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HEXAHEDRAL DISCRETISATION OF DOMAINS

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ABSTRACT

In this paper, a method to discretize the physical domain in the shape of a linear polyhedron into an assemblage of all hexahedral finite elements is discussed. The idea is to generate a coarse mesh of all tetrahedrons for the given domain, Then divide each of these tetrahedron further into a refined mesh of all tetrahedrons, if necessary. Then finally, we divide each of these tetrahedron into four hexahedra. Further each of these hexahedra is divided into 2^3 and $[(2^3)]^2$ hexahedra. A numerical scheme which decompose a arbitrary linear tetrahedron into 4, $4(2^3)$ hexahedra is presented and is applied to solve some integrals over a unit cube using Gauss Legendre Quadrature Rules.

KEYWORDS

Numerical Integration, Finite Elements, Tetrahedron, Hexahedron, Polyhedron, Irregular Heptahedron, Gauss Legendre Quadrature Rules.

INTRODUCTION

The finite element method (FEM) has become a central tool in computer graphics, and it is widely used for physically based animation of deformations, fracture, fluids, smoke, or other affects. Most methods discretize the computational domain by tetrahedral or hexahedral elements and linear or trilinear interpolants, respectively. In several earlier works[1-12], numerical integration rules for tetrahedron are already established. In studies [13], composites integration with all tetrahedron decomposition is also proposed. In a recent study [16] numerical integration over a standard tetrahedron is computed by decomposing it into four hexahedrons and applied to some typical integrals. They have not shown the application of the method to compute integrals over a linear polyhedron.

In this paper, we propose a method to discretize the physical domain in the shape of a linear polyhedron into an assemblage of all hexahedral finite elements. We have proposed numerical schemes which decompose a arbitrary linear tetrahedron into 4, $4(2^3)$ hexahedra. This is proposed in sections 2-4 of this

paper. In section 5, numerical integration scheme for a linear polyhedron which is partitioned into tetrahedra, pyramids and tetrahedra obtained by triangulating the surface of polyhedron is shown. In section 6, the above numerical schemes are applied to solve typical integrals over a unit cube using Gauss Legendre Quadrature Rules.

1. VOLUME INTEGRATION OVER AN ARBITRARY LINEAR TETRAHEDRON

Let us consider the volume integral over an arbitrary linear tetrahedron T_{1234} as

$$\text{III}_{T_{1234}}(f) = \iiint_{T_{1234}} f(X, Y, Z) dXdYdZ \quad (1)$$

Where,

T_{1234} is an arbitrary linear tetrahedron in Cartesian space with vertices $((X_i, Y_i, Z_i), i=1,2,3,4)$. We can transform the arbitrary linear tetrahedron into an orthogonal tetrahedron (standard tetrahedron) T_{1234}^{\sim} by using the following affine coordinate transformation as shown in Fig.1 and the transformation is

$$\begin{aligned} X &= X_1 + (X_2 - X_1)x + (X_3 - X_1)y + (X_4 - X_1)z, \\ Y &= Y_1 + (Y_2 - Y_1)x + (Y_3 - Y_1)y + (Y_4 - Y_1)z, \\ Z &= Z_1 + (Z_2 - Z_1)x + (Z_3 - Z_1)y + (Z_4 - Z_1)z, \end{aligned} \quad (2)$$

We now evaluate the integral

$$\iiint_{T_{1234}} f(X, Y, Z) dXdYdZ = |\det J| \iiint_{T_{1234}^{\sim}} f(X(x, y, z), Y(x, y, z), Z(x, y, z)) dx dy dz \quad (3)$$

Where, $\det J = \begin{vmatrix} X_{21} & X_{31} & X_{41} \\ Y_{21} & Y_{31} & Y_{41} \\ Z_{21} & Z_{31} & Z_{41} \end{vmatrix}$,
 $X_{pq} = X_p - X_q, Y_{pq} = Y_p - Y_q, Z_{pq} = Z_p - Z_q, \quad (4)$
 $p = 2,3,4; q = 1$

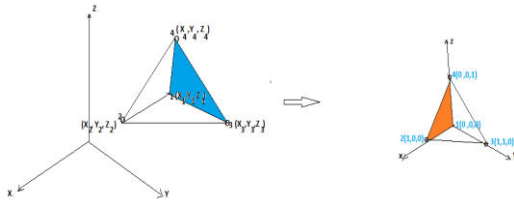


Fig.1 Three dimensional mapping of an arbitrary linear tetrahedron in XYZ-space into a unit orthogonal tetrahedron in xyz-space

