Re: approximation of function inside of hexahedron

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Three Dimensional Elementary Shapes

It is strongly advised to read about the 2-D case first, before proceeding to the more difficult algebra for three dimensions. It's in documents on the web, which can be found at:

`http://huizen.dto.tudelft.nl/deBruijn/sunall.htm`

Search for titles like "Triangle Algebra", "Quadrilateral Algebra" and "Five Point Star":

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http://hdebruijn.soo.dto.tudelft.nl/jaar2004/purified.pdf
http://hdebruijn.soo.dto.tudelft.nl/jaar2004/vierhoek.pdf
http://huizen.dto.tudelft.nl/deBruijn/article/SUNA04.NET
http://huizen.dto.tudelft.nl/deBruijn/article/SUNA10.NET
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And "Isoparametric Brick", "Seven Point Star" (3-D):

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http://huizen.dto.tudelft.nl/deBruijn/article/SUNA47.NET
http://huizen.dto.tudelft.nl/deBruijn/article/SUNA48.NET
http://hdebruijn.soo.dto.tudelft.nl/hdb_spul/belgisch.pdf
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Linear Tetrahedron

Let's consider the simplest non-trivial finite element shape in 3-D, which is a *tetrahedron*. Function behaviour inside such a tetrahedron is approximated by a *linear* interpolation between the function values at the vertices, also called nodal points. Let T be such a function, and x, y, z coordinates, then:

$$T = A.x + B.y + C.z + D$$

Where the constants A, B, C, D are yet to be determined. Substitute $x = x_k$, $y = y_k$, $z = z_k$ with $k = 0, 1, 2, 3$. Start with:

$$T_0 = A.x_0 + B.y_0 + C.z_0 + D$$

Clearly, the first of these equations can already be used to eliminate the constant D, once and forever:

$$T - T_0 = A.(x - x_0) + B.(y - y_0) + C.(z - z_0)$$

Then the constants A , B , C are determined by:

$$\begin{aligned} T_1 - T_0 &= A.(x_1 - x_0) + B.(y_1 - y_0) + C.(z_1 - z_0) \\ T_2 - T_0 &= A.(x_2 - x_0) + B.(y_2 - y_0) + C.(z_2 - z_0) \\ T_3 - T_0 &= A.(x_3 - x_0) + B.(y_3 - y_0) + C.(z_3 - z_0) \end{aligned}$$

Three equations with three unknowns. A solution can be found:

$$\begin{bmatrix} A \\ B \\ C \end{bmatrix} = \begin{bmatrix} x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \\ x_2 - x_0 & y_2 - y_0 & z_2 - z_0 \\ x_3 - x_0 & y_3 - y_0 & z_3 - z_0 \end{bmatrix}^{-1} \begin{bmatrix} T_1 - T_0 \\ T_2 - T_0 \\ T_3 - T_0 \end{bmatrix}$$

It is concluded that A, B, C and hence $(T - T_0)$ must be a linear expression in the $(T_k - T_0)$:

$$\begin{aligned} T - T_0 &= \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0) \\ &= \begin{bmatrix} \xi & \eta & \zeta \end{bmatrix} \begin{bmatrix} T_1 - T_0 \\ T_2 - T_0 \\ T_3 - T_0 \end{bmatrix} \end{aligned}$$

See above:

$$= \begin{bmatrix} \xi & \eta & \zeta \end{bmatrix} \begin{bmatrix} x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \\ x_2 - x_0 & y_2 - y_0 & z_2 - z_0 \\ x_3 - x_0 & y_3 - y_0 & z_3 - z_0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix}$$

See above:

$$= T - T_0 = \begin{bmatrix} x - x_0 & y - y_0 & z - z_0 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \end{bmatrix}$$

Hence:

$$\begin{aligned} x - x_0 &= \xi.(x_1 - x_0) + \eta.(x_2 - x_0) + \zeta.(x_3 - x_0) \\ y - y_0 &= \xi.(y_1 - y_0) + \eta.(y_2 - y_0) + \zeta.(y_3 - y_0) \\ z - z_0 &= \xi.(z_1 - z_0) + \eta.(z_2 - z_0) + \zeta.(z_3 - z_0) \end{aligned}$$

But also:

$$T - T_0 = \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0)$$

Therefore the *same* expression holds for the function T as well as for the coordinates x, y, z. This is called an *isoparametric* transformation. It is remarked without proof that the *local coordinates* ξ, η, ζ within a tetrahedron can be interpreted as sub-volumes, spanned by the vectors $\vec{r}_k - \vec{r}_0$ and $\vec{r} - \vec{r}_0$ where $\vec{r} = (x, y, z)$ and $k = 1, 2, 3$.
Reconsider the expression:

$$T - T_0 = \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0)$$

Partial differentiation to ξ , η , ζ gives:

$$\partial T/\partial\xi = T_1 - T_0 \quad ; \quad \partial T/\partial\eta = T_2 - T_0 \quad ; \quad \partial T/\partial\zeta = T_3 - T_0$$

