In[•]:=

```
(* 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[{
    (phi1 + 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,
    (nodegrads2 + nodegrads3 + nodegrads4) / 3}]];

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

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

(* Interpolate values and gradients at edge centers *)
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]],
     ((D[phi[{x, y, z}, params], z]) /. {x → x1, y → y1, z → z1}) == dofs[[1, 4]],
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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}],
Table[({D[phi[{x, y, z}, params], x], D[phi[{x, y, z}, params], y],
      D[phi[{x, y, z}, params], z]} /.
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```
        {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}]
   }];

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

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

```
(* Export element matrices as Fortran code *)

(* 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 *)
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 polynomial coeffs. to the 56 pseudo-dof\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 need the *)
(* 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"]
WriteString[str, "      double precision ggn(56,3,3)\n"]
For[i = 1, i ≤ 56, i++,
```

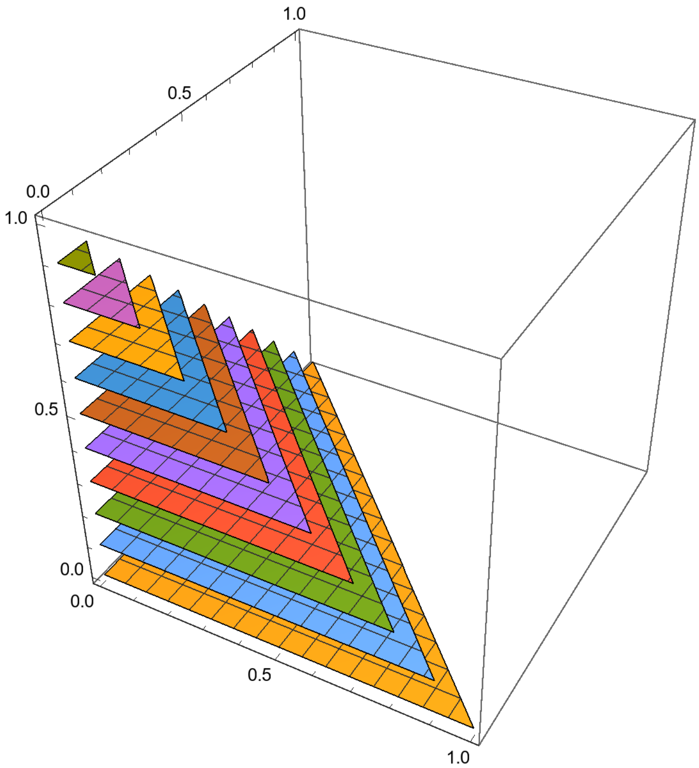
```
 For[j = 1, j ≤ 3, j++,
  For[k = 1, k ≤ 3, k++,
   WriteString[str,
    StringJoin["      ggn(", ToString[i], ",", ToString[j], ",", ToString[k],
     ")=", ToString[FortranForm[D[monome[[i]], xvek[[j]], xvek[[k]]]]], "\n"]]
  ]
 ]
]

