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In[1435]:= (* This Mathematica script generates element matrices and exports *)
(* them as fortran code for the finite element described in *)
(* https://github.com/Ra-Na/C3D4C1-Abaqus-UEL *)

(* Clear cache *)
Remove["Global`*"]

(* Define a complete 3D 5th order polynomial *)
phi[xvek_, p_] := (
  deg = 5;
  monoms = {};
  For[iii = 0, iii <= deg, iii++,
    For[jjj = 0, jjj <= deg, jjj++,
      For[kkk = 0, kkk <= deg, kkk++,
        If[iii + jjj + kkk <= deg,
          monoms = Append[monoms, xvek[[1]]^iii * xvek[[2]]^jjj * xvek[[3]]^kkk]
        ]];];
  p.monoms);

(* Create vector of polynomial coefficients *)
params = Table[ToExpression[StringJoin["p", ToString[i]]], {i, 1, 56}];

(* Create DOF as a 4x4 Matrix: First index = node number,
second index={DOF,dDOF/dx,dDOF/dy,dDOF/dz} *)
dofs = Table[0, {j, 1, 4}, {k, 1, 4}];

dofs[[1, 1]] = phi1;
dofs[[1, 2]] = phi1x;
dofs[[1, 3]] = phi1y;
dofs[[1, 4]] = phi1z;
dofs[[2, 1]] = phi2;
dofs[[2, 2]] = phi2x;
dofs[[2, 3]] = phi2y;
dofs[[2, 4]] = phi2z;
dofs[[3, 1]] = phi3;
dofs[[3, 2]] = phi3x;
dofs[[3, 3]] = phi3y;
dofs[[3, 4]] = phi3z;
dofs[[4, 1]] = phi4;
dofs[[4, 2]] = phi4x;
dofs[[4, 3]] = phi4y;
dofs[[4, 4]] = phi4z;

(* Create node coordinates *)
nodecoords1 = {x1, y1, z1};
nodecoords2 = {x2, y2, z2};
nodecoords3 = {x3, y3, z3};
nodecoords4 = {x4, y4, z4};

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(* For convenience, create DOF gradient vectors *)
nodegrads1 = {phi1x, phi1y, phi1z};
nodegrads2 = {phi2x, phi2y, phi2z};
nodegrads3 = {phi3x, phi3y, phi3z};
nodegrads4 = {phi4x, phi4y, phi4z};

(* Determine face centers *)
facecoords124 = (nodecoords1 + nodecoords2 + nodecoords4) / 3;
facecoords123 = (nodecoords1 + nodecoords2 + nodecoords3) / 3;
facecoords134 = (nodecoords1 + nodecoords3 + nodecoords4) / 3;
facecoords234 = (nodecoords2 + nodecoords3 + nodecoords4) / 3;

(* Interpolate values and gradients at face centers *)
interpol124 = FullSimplify[Flatten[{
  (bphi1 + phi2 + phi4 +
    phi1 + (facecoords124 - nodecoords1).nodegrads1 +
    phi2 + (facecoords124 - nodecoords2).nodegrads2 +
    phi4 + (facecoords124 - nodecoords4).nodegrads4) / 6,
  (nodegrads1 + nodegrads2 + nodegrads4) / 3}]]];

interpol123 = FullSimplify[Flatten[{
  (phi1 + phi2 + phi3 +
    phi1 + (facecoords123 - nodecoords1).nodegrads1 +
    phi2 + (facecoords123 - nodecoords2).nodegrads2 +
    phi3 + (facecoords123 - nodecoords3).nodegrads3) / 6,
  (nodegrads1 + nodegrads2 + nodegrads3) / 3}]]];

interpol134 = FullSimplify[Flatten[{
  (phi1 + phi3 + phi4 +
    phi1 + (facecoords134 - nodecoords1).nodegrads1 +
    phi3 + (facecoords134 - nodecoords3).nodegrads3 +
    phi4 + (facecoords134 - nodecoords4).nodegrads4) / 6,
  (nodegrads2 + nodegrads3 + nodegrads4) / 3}]]];

interpol234 = FullSimplify[Flatten[{
  (phi2 + phi3 + phi4 +
    phi2 + (facecoords234 - nodecoords2).nodegrads2 +
    phi3 + (facecoords234 - nodecoords3).nodegrads3 +
    phi4 + (facecoords234 - nodecoords4).nodegrads4) / 6,
  (nodegrads1 + nodegrads3 + nodegrads4) / 3}]]];

(* Determine edge centers *)
edgecoords12 = (nodecoords1 + nodecoords2) / 2;
edgecoords13 = (nodecoords1 + nodecoords3) / 2;
edgecoords14 = (nodecoords1 + nodecoords4) / 2;
edgecoords23 = (nodecoords2 + nodecoords3) / 2;