2. COMPOSITE INTEGRATION OVER A UNIT ORTHOGONAL LINEAR TETRAHEDRON

A composite integration by dividing the arbitrary linear tetrahedron into an all hexahedron finite element mesh is proposed. We first divide the arbitrary linear tetrahedron into four unique hexahedrons, then we refine this division into a mesh of 32 hexahedrons and finally into 256 hexahedrons. These three are connected and the give higher accuracies by using mathematical expressions of same order but higher rational constants. We now obtain the necessary coordinate transformations and their Jacobians which will transform the integration over arbitrary linear hexahedrons to the integrals over a 2-cube.

Division of a tetrahedron into four hexahedrons

We divide tetrahedron into four hexahedron as shown in the following figure; Fig.1. This is done first by joining the centroid of the tetrahedron to the centroids of four triangular surfaces which form the tetrahedron. Then we locate the centroids of the four triangular surfaces which are further joined to the mid points of the respective triangular edges of the triangular surfaces. This creates four hexahedrons $\Omega_i (i = 1,2,3,4)$ in the standard linear tetrahedron, Thus, we can write from eqn(3) for the triple integral over the arbitrary linear tetrahedron as

$$\iiint_{T_{1234}} f(X, Y, Z) dXdYdZ =$$

$$|\det J| \iiint_{T_{1234}^{\sim}} f(X(x, y, z), Y(x, y, z), Z(x, y, z)) dx dy dz = |\det J| \sum_{i=1}^4 \iiint_{\Omega_i} f(X(x, y, z), Y(x, y, z), Z(x, y, z)) dx dy dz \quad (5)$$

Where, (X, Y, Z) and (x, y, z) are different Cartesian spaces and T_{1234} , T_{1234}^{\sim} are the arbitrary linear tetrahedron and the standard orthogonal linear tetrahedron respectively. $\Omega_i (i = 1,2,3,4)$ are the hexahedrons created inside the standard linear orthogonal tetrahedron T_{1234}^{\sim} .

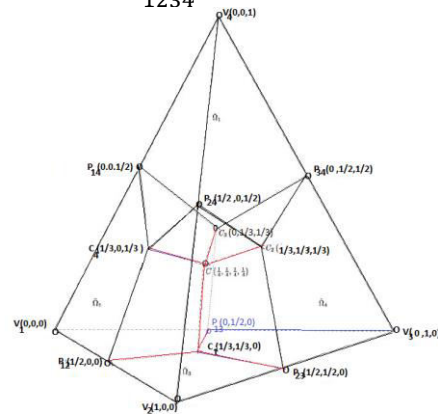


Fig.2 DIVISION OF A STANDARD TETRAHEDRON INTO FOUR HEXAHEDRONS

In Fig.2 above, $\Omega_1, \Omega_2, \Omega_3, \Omega_4$ are Hexahedrons, $C_i (i=1,2,3,4)$ are centroids of triangular faces spanned by vertices $\{V_1, V_2, V_3\}, \{V_2, V_3, V_4\}, \{V_1, V_3, V_4\}$, and $\{V_1, V_2, V_4\}$ respectively. $P_{ij}, \{(ij) = (12), (23), (13), (14), (24), (34)\}$ are the midpoints of edges joining vertices $V_i V_j$ and C is the centroid of the standard tetrahedron. The nodal coordinates for the above four hexahedrons are shown in fig.

We can transform each of these hexahedrons in physical space (x, y, z) into a standard 2-cube in a parametric space (r, s, t) by using the coordinate transformations:

$$x = \sum_{h=1}^8 N_h(r, s, t) x_h; \quad y = \sum_{h=1}^8 N_h(r, s, t) y_h; \quad z = \sum_{h=1}^8 N_h(r, s, t) z_h \quad (6)$$

Where, $N_h(r, s, t)$ are the nodal shape functions for a the standard 2-cube, $-1 \leq r, s, t \leq 1$ in the parametric space (r, s, t) and (x_h, y_h, z_h) are the nodal coordinates of the hexahedron in the Cartesian space (x, y, z)

