

White Paper:
Piecewise Linear Shape Functions on Polyhedron type cells

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Jan Vermaak
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1 Introduction - Piecewise linear shape functions on a 3D tetrahedron

For a three dimensional simulation using tetrahedral elements we seek to map a tetrahedron in cartesian space to a reference tetrahedron in natural coordinates. We do this because we can develop a method to perform integration or differentiation for the reference tetrahedron that can be mapped to a tetrahedron of any shape and location. An example of the two tetrahedron in different coordinate space is shown in Figure 1. We will denote xyz as the cartesian coordinate system and $\xi\eta\zeta$ as the “natural” coordinate system.

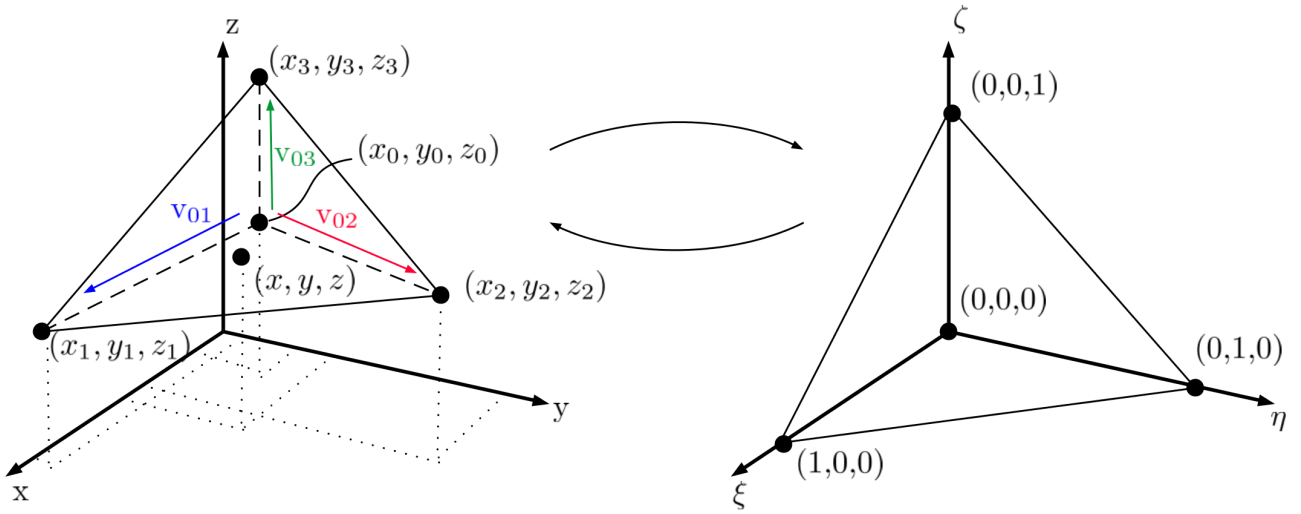


Figure 1: Mapping of a 3D tetrahedron to a reference tetrahedron in natural coordinates.

The linear basis functions for the reference tetrahedron are

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

$$N_1(\xi, \eta, \zeta) = \xi$$

$$N_2(\xi, \eta, \zeta) = \eta$$

$$N_3(\xi, \eta, \zeta) = \zeta$$

From these functions we can interpolate the point (x, y, z) with the following

$$x = N_0x_0 + N_1x_1 + N_2x_2 + N_3x_3$$

$$y = N_0y_0 + N_1y_1 + N_2y_2 + N_3y_3$$

$$z = N_0z_0 + N_1z_1 + N_2z_2 + N_3z_3$$

We can express x , y and z as functions of ξ , η and ζ by substituting the basis functions into these expression to obtain