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edgecoords24 = (nodecoords2 + nodecoords4) / 2;
edgecoords34 = (nodecoords3 + nodecoords4) / 2;

(* Interpolate values and gradients at edge centers *)
c = 2; d = 4;
interpol12 = FullSimplify[Flatten[{
  (phi1 + phi2 +
    phi1 + (edgecoords12 - nodecoords1).nodegrads1 +
    phi2 + (edgecoords12 - nodecoords2).nodegrads2) / 4,
  (nodegrads1 + nodegrads2) / 2}]]];

interpol13 = FullSimplify[Flatten[{
  (phi1 + phi3 +
    phi1 + (edgecoords13 - nodecoords1).nodegrads1 +
    phi3 + (edgecoords13 - nodecoords3).nodegrads3) / 4,
  (nodegrads1 + nodegrads3) / 2}]]];

interpol14 = FullSimplify[Flatten[{
  (phi1 + phi4 +
    phi1 + (edgecoords14 - nodecoords1).nodegrads1 +
    phi4 + (edgecoords14 - nodecoords4).nodegrads4) / 4,
  (nodegrads1 + nodegrads4) / 2}]]];

interpol23 = FullSimplify[Flatten[{
  (phi2 + phi3 +
    phi2 + (edgecoords23 - nodecoords2).nodegrads2 +
    phi3 + (edgecoords23 - nodecoords3).nodegrads3) / 4,
  (nodegrads2 + nodegrads3) / 2}]]];

interpol24 = FullSimplify[Flatten[{
  (phi2 + phi4 +
    phi2 + (edgecoords24 - nodecoords2).nodegrads2 +
    phi4 + (edgecoords24 - nodecoords4).nodegrads4) / 4,
  (nodegrads2 + nodegrads4) / 2}]]];

interpol34 = FullSimplify[Flatten[{
  (phi3 + phi4 +
    phi3 + (edgecoords34 - nodecoords3).nodegrads3 +
    phi4 + (edgecoords34 - nodecoords4).nodegrads4) / 4,
  (nodegrads3 + nodegrads4) / 2}]]];

(* Set up linear system for solving the 16 DOF +
  40 pDOF for the 56 polynomial coefficients *)
eqs = Flatten[{
  phi[nodecoords1, params] == dofs[[1, 1]],
  ((D[phi[{x, y, z}, params], x]) /. {x -> x1, y -> y1, z -> z1}) == dofs[[1, 2]],
  ((D[phi[{x, y, z}, params], y]) /. {x -> x1, y -> y1, z -> z1}) == dofs[[1, 3]],

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((D[phi[{x, y, z}, params], z]) /. {x → x1, y → y1, z → z1}) == dofs[[1, 4]],
phi[nodecoords2, params] == dofs[[2, 1]],
((D[phi[{x, y, z}, params], x]) /. {x → x2, y → y2, z → z2}) == dofs[[2, 2]],
((D[phi[{x, y, z}, params], y]) /. {x → x2, y → y2, z → z2}) == dofs[[2, 3]],
((D[phi[{x, y, z}, params], z]) /. {x → x2, y → y2, z → z2}) == dofs[[2, 4]],
phi[nodecoords3, params] == dofs[[3, 1]],
((D[phi[{x, y, z}, params], x]) /. {x → x3, y → y3, z → z3}) == dofs[[3, 2]],
((D[phi[{x, y, z}, params], y]) /. {x → x3, y → y3, z → z3}) == dofs[[3, 3]],
((D[phi[{x, y, z}, params], z]) /. {x → x3, y → y3, z → z3}) == dofs[[3, 4]],
phi[nodecoords4, params] == dofs[[4, 1]],
((D[phi[{x, y, z}, params], x]) /. {x → x4, y → y4, z → z4}) == dofs[[4, 2]],
((D[phi[{x, y, z}, params], y]) /. {x → x4, y → y4, z → z4}) == dofs[[4, 3]],
((D[phi[{x, y, z}, params], z]) /. {x → x4, y → y4, z → z4}) == dofs[[4, 4]],
phi[facecoords124, params] == interpol124[[1]],
phi[facecoords123, params] == interpol123[[1]],
phi[facecoords134, params] == interpol134[[1]],
phi[facecoords234, params] == interpol234[[1]],
Table[
  ({D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y], D[phi[{x, y, z},
    params], z]) /. {x → facecoords124[[1]], y → facecoords124[[2]],
    z → facecoords124[[3]]})[[i]] == interpol124[[i + 1]], {i, 1, 3}],
Table[({D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
  D[phi[{x, y, z}, params], z]) /. {x → facecoords123[[1]],
  y → facecoords123[[2]], z → facecoords123[[3]]})[[
  i]] == interpol123[[i + 1]], {i, 1, 3}],
Table[({D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
  D[phi[{x, y, z}, params], z]) /. {x → facecoords234[[1]],
  y → facecoords234[[2]], z → facecoords234[[3]]})[[
  i]] == interpol234[[i + 1]], {i, 1, 3}],
Table[({D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
  D[phi[{x, y, z}, params], z]) /. {x → facecoords134[[1]],
  y → facecoords134[[2]], z → facecoords134[[3]]})[[
  i]] == interpol134[[i + 1]], {i, 1, 3}],
phi[edgecoords12, params] == interpol12[[1]],
phi[edgecoords13, params] == interpol13[[1]],
phi[edgecoords14, params] == interpol14[[1]],
phi[edgecoords23, params] == interpol23[[1]],
phi[edgecoords24, params] == interpol24[[1]],
phi[edgecoords34, params] == interpol34[[1]],
Table[
  ({D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y], D[phi[{x, y, z},
    params], z]) /. {x → edgecoords12[[1]], y → edgecoords12[[2]],
    z → edgecoords12[[3]]})[[i]] == interpol12[[i + 1]], {i, 1, 3}],
Table[({D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
  D[phi[{x, y, z}, params], z]) /.
  {x → edgecoords13[[1]], y → edgecoords13[[2]], z → edgecoords13[[3]]})[[
  i]] == interpol13[[i + 1]], {i, 1, 3}],