The integrals over the hexahedrons $\Omega_i (i=1,2,3,4)$ in Cartesian space can be now expressed from the above transformations as :

$$\iiint_{\Omega_i} f(X(x, y, z), Y(x, y, z), Z(x, y, z)) dx dy dz = \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 f(X(x^i, y^i, z^i), Y(x^i, y^i, z^i), Z(x^i, y^i, z^i))$$

$$\frac{\partial(x^i, y^i, z^i)}{\partial(r, s, t)} dr ds dt \quad \dots(7)$$

Hence from eqns(5) and (7), we obtain

$$\begin{aligned} & \iiint_{T_{1234}} f(X, Y, Z) dX dY dZ = \\ & |\det J| \iiint_{T_{1234}} f(X(x, y, z), Y(x, y, z), Z(x, y, z)) dx dy dz \\ & = \\ & |\det J| \sum_{i=1}^4 \iiint_{\Omega_i} f(X(x, y, z), Y(x, y, z), Z(x, y, z)) dx dy dz \\ & = |\det J| \sum_{i=1}^4 \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 f(X(x^i, y^i, z^i), Y(x^i, y^i, z^i), Z(x^i, y^i, z^i)) \\ & \quad \frac{\partial(x^i, y^i, z^i)}{\partial(r, s, t)} dr ds dt \quad \dots(8) \end{aligned}$$

We compute the Jacobian

$$\frac{\partial(x^i, y^i, z^i)}{\partial(r, s, t)} = \begin{pmatrix} \frac{\partial x^i}{\partial r} & \frac{\partial x^i}{\partial s} & \frac{\partial x^i}{\partial t} \\ \frac{\partial y^i}{\partial r} & \frac{\partial y^i}{\partial s} & \frac{\partial y^i}{\partial t} \\ \frac{\partial z^i}{\partial r} & \frac{\partial z^i}{\partial s} & \frac{\partial z^i}{\partial t} \end{pmatrix} = J^i(r, s, t) = J^i$$

(say)(9)

Using eqn(2), the coordinate transformations over a hexahedron Ω_i can be now rewritten as

$$\begin{aligned} X(x^i, y^i, z^i) &= X_1 w^i + X_2 x^i + X_3 y^i + X_4 z^i \\ Y(x^i, y^i, z^i) &= Y_1 w^i + Y_2 x^i + Y_3 y^i + Y_4 z^i \\ Z(x^i, y^i, z^i) &= Z_1 w^i + Z_2 x^i + Z_3 y^i + Z_4 z^i \\ w^i &= 1 - x^i - y^i - z^i \quad \dots(10) \end{aligned}$$

We may now mention that the integration over an arbitrary linear tetrahedron can be computed as a sum of four integrals over the 2-cube: $-1 \leq r, s, t \leq 1$ which is shown in Fig.3, by applying Gaussian rules.

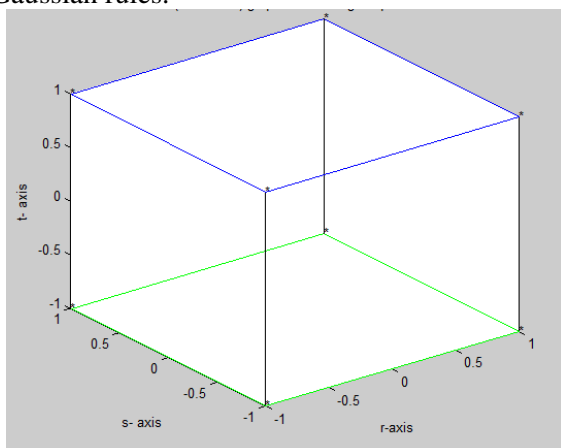


Fig.3 A 2-cube over the domain $-1 \leq r, s, t \leq 1$ in (r, s, t) space

3. DIVISION OF A TETRAHEDRON INTO THIRTY TWO HEXAHEDRONS

We divide each hexahedron into eight hexahedrons. This can be done first by

locating the centroids of the six faces of the hexahedrons and then joining the centroids to the midpoints of the respective edges. We also locate the centroid of the hexahedron and join this to the centroids of the six faces. This process can be repeated for the remaining three hexahedrons as well. This divides the tetrahedron into thirty two hexahedrons. We can then integrate over all the hexahedrons. This straight forward process is very tedious, because one has to obtain the coordinates of transformations and the respective Jacobian to apply numerical integration over the 2-cube. Instead of this we follow a more efficient method of finding the coordinates of transformations and their respective Jacobians. Using the transformations of eqn(14) and the expressions of x^i, y^i, z^i, w^i, J^i we can map the hexahedrons $\Omega_i, (i = 1, 2, 3, 4)$, into a 2-cube in (r, s, t) space. There is a one to one correspondence between 2-cube in (r, s, t) space and the hexahedron $\Omega_i, (i = 1, 2, 3, 4)$. Hence a division of 2-cube corresponds to a unique division of the hexahedra. Thus the division of hexahedra can be achieved by dividing the 2-cube. The division of a 2-cube into eight cubes of unit dimension is displayed in Fig.4