Therefore:

$$T = T(0) + \xi\frac{\partial T}{\partial\xi} + \eta\frac{\partial T}{\partial\eta} + \zeta\frac{\partial T}{\partial\zeta}$$

This is part of a Taylor series expansion around node (0). Such Taylor series expansions are very common in Finite Difference analysis. Now rewrite as follows:

$$T = (1 - \xi - \eta - \zeta).T_0 + \xi.T_1 + \eta.T_2 + \zeta.T_3$$

Here the functions $(1 - \xi - \eta - \zeta), \xi, \eta, \zeta$ are called the *shape functions* of a Finite Element. Shape functions N_k have the property that they are unity in one of the nodes (k), and zero in all other nodes. In our case:

$$N_0 = 1 - \xi - \eta - \zeta \quad ; \quad N_1 = \xi \quad ; \quad N_2 = \eta \quad ; \quad N_3 = \zeta$$

So we have two representations, which are allmost trivially equivalent:

$$\begin{array}{ll} T = T_0 + \xi.(T_1 - T_0) + \eta.(T_2 - T_0) + \zeta.(T_3 - T_0) & : \text{Finite Difference} \\ T = (1 - \xi - \eta - \zeta).T_0 + \xi.T_1 + \eta.T_2 + \zeta.T_3 & : \text{Finite Element} \end{array}$$

What kind of terms can be discretized at the domain of a linear tetrahedron? In the first place, the function $T(x, y, z)$ itself, of course. But one may also try on the first order partial derivatives $\partial T/\partial(x, y, z)$. We find:

$$\partial T/\partial x = A \quad ; \quad \partial T/\partial y = B \quad ; \quad \partial T/\partial z = C$$

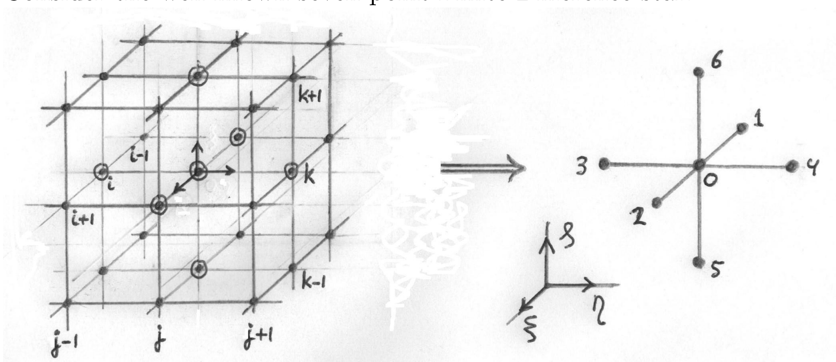
Using the expressions which were found for A, B, C:

$$\begin{bmatrix} \partial T/\partial x \\ \partial T/\partial y \\ \partial T/\partial z \end{bmatrix} = \begin{bmatrix} x_1 - x_0 & y_1 - y_0 & z_1 - z_0 \\ x_2 - x_0 & y_2 - y_0 & z_2 - z_0 \\ x_3 - x_0 & y_3 - y_0 & z_3 - z_0 \end{bmatrix}^{-1} \begin{bmatrix} T_1 - T_0 \\ T_2 - T_0 \\ T_3 - T_0 \end{bmatrix}$$

It is seen from this formula that one must determine the inverse of the above matrix first. Then add up the rows of the inverted matrix and provide the sum with a minus sign, in order to find the coefficients belonging to T_0. The result is a 3×4 *Differentiation Matrix*, which represents the gradient operator $\partial/\partial(x, y, z)$ for the function values $T_{0,1,2,3}$ at a linear tetrahedron.