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Table[{D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
      D[phi[{x, y, z}, params], z]} /.
  {x → edgecoords14[[1]], y → edgecoords14[[2]], z → edgecoords14[[3]]}][[
  i]] == interpol14[[i + 1]], {i, 1, 3}],
Table[{D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
      D[phi[{x, y, z}, params], z]} /.
  {x → edgecoords23[[1]], y → edgecoords23[[2]], z → edgecoords23[[3]]}][[
  i]] == interpol23[[i + 1]], {i, 1, 3}],
Table[{D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
      D[phi[{x, y, z}, params], z]} /.
  {x → edgecoords24[[1]], y → edgecoords24[[2]], z → edgecoords24[[3]]}][[
  i]] == interpol24[[i + 1]], {i, 1, 3}],
Table[{D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
      D[phi[{x, y, z}, params], z]} /.
  {x → edgecoords34[[1]], y → edgecoords34[[2]], z → edgecoords34[[3]]}][[
  i]] == interpol34[[i + 1]], {i, 1, 3}]
}];

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(* Extract linear system components *)
coeffs = CoefficientArrays[eqs, params]

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Out[1485]= {SparseArray[ Specified elements: 56  
Dimensions: {56}], SparseArray[ Specified elements: 2254  
Dimensions: {56, 56}]}

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In[1486]:= (* Export element matrices as Fortran code *)

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(* right hand side =
   56 expressions involving the DOF and the node's coordinates *)
(* rhs is linear in the DOF and nonlinear in the node's coordinates *)
rhs = -FullSimplify[Normal[coeffs[[1]]]];
(* DOF vector as intended to use in UEL *)
dofvek = {phi1, phi1x, phi1y, phi1z, phi2, phi2x, phi2y,
          phi2z, phi3, phi3x, phi3y, phi3z, phi4, phi4x, phi4y, phi4z};
(* now we produce the 16x56 matrix which maps the vector
   of degrees of freedom to rhs *)
map = CoefficientArrays[rhs, dofvek];
str = OpenWrite["~/code56.txt"];
WriteString[str, "\n! matrix2 maps from the 16 dof to the 56 pseudo-dof \n"];
WriteString[str, "      double precision matrix2(56,16)\n"];
For[i = 1, i ≤ 56, i++,
  For[j = 1, j ≤ 16, j++,
    WriteString[str, StringJoin["      matrix2(", ToString[i], ",", ToString[j],
      ")=", ToString[FortranForm[ FullSimplify[map[[2, i, j]] ]], "\n" ]]]
  ]
]

(* coefficient matrix that maps polynomial coefficients p1...
   p56 onto the rhs *)

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matrix = FullSimplify[Normal[coeffs[[2]]]];
(* we need the inverse of this matrix to
   calculate the polynomial coefficients from rhs(dof) *)
(* this is done numerically in Fortran,
   here we export only the 56x56 matrix *)
WriteString[str, "\n! the q-matrix maps
   from the 56 pseudo-dof to the 56 polynomial coeffs. \n"]
WriteString[str, "      double precision q(56,56)\n"]
For[i = 1, i ≤ 56, i++,
  For[j = 1, j ≤ 56, j++,
    WriteString[str, StringJoin["      q(", ToString[i], ",",
      ToString[j], ")=", ToString[FortranForm[matrix[[i, j]]]], "\n" ]]
  ]
]

