10 The Quadratic Tetrahedron

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§10.1. Introduction

The four-node, linear tetrahedron introduced in the previous Chapter is easy to formulate and implement. It is the workhorse of most 3D mesh generators. It performs poorly, however, for stress analysis in structures and solid mechanics. The quadratic tetrahedron covered in this Chapter is significantly better in that regard. In addition, it retains the geometry favored in 3D mesh generation, and allows for curved faces and sides. The element has several drawbacks: more complicated formulation, increased formation time (about 15 to 30 times that of the linear tetrahedron) and increasing connectivity in the master stiffness matrix.

§10.2. The Ten-Node Tetrahedron

The ten-node tetrahedron, also called *quadratic tetrahedron*, is shown in Figure 10.1. In programming contexts it will be called Tet10. This is the second complete-polynomial member of the isoparametric tetrahedron family. As noted above, for stress calculations it behaves significantly better than the four-node (linear) tetrahedron.¹ It takes advantage of the existence of fully automatic tetrahedral meshers, something still missing for bricks.

The element has four corner nodes with *local* numbers 1 through 4, which must be traversed following the same convention explained for the four node tetrahedron in the previous Chapter. It has six side nodes, with local numbers 5 through 10. Nodes 5,6,7 are located on sides 12, 23 and 31, respectively, while nodes 8,9,10 are located on sides 14, 24, and 34, respectively. The side nodes are not necessarily placed at the midpoints of the sides but may deviate from those locations, subjected to positive-Jacobian-determinant constraints. Each element face is defined by six nodes. These do not necessarily lie on a plane, but they should not deviate too much from it. This freedom allows the element to have curved sides and faces; see Figure 10.1(b).

The tetrahedral natural coordinates ζ_1 through ζ_4 are introduced in a fashion similar to that described in the previous Chapter for the linear tetrahedron. If the element has variable metric (VM), as discussed below, there are some differences:

- 1. $\zeta_i = constant$ is not necessarily the equation of a plane;
- 2. Geometric definitions in terms of either distance or volume ratios are no longer valid.

§10.2.1. Element Definition

The definition of the quadratic tetrahedron as an isoparametric element is

$$\begin{bmatrix} 1 \\ x \\ y \\ z \\ u_x \\ u_y \\ u_z \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & x_4 & x_5 & \dots & x_{10} \\ y_1 & y_2 & y_3 & y_4 & y_5 & \dots & y_{10} \\ z_1 & z_2 & z_3 & z_4 & z_5 & \dots & z_{10} \\ u_{x1} & u_{x2} & u_{x3} & u_{x4} & u_{x5} & \dots & u_{x10} \\ u_{y1} & u_{y2} & u_{y3} & u_{y4} & u_{y5} & \dots & u_{y10} \\ u_{z1} & u_{z2} & u_{z3} & u_{z4} & u_{z5} & \dots & u_{z10} \end{bmatrix} \begin{bmatrix} N_1^e \\ N_2^e \\ N_3^e \\ N_5^e \\ \vdots \\ N_{10}^e \end{bmatrix}.$$

$$(10.1)$$

A mesh of quadratic tetrahedra exhibits wider connectivity than a corresponding mesh of linear tetrahedra with the *same number of nodes*. Consequently the solution of the master stiffness equations will be costlier for the former.

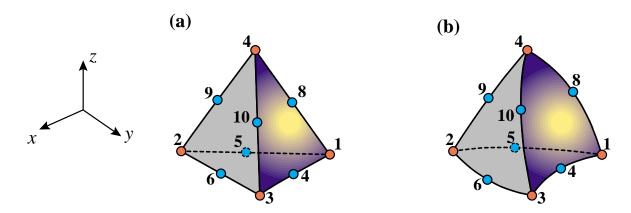


FIGURE 10.1. The quadratic (ten-node) tetrahedron. (a): element with planar faces and side nodes located at side midpoints; (b): element with curved faces and sides.

The conventional (non-hierarchical) shape functions are given by

$$N_{1}^{e} = \zeta_{1}(2\zeta_{1} - 1), \ N_{2}^{e} = \zeta_{2}(2\zeta_{2} - 1), \ N_{3}^{e} = \zeta_{3}(2\zeta_{3} - 1), \ N_{4}^{e} = \zeta_{4}(2\zeta_{4} - 1),$$

$$N_{5}^{e} = 4\zeta_{1}\zeta_{2}, \ N_{6}^{e} = 4\zeta_{2}\zeta_{3}, \ N_{7}^{e} = 4\zeta_{3}\zeta_{1}, \ N_{8}^{e} = 4\zeta_{1}\zeta_{4}, \ N_{9}^{e} = 4\zeta_{2}\zeta_{4}, \ N_{10}^{e} = 4\zeta_{3}\zeta_{4}.$$

$$(10.2)$$

These shape functions can be readily built by inspection, using the "product guessing" technique explained in Chapter 18 of IFEM. They closely resemble those of the six node quadratic triangle discussed in that Chapter. If the element is curved (that is, the six nodes that define each face are not on a plane and/or the side nodes are not located at the side midpoints), constant tetrahedron coordinates no longer define planes, but form a curvilinear system. More on that topic later.

§10.2.2. Constant Versus Variable Metric

A constant metric (abbreviation: CM) tetrahedron is mathematically defined as one in which the Jacobian determinant J over the element domain is constant.² Otherwise the element is said to be of variable metric (abbreviation: VM). The linear tetrahedron is always a CM element because J = 6V is constant over it. The quadratic tetrahedron is CM if and only if the six midside modes are collocated at the midpoints between adjacent corners. Mathematically:

$$x_5 = \frac{1}{2}(x_1 + x_2), \quad x_6 = \frac{1}{2}(x_2 + x_3), \quad \dots \quad x_{10} = \frac{1}{2}(x_3 + x_4),$$

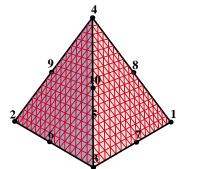
$$y_5 = \frac{1}{2}(y_1 + y_2), \quad y_6 = \frac{1}{2}(y_2 + y_3), \quad \dots \quad y_{10} = \frac{1}{2}(y_3 + y_4),$$

$$z_5 = \frac{1}{2}(z_1 + z_2), \quad z_6 = \frac{1}{2}(z_2 + z_3), \quad \dots \quad z_{10} = \frac{1}{2}(z_3 + z_4).$$
(10.3)

If the conditions (10.3) are imposed upon the first four rows of the iso-P definition (10.1), that portion reduces to

$$\begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ z_1 & z_2 & z_3 & z_4 \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \end{bmatrix}.$$
(10.4)

² The expression of J for an arbitrary iso-P tetrahedron is worked out in §10.3.1.



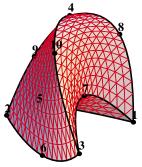




FIGURE 10.2. Illustrating differences between constant metric (CM) and variable metric (VM) tetrahedra. (a) CM quadratic tetrahedron; (b) VM quadratic tetrahedron with the same corner locations as the CM one; (c) the isocoordinate surfaces $\zeta_4=0$, $\zeta_4=\frac{1}{4}$, $\zeta_4=\frac{1}{2}$, $\zeta_4=\frac{3}{4}$ and $\zeta_4=\frac{49}{50}$ for the VM tetrahedron. Plots produced by module PlotTet10Element listed in Figure 10.4.

This is exactly the geometric definition (9.10) of the linear tetrahedron. Therefore J is the same at all points, and expressed in terms of the corner coordinates by (9.3) or (9.4). Consequences: the four faces are planar, and the six sides straight.³ If at least one midside node deviates from (10.3), J will be a function of position and the element is VM.

Figure 10.2(a,b) visually contrasts two quadratic tetrahedra of constant and variable metric, respectively. Both tetrahedra have the *same corner locations*. For the VM one, Figure 10.2(c) pictures the five isocoordinate surfaces $\zeta_4 = 0$, $\zeta_4 = \frac{1}{4}$, $\zeta_4 = \frac{1}{2}$, $\zeta_4 = \frac{3}{4}$, and $\zeta_4 = \frac{49}{50}$ (a plot of $\zeta_4 = 1$ would be invisible, as it collapses to a point). This plot illustrates the fact that the tetrahedral coordinates ζ_i form a system of *curvilinear coordinates* if the element has VM geometry. These plots were produced by the module PlotTet10Element described in the next subsection.

Why is CM versus VM important? Implementation side effects. If the tetrahedron is CM,

- 1. Computation of partial derivatives such as $\partial \zeta_i / \partial x$ is easy because (9.18) can be reused.
- 2. Analytical integration (over volume, faces or sides) is straightforward, as long as integrands are polynomials in tetrahedral coordinates. See §9.1.10 about how to do it.

For VM elements the computation of partial derivatives is considerably more laborious.⁴ In addition, numerical integration is necessary. So a key implementation question is: are VM tetrahedra allowed? In the sequel we shall assume that to be the case. Consequently the more general formulation is presented.

Remark 10.1. Elements whose geometric definition is of lower order (in the sense of polynomial variation in natural coordinates) than the displacement interpolation are called *subparametric* in the FEM literature. Pre-1967 triangular and tetrahedral elements were subparametric until isoparametric models came along. The opposite case: elements whose geometry is of higher order (again, polynomial-wise) than the displacement field interpolation are called *superparametric*. These are comparatively rare.

³ The converse is not true: even if a quadratic tetrahedron has planar faces and straight sides, it is not necessarily CM, since deviations from (10.3) could be such that midside nodes remain on the straight line passing through adjacent corners.

⁴ Reason: if one tries to directly express the ζ_i in terms of $\{x, y, z\}$ from the first four rows of the Iso-P definition (10.1), it would entail solving 4 quadratic polynomial equations for 4 coupled unknowns. A closed form solution comparable to (9.11) does not generally exist. But such a solution is possible for the differentials, as shown in §10.3.1.

§10.2.3. Hierarchical Geometric Formulation

An alternative geometric descrition of the tetrahedral element uses *deviations from midpoint locations* to establish the position of the midside nodes:

$$x_{5} = \frac{1}{2}(x_{1} + x_{2}) + \Delta x_{5}, \quad y_{5} = \frac{1}{2}(y_{1} + y_{2}) + \Delta y_{5}, \quad z_{5} = \frac{1}{2}(z_{1} + z_{2}) + \Delta z_{5},$$

$$x_{6} = \frac{1}{2}(x_{2} + x_{3}) + \Delta x_{6}, \quad y_{6} = \frac{1}{2}(y_{2} + y_{3}) + \Delta y_{6}, \quad z_{6} = \frac{1}{2}(z_{2} + z_{3}) + \Delta z_{6},$$

$$\dots$$

$$x_{10} = \frac{1}{2}(x_{3} + x_{4}) + \Delta x_{10}, \quad y_{10} = \frac{1}{2}(y_{3} + y_{4}) + \Delta y_{10}, \quad z_{10} = \frac{1}{2}(z_{3} + z_{4}) + \Delta z_{10}.$$

$$(10.5)$$

in which Δx_i , Δy_i , and Δz_i are the *midpoint coordinate deviations*. Rewriting the geometry definition from (10.1) in terms of these deviations yields

$$\begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & \dots & 0 \\ x_1 & x_2 & x_3 & x_4 & \Delta x_5 & \dots & \Delta x_{10} \\ y_1 & y_2 & y_3 & y_4 & \Delta y_5 & \dots & \Delta y_{10} \\ z_1 & z_2 & z_3 & z_4 & \Delta z_5 & \dots & \Delta z_{10} \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \zeta_4 \\ N_5^e \\ \vdots \\ N_{10}^e \end{bmatrix}.$$
(10.6)

The four corner shape functions change from $\zeta_i(2\zeta_i - 1)$ to just ζ_i , which are the shape functions of the linear tetrahedron. The shape functions associated with the coordinate deviations remain unchanged. This reformulation is called a *geometry-hierarchical element*. It has certain implementation merits. The chief advantage: for a CM element all midpoint deviations vanish, allowing immediate regression to linear tetrahedron formulas. In addition the expression of the Jacobian derived in §10.3 is simpler.

If midside nodal displacements are similarly adjusted, the model is called a *iso-P hierarchical element*. It offers certain advantages (as well as shortcomings) that are not elaborated upon here.