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

In terms of the vectors from vertex 0 to the other three vertices (refer to Figure 1) we can write this as

$$x = x_0 + v_{01x}\xi + v_{02x}\eta + v_{03x}\zeta \quad (1)$$

$$y = y_0 + v_{01y}\xi + v_{02y}\eta + v_{03y}\zeta \quad (2)$$

$$z = z_0 + v_{01z}\xi + v_{02z}\eta + v_{03z}\zeta \quad (3)$$

which is in the form of linear transformation and from which we can determine the very important Jacobian matrix

$$\mathbf{J} = \begin{bmatrix} \frac{dx}{d\xi} & \frac{dx}{d\eta} & \frac{dx}{d\zeta} \\ \frac{dy}{d\xi} & \frac{dy}{d\eta} & \frac{dy}{d\zeta} \\ \frac{dz}{d\xi} & \frac{dz}{d\eta} & \frac{dz}{d\zeta} \end{bmatrix} = \begin{bmatrix} v_{01x} & v_{02x} & v_{03x} \\ v_{01y} & v_{02y} & v_{03y} \\ v_{01z} & v_{02z} & v_{03z} \end{bmatrix} = \begin{bmatrix} (x_1 - x_0) & (x_2 - x_0) & (x_3 - x_0) \\ (y_1 - y_0) & (y_2 - y_0) & (y_3 - y_0) \\ (z_1 - z_0) & (z_2 - z_0) & (z_3 - z_0) \end{bmatrix}. \quad (4)$$

As was the case with the triangle we now seek

$$\begin{bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{bmatrix} = (\mathbf{J}^T)^{-1} \begin{bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{bmatrix} \quad (5)$$

where we need to find the inverse of transpose of the Jacobian, with the transpose given by

$$\mathbf{J}^T = \begin{bmatrix} v_{01x} & v_{01y} & v_{01z} \\ v_{02x} & v_{02y} & v_{02z} \\ v_{03x} & v_{03y} & v_{03z} \end{bmatrix} \quad (6)$$

And then we can use a suitable method in literature for obtaining the inverse of a 3×3 matrix:

$$(\mathbf{J}^T)^{-1} = \begin{bmatrix} \frac{dx}{d\xi} & \frac{dy}{d\xi} & \frac{dz}{d\xi} \\ \frac{dx}{d\eta} & \frac{dy}{d\eta} & \frac{dz}{d\eta} \\ \frac{dx}{d\zeta} & \frac{dy}{d\zeta} & \frac{dz}{d\zeta} \end{bmatrix} \quad (7)$$

With the Jacobian and inverse of the Jacobian-transpose in-hand we can perform integration and differentiation on the reference tetrahedron (in “natural” coordinates) and simply map the result to cartesian coordinates.

2 Piecewise linear shape functions on a 3D Polyhedron

The same methodology as depicted in [1] was used where the shape function for each vertex i of the polyhedron is given by

$$P_i(x, y, z) = N_i(x, y, z) + \sum_{\text{faces at } i} \beta_f N_f(x, y, z) + \alpha_c N_c(x, y, z) \quad (8)$$

where the functions $N(x, y, z)$ are the standard linear shape functions defined on a tetrahedron. β_s and α_c is the weight that gives the face midpoint, \bar{r}_{fc} , and cell mid-point, \bar{r}_{cc} , respectively from the sum of the vertices that constitute them. i.e.

$$\bar{r}_{fc} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}_{fc} = \sum_{v=0}^{N_{vf}} \beta_f \begin{bmatrix} x \\ y \\ z \end{bmatrix}_v \quad (9)$$

$$\bar{r}_{cc} = \begin{bmatrix} x \\ y \\ z \end{bmatrix}_{cc} = \sum_{v=0}^{N_{vc}} \alpha_c \begin{bmatrix} x \\ y \\ z \end{bmatrix}_v \quad (10)$$

where N_{vf} is the number of vertices for the given face and N_{vc} is the number of vertices for the entire cell. Naturally it follows that $\beta_f = \frac{1}{N_{vf}}$ and $\alpha_c = \frac{1}{N_{vc}}$. The format of equation 8 is not intuitive at first sight ... it is hard to comprehend the summation over faces “at j”, but let us try to clarify this with a diagram (see Figure 2).