Seven Point Star

Consider the well known seven point Finite Difference star:



The Finite Difference grid labels $(i{\pm}1, j{\pm}1, k{\pm}1)$ are replaced by Finite Element node numbers. Function values $(T_0, T_1, T_2, T_3, T_4, T_5, T_6)$ can be defined then at the nodal points. These values can be interpolated by a (Finite Element like) polynomial, which is defined by:

$$T(\xi, \eta, \zeta) = a_0 + a_1.\xi + a_2.\xi^2 + a_3.\eta + a_4.\eta^2 + a_5.\zeta + a_6.\zeta^2$$

Specify $T(\xi, \eta, \zeta)$ for the nodes $(0, 1, 2, 3, 4, 5, 6)$:

$$(0, 0, 0), (-1, 0, 0), (+1, 0, 0), (0, -1, 0), (0, +1, 0), (0, 0, -1), (0, 0, +1)$$

This results in 7 equations for the 7 unknowns $(a_0, a_1, a_2, a_3, a_4, a_5, a_6)$:

$$\begin{array}{llll} T_0 = a_0 & ; \quad T_1 = a_0 - a_1 + a_2 & ; & T_2 = a_0 + a_1 + a_2 \\ & \quad\; T_3 = a_0 - a_3 + a_4 & ; & T_4 = a_0 + a_3 + a_4 \\ & \quad\; T_5 = a_0 - a_5 + a_6 & ; & T_6 = a_0 + a_5 + a_6 \end{array}$$

From which it follows that:

$$a_0 = T_0 \quad ; \quad a_1 = (T_2 - T_1)/2 \quad ; \quad a_3 = (T_4 - T_3)/2 \quad ; \quad a_5 = (T_6 - T_5)/2$$

$$a_2 = (T_2 - 2T_0 + T_1)/2 \quad ; \quad a_4 = (T_4 - 2T_0 + T_3)/2 \quad ; \quad a_6 = (T_6 - 2T_0 + T_5)/2$$

These are the well known finite difference schemes for the zero'th, first and second order partial derivatives at the seven point star. By substitution of the a's, the function T is expressed as follows:

$$\begin{aligned} T(\xi, \eta, \zeta) = T_0 \quad & + \quad \frac{T_2 - T_1}{2}\xi + \frac{T_2 - 2T_0 + T_1}{2}\xi^2 \\ & + \quad \frac{T_4 - T_3}{2}\eta + \frac{T_4 - 2T_0 + T_3}{2}\eta^2 \\ & + \quad \frac{T_6 - T_5}{2}\zeta + \frac{T_6 - 2T_0 + T_5}{2}\zeta^2 \end{aligned}$$

Which can be rewritten as:

$$\begin{aligned} T(\xi,\eta,\zeta) &= (1-\xi^2-\eta^2-\zeta^2)T_0 \\ &+ \frac{\xi^2-\xi}{2}T_1 + \frac{\eta^2-\eta}{2}T_3 + \frac{\zeta^2-\zeta}{2}T_5 \\ &+ \frac{\xi^2+\xi}{2}T_2 + \frac{\eta^2+\eta}{2}T_4 + \frac{\zeta^2+\zeta}{2}T_6 \end{aligned}$$

Sic! Here we have found Finite Element *Shape Functions* for the seven point Finite Difference Star! They are:

$$N_0(\xi,\eta,\zeta) = 1-\xi^2-\eta^2-\zeta^2$$

$$N_1(\xi,\eta,\zeta) = \frac{1}{2}(-\xi+\xi^2) \quad ; \quad N_2(\xi,\eta,\zeta) = \frac{1}{2}(+\xi+\xi^2)$$

$$N_3(\xi,\eta,\zeta) = \frac{1}{2}(-\eta+\eta^2) \quad ; \quad N_4(\xi,\eta,\zeta) = \frac{1}{2}(+\eta+\eta^2)$$

$$N_5(\xi,\eta,\zeta) = \frac{1}{2}(-\zeta+\zeta^2) \quad ; \quad N_6(\xi,\eta,\zeta) = \frac{1}{2}(+\zeta+\zeta^2)$$

Until now, the coordinates (ξ,η,ζ) actually have been interpreted as *global* Cartesian coordinates. But it's more advantageous to look upon them as *local* coordinates. Then a (Finite Element) *isoparametric mapping* $(\xi,\eta,\zeta) \rightarrow (x,y,z)$ from the local to the global coordinate system (x,y,z) can be defined, as follows:

$$\begin{aligned} x &= N_0x_0 + N_1x_1 + N_2x_2 + N_3x_3 + N_4x_4 + N_5x_5 + N_6x_6 \\ y &= N_0y_0 + N_1y_1 + N_2y_2 + N_3y_3 + N_4y_4 + N_5y_5 + N_6y_6 \\ z &= N_0z_0 + N_1z_1 + N_2z_2 + N_3z_3 + N_4z_4 + N_5z_5 + N_6z_6 \end{aligned}$$

So now it has become clear why we adopted the (ξ,η,ζ) notation in the first place. For any other function $f(x,y,z)$ we can write:

$$f = N_0f_0 + N_1f_1 + N_2f_2 + N_3f_3 + N_4f_4 + N_5f_5 + N_6f_6$$

Disclaimers

Anything free comes without referee :-(
My English may be better than your Dutch :-)