(* To determine the approximation and its
   first and second gradient at any given point *)
(* which is needed for the numerical integration we *)
(* polynomial coefficients and the monomials as 56-vectors *)
xvek = {x, y, z};
monome = {};
deg = 5;
For[iii = 0, iii ≤ deg, iii++,
  For[jjj = 0, jjj ≤ deg, jjj++,
    For[kkk = 0, kkk ≤ deg, kkk++,
      If[iii + jjj + kkk ≤ deg,
        monome = Append[monome, xvek[[1]]^iii * xvek[[2]]^jjj * xvek[[3]]^kkk]
      ]
    ]
  ];

(* export shape func monomials *)
WriteString[str, "\n! the shape function monomials \n"]
WriteString[str, "      double precision n(56)\n"]
For[i = 1, i ≤ 56, i++,
  WriteString[str, StringJoin["      n(",
    ToString[i], ")=", ToString[FortranForm[monome[[i]]]], "\n"]]
]

(* export first gradient of shape func monomials *)
WriteString[str, "\n! the shape function monomials first gradients \n"]
WriteString[str, "      double precision gn(56,3)\n"]
For[i = 1, i ≤ 56, i++,
  For[j = 1, j ≤ 3, j++,
    WriteString[str, StringJoin["      gn(", ToString[i], ",", ToString[j],
      ")=", ToString[FortranForm[D[monome[[i]], xvek[[j]]]]], "\n"]]
  ]
]

(* export second gradient of shape func monomials *)
WriteString[str, "\n! the shape function monomials second gradients \n"]

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WriteString[str, "      double precision ggn(56,3,3)\n"]
For[i = 1, i ≤ 56, i++,
  For[j = 1, j ≤ 3, j++,
    For[k = 1, k ≤ 3, k++,
      WriteString[str,
        StringJoin["      ggn(", ToString[i], ",", ToString[j], ",", ToString[k],
          ")=", ToString[FortranForm[D[monome[[i]], xvek[[j]], xvek[[k]]]]], "\n"]]]
    ]
  ]
]

Close[str]

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Out[1510]= /home/gluege/code56.txt

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In[1511]:= (* Plot interpolation for some a test cases *)
(* Coordinates for the reference tetrahedron *)
x1 = 0; y1 = 0; z1 = 0;
x2 = 1; y2 = 0; z2 = 0;
x3 = 0; y3 = 1; z3 = 0;
x4 = 0; y4 = 0; z4 = 1;
DOFsToPolyCoeffs = Inverse[matrix].map[[2]];
(* constant gradient in <0,0,1> direction, linear field *)
(* DOF-vector: phi1, phi1x, phi1y, phi1z, phi2, ... *)
DOFS = {0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 1, 0, 0, 1};
PolyCoeffs = DOFsToPolyCoeffs.DOFS;
phi[x_, y_, z_] = monome.PolyCoeffs;
gphi[x_, y_, z_] = {D[phi[x, y, z], x], D[phi[x, y, z], y], D[phi[x, y, z], z]};
ContourPlot3D[phi[x, y, z], {x, 0, 1}, {y, 0, 1}, {z, 0, 1},
  RegionFunction → Function[{x, y, z}, Evaluate[x + y + z < 1]],
  Contours → {0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1}]
(* constant gradient in <1,1,1> direction, linear field *)
DOFS = {0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1};
PolyCoeffs = DOFsToPolyCoeffs.DOFS;
phi[x_, y_, z_] = monome.PolyCoeffs;
gphi[x_, y_, z_] = {D[phi[x, y, z], x], D[phi[x, y, z], y], D[phi[x, y, z], z]};
ContourPlot3D[phi[x, y, z], {x, 0, 1}, {y, 0, 1}, {z, 0, 1},
  RegionFunction → Function[{x, y, z}, Evaluate[x + y + z < 1]],
  Contours → {0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1}]
(* linear gradient in <0,0,1> direction, quadratic field *)
DOFS = {0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 2};
PolyCoeffs = DOFsToPolyCoeffs.DOFS;
phi[x_, y_, z_] = monome.PolyCoeffs;
gphi[x_, y_, z_] = {D[phi[x, y, z], x], D[phi[x, y, z], y], D[phi[x, y, z], z]};
ContourPlot3D[phi[x, y, z], {x, 0, 1}, {y, 0, 1}, {z, 0, 1},
  RegionFunction → Function[{x, y, z}, Evaluate[x + y + z < 1]],
  Contours → {0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1}]

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