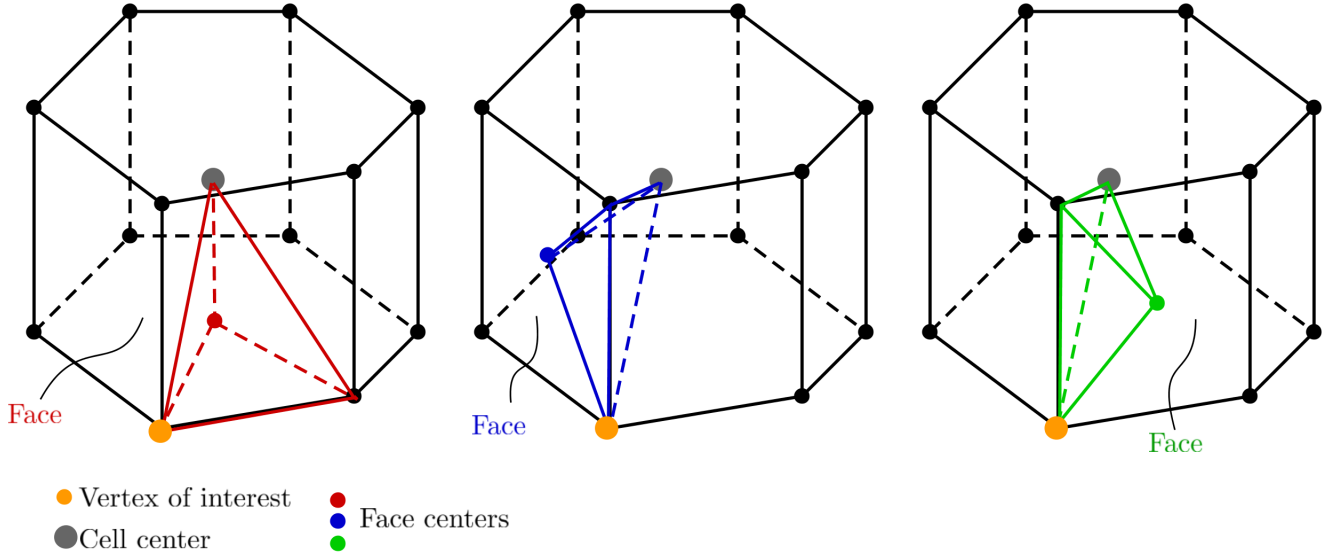


Figure 2: Connection of the vertex of interest to the tetrahedrons that comprise the cell.

Firstly we split the polyhedron into faces, where each face can be a polygonal face. Each face is then split into a number of sides. A side is a tetrahedron, corresponding to a face, which is formed from each edge of the polygonal face where the vertex collection are the two vertices of the edge, the face center and the cell center. In other words the face center and the two vertices of the edge forms a triangle, and the cell center makes it a tetrahedron.

As was the case with the polygon, all the other vertices j (not i) are connected to the vertex of interest i through the cell center. Again, we don't include the cell center as a point in the simulation so we have to spread its effect through to each of the vertices using the α_c factor. We also have face centered shape functions associated with the division of each polygonal face into sides. On each face, to which vertex i belongs, the shape functions defined on the face centers will protrude into the tetrahedron under consideration (i.e. the tetrahedron associated with vertex i associated with face f , side s). Therefore more clearly we can express the shape functions on a tetrahedron-by-tetrahedron basis

$$P_i^{tet}(x, y, z) = \begin{cases} \alpha_c N_c(x, y, z) & \text{no matter which tetrahedron} \\ +\beta_f N_f(x, y, z) & \text{if vertex } i \text{ is part of the face} \\ +N_i(x, y, z) & \text{if vertex } i \text{ is part of the face-side pair} \end{cases} \quad (11)$$

Figure 3 shows the influence of a shape function (centered on a specific point as denoted by the start of an arrow) from a specific vertex (color). The orange colored vertex's influence is shown on the left most figure where the shape function is then the full equation because all of the conditions are met; i.e. $\alpha_c N_c$ is always present, vertex i is indeed part of the face where this tetrahedron is defined and therefore $\beta_f N_f$

is present, finally it is also part of the side of the tetrahedron and therefore its basic shape function N_i is present.

The middle figure shows the red vertex as a vertex that only has the contribution of $\alpha_c N_c$ and $\beta_f N_f$ because the red vertex is not on the side composing the tetrahedron of interest. The rightmost figure shows only the contribution of $\alpha_c N_c$ because the blue vertex is not part of any adjacent face.