§10.2.4. *Geometric Visualization

Picturing VM tetrahedra is useful to visually understand concepts such as curved sides and faces, as well as tetrahedral coordinate isosurfaces. The plots shown in Figure 10.3 were produced by the *Mathematica* module PlotTet10Element listed in Figure 10.4. That module is invoked as

The arguments are:

xyztet Tetrahedon $\{x, y, z\}$ nodal coordinates stored node-by-node as a two-dimensional list: $\{\{x1,y1,z1\},\{x2,y2,z2\},\{x3,y3,z3\},\ldots \{x10,y10,z10\}\}.$

Plotwhat A list specifying what is to be plotted. List items must be of one of three forms: $\{i,c\}$, where i=1,2,3,4, and c a real number $c\in[0,1]$: plot surface $\zeta_i=c$. 10*i+j, where i,j=1,2,3,4: plot side joining corners i and j, n, where $n=1,2,\ldots 10$: plot element node n as dark dot and write its number nearby. The plotwhat configurations used to generate the plots of Figure 10.4 are given below.

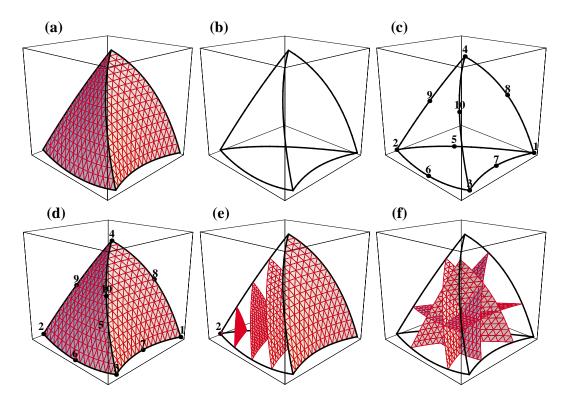


FIGURE 10.3. Sample plots for a variable metric (VM) quadratic tetrahedron, produced by *Mathematica* module PlotTet10Element. (a): sides and faces; (b) sides only; (c) sides and nodes; (d) sides, faces and nodes; (e) the five surfaces $\zeta_2 = 0$ (face 2), $\zeta_2 = \frac{1}{4}$, $\zeta_2 = \frac{1}{2}$, $\zeta_2 = \frac{3}{4}$, and $\zeta_2 = .98$ ($\zeta_2 = 1$ would produce only a point as it reduces to node 2.); (e) the four surfaces $\zeta_1 = 1/4$ for i = 1, 2, 3, 4 showing intersection at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ (which is not necessarily the centroid if tetrahedron is VM). For plot input data see text.

Nsub Number of subdivisions along sides used to triangulate faces. If tetrahedron is constant metric (CM), Nsub=1 is enough, but if it has curved faces a pleasing value of Nsub should be determined by trial and error. The plots of Figure 10.4 use Nsub=16.

aspect Specifies the *z* aspect ratio of the plot box frame. Normally 1.

The coordinates of a point in space from which the objects plotted are to be viewed. Used to set the option ViewPoint->view in *Mathematica*. Typically determined by trial and error. The plots of Figure 10.4 were done with $view = \{-2, -2, 1\}$.

A logical flag. Set box to True to get a coordinates aligned box-frame drawn around the tetrahedron, as illustrated by the plots of Figure 10.4. If set to False, no box is drawn.

The function PlotTet10Element does not return a value.

The tetrahedron geometry plotted in Figure 10.3 is defined by the node coordinates

Further Nsub=16, view={-2,-2,1}, aspect=1, and box=True for all six plots, which are produced by

- (a) PlotTet10Element[xyztet,{{1,0},{2,0},{3,0},{4,0},12,23,31,14,24,34}, Nsub,aspect,view,box];
- (b) PlotTet10Element[xyztet,{12,23,31,14,24,34},Nsub,aspect,view,box];

```
PlotTet10Element[xyztet_,plotwhat_,Nsub_,aspect_,view_,box_]:=
  Module[{Ne,m,i,k,x1,x2,x3,x4,x5,x6,x7,x8,x9,x10,y1,y2,y3,y4,y5,}
  y6,y7,y8,y9,y10,z1,z2,z3,z4,z5,z6,z7,z8,z9,z10,ζ1,ζ2,ζ3,ζ4,c,d,
  c1,c2,c3,Ne1,Ne2,Ne3,xyz1,xyz2,xyz3,i1,i2,i3,nplot,iplot,what,
  \(\zeta_i,\ni=3*\nsub,\xyzn,\exyz,\nlab,\style, lines=\{\},\npolys=\{\},\sides=\{\},\)
  nodlab={},nodcir={},DisplayChannel,modname="PlotTet10Element: "},
  Ne[\{\zeta1\_,\zeta2\_,\zeta3\_,\zeta4\_\}] := \{\zeta1*(2*\zeta1-1),\zeta2*(2*\zeta2-1),\zeta3*(2*\zeta3-1),
        $\delta\(2*\zeta\),4*\zeta\(2\),4*\zeta\(2\),4*\zeta\(3\),4*\zeta\(1\),4*\zeta\(2\),4*\zeta\(3\);
 {{x1,y1,z1},{x2,y2,z2},{x3,y3,z3},{x4,y4,z4},{x5,y5,z5},{x6,y6,z6},
{x7,y7,z7},{x8,y8,z8},{x9,y9,z9},{x10,y10,z10}}=Take[xyztet,10];
   xn={x1,x2,x3,x4,x5,x6,x7,x8,x9,x10};
   yn={y1,y2,y3,y4,y5,y6,y7,y8,y9,y10};
    zn={z1,z2,z3,z4,z5,z6,z7,z8,z9,z10};
    style=TextStyle->{FontFamily->"Times",FontSize->15,
                           FontWeight->"Bold" };
    nplot=Length[plotwhat]; If [nplot<=0,Return[]];
    For [iplot=1,iplot<=nplot,iplot++, what=plotwhat[[iplot]];</pre>
       If [Length[what] == 2, \{i, \zeta i\} = what;
             If [Count[{1,2,3,4},i]<=0, Print[modname,</pre>
                 "Bad face index in plotwhat"]; Return[]]; c=(1-\zeta i)/Ni;
            For [i1=1,i1<=Ni,i1++, For [i2=1,i2<=Ni-i1,i2++,
                  i3=Ni-i1-i2; If [i3<=0, Continue[]]; d=0;
                  If [Mod[i1+2,3]==0&&Mod[i2-1,3]==0, d= 1];
                  If [Mod[i1-2,3]==0&&Mod[i2+1,3]==0, d=-1];
                  If [d==0, Continue[]]; k=i-1;
                  c1=RotateRight[N[\{\zeta_{i,(i1+d+d)*c,(i2-d)*c,(i3-d)*c}\}],k];
                  \begin{array}{l} \text{c2=RotateRight[N[\{\zeta i,(i1-d)*c,(i2+d+d)*c,(i3-d)*c\}],k];} \\ \text{c3=RotateRight[N[\{\zeta i,(i1-d)*c,(i2-d)*c,(i3+d+d)*c\}],k];} \\ \text{Ne1=Ne[c1]; } \text{xyz1=} & \{\text{xn.Ne1,yn.Ne1,zn.Ne1}\}; \\ \end{array} 
                 Ne2=Ne[c2]; xyz2=\{xn.Ne2,yn.Ne2,zn.Ne2\};
                  Ne3=Ne[c3]; xyz3={xn.Ne3,yn.Ne3,zn.Ne3};
                  AppendTo[polys,Polygon[{xyz1,xyz2,xyz3}]];
                  AppendTo[lines,Line[{xyz1,xyz2,xyz3,xyz1}]];
                  ]]; Continue[];
            ]; m=what;
       If [m>0&&m<=10, nlab=ToString[m];</pre>
            xyzn={xn[[m]],yn[[m]],zn[[m]]}; exyz={0.02,0,.06};
            AppendTo[nodlab,Graphics3D[Text[nlab,xyzn+exyz,style]]];
            AppendTo[nodcir,Graphics3D[Point[xyzn]]]; Continue[]];
       If [Count[{12,21,13,31,14,41,23,32,24,42,34,43},m]<=0,
             Print[modname," Bad side id in plotwhat"]; Return[]];
            For [i1=1,i1<=Nsub,i1++, i2=i1+1;
                   \zeta_{1=N[(i1-1)/Nsub]}; \zeta_{2=N[(i2-1)/Nsub]};
                   If [m==12 \mid |m==21,c1=\{\zeta 1,1-\zeta 1,0,0\}; c2=\{\zeta 2,1-\zeta 2,0,0\}];
                   If [m=13] |m=31,c1=\{\zeta_1,0,1-\zeta_1,0\}; c2=\{\zeta_2,0,1-\zeta_2,0\}]; If [m=14] |m=41,c1=\{\zeta_1,0,0,1-\zeta_1\}; c2=\{\zeta_2,0,0,1-\zeta_2\}]; If [m=23] |m=32,c1=\{0,\zeta_1,1-\zeta_1,0\}; c2=\{0,\zeta_2,1-\zeta_2,0\}]; If [m=24] |m=42,c1=\{0,\zeta_1,0,1-\zeta_1\}; c2=\{0,\zeta_2,0,1-\zeta_2\}];
                   If [m=34 | m=43,c1=\{0,0,\zeta1,1-\zeta1\}; c2=\{0,0,\zeta2,1-\zeta2\}];
                   Ne1=Ne[c1]; xyz1={xn.Ne1,yn.Ne1,zn.Ne1};
                   Ne2=Ne[c2]; xyz2={xn.Ne2,yn.Ne2,zn.Ne2};
                   AppendTo[sides,Line[{xyz1,xyz2}]]];
           1:
   DisplayChannel=$DisplayFunction;
    If [$VersionNumber>=6.0, DisplayChannel=Print];
    Show[Graphics3D[RGBColor[1,0,0]],Graphics3D[polys],
          Graphics3D[AbsoluteThickness[1]],Graphics3D[lines],
          Graphics3D[RGBColor[0,0,0]],Graphics3D[AbsoluteThickness[2]],
          Graphics3D[sides],
          Graphics3D[AbsolutePointSize[6]],nodcir,nodlab,
          PlotRange->All, ViewPoint->view,
          AmbientLight->GrayLevel[0],BoxRatios->{1,1,aspect},
          Boxed->box,DisplayFunction->DisplayChannel];
    ClearAll[polys,lines,sides,nodlab,nodcir]];
```

FIGURE 10.4. Quadratic tetrahedron plotting module. See text for usage.

- (d) PlotTet10Element[xyztet,{{1,0},{2,0},{3,0},{4,0},12,23,31,14,24,34,1,2,3,4,5,6,7,8,9,10},Nsub,aspect,view,box];
- (f) PlotTet10Element[xyztet,{{1,1/4},{2,1/4},{3,1/4},{4,1/4}, 12,23,31,14,24,34},Nsub,aspect,view,box];

See legend of Figure 10.3 for description of what the plots show.

Implementation Considerations. Several plot options and details are built in the module; for example lighting, face colors, node number fonts, line thicknesses, etc. Those could be externally controlled with additional arguments, but it is just as easy to go in and modify the module. The Show statement contains a specification, namely, DisplayFunction->DisplayChannel, that is Mathematica version dependent.

§10.3. Partial Derivative Calculations

The problem considered in this section is: given a smooth scalar function $F(\zeta_1, \zeta_2, \zeta_3, \zeta_4)$ expressed in tetrahedral coordinates and interpolated by the shape functions in terms of nodal values, find $\partial F/\partial x$, $\partial F/\partial y$, and $\partial F/\partial z$ at any point in the element. This requires finding the partial derivatives $\partial \zeta_i/\partial x$, $\partial \zeta_i/\partial y$, and $\partial \zeta_i/\partial z$ in order to apply the chain rule. The following derivation assumes that the tetrahedron has variable metric (VM). Simplifications for the constant metric (CM) case are noted as appropriate. All stated derivatives are assumed to exist.

The derivation given in $\S 10.3.1$ is *general* in the sense that it applies to *any* VM, isoparametric tetrahedral element with n nodes. The results are specialized to the quadratic tetrahedron in $\S 10.3.2$.

