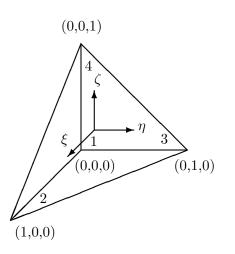
Master of Science on Computational Science

Institute of Computational Science

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The 3D reference tetrahedral element



$$\begin{aligned} N_1 &= (1 - \xi - \eta - \zeta) \\ N_2 &= \xi \\ N_3 &= \eta \\ N_4 &= \zeta \end{aligned}$$

The affine mapping

The mapping from the reference triangle T_0 to the current triangle T_e with coordinates $(x_0, y_0, z_0), (x_1, y_1, z_1), (x_2, y_2, z_2), (x_3, y_3, z_3)$ is

$$x = x_0 + (x_1 - x_0)\xi + (x_2 - x_0)\eta + (x_3 - x_0)\zeta$$

$$y = y_0 + (y_1 - y_0)\xi + (y_2 - y_0)\eta + (y_3 - y_0)\zeta$$

$$z = z_0 + (z_1 - z_0)\xi + (z_2 - z_0)\eta + (z_3 - z_0)\zeta.$$

Now for any function $f(x, y, z) = f(x(\xi, \eta, \zeta), y(\xi, \eta, \zeta), z(\xi, \eta, \zeta))$ using the chain rule of differentiation, we have

$$\begin{split} \frac{\partial f}{\partial \xi} &= \frac{\partial f}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \xi} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \xi} \\ \frac{\partial f}{\partial \eta} &= \frac{\partial f}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \eta} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \eta} \\ \frac{\partial f}{\partial \zeta} &= \frac{\partial f}{\partial x} \frac{\partial x}{\partial \zeta} + \frac{\partial f}{\partial y} \frac{\partial y}{\partial \zeta} + \frac{\partial f}{\partial z} \frac{\partial z}{\partial \zeta} \end{split}$$

From the current to the reference

or in more compact form

$$J = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{pmatrix} dx dy dz = |J| d\xi d\eta d\zeta$$

Even more compact, when we differentiate we should keep in mind

$$\nabla_{\boldsymbol{\xi}} = J \ \nabla_{\mathbf{x}}$$
$$\nabla_{\mathbf{x}} = J^{-1} \ \nabla_{\boldsymbol{\xi}}$$

The entries of the matrix J

We can map a point (ξ, η, ζ) in the reference tetrahedron to the point (x, y, z) in the current tetrahedron using the equations

$$x = x_0 + (x_1 - x_0)\xi + (x_2 - x_0)\eta + (x_3 - x_0)\zeta$$

$$y = y_0 + (y_1 - y_0)\xi + (y_2 - y_0)\eta + (y_3 - y_0)\zeta$$

$$z = z_0 + (z_1 - z_0)\xi + (z_2 - z_0)\eta + (z_3 - z_0)\zeta.$$

Then it is easy to see that the entries of the Jacobian of J are

$$J = \begin{pmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{pmatrix} = \begin{pmatrix} x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \\ x_2 - x_0 & y_2 - y_0 & z_2 - z_0 \\ x_3 - x_0 & y_3 - y_0 & z_3 - z_0 \end{pmatrix}$$