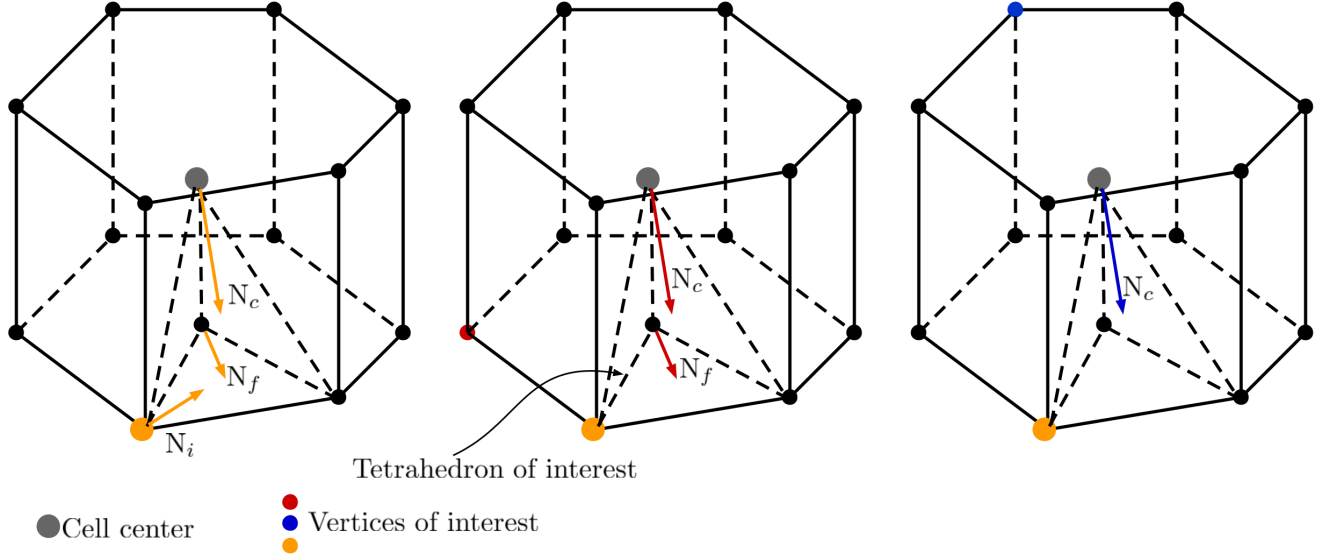


Figure 3: Influence of different vertices on the shape functions of within a tetrahedral portion of the cell.

3 Volume integrals

`IntV_gradShapeI_gradShapeJ[i][j]`
`IntV_shapeI_gradshapeJ[i][j]`
`IntV_shapeI_shapeJ[i][j]`
`IntV_shapeI[i]`

The finite element method requires the integration of the shape functions over the volume and surface of the cell. These integrations can easily be made analytically but for the purpose of being easy to follow we will revert to integration using a Gaussian quadrature. Let us discuss the assembly of the volume integrals. Before we do so we have to understand the assembly of the integrals in a tetrahedron-by-tetrahedron fashion. Volume integrals therefore take the form

$$\begin{aligned} \int_V P_i P_j . dV &= \int_V \left[\alpha_c N_c + \beta_{fi} N_{fi} + N_i \right] \left[\alpha_c N_c + \beta_{fj} N_{fj} + N_j \right] . dV \\ &= \sum_{tets} \int_{V_{tet}} \left[\alpha_c N_c + \beta_{fi} N_{fi} + N_i \right] \left[\alpha_c N_c + \beta_{fj} N_{fj} + N_j \right] . dV_{tet}. \end{aligned} \quad (12)$$

Now let

$$F(x, y, z) = \left[\alpha_c N_c + \beta_{fi} N_{fi} + N_i \right] \left[\alpha_c N_c + \beta_{fj} N_{fj} + N_j \right].$$

With this definition we now have the more general form of a function evaluated tetrahedron-by-tetrahedron which is represented by

$$\int_V P_i P_j . dV = \int_V F(x, y, z) . dV = \sum_{tets} \int_{V_{tet}} F(x, y, z) . dV_{tet} \quad (13)$$

for which we can first transform the integral over the cartesian coordinate version of a tetrahedron (V_{tet}) to an integral over the natural coordinates version (V_τ) as

$$\int_{V_{tet}} F(x, y, z) . dV_{tet} = \int_{V_\tau} F(\xi, \eta, \zeta) . dV_\tau . |J|_{tet} \quad (14)$$

and then apply an appropriate Gaussian quadrature for the volume integral

$$\int_{V_\tau} F(\xi, \eta, \zeta) . dV_\tau . |J|_{tet} = \sum_q^Q F((\xi, \eta, \zeta)_q) . w_q . |J|_{tet} \quad (15)$$

where w_q is the quadrature weight associated with quadrature abscissa q , a unique combination of ξ , η and ζ . These weights and abscissae are tabulated in Appendix A.