§10.3.1. Arbitrary Iso-P Tetrahedron

Consider a generic *scalar* function $F(\zeta_1, \zeta_2, \zeta_3, \zeta_4)$ that is interpolated as

$$F = [F_1 \quad F_2 \quad F_3 \quad F_4 \quad \dots \quad F_n] \begin{bmatrix} N_1^e \\ N_2^e \\ \vdots \\ N_n^e \end{bmatrix} = F_k N_k^e.$$
 (10.8)

Here F_k denotes the value of $F(\zeta_1, \zeta_2, \zeta_3, \zeta_4)$ at the k^{th} node, while $N_k^e = N_k^e(\zeta_i)$ are the appropriate shape functions. The summation convention applies to the last expression over $k = 1, 2, \ldots n$. Symbol F may stand for 1, x, y, z, u_x , u_y or u_z in the isoparametric representation, or other element-varying quantities such as temperature or body force components. On taking partials with respect to x, y and z, and applying the chain rule twice we get

$$\frac{\partial F}{\partial x} = F_k \frac{\partial N_k}{\partial x} = F_k \left(\frac{\partial N_k}{\partial \zeta_1} \frac{\partial \zeta_1}{\partial x} + \frac{\partial N_k}{\partial \zeta_2} \frac{\partial \zeta_2}{\partial x} + \frac{\partial N_k}{\partial \zeta_3} \frac{\partial \zeta_3}{\partial x} + \frac{\partial N_k}{\partial \zeta_4} \frac{\partial \zeta_4}{\partial x} \right) = F_k \frac{\partial N_k}{\partial \zeta_i} \frac{\partial \zeta_i}{\partial x},$$

$$\frac{\partial F}{\partial y} = F_k \frac{\partial N_k}{\partial y} = F_k \left(\frac{\partial N_k}{\partial \zeta_1} \frac{\partial \zeta_1}{\partial y} + \frac{\partial N_k}{\partial \zeta_2} \frac{\partial \zeta_2}{\partial y} + \frac{\partial N_k}{\partial \zeta_3} \frac{\partial \zeta_3}{\partial y} + \frac{\partial N_k}{\partial \zeta_4} \frac{\partial \zeta_4}{\partial x} \right) = F_k \frac{\partial N_k}{\partial \zeta_i} \frac{\partial \zeta_i}{\partial y}, \quad (10.9)$$

$$\frac{\partial F}{\partial z} = F_k \frac{\partial N_k}{\partial y} = F_k \left(\frac{\partial N_k}{\partial \zeta_1} \frac{\partial \zeta_1}{\partial z} + \frac{\partial N_k}{\partial \zeta_2} \frac{\partial \zeta_2}{\partial z} + \frac{\partial N_k}{\partial \zeta_3} \frac{\partial \zeta_3}{\partial z} + \frac{\partial N_k}{\partial \zeta_4} \frac{\partial \zeta_4}{\partial x} \right) = F_k \frac{\partial N_k}{\partial \zeta_i} \frac{\partial \zeta_i}{\partial z},$$

in which sums run over k = 1, 2, ...n and i = 1, 2, 3, 4, and element superscripts on the shape functions have been suppressed for clarity. In matrix form:

$$\begin{bmatrix} \frac{\partial F}{\partial x} \\ \frac{\partial F}{\partial y} \\ \frac{\partial F}{\partial z} \end{bmatrix} = \begin{bmatrix} \frac{\partial \zeta_{1}}{\partial x} & \frac{\partial \zeta_{2}}{\partial x} & \frac{\partial \zeta_{3}}{\partial x} & \frac{\partial \zeta_{4}}{\partial x} \\ \frac{\partial \zeta_{1}}{\partial y} & \frac{\partial \zeta_{2}}{\partial y} & \frac{\partial \zeta_{3}}{\partial y} & \frac{\partial \zeta_{4}}{\partial y} \\ \frac{\partial \zeta_{1}}{\partial z} & \frac{\partial \zeta_{2}}{\partial z} & \frac{\partial \zeta_{3}}{\partial z} & \frac{\partial \zeta_{4}}{\partial z} \end{bmatrix} \begin{bmatrix} F_{k} \frac{\partial N_{k}}{\partial \zeta_{1}} \\ F_{k} \frac{\partial N_{k}}{\partial \zeta_{2}} \\ F_{k} \frac{\partial N_{k}}{\partial \zeta_{3}} \\ F_{k} \frac{\partial N_{k}}{\partial \zeta_{4}} \end{bmatrix}$$

$$(10.10)$$

Transpose both sides of (10.10), and switch the left and right hand sides to get

$$\begin{bmatrix} F_k \frac{\partial N_k}{\partial \zeta_1} & F_k \frac{\partial N_k}{\partial \zeta_2} & F_k \frac{\partial N_k}{\partial \zeta_3} & F_k \frac{\partial N_k}{\partial \zeta_4} \end{bmatrix} \begin{bmatrix} \frac{\partial \zeta_1}{\partial x} & \frac{\partial \zeta_1}{\partial y} & \frac{\partial \zeta_1}{\partial z} \\ \frac{\partial \zeta_2}{\partial x} & \frac{\partial \zeta_2}{\partial y} & \frac{\partial \zeta_2}{\partial z} \\ \frac{\partial \zeta_3}{\partial x} & \frac{\partial \zeta_3}{\partial y} & \frac{\partial \zeta_3}{\partial z} \\ \frac{\partial \zeta_4}{\partial x} & \frac{\partial \zeta_4}{\partial y} & \frac{\partial \zeta_4}{\partial z} \end{bmatrix} = \begin{bmatrix} \frac{\partial F}{\partial x} & \frac{\partial F}{\partial y} & \frac{\partial F}{\partial z} \end{bmatrix}. (10.11)$$

Next, set F to x, y and z, stacking results row-wise. To make the coefficient matrix square, differentiate both sides of $\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 1$ with respect to x, y and z, and insert as first row:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ x_k \frac{\partial N_k}{\partial \zeta_1} & x_k \frac{\partial N_k}{\partial \zeta_2} & x_k \frac{\partial N_k}{\partial \zeta_3} & x_k \frac{\partial N_k}{\partial \zeta_4} \\ y_k \frac{\partial N_k}{\partial \zeta_1} & y_k \frac{\partial N_k}{\partial \zeta_2} & y_k \frac{\partial N_k}{\partial \zeta_3} & y_k \frac{\partial N_k}{\partial \zeta_4} \\ z_k \frac{\partial N_k}{\partial \zeta_1} & z_k \frac{\partial N_k}{\partial \zeta_2} & z_k \frac{\partial N_k}{\partial \zeta_3} & z_k \frac{\partial N_k}{\partial \zeta_4} \end{bmatrix} \begin{bmatrix} \frac{\partial \zeta_1}{\partial x} & \frac{\partial \zeta_1}{\partial y} & \frac{\partial \zeta_1}{\partial z} \\ \frac{\partial \zeta_2}{\partial x} & \frac{\partial \zeta_2}{\partial y} & \frac{\partial \zeta_2}{\partial z} \\ \frac{\partial \zeta_3}{\partial x} & \frac{\partial \zeta_3}{\partial y} & \frac{\partial \zeta_3}{\partial z} \end{bmatrix} = \begin{bmatrix} \frac{\partial 1}{\partial x} & \frac{\partial 1}{\partial y} & \frac{\partial 1}{\partial z} \\ \frac{\partial x}{\partial x} & \frac{\partial x}{\partial y} & \frac{\partial x}{\partial z} \\ \frac{\partial \zeta_3}{\partial x} & \frac{\partial \zeta_3}{\partial y} & \frac{\partial \zeta_3}{\partial z} \end{bmatrix} = \begin{bmatrix} \frac{\partial 1}{\partial x} & \frac{\partial 1}{\partial y} & \frac{\partial 1}{\partial z} \\ \frac{\partial x}{\partial x} & \frac{\partial x}{\partial y} & \frac{\partial x}{\partial z} \\ \frac{\partial x}{\partial x} & \frac{\partial x}{\partial y} & \frac{\partial x}{\partial z} \\ \frac{\partial x}{\partial x} & \frac{\partial x}{\partial y} & \frac{\partial x}{\partial z} \end{bmatrix}. \quad (10.12)$$

But $\partial x/\partial x = \partial y/\partial y = \partial z/\partial z = 1$, and $\partial 1/\partial x = \partial 1/\partial y = \partial 1\partial z = \partial x/\partial y = \partial x/\partial z = \partial y/\partial x = \partial y/\partial z = \partial z/\partial x = \partial z/\partial y = 0$, because x, y and z are independent coordinates. Thus

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ x_{k} \frac{\partial N_{k}}{\partial \zeta_{1}} & x_{k} \frac{\partial N_{k}}{\partial \zeta_{2}} & x_{k} \frac{\partial N_{k}}{\partial \zeta_{3}} & x_{k} \frac{\partial N_{k}}{\partial \zeta_{4}} \\ y_{k} \frac{\partial N_{k}}{\partial \zeta_{1}} & y_{k} \frac{\partial N_{k}}{\partial \zeta_{2}} & y_{k} \frac{\partial N_{k}}{\partial \zeta_{3}} & y_{k} \frac{\partial N_{k}}{\partial \zeta_{4}} \\ z_{k} \frac{\partial N_{k}}{\partial \zeta_{1}} & z_{k} \frac{\partial N_{k}}{\partial \zeta_{2}} & z_{k} \frac{\partial N_{k}}{\partial \zeta_{3}} & z_{k} \frac{\partial N_{k}}{\partial \zeta_{3}} & z_{k} \frac{\partial N_{k}}{\partial \zeta_{4}} \end{bmatrix} \begin{bmatrix} \frac{\partial \zeta_{1}}{\partial x} & \frac{\partial \zeta_{1}}{\partial y} & \frac{\partial \zeta_{1}}{\partial z} \\ \frac{\partial \zeta_{2}}{\partial x} & \frac{\partial \zeta_{2}}{\partial y} & \frac{\partial \zeta_{2}}{\partial z} \\ \frac{\partial \zeta_{3}}{\partial x} & \frac{\partial \zeta_{3}}{\partial y} & \frac{\partial \zeta_{3}}{\partial z} \\ \frac{\partial \zeta_{3}}{\partial x} & \frac{\partial \zeta_{3}}{\partial y} & \frac{\partial \zeta_{3}}{\partial z} \\ \frac{\partial \zeta_{4}}{\partial x} & \frac{\partial \zeta_{4}}{\partial y} & \frac{\partial \zeta_{4}}{\partial z} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$
 (10.13)

This can be expressed in compact matrix notation as

$$\mathbf{JP} = \mathbf{I}_{aug}.\tag{10.14}$$

Here **P** is the 4 × 3 matrix of ζ_i Cartesian partial derivatives, \mathbf{I}_{aug} is the order 3 identity matrix augmented with a zero first row, and

$$\mathbf{J} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ J_{x1} & J_{x2} & J_{x3} & J_{x4} \\ J_{y1} & J_{y2} & J_{y3} & J_{y4} \\ J_{z1} & J_{z2} & J_{z3} & J_{z4} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ x_k \frac{\partial N_k}{\partial \zeta_1} & x_k \frac{\partial N_k}{\partial \zeta_2} & x_k \frac{\partial N_k}{\partial \zeta_3} & x_k \frac{\partial N_k}{\partial \zeta_4} \\ y_k \frac{\partial N_k}{\partial \zeta_1} & y_k \frac{\partial N_k}{\partial \zeta_2} & y_k \frac{\partial N_k}{\partial \zeta_3} & y_k \frac{\partial N_k}{\partial \zeta_4} \\ z_k \frac{\partial N_k}{\partial \zeta_1} & z_k \frac{\partial N_k}{\partial \zeta_2} & z_k \frac{\partial N_k}{\partial \zeta_2} & z_k \frac{\partial N_k}{\partial \zeta_3} & z_k \frac{\partial N_k}{\partial \zeta_4} \end{bmatrix}.$$
 (10.15)

is called the *Jacobian matrix*. To express its determinant and inverse it is convenient to introduce the abbreviations

$$J_{xij} = J_{xi} - J_{xj}, \quad J_{vij} = J_{vi} - J_{vj}, \quad J_{zij} = J_{zi} - J_{zj}, \quad i, j = 1, \dots 4.$$
 (10.16)

With the abbreviations (10.16), the *Jacobian determinant* $J = \det(\mathbf{J})$ can be compactly stated as

$$J = J_{x21} (J_{y23} J_{z34} - J_{y34} J_{z23}) + J_{x32} (J_{y34} J_{z12} - J_{y12} J_{z34}) + J_{x43} (J_{y12} J_{z23} - J_{y23} J_{z12}).$$
(10.17)