The tetrahedral element using barycentric coordinates

$$\begin{array}{lll} a_1^ex_1^e+b_1^ey_1^e+c_1^ez_1^e+d_1^e=1 & a_2^ex_1^e+b_2^ey_1^e+c_2^ez_1^e+d_2^e=0 \\ a_1^ex_2^e+b_1^ey_2^e+c_1^ez_2^e+d_1^e=0 & a_2^ex_2^e+b_2^ey_2^e+c_2^ez_2^e+d_2^e=1 \\ a_1^ex_3^e+b_1^ey_3^e+c_1^ez_3^e+d_1^e=0 & a_2^ex_3^e+b_2^ey_3^e+c_2^ez_3^e+d_2^e=0 \\ a_1^ex_4^e+b_1^ey_4^e+c_1^ez_4^e+d_1^e=0 & a_2^ex_4^e+b_2^ey_4^e+c_2^ez_4^e+d_2^e=0 \\ a_3^ex_1^e+b_3^ey_1^e+c_3^ez_1^e+d_3^e=0 & a_4^ex_1^e+b_4^ey_1^e+c_4^ez_1^e+d_4^e=0 \\ a_3^ex_2^e+b_3^ey_2^e+c_3^ez_2^e+d_3^e=0 & a_4^ex_2^e+b_4^ey_2^e+c_4^ez_2^e+d_4^e=0 \\ a_3^ex_1^e+b_3^ey_2^e+c_3^ez_3^e+d_3^e=1 & a_4^ex_1^e+b_4^ey_1^e+c_4^ez_2^e+d_4^e=0 \\ a_3^ex_1^e+b_3^ey_2^e+c_3^ez_2^e+d_3^e=0 & a_4^ex_1^e+b_4^ey_2^e+c_4^ez_2^e+d_4^e=0 \\ a_3^ex_1^e+b_3^ey_2^e+c_3^ez_2^e+d_3^e=0 & a_4^ex_1^e+b_4^ey_1^e+c_4^ez_2^e+d_4^e=0 \\ a_3^ex_1^e+b_3^ey_2^e+c_3^ez_2^e+d_3^e=0 & a_4^ex_1^e+b_4^ey_1^e+c_4^ez_2^e+d_4^e=0 \\ a_3^ex_1^e+b_3^ey_2^e+c_3^ez_2^e+d_3^e=0 & a_4^ex_1^e+b_4^ey_1^e+c_4^ez_2^e+d_4^e=0 \\ a_4^ex_1^e+b_2^ex_1^e+c_2^e+d_2^e=0 \\ a_4^ex_1^e+b_2^ex_1^e+c_2^ex_1^e+d_2^e=0 \\ a_4^ex_1^e+b_2^ex_1^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e+a_2^e$$

$$\begin{pmatrix} x_1^e & y_1^e & z_1^e & 1 \\ x_2^e & y_2^e & z_2^e & 1 \\ x_3^e & y_3^e & z_3^e & 1 \\ x_4^e & y_4^e & z_4^e & 1 \end{pmatrix} \begin{pmatrix} a_1^e & a_2^e & a_3^e & a_4^e \\ b_1^e & b_2^e & b_3^e & b_4^e \\ c_1^e & c_2^e & c_3^e & c_4^e \\ d_1^e & d_2^e & d_3^e & d_4^e \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The 3D tetrahedral element

$$\begin{pmatrix} a_1^e & a_2^e & a_3^e & a_4^e \\ b_1^e & b_2^e & b_3^e & b_4^e \\ c_1^e & c_2^e & c_3^e & c_4^e \\ d_1^e & d_2^e & d_3^e & d_4^e \end{pmatrix} = \begin{pmatrix} x_1^e & y_1^e & z_1^e & 1 \\ x_2^e & y_2^e & z_2^e & 1 \\ x_3^e & y_3^e & z_3^e & 1 \\ x_4^e & y_4^e & z_4^e & 1 \end{pmatrix}^{-1}$$

Barycentric coordinates

$$N_i^e = a_i^e x + b_i^e y + c_i^e z + d_i^e$$

Local approximation

$$u^e(x,y,z) = u^e_1 N^e_1(x,y,z) + u^e_2 N^e_2(x,y,z) + u^e_3 N^e_3(x,y,z) + u^e_4 N^e_4(x,y,z) \label{eq:ue}$$

Local mass matrix

Integration on a simplex

$$\int_{V_e} N_1^i N_2^j N_3^k N_4^l dV_e = \frac{i! j! k! l!}{(d+i+j+k+l!)!} d! V_e$$

Local mass matrix

$$M_{ij}^{e} = \int_{V_{e}} N_{i}^{e} N_{j}^{e} dV_{e} = \begin{cases} \frac{V_{e}}{20}, & i \neq j \\ \frac{V_{e}}{10}, & i = j \end{cases}$$