When derivatives are encountered the result will be a vector and the integral over each tetrahedron needs to be multiplied from the left by the inverse of the Jacobian-transpose.

$$\int_{V_{tet}} \nabla F(x, y, z) \cdot dV_{tet} = (J^T)_{tet}^{-1} \int_{V_\tau} \nabla F(\xi, \eta, \zeta) \cdot dV_\tau \cdot |J|_{tet} = (J^T)_{tet}^{-1} \sum_q^Q \nabla F((\xi, \eta, \zeta)_q) \cdot w_q \cdot |J|_{tet} \quad (16)$$

4 Surface integrals

`IntS_shapeI_shapeJ[f][i][j]`

`IntS_shapeI[f][i]`

`IntS_shapeI_gradshapeJ[f][i][j]`

The same form of volume integrals can be encountered on surfaces but here instead of being integrals over the volume of a tetrahedron it will be the integral over a triangular face of a tetrahedron. To this end we can use a simple convention as shown in 4 below. This figure depicts that the root coordinate of the reference tetrahedron is taken as the first vertex of the edge that defines the face's side. The first leg of the reference tetrahedron is then taken to be the vector to the face center (along ξ). The second leg (along η) is taken to be vector to the second vertex of the edge mentioned before, and finally the third leg (along ζ) is taken to be the vector to the cell-centre. The benefit of this convention is that we can use a 2D triangular quadrature without the need to define new reference shape functions since any coordinate in reference xy-space can be mapped to $\xi\eta$ -space and will still be valid on the surface.

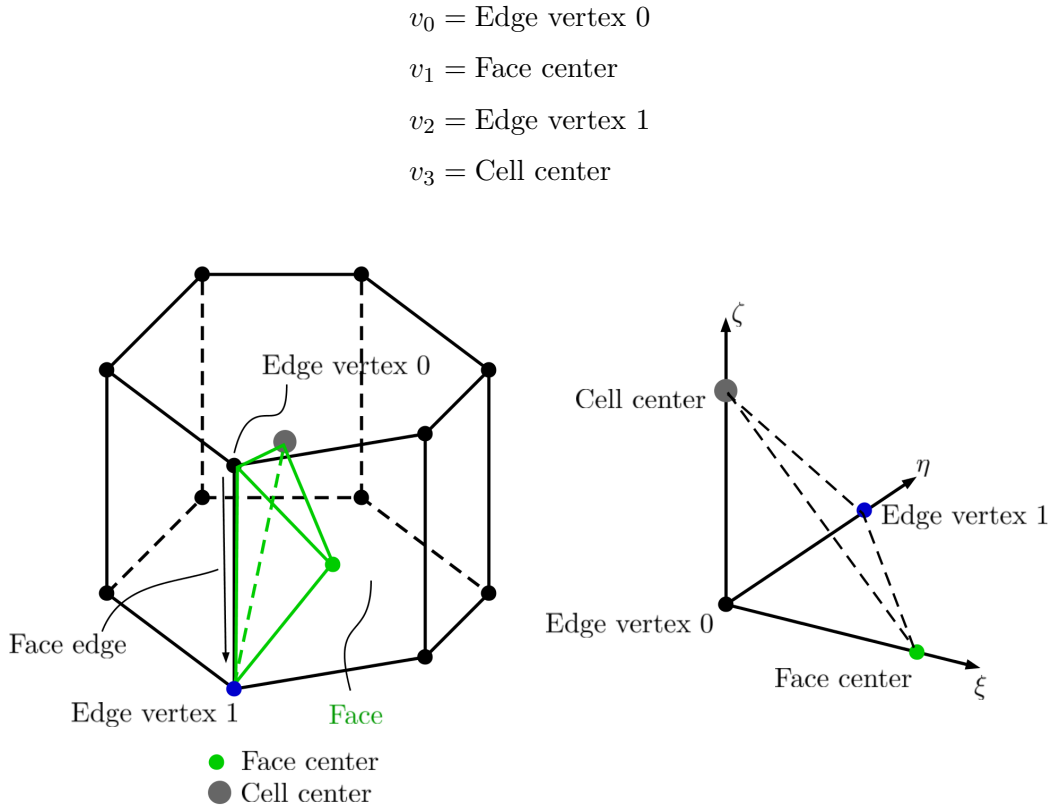


Figure 4: Convention used for defining tetrahedrons by side.