If $J \neq 0$, explicit inversion gives

$$\mathbf{J}^{-1} = \frac{1}{J} \begin{bmatrix} 6V_{01} & J_{y42} J_{z32} - J_{y32} J_{z42} & J_{x32} J_{z42} - J_{x42} J_{z32} & J_{x42} J_{y32} - J_{x32} J_{y42} \\ 6V_{02} & J_{y31} J_{z43} - J_{y34} J_{z13} & J_{x43} J_{z31} - J_{x13} J_{z34} & J_{x31} J_{y43} - J_{x34} J_{y13} \\ 6V_{03} & J_{y24} J_{z14} - J_{y14} J_{z24} & J_{x14} J_{z24} - J_{x24} J_{z14} & J_{x24} J_{y14} - J_{x14} J_{y24} \\ 6V_{04} & J_{y13} J_{z21} - J_{y12} J_{z31} & J_{x21} J_{z13} - J_{x31} J_{z12} & J_{x13} J_{y21} - J_{x12} J_{y31} \end{bmatrix}.$$

$$(10.18)$$

The solution $\mathbf{P} = \mathbf{J}^{-1} \mathbf{I}_{aug}$ of (10.14) for the ζ_i partials is supplied by the last 3 columns of \mathbf{J}^{-1} :

$$\mathbf{P} = \begin{bmatrix} \frac{\partial \zeta_{1}}{\partial x} & \frac{\partial \zeta_{1}}{\partial y} & \frac{\partial \zeta_{1}}{\partial z} \\ \frac{\partial \zeta_{2}}{\partial x} & \frac{\partial \zeta_{2}}{\partial y} & \frac{\partial \zeta_{2}}{\partial z} \\ \frac{\partial \zeta_{3}}{\partial x} & \frac{\partial \zeta_{3}}{\partial y} & \frac{\partial \zeta_{3}}{\partial z} \\ \frac{\partial \zeta_{3}}{\partial x} & \frac{\partial \zeta_{3}}{\partial y} & \frac{\partial \zeta_{3}}{\partial z} \\ \frac{\partial \zeta_{4}}{\partial x} & \frac{\partial \zeta_{4}}{\partial y} & \frac{\partial \zeta_{4}}{\partial z} \end{bmatrix} = \frac{1}{J} \begin{bmatrix} J_{y42} J_{z32} - J_{y32} J_{z42} & J_{x32} J_{z42} - J_{x42} J_{z32} & J_{x42} J_{y32} - J_{x32} J_{y42} \\ J_{y31} J_{z43} - J_{y34} J_{z13} & J_{x43} J_{z31} - J_{x13} J_{z34} & J_{x31} J_{y43} - J_{x34} J_{y13} \\ J_{y24} J_{z14} - J_{y14} J_{z24} & J_{x14} J_{z24} - J_{x24} J_{z14} & J_{x24} J_{y14} - J_{x14} J_{y24} \\ J_{y13} J_{z21} - J_{y12} J_{z31} & J_{x21} J_{z13} - J_{x31} J_{z12} & J_{x13} J_{y21} - J_{x12} J_{y31} \end{bmatrix}.$$

$$(10.19)$$

With (10.19) available, the Cartesian partial derivatives of any function $F(\zeta_1, \zeta_2, \zeta_3, \zeta_4)$ follow from the chain rule expression (10.9). As in the previous Chapter, to facilitate use of the summation convention it is convenient to represent entries of **P** using a more compact notation:

$$\mathbf{P} = \begin{bmatrix} \frac{\partial \zeta_1}{\partial x} & \frac{\partial \zeta_1}{\partial y} & \frac{\partial \zeta_1}{\partial z} \\ \frac{\partial \zeta_2}{\partial x} & \frac{\partial \zeta_2}{\partial y} & \frac{\partial \zeta_2}{\partial z} \\ \frac{\partial \zeta_3}{\partial x} & \frac{\partial \zeta_3}{\partial y} & \frac{\partial \zeta_3}{\partial z} \\ \frac{\partial \zeta_4}{\partial x} & \frac{\partial \zeta_4}{\partial y} & \frac{\partial \zeta_4}{\partial z} \end{bmatrix} = \frac{1}{J} \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \\ a_4 & b_4 & c_4 \end{bmatrix}$$
(10.20)

Thus $\partial \zeta_i/\partial x = a_i/J$, $\partial \zeta_i/\partial y = b_i/J$, and $\partial \zeta_i/\partial z = c_i/J$, and from (10.9) and the abbreviations (10.20) we get

$$\frac{\partial F}{\partial x} = F_k \frac{\partial N_k}{\partial \zeta_i} \frac{a_i}{J}, \qquad \frac{\partial F}{\partial y} = F_k \frac{\partial N_k}{\partial \zeta_i} \frac{b_i}{J}, \qquad \frac{\partial F}{\partial z} = F_k \frac{\partial N_k}{\partial \zeta_i} \frac{c_i}{J}.$$
 (10.21)

where sums run over i = 1, 2, 3, 4 and k = 1, 2, ... n. This shows that these partials are rational functions in the triangular coordinates.

Remark 10.2. Entries of the first column of J^{-1} are rarely of interest, but if necessary they can be obtained explicitly from

$$6V_{01} = J_{x2} (J_{y3} J_{z4} - J_{y4} J_{z3}) + J_{x3} (J_{y4} J_{z2} - J_{y2} J_{z4}) + J_{x4} (J_{y2} J_{z3} - J_{y3} J_{z2}),$$

$$6V_{02} = J_{x1} (J_{y4} J_{z3} - J_{y3} J_{z4}) + J_{x3} (J_{y1} J_{z4} - J_{y4} J_{z1}) + J_{x4} (J_{y3} J_{z1} - J_{y1} J_{z3}),$$

$$6V_{03} = J_{x1} (J_{y2} J_{z4} - J_{y4} J_{z2}) + J_{x2} (J_{y4} J_{z1} - J_{y1} J_{z4}) + J_{x4} (J_{y1} J_{z2} - J_{y2} J_{z1}),$$

$$6V_{04} = J_{x1} (J_{y3} J_{z2} - J_{y2} J_{z3}) + J_{x2} (J_{y1} J_{z3} - J_{y3} J_{z1}) + J_{x3} (J_{y2} J_{z1} - J_{y1} J_{z2}).$$

$$(10.22)$$

These are the analog of (?) for the linear tetrahedron, and become identical for a CM element.

Remark 10.3. The Jacobian matrix **J** given in (10.15) is valid for *any* variable metric (VM) iso-P tetrahedron. If the element is of constant metric (CM), **J** may be expected to collapse to that of the linear tetrahedron, given in (9.3), which depends only on corner coordinates. As discussed in §10.6, those expectations are *not* necessarily realized. The outcome depends on geometric definition details. What is true is that the CM Jacobian determinant, which is explicitly given by (9.4), is always obtained regardless of definition.

Remark 10.4. The Jacobian determinant appears in the transformation of element volume integrals from Cartesian to tetrahedral coordinates through the replacement $dx dy dz = \frac{1}{6} J d\zeta_1 d\zeta_2 d\zeta_3 d\zeta_4$. Thus

$$\int_{\Omega^e} F(x, y, z) d\Omega^e = \int_{\Omega^e} F(x, y, z) dx dy dz = \int_{\Omega^e} F(\zeta_1, \zeta_2, \zeta_3, \zeta_4) \frac{1}{6} J d\zeta_1 d\zeta_2 d\zeta_3 d\zeta_4.$$
 (10.23)

§10.3.2. Specialization To Quadratic Tetrahedron

We now specialize the foregoing results to the quadratic tetrahedron, for which n = 10 and the shape functions are given by (10.2). It is convenient to built a table of shape function derivatives

$$\nabla \mathbf{N} = \begin{bmatrix} 4\zeta_1 - 1 & 0 & 0 & 0 & 4\zeta_2 & 0 & 4\zeta_3 & 4\zeta_4 & 0 & 0 \\ 0 & 4\zeta_2 - 1 & 0 & 0 & 4\zeta_1 & 4\zeta_3 & 0 & 0 & 4\zeta_4 & 0 \\ 0 & 0 & 4\zeta_3 - 1 & 0 & 0 & 4\zeta_2 & 4\zeta_1 & 0 & 0 & 4\zeta_4 \\ 0 & 0 & 0 & 4\zeta_4 - 1 & 0 & 0 & 0 & 4\zeta_1 & 4\zeta_2 & 4\zeta_3 \end{bmatrix}$$
 (10.24)

where the $\{i, j\}$ entry is $\partial N_k/\partial \zeta_i$. Taking dot products with the node coordinates $\{x_k, y_k, z_k\}$ yields

$$\mathbf{J} = 4 \begin{bmatrix} \frac{1}{4} & x_1\bar{\zeta}_1 + x_5\zeta_2 + x_7\zeta_3 + x_8\zeta_4 & y_1\bar{\zeta}_1 + y_5\zeta_2 + y_7\zeta_3 + y_8\zeta_4 & z_1\bar{\zeta}_1 + z_5\zeta_2 + z_7\zeta_3 + z_8\zeta_4 \\ \frac{1}{4} & x_5\zeta_1 + x_2\bar{\zeta}_2 + x_6\zeta_3 + x_9\zeta_4 & y_5\zeta_1 + y_2\bar{\zeta}_2 + y_6\zeta_3 + y_9\zeta_4 & z_5\zeta_1 + z_2\bar{\zeta}_2 + z_6\zeta_3 + z_9\zeta_4 \\ \frac{1}{4} & x_7\zeta_1 + x_6\zeta_2 + x_3\bar{\zeta}_3 + x_{10}\zeta_4 & y_7\zeta_1 + y_6\zeta_2 + y_3\bar{\zeta}_3 + y_{10}\zeta_4 & z_7\zeta_1 + z_6\zeta_2 + z_3\bar{\zeta}_3 + z_{10}\zeta_4 \\ \frac{1}{4} & x_8\zeta_1 + x_9\zeta_2 + x_{10}\zeta_3 + x_4\bar{\zeta}_4 & y_8\zeta_1 + y_9\zeta_2 + y_{10}\zeta_3 + y_4\bar{\zeta}_4 & z_8\zeta_1 + z_9\zeta_2 + z_{10}\zeta_3 + z_4\bar{\zeta}_4 \end{bmatrix}^T$$

$$(10.25)$$

in which $\bar{\zeta}_1 = \zeta_1 - 1/4$, $\bar{\zeta}_2 = \zeta_2 - 1/4$, $\bar{\zeta}_3 = \zeta_3 - 1/4$, and $\bar{\zeta}_4 = \zeta_4 - 1/4$. (Matrix **J** is displayed in transposed form to fit within page width.) The entries of **P** follow from (10.19).

The shape function Cartesian derivatives are explicitly given by

$$\frac{\partial N_n}{\partial x} = (4\zeta_n - 1)\frac{a_n}{J}, \quad \frac{\partial N_n}{\partial y} = (4\zeta_n - 1)\frac{b_n}{J}, \quad \frac{\partial N_n}{\partial z} = (4\zeta_n - 1)\frac{c_n}{J},
\frac{\partial N_m}{\partial x} = 4\frac{a_i\zeta_j + a_j\zeta_i}{J}, \quad \frac{\partial N_m}{\partial y} = 4\frac{b_i\zeta_j + b_j\zeta_i}{J}, \quad \frac{\partial N_m}{\partial z} = 4\frac{c_i\zeta_j + c_j\zeta_i}{J},$$
(10.26)

For the corner node shape functions, n = 1, 2, 3, 4. For the side node shape functions, m = 5, 6, 7, 8, 9, 10; the corresponding RHS indices being i = 1, 2, 3, 1, 2, 3, and j = 2, 3, 1, 4, 4, 4.

§10.3.3. Shape Function Module

A shape function module called IsoTet10ShapeFunDer, which returns shape function values and their derivatives with respect to $\{x, y, z\}$, is listed in Figure 10.5, The module is referenced as

The arguments are:

xyztet Tetrahedral node coordinates, supplied as the two-dimensional list $\{\{x1,y1,z1\},\{x2,y2,z2\},\{x3,y3,z3\},\ldots\{x10,y10,z10\}\}.$

Tetrahedral coordinates of the point at which shape functions and their derivatives will be evaluated, supplied as a list: $\{\zeta_1, \zeta_2, \zeta_3, \zeta_4\}$

numer A logical flag. True to carry out floating-point numeric computations, else False.

The function returns are:

Nfx List of scaled shape function partial derivatives $J \partial N_i / \partial x$, i = 1, 2, ... 10

Nfy List of scaled shape function partial derivatives $J \partial N_i / \partial y$, i = 1, 2, ... 10

Nfz List of scaled shape function partial derivatives $J \partial N_i / \partial z$, i = 1, 2, ... 10

Jdet Jacobian matrix determinant J at the evaluation point.