Close[str]
```

Out[•]= /home/gluege/code56.txt

```
In[•]:= (* 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]];
```

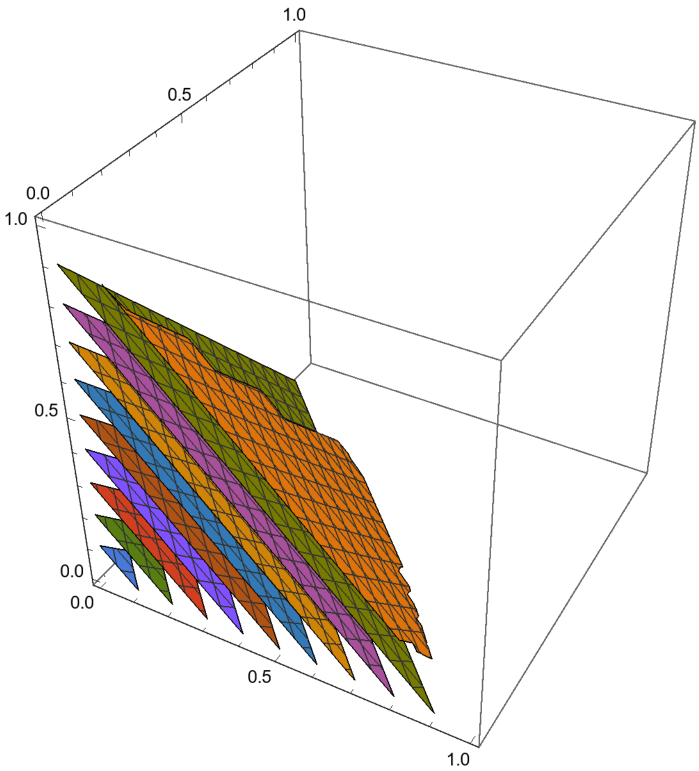
In[•]:=
```
(* constant gradient in <0,0,1> direction, linear field *)
(* DOF-vector: phi1, phi1x,phi1y,phi1z, phi2, ... *)
DOFS = {0, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 1, 0, 0, 1};
PolyCoeffs = DOFsToPolyCoeffs.DOFS;
phi[x_, y_, z_] = monome.PolyCoeffs;
ContourPlot3D[phi[x, y, z], {x, 0, 1}, {y, 0, 1}, {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}]
```

Out[•]=



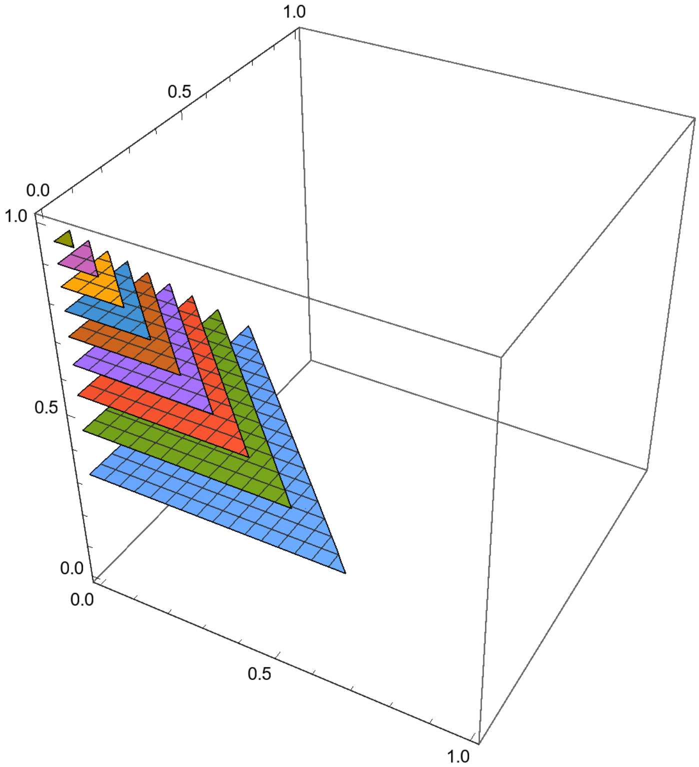
In[∘]:=
```
(* constant gradient in <1,1,1> direction, linear field *)
DOFS = {0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1};
PolyCoeffs = DOFsToPolyCoeffs.DOFS;
phi[x_, y_, z_] = monome.PolyCoeffs;
ContourPlot3D[phi[x, y, z], {x, 0, 1}, {y, 0, 1}, {z, 0, 1},
 RegionFunction → Function[{x, y, z}, Evaluate[x + y + z < 1]],
 Contours → {0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1}]
```

Out[∘]=



In[•]:=
```
(* 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;
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}]
```

Out[•]=



In[•]:=
```
(* Radial field *)
DOFS = {0, 0, 0, 0,
   1, 2, 0, 0,
   1, 0, 2, 0,
   1, 0, 0, 2};
PolyCoeffs = DOFsToPolyCoeffs.DOFS;
phi[x_, y_, z_] = monome.PolyCoeffs;
k = 10;
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 → Table[0.1 i, {i, 0, k}]]
```

Out[•]=