There is one complication of integrating over the surface without using different definitions of the shape functions and that is the different Jacobian form used in the integration process. Fortunately though the developed convention greatly assists us in this regards. We simply need to rotate the v_{01} - and v_{02} legs to the 2D plane and compute the surface Jacobian in this 2D reference frame.

Let the **normal-vector**, n , be the negative of the face's geometric normal (which should be pointing outwards), let b be the **binorm-vector** defined by normalizing the η leg of the tetrahedron (i.e. v_{02}) as

$$b = \frac{1}{||v_{02}||} \cdot v_{02}$$

Now the **tangent-vector**, t , is simply defined by

$$t = b \times n$$

The **rotation matrix**, R , for rotating any vector in the 2D plane to the reference surface is given by

$$R = \begin{bmatrix} t_x & b_x & n_x \\ t_y & b_y & n_y \\ t_z & b_z & n_z \end{bmatrix}. \quad (17)$$

For our purposes we need to rotate 3D vectors to the 2D plane and therefore we require the inverse of this matrix. When applied to the first and second legs of our tetrahedron we get

$$\begin{aligned} v'_{01} &= R^{-1} v_{01} \\ v'_{02} &= R^{-1} v_{02} \end{aligned} \quad (18)$$

And then

$$J_{surf} = \begin{bmatrix} v'_{01x} & v'_{02x} \\ v'_{01y} & v'_{02y} \end{bmatrix}$$

and therefore

$$|J|_{surf} = v'_{01x} \cdot v'_{02y} - v'_{01y} \cdot v'_{02x} \quad (19)$$

Surface integrals can now take the simple form of the volume integrals without any special treatment

$$\int_{S_{side}} F(x, y, z) \cdot dA_{side} = \sum_q^Q F((\xi, \eta, 0)_q) \cdot w_q \cdot |J|_{surf} \quad (20)$$

Quadrature weights and abscissae for this integration are depicted in Appendix B.

5 Coding Implementation

5.1 Constructor `00_constrdestr.cc`

In the constructor we receive the basic cell information (i.e. information about vertices and faces), a reference to the grid (holding actual vertex values) and the discretization method (holding quadrature information).

```
PolyhedronFEView(chi_mesh::CellPolyhedron *polyh_cell,
                  chi_mesh::MeshContinuum *vol_continuum,
                  CHI_DISCRETIZATION_PWL *discretization)
```

- We immediately make reference copies of the quadrature sets and then assign the cell centre, v_{cc} , and compute α_c .
- We then construct our tetrahedrons by firstly looping over the faces and then internally over edges of the face.
 - For each face we instantiate a new data structure, `FEface_data`, which holds the tetrahedron “side”-information. It also holds the face center v_{fc} .
 - Loop over face edges.
 - * For each edge we define a side with the data structure `FEside_data`. This essentially stores all the information related to a tetrahedron.
 - * We assign the vertices and compute the legs v_{01} to v_{02} .
 - * We compute the single surface Jacobian $|J|_{surf}$ associated with each tetrahedron.
 - * We assemble the Jacobian from the legs, we compute the Jacobian-transpose and then the inverse of the Jacobian-transpose.
 - * We receive quadrature point data for each of the cell’s degrees of freedom on this side data structure.
 - * Finally we push the side data to the face data structure.
- In order to determine whether N_f or N_i applies to a specific side when given degree of freedom i we need to develop a mapping of each cell degree of freedom to each face-side pair.
- In other words ... given face f and side s :
 - N_c (or N_3 for the given tet) is always applied so we don’t need to check for it.
 - Is dof_i part of face f ? If yes then N_f applies (the tet’s N_1).
 - Is dof_i part of the face-side pair, determined by checking if dof_i is equal to either this tetrahedron’s v_0 or v_2 . Then N_0 or N_2 needs to be applied accordingly.
- We then compute a cell DOF to face DOF mapping which is convenient purely for codes using integrations over surfaces. i.e. like a transport sweep code.