Note that it is convenient to return, say, $J\partial N_i/\partial x$ and not $\partial N_i/\partial x$ to avoid zero-J exceptions inside IsoTet10ShapeFunDer; expressions in (10.26) make this clear. Consequently the module *always* returns the above data, even if Jdet is zero or negative. It is up to the calling program to proceed upon testing whether Jdet ≤ 0 .

§10.4. The Quadratic Tetrahedron As Iso-P Elasticity Element

The derivation of the quadratic tetrahedron as an iso-P displacement model based on the Total Potential Energy (TPE) principle as source variational form, largely follows the description of §9.2 in the previous Chapter. Only several implementation differences are highlighted here.

```
IsoTet10ShapeFunDer[xyztet_,tcoor_,numer_]:= Module[{
    x1,y1,z1,x2,y2,z2,x3,y3,z3,x4,y4,z4,
    x5,y5,z5,x6,y6,z6,x7,y7,z7,x8,y8,z8,
    x9,y9,z9,x10,y10,z10,\zeta1,\zeta2,\zeta3,\zeta4,ncoor=xyztet,
    Jx1,Jx2,Jx3,Jx4,Jy1,Jy2,Jy3,Jy4,Jz1,Jz2,Jz3,Jz4,
    Jx12,Jx13,Jx14,Jx23,Jx24,Jx34,Jx21,Jx41,Jx31,Jx32,Jx42,Jx43,
    Jy12, Jy13, Jy14, Jy23, Jy24, Jy34, Jy21, Jy41, Jy31, Jy32, Jy42, Jy43,
    Jz12,Jz13,Jz14,Jz23,Jz24,Jz34,Jz21,Jz41,Jz31,Jz32,Jz42,Jz43,
    a1,a2,a3,a4,b1,b2,b3,b4,c1,c2,c3,c4,Nfx,Nfy,Nfz,Jdet},
    If [numer, ncoor=N[xyztet]];
     \{\{x1,y1,z1\},\{x2,y2,z2\},\{x3,y3,z3\},\{x4,y4,z4\},
        {x5,y5,z5},{x6,y6,z6},{x7,y7,z7},{x8,y8,z8},
       \{x9,y9,z9\},\{x10,y10,z10\}\}=ncoor; \{\zeta1,\zeta2,\zeta3,\zeta4\}=tcoor;
    Jx1=4*(x1*(\zeta1-1/4)+x5*\zeta2+x7*\zeta3+x8*\zeta4);
    Jy1=4*(y1*(\zeta1-1/4)+y5*\zeta2+y7*\zeta3+y8*\zeta4);
    Jz1=4*(z1*(\zeta1-1/4)+z5*\zeta2+z7*\zeta3+z8*\zeta4);
    Jx2=4*(x5*\zeta1+x2*(\zeta2-1/4)+x6*\zeta3+x9*\zeta4);
Jy2=4*(y5*\zeta1+y2*(\zeta2-1/4)+y6*\zeta3+y9*\zeta4);
Jz2=4*(z5*\zeta1+z2*(\zeta2-1/4)+z6*\zeta3+z9*\zeta4);
    Jx3=4*(x7*\zeta1+x6*\zeta2+x3*(\zeta3-1/4)+x10*\zeta4);

Jy3=4*(y7*\zeta1+y6*\zeta2+y3*(\zeta3-1/4)+y10*\zeta4);

Jz3=4*(z7*\zeta1+z6*\zeta2+z3*(\zeta3-1/4)+z10*\zeta4);
    Jx4=4*(x8*\zeta1+x9*\zeta2+x10*\zeta3+x4*(\zeta4-1/4));
    Jy4=4*(y8*\mathring{\zeta}1+y9*\mathring{\zeta}2+y10*\mathring{\zeta}3+y4*(\mathring{\zeta}4-1/4));
    Jz4=4*(z8*\zeta1+z9*\zeta2+z10*\zeta3+z4*(\zeta4-1/4));
    Jx12=Jx1-Jx2; Jx13=Jx1-Jx3; Jx14=Jx1-Jx4; Jx23=Jx2-Jx3;
    Jx24=Jx2-Jx4; Jx34=Jx3-Jx4; Jy12=Jy1-Jy2; Jy13=Jy1-Jy3;
    Jy14=Jy1-Jy4; Jy23=Jy2-Jy3; Jy24=Jy2-Jy4; Jy34=Jy3-Jy4;
    Jz12=Jz1-Jz2; Jz13=Jz1-Jz3; Jz14=Jz1-Jz4;
    Jz23=Jz2-Jz3; Jz24=Jz2-Jz4; Jz34=Jz3-Jz4;
    Jx21=-Jx12; Jx31=-Jx13; Jx41=-Jx14; Jx32=-Jx23; Jx42=-Jx24;
    Jx43=-Jx34; Jy21=-Jy12; Jy31=-Jy13; Jy41=-Jy14; Jy32=-Jy23;
    Jy42=-Jy24; Jy43=-Jy34; Jz21=-Jz12; Jz31=-Jz13; Jz41=-Jz14;
    Jz32=-Jz23; Jz42=-Jz24; Jz43=-Jz34;
    Jdet=Jx21*(Jy23*Jz34-Jy34*Jz23)+Jx32*(Jy34*Jz12-
                               Jy12*Jz34)+Jx43*(Jy12*Jz23-Jy23*Jz12);
    a1=Jy42*Jz32-Jy32*Jz42; a2=Jy31*Jz43-Jy34*Jz13;
    a3=Jy24*Jz14-Jy14*Jz24; a4=Jy13*Jz21-Jy12*Jz31;
    b1=Jx32*Jz42-Jx42*Jz32; b2=Jx43*Jz31-Jx13*Jz34;
    b3=Jx14*Jz24-Jx24*Jz14; b4=Jx21*Jz13-Jx31*Jz12;
    c1=Jx42*Jy32-Jx32*Jy42; c2=Jx31*Jy43-Jx34*Jy13;
    c3=Jx24*Jy14-Jx14*Jy24; c4=Jx13*Jy21-Jx12*Jy31;
    Nfx=\{(4*\zeta_1-1)*a_1, (4*\zeta_2-1)*a_2, (4*\zeta_3-1)*a_3, (4*\zeta_4-1)*a_4,
                   4*(\zeta_{1*a2+\zeta_{2*a1}}, 4*(\zeta_{2*a3+\zeta_{3*a2}}, 4*(\zeta_{3*a1+\zeta_{1*a3}}),
                   4*(\zeta_1*a_4+\zeta_4*a_1), 4*(\zeta_2*a_4+\zeta_4*a_2), 4*(\zeta_3*a_4+\zeta_4*a_3);
    Nfy=\{(4*\zeta 1-1)*b1, (4*\zeta 2-1)*b2, (4*\zeta 3-1)*b3, (4*\zeta 4-1)*b4,
                   4*(\zeta_{1}*b_{2}+\zeta_{2}*b_{1}), 4*(\zeta_{2}*b_{3}+\zeta_{3}*b_{2}), 4*(\zeta_{3}*b_{1}+\zeta_{1}*b_{3}),
                   4*(\zeta_1*b_4+\zeta_4*b_1), 4*(\zeta_2*b_4+\zeta_4*b_2), 4*(\zeta_3*b_4+\zeta_4*b_3);
    Nfz=\{(4*\zeta 1-1)*c1, (4*\zeta 2-1)*c2, (4*\zeta 3-1)*c3, (4*\zeta 4-1)*c4, (4*\zeta 4-1)
                   Return[Simplify[{Nfx,Nfy,Nfz,Jdet}]]];
```

FIGURE 10.5. Quadratic tetrahedron shape function module IsoTet10ShapeFunDer.

§10.4.1. Displacements, Strains, Stresses

The element displacement field is defined by the three components u_x , u_y and u_z . These are quadratically interpolated from their node values as shown in the last three rows of the element definition (10.1).

The 30×1 node displacement vector is configured node-wise as

$$\mathbf{u}^e = [u_{x1} \quad u_{y1} \quad u_{z1} \quad u_{x2} \quad u_{y2} \quad u_{z2} \quad \dots \quad u_{z10}]^T.$$
 (10.28)

It is easily shown that the resulting element is C^0 inter-element conforming. It is also complete for the TPE functional, which has a variational index of one. Consequently, the element is *consistent* in the sense discussed in Chapter 19 of IFEM.

The element strain field is strongly connected to the displacements by the strain-displacement equations, which are listed as (9.30), (9.31), and (9.32) in the previous Chapter. The **B** matrix is now 6×30 : and takes the following configuration:

$$\mathbf{B} = \frac{1}{J} \begin{bmatrix} \frac{\partial N_1}{\partial x} & 0 & 0 & \frac{\partial N_2}{\partial x} & 0 & 0 & \dots & \frac{\partial N_{10}}{\partial x} & 0 & 0 \\ 0 & \frac{\partial N_1}{\partial y} & 0 & 0 & \frac{\partial N_2}{\partial y} & 0 & \dots & 0 & \frac{\partial N_{10}}{\partial y} & 0 \\ 0 & 0 & \frac{\partial N_1}{\partial z} & 0 & 0 & \frac{\partial N_2}{\partial z} & \dots & 0 & 0 & \frac{\partial N_{10}}{\partial z} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_1}{\partial x} & 0 & \frac{\partial N_2}{\partial y} & \frac{\partial N_2}{\partial x} & 0 & \dots & \frac{\partial N_{10}}{\partial y} & \frac{\partial N_{10}}{\partial z} & 0 \\ 0 & \frac{\partial N_1}{\partial z} & \frac{\partial N_1}{\partial y} & 0 & \frac{\partial N_2}{\partial z} & \frac{\partial N_2}{\partial z} & 0 & \dots & \frac{\partial N_{10}}{\partial z} & \frac{\partial N_{10}}{\partial z} & \frac{\partial N_{10}}{\partial y} \\ \frac{\partial N_1}{\partial z} & 0 & \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial z} & 0 & \frac{\partial N_2}{\partial z} & \dots & \frac{\partial N_{10}}{\partial z} & 0 & \frac{\partial N_{10}}{\partial z} \end{bmatrix}.$$
 (10.29)

Note that this matrix varies over the element.

The stress field is defined by the stress vector (9.35). This is linked to the strains by the matrix elasticity constitutive equations (9.34). For a general anisotropic material the detailed stress-strain equations are (9.37), which reduce to (9.38) for the isotropic case.

§10.4.2. Numerically Integrated Stiffness Matrix

Introducing $\mathbf{e} = \mathbf{B}\mathbf{u}$ and $\sigma = \mathbf{E}\mathbf{e}$ into the TPE functional restricted to the element volume and rendering the resulting algebraic form stationary with respect to the node displacements \mathbf{u}^e we get the usual expression for the element stiffness matrix

$$\mathbf{K}^e = \int_{\Omega^e} \mathbf{B}^T \mathbf{E} \mathbf{B} \ d\Omega^e. \tag{10.30}$$

Unlike the linear tetrahedron, the integrand varies over the element, and numerical integration by Gauss rules is recommended. To apply these rules it is necessary to express (10.30) in terms of tetrahedral coordinates. Since **B** is already a function of the ζ_i while **E** is taken to be constant, the only adjustment needed is onthe volume differential $d\Omega^e$ and the integration limits. Using (10.23) we get

$$\mathbf{K}^{e} = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \mathbf{B}^{T} \mathbf{E} \mathbf{B} \, \frac{1}{6} J \, d\zeta_{1} \, d\zeta_{2} \, d\zeta_{3} \, d\zeta_{4}.$$
 (10.31)

Denote the 30 × 30 matrix integrand by $\mathbf{F}(\zeta_1, \zeta_2, \zeta_3, \zeta_4) = \mathbf{B}^T \mathbf{E} \mathbf{B} \frac{1}{6} J$. Application of a *p*-point Gauss integration rule with abcissas $\{\zeta_{1k} \zeta_{2k} \zeta_{3k} \zeta_{4k}\}$ and weights w_k with k = 1, 2, ... p, gives

$$\mathbf{K}^{e} = \sum_{k=1}^{p} w_{k} \mathbf{F}(\zeta_{1k} \zeta_{2k} \zeta_{3k} \zeta_{4k}).$$
 (10.32)

The target rank of K^e is 30 - 6 = 24. Since each Gauss point adds 6 to the rank up to a maximum of 24, the number of Gauss points should be 4 or higher. There is actually a tetrahedron Gauss rule with 4 points and degree 2,⁵ which is the default one. For additional details on Gauss integration rules over tetrahedra, see §10.7.