Local Laplacian matrix

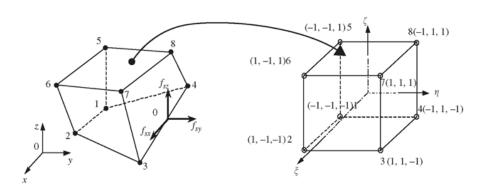
Barycentric coordinates

$$N_i^e = a_i^e x + b_i^e y + c_i^e z + d_i^e, \quad i = 1, 2, 3, 4$$

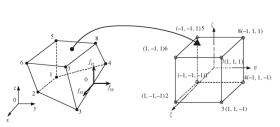
Laplacian

$$K_{ij}^{e} = \int_{V_{e}} \nabla N_{i}^{e} \cdot \nabla N_{j}^{e} dV_{e} = (a_{i}^{e} a_{j}^{e} + b_{i}^{e} b_{j}^{e} + c_{i}^{e} c_{j}^{e}) V_{e}$$

Mapping to the reference element 3D



Trilinear hexahedral element



$$N_{1} = \frac{1}{8}(1 - \xi)(1 - \eta)(1 - \zeta)$$

$$N_{2} = \frac{1}{8}(1 + \xi)(1 - \eta)(1 - \zeta)$$

$$N_{3} = \frac{1}{8}(1 + \xi)(1 + \eta)(1 - \zeta)$$

$$N_{4} = \frac{1}{8}(1 - \xi)(1 + \eta)(1 - \zeta)$$

$$N_{5} = \frac{1}{8}(1 - \xi)(1 - \eta)(1 + \zeta)$$

$$N_{6} = \frac{1}{8}(1 + \xi)(1 - \eta)(1 + \zeta)$$

$$N_{7} = \frac{1}{8}(1 + \xi)(1 + \eta)(1 + \zeta)$$

$$N_{8} = \frac{1}{8}(1 - \xi)(1 + \eta)(1 + \zeta)$$

$$N_{i} = \frac{1}{8}(1 + \xi_{i}\xi)(1 + \eta_{i}\eta)(1 + \zeta_{i}\zeta)$$

3D integrals

Gaussian quadrature in 1D: n points can integrate exactly a polynomial of degree equal to 2n-1

$$I = \int_{-1}^{1} f(\xi)d\xi$$
$$I \approx \sum_{k=1}^{n} w_k f(\xi_k)$$

Gaussian cubature

$$I = \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} f(\xi, \eta, \zeta) d\xi d\eta d\zeta$$
$$I \approx \sum_{k_1=1}^{n} \sum_{k_2=1}^{n} \sum_{k_3=1}^{n} w_{k_1} w_{k_2} w_{k_3} f(\xi_{k_1}, \eta_{k_2}, \zeta_{k_3})$$

3D integrals ...

Integrating the Laplacian on the reference element

$$I = \int_{\Omega} \nabla N_i(x, y, z) \cdot \nabla N_j(x, y, z) d\Omega$$

$$I = \int_{\Omega_0} J^{-1} \nabla N_i(\xi, \eta, \zeta) \cdot J^{-1} \nabla N_j(\xi, \eta, \zeta) |J| d\Omega_0$$

$$I = \int_{-1}^{1} \int_{-1}^{1} J^{-1} \nabla N_i(\xi, \eta, \zeta) \cdot J^{-1} \nabla N_j(\xi, \eta, \zeta) |J| d\xi \, d\eta \, d\zeta$$

$$I \approx \sum_{k_1, k_2, k_3 = 1}^{n} (w_{k_1} w_{k_2} w_{k_3} J_{k_1, k_2, k_3}^{-1} \nabla N_i(\xi_{k_1}, \eta_{k_2}, \zeta_{k_3}) \cdot J_{k_1, k_2, k_3} \nabla N_j(\xi_{k_1}, \eta_{k_2}, \zeta_{k_3}) |J_{k_1, k_2, k_3}|)$$