5.2 Precomputing the integrals

The precompute function, also called the phase of computing cell matrices, is a function which pre-computes the quadrature rule based integrals. For its first phase it computes the values of the different shape functions on every tetrahedron and every quadrature point. To this end the code relies on the following functions:

Defined in [03.compcellmat.cc](#)

```
double PreShape(int face_index, int side_index, int i, int qpoint_index,
                bool on_surface = false);

double PreGradShape_x(int face_index, int side_index, int i, int qpoint_index);
double PreGradShape_y(int face_index, int side_index, int i, int qpoint_index);
double PreGradShape_z(int face_index, int side_index, int i, int qpoint_index);
```

These functions use the developed [FESide.data](#) data structure to evaluate the side shape functions from the reference tetrahedron function and therefore each of these functions in turn use the reference tetrahedron functions:

Defined in [01.refitet.cc](#)

```
double TetShape(int index, int qpoint_index, bool on_surface = false);
double TetGradShape_x(int index, int qpoint_index);
double TetGradShape_y(int index, int qpoint_index);
double TetGradShape_z(int index, int qpoint_index);
```

As an example consider [PreGradShape_x](#) :

Defined in [03.compcellmat.cc](#)

```
double PreGradShape_x(int face_index,
                      int side_index,
                      int i, int qpoint_index)
{
    double value = 0.0;
    double tetdfox = 0.0;
    double tetdfdy = 0.0;
    double tetdfdz = 0.0;
    int index = node_maps[i]->face_map[face_index]->
                side_map[side_index]->index;
    double betaf = face_betaf[face_index];

    tetdfox += TetGradShape_x(index, qpoint_index);
    if (node_maps[i]->face_map[face_index]->side_map[side_index]->part_of_face){
        tetdfox += betaf* TetGradShape_x(1, qpoint_index);}
    tetdfox += alphac* TetGradShape_x(3, qpoint_index);

    tetdfdy += TetGradShape_y(index, qpoint_index);
    if (node_maps[i]->face_map[face_index]->side_map[side_index]->part_of_face){
        tetdfdy += betaf* TetGradShape_y(1, qpoint_index);}
    tetdfdy += alphac* TetGradShape_y(3, qpoint_index);

    tetdfdz += TetGradShape_z(index, qpoint_index);
    if (node_maps[i]->face_map[face_index]->side_map[side_index]->part_of_face){
        tetdfdz += betaf* TetGradShape_z(1, qpoint_index);}
    tetdfdz += alphac* TetGradShape_z(3, qpoint_index);
```

```

    value += faces[face_index]->sides[side_index]->JTinv.GetIJ(0,0)*tetdfdx;
    value += faces[face_index]->sides[side_index]->JTinv.GetIJ(0,1)*tetdfdy;
    value += faces[face_index]->sides[side_index]->JTinv.GetIJ(0,2)*tetdfdzt;

    return value;
}

```

This entire trail culminates in the following portion of the [PreCompute](#) phase:

Defined in [03_compcellmat.cc](#)

```

for (int f=0; f<faces.size(); f++)
{
    for (int s=0; s<faces[f]->sides.size(); s++)
    {
        for (int i=0; i<dofs; i++)
        {
            FEqp_data* pernode_data = new FEqp_data;

            //Prestore GradVarphi_xyz
            for (int qp=0; qp<quadratures[DEG3]->qpoints.size(); qp++)
            {
                pernode_data->gradshapex_qp.push_back(PreGradShape_x(f, s, i, qp));
                pernode_data->gradshapex_qp.push_back(PreGradShape_y(f, s, i, qp));
                pernode_data->gradshapex_qp.push_back(PreGradShape_z(f, s, i, qp));
            }
            //Prestore Varphi
            for (int qp=0; qp<quadratures[DEG3]->qpoints.size(); qp++)
            {
                pernode_data->shape_qp.push_back(PreShape(f, s, i, qp));
            }
            //Prestore Varphi on surface
            for (int qp=0; qp<quadratures[DEG3_SURFACE]->qpoints.size(); qp++)
            {
                pernode_data->shape_qp_surf.push_back(PreShape(f, s, i, qp, ON_SURFACE));
            }

            faces[f]->sides[s]->qp_data.push_back(pernode_data);
        } // for i
    } //for side
} //for face

```

With the values of the shape functions evaluated at the quadrature points second phase of the [PreCompute](#) function assembles the integrals as if we were assembling a matrix by using the quadrature points. It has many facets and a number of utility functions but should be intuitive to follow.