§10.5. Element Stiffness Matrix

An implementation of the quadratic tetrahedron stiffness matrix computations as a *Mathematica* module is listed in Figure 10.6. The module is invoked as

The arguments are

xyztet Element node coordinates, arranged as a two-dimensional list:

 $\{\{x1,y1,z1\},\{x2,y2,z2\},\{x3,y3,z3\},\ldots\{x10,y10,z10\}\}.$

Emat The 6×6 matrix of elastic moduli (?) provided as a two-dimensional list:

 $\{\{E11,E12,E13,E14,E15,E16\}, \dots \{E16,E26,E36,E46,E56,E66\}\}.$

options A list containing optional additional information. For this element:

options={numer,p,e}, in which

numer A logical flag: True to specify floating-point numeric work, False to request exact calculations. If omitted, False is assumed.

- p Gauss integration rule identifier. See §10.7 for instructions on how to designate rules. If omitted, p=4 is assumed.
- e Element number. Only used in error messages. If omitted, 0 is assumed.

The third argument is a placeholder and should be set to the empty list { }.

The stiffness module calls IsoTet10ShapeFunDer, which was described in §10.3.3, and listed in Figure 10.5, to get the Cartesian partial derivatives of the shape functions as well as the Jacobian determinant. Note that in the implementation of Figure 10.6, Be is J B and not B. The correct scaling is restored in the Ke+=(wk/(6*Jdet))*Transpose[Be]. (Emat.Be) statement. (For the provenance of the $\frac{1}{6}$ factor, see (10.31).)

Module IsoTet10Stiffness is exercised by the *Mathematica* script listed in Figure 10.7, which forms the stiffness matrix of a linear tetrahedron with corner coordinates

$$xyztet=\{\{2,3,4\},\{6,3,2\},\{2,5,1\},\{4,3,6\}\}.$$
 (10.34)

⁵ Meaning that it integrates exactly polynomials of degree 2 or higher in tetrahedral coordinates if the tetrahedron is CM.

```
IsoTet10Stiffness[xyztet_,Emat_,{},options_]:= Module[{e=0,
 k,ip,p=4,tcoork,wk,numer=False,Nfx,Nfy,Nfz,
 Jdet,Be,Ke}, Ke=Table[0,{30},{30}];
 If [Length[options]>=1, numer=options[[1]]];
  If [Length[options]>=2, p=options[[2]]];
 If [Length[options]>=3, e=options[[3]]];
  For [k=1,k<=Abs[p],k++,
    {tcoork,wk}=TetrGaussRuleInfo[{p,numer},k];
    {Nfx,Nfy,Nfz,Jdet}=IsoTet10ShapeFunDer[xyztet,tcoork,numer];
    If [numer&&(Jdet<=0), Print["IsoTet10Stiffness: Neg "</pre>
        "or zero Jacobian, element," e]; Return[Null]];
   Be= {Flatten[Table[{Nfx[[i]],0,0},{i,1,10}]],
     Flatten[Table[{0,Nfy[[i]],0},{i,1,10}]],
         Flatten[Table[{0,0,Nfz[[i]]},{i,1,10}]],
         Flatten[Table[{Nfy[[i]],Nfx[[i]],0},{i,1,10}]],
         Flatten[Table[{0,Nfz[[i]],Nfy[[i]]},{i,1,10}]],
         Flatten[Table[{Nfz[[i]],0,Nfx[[i]]},{i,1,10}]]};
   Ke+=(wk/(6*Jdet))*Transpose[Be].(Emat.Be)];
 If [!numer,Ke=Simplify[Ke]]; Return[Ke] ];
```

FIGURE 10.6. Quadratic tetrahedron stiffness matrix module.

FIGURE 10.7. Test script for stiffness matrix module.

Midpoint node coordinates are set by averaging coordinates of adjacent corner nodes; consequently this test element has constant metric. Its volume is +24. The material is isotropic with E=480 and $\nu=1/3$. The results are shown in Figure 10.8. The computation of stiffness matrix eigenvalues is always a good programming test, since six eigenvalues (associated with rigid body modes) must be exactly zero while the other six must be real and positive. This is verified by the results shown at the bottom of Figure 10.8.

§10.6. *The Jacobian Matrix Paradox

There are some dark alleys in the Jacobian matrix computations covered in (§10.3). Those are elucidated here in some detail, since they are not discussed in the FEM literature. They are manifested when the general tetrahedral geometry is specialized to the constant metric (CM) case. If so the Jacobian matrix **J** should be *constant and reduce to that of the linear tetrahedron*. Which will not necessarily happen. This mismatch may cause grief to element implementors, and prompt a fruitless search for bugs. But it is *not* a bug: only a side

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	324 72	324 1032 162	72 162 339	1 24 0	-6 -104 -30	-12 -42 -35	54 24 0	48 216 24	0 12 54	94 60 24	66 232 60			-90 -32 36	12 72 -8
	1	24	0	87	-50 -54	-35 -36	18	-24 -24	0	10	-18	-12		-54	-8 12
	-6	-104	-30	-54	132	54	-12	72	12	0	76	36		268	72
	-12	-42	-35	-36	54	87	0	24	18	0	36	46		108	76
	54	24	0	18	-12	0	108	0	0	-36	-12	0	72	12	0
	48	216	24	-24	72	24	0	432	0	-24	-144	-48		288	48
	0	12	54	0	12	18	0	0	108	0	-24	-36	0	24	72
	94	60	24	10	0	0	-36	-24	0	204	108	72	104	60	24
	66	232	60	-18	76	36	-12	-144	-24	108	492	216	48	308	96
	36	84	94	-12	36	46	0	-48	-36	72	216	312	24	120	140
	-152	-180	-24	-32	36	48	72	24	0	104	48	24	1416	648	144
	-90	-32	36	-54	268	108	12	288	24	60	308	120	648	3936	364
e=	12	72	-8	12	72	76	0	48	72	24	96	140	144	864 1	416
	55	48	0	-83	54	12	-90	72	0	-26	-30	-12	-392 -	-312 -	-48
	42	112	-6	90	-260	-90	36	-360	-36	-24	-68	-12	-336 -	1424 -	-96
	-12	-30	19	12	-54	-83	0	-72	-90	0	12	10	0	96 -	248
	-311	-180	-24	19	-18	-12	-198	-144	0	58	54	36	232	456	144
	-252	-992	-126	0	-32	-18	-72	-792	-36	36	88	36	336	352	96
	-24	-90	-275	0	-18	-17	0	-72	-198	24	36	58	96	192	232
	-431	-288	-96	11	-6	-12	18	24	0	-350	-234	-132	136	216	48
	-306	-1040	-234	6	-28	-6	12	72	-12	-216	-860	-324	216	256 -	144
	-132	-306	-395	-12	6	11	0	-24	18	-96	-252	-386	48 -	-288 -	152
	95	84	24	-59	18	12	-18	-48	0	-98	18	12	-680 -	-648 -	240
	60	128	30	72	-272	-126	-24	-72	-12	-36	-392	-180	-504 -	1568 -	432
	24	42	59	48	-126	-167	0	-24	-18	-24	-180	-242	-240 -	-576 -	680
	148	84	24	28	-12	0	72	72	0	40	0	-24	-704 -	-288 -	-96
	114	448	84	-42	148	60	36	288	72	36	268	72	-288 $-$	2384 -	576
	36	96	148	-12	48	64	0	144	72	-24	0	4	-96 -	-576 –	848
	55	42	-12	-311	-252	-24	-431	-306	-132	95	60	24		114	36
	48	112	-30	-180	-992	-90	-288	-1040	-306	84	128			448	96
	0	-6	19	-24	-126	-275	-96	-234	-395	24	30	59		84 -42	148
	-83 54	90 -260	12 -54	19	0 -32	0 -18	11	6	-12 6	-59 18	72 -27	48		-42 148	-12
	12	-200 -90	-34 -83	-18 -12	-32 -18	-18 -17	-6 -12	-28 -6	11	12	-120			60	48 64
	-90	36	0	-12	-72	0	18	12	0	-18	-24			36	0
	-90 72	-360	-72	-144	-792	-72	24	72	-24	-48	-72 -72			288	144
	0	-36	-72 -90	0	-36	-198	0	-12	18	0	-12			72	72
	-26	-30 -24	0	58	36	24	-350	-216	-96	-98	-36			36	-24
	-30	-68	12	54	88	36	-234	-860	-252	18	-392			268	0
	-12	-12	10	36	36	58	-132	-324	-386	12	-180			72	4
	-392	-336	0	232	336	96	136	216	48	-680				-288	-96
		-330 -1424	96	456	352	192	216	256	-288	-648				-2384	-576
	-48		-248	144	96	232	48	-144	-152	-240				-576	-848
	376	0	-96	-152	-192	0	-116	-72	48	292	144			288	96
	0	928	0	-96	256	96	-72	-176	72	216	736			256	-144
	-96	0	376	96	192	136	48	72	-116	-48	72			-288	-152
	-152	-96	96	1048	576	192	292	168	-48	-308				-672	-288
	-192	256	192	576	2176	288	192	736	168	-144				-1568	-528
	0	96	136	192	288	760	0	120	148	-96				-480	-680
	-116	-72	48	292	192	0	984	648	144	-152				-408	-48
	-72	-176	72	168	736	120	648	2208	432	-216				-1424	-48
	48	72	-116	-48	168	148	144	432	984	48	144			48	-248
	292	216	-48	-308	-144	-96	-152	-216	48	696	216			504	144
	144	736	72	-144	-224	-72	-72	256	144	216	1056			352	144
	0	216	148	-96	-72	-164	48	144	136	144	432			144	232
	136	144	0	-680	-480	-192	-392	-240	0	232	288			432	192
	288	256	-288	-672	-1568	-480	-408	-1424	48	504	352			3616	864
	96		-152	-288	-528	-680	-48	-48	-248	144	144			864	1408

FIGURE 10.8. Result from stiffness matrix test.

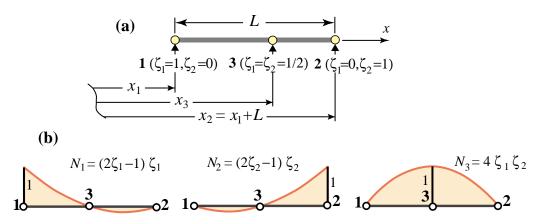


FIGURE 10.9. Three-node bar element for case study in ?.

effect of the use of *non-independent natural coordinates*. In fact, the phenomenon may occur in all higher order iso-P elements developed with that kind of coordinates. For instance, the six-node plane stress triangle.

Covering this topic for the quadratic tetrahedron leads to an algebraic maze. It is more readily illustrated with the simplest quadratic iso-P element: the three-node bar introduced in Chapter 16 of IFEM. See Figure 10.9. Instead of the single iso-P natural coordinate ξ employed there, we will use *two* natural coordinates: ζ_1 and ζ_2 , defined as shown in Figure 10.9(a). Both coordinates vary from 0 to 1, and are linked by $\zeta_1 + \zeta_2 = 1$. Quick preview of what may happen: $F = \zeta_1$ and $G = \zeta_1(\zeta_1 + \zeta_2)$, say, are obviously the same function. But the formal partial derivatives $\partial F/\partial \zeta_1 = 1$ and $\partial G/\partial \zeta_1 = 2\zeta_1 + \zeta_2 = 1 + \zeta_1$ are plainly different. The discrepancy comes from the constraint $\zeta_1 + \zeta_2 = 1$ not being properly accounted for in the differentiation.

For the element of Figure 10.9(a), define for convenience

$$x_0 = \frac{x_1 + x_2}{2}, \qquad x_3 = \frac{x_1 + x_2}{2} + \alpha (x_2 - x_1) = x_0 + \alpha L.$$
 (10.35)

The last relation defines the position of node 3 hierarchically, in terms of the *midpoint deviation* $\Delta x_3 = \alpha L$. Here $-1/2 < \alpha < 1/2$. The element is of constant metric (CM) if $\alpha = 0$. The shape functions, depicted in Figure 10.9(b), are $N_1 = (2\zeta_1 - 1)\zeta_1$, $N_2 = (2\zeta_2 - 1)\zeta_2$, and $N_3 = 4\zeta_1\zeta_2$. Two iso-P definitions for the axial coordinate x are examined. The conventional (C) definition is

$$x_C = x_1 N_1 + x_2 N_2 + x_3 N_3 = x_1 (2\zeta_1 - 1)\zeta_1 + x_2 (2\zeta_2 - 1)\zeta_2 + 4x_3 \zeta_1 \zeta_2, \tag{10.36}$$

The hierarchical (H) definition is

$$x_H = x_1 \left(N_1 + \frac{1}{2} N_3 \right) + x_2 \left(N_2 + \frac{1}{2} N_3 \right) + \alpha \left(x_2 - x_1 \right) N_3 = x_1 \zeta_1 + x_2 \zeta_2 + 4 \alpha L \zeta_1 \zeta_2. \tag{10.37}$$

The difference is

$$x_C - x_H = \lambda_{CH}(\zeta_1 + \zeta_2 - 1), \qquad \lambda_{CH} = 2(x_1\zeta_1 + x_2\zeta_2).$$
 (10.38)

in which λ_{CH} may be viewed as a Lagrange multiplier operating on the constraint $\lambda_1 + \lambda_2 = 1$.

