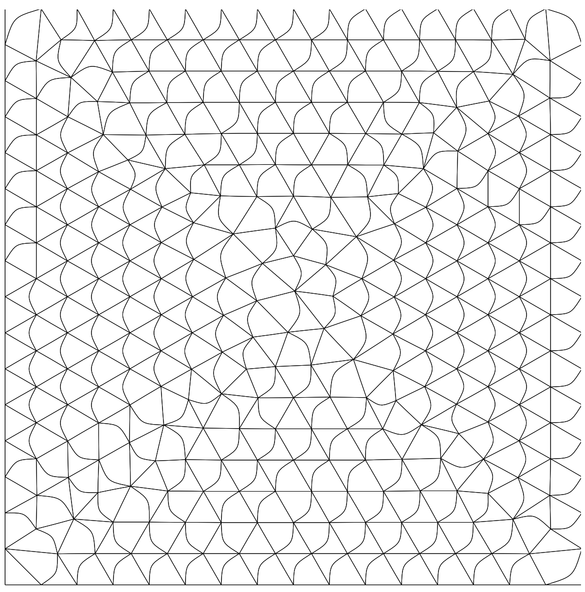
$$S = \sqrt{\vec{\omega}\cdot\vec{\omega}} \qquad \widehat{S} = \frac{\upsilon\psi}{\kappa_T^2 d^2} f_{v2} \qquad f_{v1} = \frac{\psi^3}{\psi^3 + c_{v1}^3} \qquad f_{v2} = 1 - \frac{\psi}{1 + \psi f_{v1}}$$

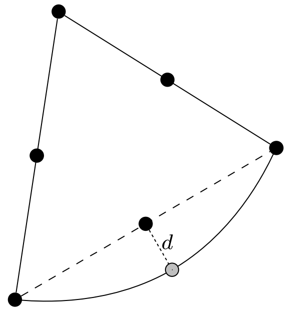
$$\psi = \begin{cases} 0.05\ln\left(1 + e^{20\chi}\right) & \text{if } \chi \leq 10 \\ \chi & \text{if } \chi > 10 \end{cases} \qquad r = \frac{\upsilon\psi}{\tilde{S}\kappa_T^2 d^2} \qquad f_w = g\left(\frac{1 + c_{w3}^6}{g + c_{w3}^6}\right)^{1/6}$$

$$g = r + c_{w2}\left(r^6 - r\right) \qquad \chi = \frac{\tilde{\upsilon}}{\upsilon}$$

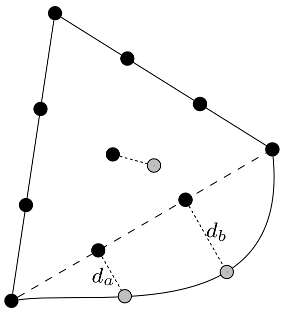
Curved Elements

- On boundaries (e.g. cylinder), distances are reduced quadratically implying loss of accuracy
- Can verify using discontinuous Galerkin or Petrov Galerkin

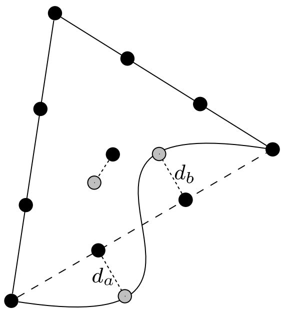




Quadratic



Cubic “H-Bend”



Cubic “S-Bend”

Curved Elements

Nodes in Mesh	Variation with order h		Variation with order h**2	
	P2	P3	P2	P3
322/1,239	1.96	2.54	2.99	4.35
1,239/4,837	1.91	2.18	2.94	4.16
4,837/19,139	2.01	2.16	2.96	4.13

Nodes in Mesh	Variation with order h		Variation with order h**2	
	S-Bend	H-Bend	S-Bend	H-Bend
322/1,239	3.28	3.37	4.25	4.30
1,239/4,837	3.18	3.21	4.20	4.27
4,837/19,139	3.13	3.14	4.14	4.19

- Also verified using