6 Using the interpolation [02_xyz_shapefuncs.cc](#)

Two utility functions are available for use by field function interpolators:

Defined in [02_xyz_shapefuncs.cc](#)

```
double          Shape_xyz(int i, chi_mesh::Vector xyz);  
chi_mesh::Vector GradShape_xyz(int i, chi_mesh::Vector xyz);
```

These functions are used with cartesian coordinates and returns the values of the shape functions in the cartesian reference frames.

Appendix A Quadrature rule for integration of tetrahedron space

The study of quadratures for tetrahedrons is a deeply mathematical topic one that is outside the scope of this study. As with the two dimensional case, and since we will limit our study to piece-wise linear shape functions we will limit our quadrature set to a minimum degree of precision of 2. Meaning we only need to exactly integrate polynomials of to the second degree. For tetrahedons, in natural coordinates, quadrature sets are available in [2]. For this study the weights and quadrature points as shown in Table below will be used.

Point	weights	X	Y	Z
0	0.25	0.585410197	0.138196601	0.138196601
1	0.25	0.138196601	0.138196601	0.138196601
2	0.25	0.138196601	0.138196601	0.585410197
3	0.25	0.138196601	0.585410197	0.138196601

Table 1: Quadrature points and weights used for tetrahedron elements.

Appendix B Quadrature rule for integration of triangle space

We seek an integral of a function in triangle space T_{sp} in the form

$$\int \int_{T_{sp}} f(x, y).dx.dy = \sum_{i=0}^{N-1} w_i f(x_i, y_i).$$

Furthermore we know that in the finite element method with only linear shape functions we will at most have polynomials of degree 2 therefore we can devise a set of test functions

$$\begin{aligned} f(x, y) = 1 & \quad \int_0^1 \int_0^{1-y} 1.dx.dy = \frac{1}{2} = \sum_{i=0}^{N-1} w_i \\ f(x, y) = x & \quad \int_0^1 \int_0^{1-y} x.dx.dy = \frac{1}{6} = \sum_{i=0}^{N-1} w_i x_i \\ f(x, y) = y & \quad \int_0^1 \int_0^{1-y} y.dx.dy = \frac{1}{6} = \sum_{i=0}^{N-1} w_i y_i \\ f(x, y) = xy & \quad \int_0^1 \int_0^{1-y} xy.dx.dy = \frac{1}{24} = \sum_{i=0}^{N-1} w_i x_i y_i \\ f(x, y) = x^2 & \quad \int_0^1 \int_0^{1-y} x^2.dx.dy = \frac{1}{12} = \sum_{i=0}^{N-1} w_i x_i^2 \\ f(x, y) = y^2 & \quad \int_0^1 \int_0^{1-y} y^2.dx.dy = \frac{1}{12} = \sum_{i=0}^{N-1} w_i y_i^2 \end{aligned}$$

With $N = 3$ a symmetric solution is obtained with

$$\begin{aligned} w_i &= \frac{1}{6} \\ x_0, y_0 &= \left(\frac{1}{6}, \frac{1}{6}\right) \\ x_1, y_1 &= \left(\frac{4}{6}, \frac{1}{6}\right) \\ x_2, y_2 &= \left(\frac{1}{6}, \frac{4}{6}\right) \end{aligned}$$

which is not a unique solution.

References

- [1] Bailey T.S., Adams M.L., Yang B., Zika M.R., *A piecewise linear finite element discretization of the diffusion equation for arbitrary polyhedral grids*, Journal of Computational Physics 227 (2008) 3738–3757, 2007
- [2] Engels H., Zienkiewicz O., *Quadrature Rules for Tetrahedrons*, http://people.sc.fsu.edu/~jburkardt/datasets/quadrature_rules_tet/quadrature_rules_tet.html, accessed January 1, 2019.