The Jacobian entries associated with (10.36) are

$$J_{Cx1} = \frac{\partial x_C}{\partial \zeta_1} = x_1(4\zeta_1 - 1) + 4x_3\zeta_2, \quad J_{Cx2} = \frac{\partial x_C}{\partial \zeta_2} = x_2(4\zeta_2 - 1) + 4x_3\zeta_1.$$
 (10.39)

On introducing $x_3 = (x_1 + x_2)/2 + \alpha L$, and replacing $1 - \zeta_1$ and $1 - \zeta_2$ as appropriate, the Jacobian matrix emerges as

$$\mathbf{J}_{C} = \begin{bmatrix} 1 & 1 \\ J_{Cx1} & J_{Cx2} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ x_{1}(3 - 2\zeta_{2}) + 2(x_{2} + \alpha L)\zeta_{2} & 2(x_{1} + \alpha L)\zeta_{1} + x_{2}(3 - 2\zeta_{1}) \end{bmatrix}$$
(10.40)

Setting $\alpha = 0$, the resulting \mathbf{J}_C differs substantially from the expected constant-metric result:

$$\mathbf{J}_{C|_{\alpha \to 0}} = \begin{bmatrix} 1 & 1 \\ x_1(3+2\zeta_2) + 2x_2\zeta_2 & 2x_1\zeta_1 + x_2(3+2\zeta_1) \end{bmatrix} \neq \mathbf{J}_{CM} = \begin{bmatrix} 1 & 1 \\ x_1 & x_2 \end{bmatrix}.$$
(10.41)

On the other hand, going through the same process with x_H as defined in (10.37) yields

$$\mathbf{J}_{H} = \begin{bmatrix} 1 & 1 \\ J_{H_{X1}} & J_{H_{X2}} \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ x_{1} + 4\alpha L \zeta_{2} & x_{2} + 4\alpha L \zeta_{1} \end{bmatrix}.$$
(10.42)

On setting $\alpha = 0$, \mathbf{J}_H reduces to \mathbf{J}_{CM} , as expected. Lesson: application of metric constraints on shape functions and differentiation do not commute when natural coordinates are not independent. However, the Jacobian determinants do agree:

$$J_C = \det(\mathbf{J}_C) = L\left(1 + \alpha(\zeta_1 - \zeta_2)\right), \qquad J_H = \det(\mathbf{J}_H) = J_C, \tag{10.43}$$

so we may simply denote $J = J_C = J_H$. Taking inverses gives

$$\mathbf{J}_{C}^{-1} = \frac{1}{J} \begin{bmatrix} 2(x_{1} + 2\alpha L)\zeta_{1} + x_{2}(3 - 2\zeta_{1}) & -1 \\ x_{1}(3 - 2\zeta_{2}) + 2(x_{2} + 2\alpha L)\zeta_{2} & 1 \end{bmatrix}, \quad \mathbf{J}_{H}^{-1} = \frac{1}{J} \begin{bmatrix} x_{2} + 4\alpha L \zeta_{1} & -1 \\ -x_{1} - 4\alpha L \zeta_{2} & 1 \end{bmatrix}$$
(10.44)

The crucial portion of \mathbf{J}^{-1} is the last column, which stores $\partial \zeta_1/\partial x = -1/J$ and $\partial \zeta_2/\partial x = 1/J$. As can be seen, this portion is the same for both definitions. This coincidence is not accidental. Jacobian matrices produced by different iso-P geometric definitions in any number of dimensions obey a common configuration:

1D:
$$\mathbf{J} = \begin{bmatrix} 1 & 1 \\ J_{x1} - \Delta J_x & J_{x2} - \Delta J_x \end{bmatrix}$$
, 2D: $\mathbf{J} = \begin{bmatrix} 1 & 1 & 1 \\ J_{x1} - \Delta J_x & J_{x2} - \Delta J_x & J_{x3} - \Delta J_x \\ J_{y1} - \Delta J_y & J_{y2} - \Delta J_y & J_{y3} - \Delta J_y \end{bmatrix}$, ... etc. (10.45)

where the ΔJ 's come from differentiating Lagrange multiplier terms such as that shown in (10.38). These terms do not change the shape functions; only their derivatives. It is readily verified through matrix algebra that in k space dimensions, the Jacobian determinant J and the last k columns of the inverse Jacobian matrix \mathbf{J}^{-1} do not depend on the ΔJ 's. Hence all definitions coalesce. Conclusions for element work:

- 1. If only J and/or the ζ_i -partials portion of \mathbf{J}^{-1} are needed, the iso-P geometric definition: conventional or hierarchical (or any combination thereof) makes no difference.
- 2. If **J** is needed, and getting the expected \mathbf{J}_{CM} for a CM element is important, use of the hierarchical definition is recommended. However, the direct use of **J** (as opposed to its determinant) in element development is rare.

§10.7. *Gauss Integration Rules For Tetrahedra

For convenience we restate here two key properties that a Gauss integration rule must have to be useful in finite element work:

- 1. *Full Symmetry*. The same result must be obtained if the local element numbers are cyclically renumbered, which modifies the natural coordinates.⁶
- 2. Positivity. All integration weights must be positive.

As in the case of the triangle discussed in IFEM, fully symmetric integration rules over tetrahedra must be of non-product type.

⁶ Stated mathematically: the numerically evaluated integral must remain invariant under all affine transformations of the element domain onto itself.

Ident	Stars	Points	Degree	Comments					
1	S_4	1	1	Centroid formula, useful for Tet4 stiffness					
4	S_{31}	4	2	Useful for Tet4 mass and Tet10 stiffness					
8	$2S_{31}$	8	3						
-8	$2S_{31}$	8	3	Has corners and face centers as sample points					
14	$2S_{31} + S_{22}$	14	4	Useful for Tet10 mass; exact form unavailable					
-14	$2S_{31} + S_{22}$	14	3	Has edge midpoints as sample points					
15	$S_4 + 2S_{31} + S_{22}$	15	5	Useful for Tet21 stiffness					
-15	$S_4 + 2S_{31} + S_{22}$	15	4	Less accurate than above one					
24	$3S_{21} + S_{211}$	24	6	Useful for Tet21 mass; exact form unavailable					
The 5	The 5-point, degree-3, symmetric rule listed in some FEM textbooks has one negative weight.								

Table §10.1. Tetrahedron Integration Formulas

To illustrate the first requirement, suppose that the i^{th} sample point has tetrahedral coordinates $\{\zeta_{1i}, \zeta_{2i}, \zeta_{3i}\zeta_{4i}\}$ linked by $\zeta_{1i} + \zeta_{2i} + \zeta_{3i} + \zeta_{4i} = 1$. Then all points obtained by permuting the 4 indices must be also sample points and have the same weight w_i . If the four values are different, permutations provide 24 sample points:

$$\{\zeta_{1i}, \zeta_{2i}, \zeta_{3i}, \zeta_{4i}\}, \{\zeta_{1i}, \zeta_{2i}, \zeta_{4i}, \zeta_{3i}\}, \{\zeta_{1i}, \zeta_{3i}, \zeta_{2i}, \zeta_{4i}\}, \{\zeta_{1i}, \zeta_{3i}, \zeta_{4i}, \zeta_{2i}\}, \dots \{\zeta_{4i}, \zeta_{3i}, \zeta_{2i}, \zeta_{1i}\}.$$
 (10.46)

This set of points is said to form a *sample point star* or simple *star*, which is denoted by S_{1111} . If two values are equal, the set (10.46) coalesces to 12 different points, and the star is denoted by S_{211} . If two point pairs coalesce, the set (10.46) reduces to 6 points, and the star is denoted by S_{22} . If three values coalesce, the set (10.46) reduces to 4 points and the star is denoted by S_{31} . Finally if the four values coalesce, which can only happen for $\zeta_{1i} = \zeta_{2i} = \zeta_{3i} = \zeta_{4i} = \frac{1}{4}$, the set (10.46) coalesces to one point and the star is denoted by S_4

Sample point stars S_4 , S_{31} , S_{22} , S_{211} and S_{1111} have 1, 4, 6, 12 or 24 points, respectively. Thus possible rules can have i + 4j + 6k + 12l + 24m points, where i, j, k, l, m are nonegative integers and i is 0 or 1. This restriction exclude rules with 2, 3, 8 and 11 points. Table 10.1 lists nine FEM-useful rules for the tetrahedral geometry, all of which comply with the requirements listed above. Several of these are well known while others were derived by the author.

The nine rules listed in Table 10.1 are implemented in a self-contained *Mathematica* module called TetrGaussRuleInfo. Because of its length the module logic is split in two Figures: 10.10 and 10.11. It is invoked as

The module has three arguments: rule, numer and i. The first two are grouped in a two-item list.

Argument rule, which can be 1, 4, 8, -8, 14, -14, 15, -15 or 24, identifies the integration formula as follows. Abs [rule] is the number of sample points. If there are two useful rules with the same number of points, the most accurate one is identified with a positive value and the other one with a minus value. For example, there are two useful 8-point rules. If rule=8 a formula with all interior points is chosen. If rule=-8 a formula with sample points at the 4 corners and the 4 face centers (less accurate but simpler and easy to remember) is picked.

Logical flag numer is set to True or False to request floating-point or exact information, respectively, for rules other than +14 or +24. For the latter see below.

```
TetrGaussRuleInfo[{rule_,numer_},point_]:= Module[{
   jk6= {{1,2},{1,3},{1,4},{2,3},{2,4},{3,4}},
jk12={{1,2},{1,3},{1,4},{2,3},{2,4},{3,4},
          \{2,1\},\{3,1\},\{4,1\},\{3,2\},\{4,2\},\{4,3\}\},
   i=point,j,k,g1,g2,g3,g4,h1,w1,w2,w3,eps=10.^(-16),
   info={{Null,Null,Null},0}
   If [rule==1, info={{1/4,1/4,1/4,1/4},1}];
   If [rule==4, g1=(5-Sqrt[5])/20; h1=(5+3*Sqrt[5])/20;
      info={{g1,g1,g1,g1},1/4}; info[[1,i]]=h1];
   If [rule==8, j=i-4;
      g1=(55-3*Sqrt[17]+Sqrt[1022-134*Sqrt[17]])/196;
      g2=(55-3*Sqrt[17]-Sqrt[1022-134*Sqrt[17]])/196;
      w1=1/8+Sqrt[(1715161837-406006699*Sqrt[17])/23101]/3120;
      w2=1/8-Sqrt[(1715161837-406006699*Sqrt[17])/23101]/3120;
      If [j<=0,info={{g1,g1,g1,g1},w1}; info[[1,i]]=1-3*g1];
If [j> 0,info={{g2,g2,g2,g2},w2}; info[[1,j]]=1-3*g2]];
   If [rule==-8, j=i-4;
      If [j <= 0, info = \{\{0,0,0,0\}, 1/40\}; info[[1,i]] == 1];
      If [j> 0, info=\{\{1,1,1,1\}/3,9/40\}; info[[1,j]]=0]];
   If [rule==14, (* g1,g2 + roots of P(g)=0, P=9+96*g-
         1712*g^2-30464*g^3-127232*g^4+86016*g^5+1060864*g^6 *)
      g1=0.09273525031089122640232391373703060;
      g2=0.31088591926330060979734573376345783;
      g3=0.45449629587435035050811947372066056;
      If [!numer,{g1,g2,g3}=Rationalize[{g1,g2,g3},eps]];
      w1=(-1+6*g2*(2+g2*(-7+8*g2))+14*g3-60*g2*(3+4*g2*)
           (-3+4*g2))*g3+4*(-7+30*g2*(3+4*g2*(-3+4*g2)))*g3^2)/
           (120*(g1-g2)*(g2*(-3+8*g2)+6*g3+8*g2*(-3+4*g2)*g3-4*
           (3+4*g2*(-3+4*g2))*g3^2+8*g1^2*(1+12*g2*
           (-1+2*g2)+4*g3-8*g3^2)+g1*(-3-96*g2^2+24*g3*(-1+2*g3)+
          g2*(44+32*(1-2*g3)*g3))));
      w2=(-1-20*(1+12*g1*(2*g1-1))*w1+20*g3*(2*g3-1)*(4*w1-1))/(2*g1-1)
         (20*(1+12*g2*(2*g2-1)+4*g3-8*g3^2));
      If [i<5,
                    info={{g1,g1,g1,g1},w1};info[[1,i]]=1-3*g1];
      If [i>4&&i<9, info=\{\{g2,g2,g2,g2\},w2\};info[[1,i-4]]=1-3*g2];
                     info=\{\{g3,g3,g3,g3\},1/6-2*(w1+w2)/3\};
      If [i>8,
           {j,k}=jk6[[i-8]]; info[[1,j]]=info[[1,k]]=1/2-g3] ];
   If [rule==-14,
      g1=(243-51*Sqrt[11]+2*Sqrt[16486-9723*Sqrt[11]/2])/356;
      g2=(243-51*Sqrt[11]-2*Sqrt[16486-9723*Sqrt[11]/2])/356;
      w1=31/280+Sqrt[(13686301-3809646*Sqrt[11])/5965]/600;
      w2=31/280-Sqrt[(13686301-3809646*Sqrt[11])/5965]/600;
                     info={{g1,g1,g1,g1},w1};info[[1,i]]=1-3*g1];
      If [i<5,
      If [i>4&&i<9, info={{g2,g2,g2,g2},w2};info[[1,i-4]]=1-3*g2];
If [i>8&&i<15,info={{0,0,0,0},2/105};</pre>
           {j,k}=jk6[[i-8]]; info[[1,j]]=info[[1,k]]=1/2]];
```

FIGURE 10.10. Tetrahedral integration rule information module, Part 1 of 2.

Argument i is the index of the sample point, which may range from 1 through Abs[rule].

The module returns the list $\{\{\zeta_1, \zeta_2, \zeta_3, \zeta_4\}, w\}$, where $\zeta_1, \zeta_2, \zeta_3, \zeta_4$ are the natural coordinates of the sample point, and w is the integration weight. For example, TetrGaussRuleInfo[{4,False},2] returns $\{\{(5-\text{Sqrt}[5])/20, (5+3*\text{Sqrt}[5])/20, (5-\text{Sqrt}[5])/20\}, (5+3*\text{Sqrt}[5])/20\}$

If rule is not implemented the module returns { { Null, Null, Null, Null}, 0 }.

Exact information for rules +14 and +24 is either unknown or only partly known. For these the abscissas are given in floating-point form with 36 exact digits. If flag numer is False, the abscissas are converted to rational numbers that represent the data to 16 place accuracy, using the built-in function Rationalize. Weights are recovered from the abscissas. The conversion precision can be changed by adjusting the value of internal variable eps, which is set in the module preamble.

We specifically mention the two simplest numerical integration rules, which find applications in the evaluation

```
If [rule==15,
      g1=(7-Sqrt[15])/34; g2=7/17-g1; g3=(10-2*Sqrt[15])/40;
      w1=(2665+14*Sqrt[15])/37800; w2=(2665-14*Sqrt[15])/37800;
      If [i<5,
                      info={{g1,g1,g1,g1},w1};info[[1,i]]=1-3*g1];
      If [i>4&&i<9, info={{g2,g2,g2},w2};info[[1,i-4]]=1-3*g2];
If [i>8&&i<15,info={{g3,g3,g3,g3},10/189};
    {j,k}=jk6[[i-8]]; info[[1,j]]=info[[1,k]]=1/2-g3];</pre>
      If [i==15,info={{1/4,1/4,1/4},16/135}] ];
   If [rule==-15,
                      g1=(13-Sqrt[91])/52;
      If [i<5, info={{1,1,1,1}/3,81/2240};info[[1,i]]=0];
If [i>4&&i<9, info={{1,1,1,1}/11,161051/2304960};</pre>
                      info[[1,i-4]]=8/11];
      If [i>8&&i<15,info={{g1,g1,g1,g1},338/5145};</pre>
           {j,k}=jk6[[i-8]]; info[[1,j]]=info[[1,k]]=1/2-g1];
      If [i==15,info={{1/4,1/4,1/4},6544/36015}] ];
   If [rule==24,
       g1=0.214602871259152029288839219386284991;
       g2=0.040673958534611353115579448956410059;
       g3=0.322337890142275510343994470762492125;
       If [!numer,{g1,g2,g3}=Rationalize[{g1,g2,g3},eps]];
       w1= (85+2*g2*(-319+9*Sqrt[5]+624*g2)-638*g3-
             24*g2*(-229+472*g2)*g3+96*(13+118*g2*(-1+2*g2))*g3^2+
             9*Sqrt[5]*(-1+2*g3))/(13440*(g1-g2)*(g1-g3)*(3-8*g2+
             8*g1*(-1+2*g2)-8*g3+16*(g1+g2)*g3));
       w2 = -(85+2*g1*(-319+9*Sqrt[5]+624*g1)-638*g3-
             24*g1*(-229+472*g1)*g3+96*(13+118*g1*(-1+2*g1))*g3^2+
             9*Sqrt[5]*(-1+2*g3))/(13440*(g1-g2)*(g2-g3)*(3-8*g2+
             8*g1*(-1+2*g2)-8*g3+16*(g1+g2)*g3));
       w3= (85+2*g1*(-319+9*Sqrt[5]+624*g1)-638*g2-
             24*g1*(-229+472*g1)*g2+96*(13+118*g1*(-1+2*g1))*g2^2+
             9*Sqrt[5]*(-1+2*g2))/(13440*(g1-g3)*(g2-g3)*(3-8*g2+
             8*g1*(-1+2*g2)-8*g3+16*(g1+g2)*g3));
      g4=(3-Sqrt[5])/12; h4=(5+Sqrt[5])/12; p4=(1+Sqrt[5])/12;
                      info={{g1,g1,g1,g1},w1};info[[1,i]]= 1-3*g1];
      If [i<5,
      If [i>4\&i<9, info=\{\{g2,g2,g2,g2\},w2\};info[[1,i-4]]=1-3*g2];
      If [i>8&&i<13,info={{g3,g3,g3,g3},w3};info[[1,i-8]]=1-3*g3];</pre>
      If [i>12,info={{g4,g4,g4,g4},27/560};
           {j,k}=jk12[[i-12]];info[[1,j]]=h4;info[[1,k]]=p4] ];
   If [numer, Return[N[info]], Return[Simplify[info]]];
];
```

FIGURE 10.11. Tetrahedral integration rule information module, Part 2 of 2.

of the element stiffness matrix and consistent force vector for the quadratic tetrahedron.

One point rule (exact for constant and linear polynomials over CM tetrahedra):

$$\frac{1}{V} \int_{\Omega^e} F(\zeta_1, \zeta_2, \zeta_3, \zeta_4) d\Omega^e \approx F(\frac{1}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}). \tag{10.48}$$

Four-point rule (exact for constant through quadratic polynomials over CM tetrahedra):

$$\frac{1}{V} \int_{\Omega^e} F(\zeta_1, \zeta_2, \zeta_3, \zeta_4) d\Omega^e \approx \frac{1}{4} F(\alpha, \beta, \beta, \beta) + \frac{1}{4} F(\beta, \alpha, \beta, \beta) + \frac{1}{4} F(\beta, \beta, \alpha, \beta) + \frac{1}{4} F(\beta, \beta, \beta, \alpha), \quad (10.49)$$

in which $\alpha = (5 + 3\sqrt{5})/20 = 0.58541020$, $\beta = (5 - \sqrt{5})/20 = 0.13819660$.

(More material to be added, especially timing results)

Notes and Bibliography

The 10-node quadratic tetrahedron is the natural 3D generalization of the 6-node quadratic triangle. Once the latter was formulated by Fraeijs de Veubeke [278] the road to high order elements was open. The constant metric (CM) version was first published by Argyris in 1965 [27], in which natural coordinates and exact integration were used. Extensions to variable metric (VM) had to wait until the isoparametric formulation was developed by Bruce Irons within Zienkiewicz' group at Swansea. Once that formulation become generally known by 1966 [398], VM tetrahedra of arbitrary order could be fitted naturally into one element family. The first comprehensive description of the 2D and 3D iso-P families may be found in [830].

Examination of the publications of this period brings up some interesting quirks, which occasionally reveal more about "non invented here" territorial hubris than actual contributions to FEM.

The calculation of partial derivatives of functions expressed in tetrahedral coordinates, covered in §10.3, is not available in the literature. For the plane stress 6-node triangle it was formulated by the author during a 1975 software project at Lockheed Palo Alto Research Labs, which was published in [224], as well as in the IFEM notes [257, Ch 24]. The extension from triangles to tetrahedra is immediate. As discussed in §10.6, the Jacobian matrix that emerges from such calculations is not unique, but if correctly programmed all variants lead to the same element equations.

The simplest Gauss integration rules for tetrahedra may be found in the monograph by Stroud and Secrest [713], along with extensive references to original sources. Rules for 14 or more points cited in Table 10.1 and implemented in the *Mathematica* module of Figures 10.10 and 10.11 are taken from the compendium [244].

Homework Exercises for Chapter 10

The Quadratic Tetrahedron

EXERCISE 10.1 [A:15] The iso-P 10-node tetrahedron element (Tet10) is converted into an 11-point tetrahedron (abbreviation: Tet11) by adding an interior node point 11 located at the element center $\zeta_1 = \zeta_2 = \zeta_3 = \zeta_4 = 1/4$. Construct the shape functions N_1^e , N_5^e and and N_{11}^e . (You do not need to write down the full element definition).

Hint: add a "correction bubble" by trying $N_1^e = \hat{N}_1^e + c_1\zeta_1\zeta_2\zeta_3\zeta_4$, in which \hat{N}_1^e is the 10-node tetrahedron shape function given in (10.2); you just need to find c_1 . Likewise for N_5^e . For N_{11}^e , think a while.

Interesting tidbit: why does the quartic $\hat{N}_1^e + c_1 \zeta_1 \zeta_2 \zeta_3 \zeta_4$ satisfies interelement compatibility but the obvious cubic $N_1^e = c_1 \hat{N}_1^e (\zeta_1 - \frac{1}{4})$ does not? (Think of the polynomial variation along edges.)

EXERCISE 10.2 [A:20] Obtain the 11 shape functions of the Tet11 tetrahedron of the previous Exercise, and verify that its sum is identically one (use the constraint $\zeta_1 + \zeta_2 + \zeta_3 + \zeta_4 = 1$ when proving that).

EXERCISE 10.3 [A:15] The next full-polynomial, iso-P member of the tetrahedron family is the cubic tetrahedron (abbreviation: Tet20), which has 20 node points and 60 degrees of freedom. Where do you think the nodes are located?

Hint: the last four: numbered 17, 18, 19, and 20, are located at the face centers; those are called face nodes.

EXERCISE 10.4 [A:20] Derive the corner-node shape function N_1 and the face-node shape function N_{17} for the 20-node cubic tetrahedron. *Note*: node 17 lies at the centroid of face 1-2-3. Assume the element has constant metric (CM) to facilitate visualization.

Hint for N_1 : cross all 20 nodes except 1 with three planes; those planes have equations $\zeta_1 = C$ where the constant C varies for each plane.

Hint for N_{17}^e : find 3 planes that cross all 20 nodes except 17.

EXERCISE 10.5 [A/C:25] Derive the 20 shape functions for the 20-node cubic tetrahedron, and verify that their sum is exactly one. (Only possible in reasonable time with a computer algebra system).

EXERCISE 10.6 [A/C:20] Compute \mathbf{f}^e for a constant-metric (CM) 10-node tetrahedron if the body forces b_x and b_y vanish, while $b_z = -\rho g$ (g is the acceleration of gravity) is constant over the element. Use the 4-point Gauss rule (10.49) to evaluate the integral that gives the consistent node force expression

$$\mathbf{f}^e = \int_{\Omega^e} \mathbf{N}^T \mathbf{b} \ d\Omega^e, \quad \text{in which} \quad \mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ -\rho g \end{bmatrix}, \tag{E10.1}$$

using the exact expressions for $\alpha=(5+3\sqrt{5})/20$ and $\beta=(5-\sqrt{5})/20$ in the 4-point rule, and $V\to V^e$. You need to list only the z force components. Check that the sum of the z force components is $-\rho g V^e$. The result for the corner nodes is physically unexpected.