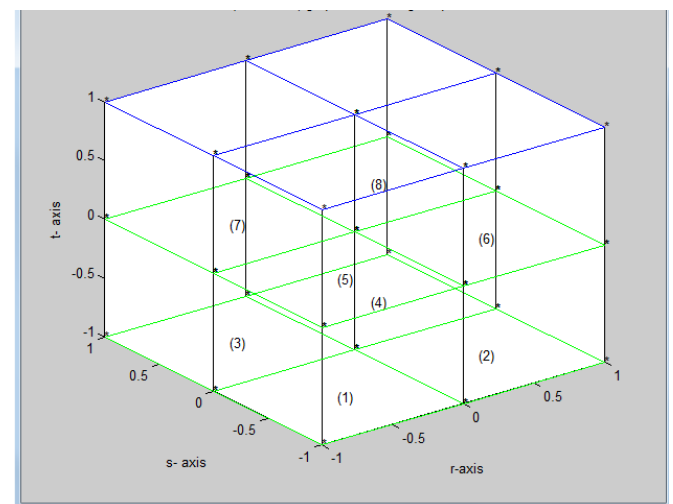


Fig.4 Division of a 2-cube into eight cubes of unit dimension

We now consider the integration over a 2-cube by dividing the 2-cube into eight unit cubes.

Let

$$F(r, s, t) =$$

$$f(X(x^i, y^i, z^i), Y(x^i, y^i, z^i), Z(x^i, y^i, z^i)) \frac{\partial(x^i, y^i, z^i)}{\partial(r, s, t)}$$

.....(11)

$$\iiint_{\Omega_i} f(X(x, y, z), Y(x, y, z), Z(x, y, z)) dx dy dz$$

$$= \iiint_{\Omega_i} f(X(x^i, y^i, z^i), Y(x^i, y^i, z^i), Z(x^i, y^i, z^i)) \frac{\partial(x^i, y^i, z^i)}{\partial(r, s, t)} dr ds dt \dots\dots\dots(12a)$$

$$= \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F(r, s, t) dr ds dt$$

$$= \sum_{j=1}^8 \iiint_{\Omega_{i,j}} f(X(x^{i,j}, y^{i,j}, z^{i,j}), Y(x^{i,j}, y^{i,j}, z^{i,j}), Z(x^{i,j}, y^{i,j}, z^{i,j})) J^{i,j}(r, s, t) dr ds dt \dots\dots\dots(12b)$$

$$= \int_{-1}^0 \int_{-1}^0 \int_{-1}^0 F(r, s, t) dr ds dt +$$

$$\int_{-1}^0 \int_{-1}^0 \int_0^1 F(r, s, t) dr ds dt +$$

$$+ \int_{-1}^0 \int_0^1 \int_{-1}^0 F(r, s, t) dr ds dt +$$

$$\int_{-1}^0 \int_0^1 \int_0^1 F(r, s, t) dr ds dt +$$

$$+ \int_0^1 \int_{-1}^0 \int_{-1}^0 F(r, s, t) dr ds dt +$$

$$\int_{-1}^0 \int_{-1}^0 \int_0^1 F(r, s, t) dr ds dt + \int_0^1 \int_0^1 \int_{-1}^0 F(r, s, t) dr ds dt$$

.....(12c)

$$= \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{-1}{2} + \frac{1}{2}r, \frac{-1}{2} + \frac{1}{2}s, \frac{-1}{2} + \frac{1}{2}t\right) dr ds dt$$

$$+ \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{1}{2} + \frac{1}{2}r, \frac{-1}{2} + \frac{1}{2}s, \frac{-1}{2} + \frac{1}{2}t\right) dr ds dt$$

$$+ \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{-1}{2} + \frac{1}{2}r, \frac{1}{2} + \frac{1}{2}s, \frac{-1}{2} + \frac{1}{2}t\right) dr ds dt$$

$$+ \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{1}{2} + \frac{1}{2}r, \frac{1}{2} + \frac{1}{2}s, \frac{-1}{2} + \frac{1}{2}t\right) dr ds dt$$

$$+ \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{-1}{2} + \frac{1}{2}r, \frac{-1}{2} + \frac{1}{2}s, \frac{1}{2} + \frac{1}{2}t\right) dr ds dt$$

$$+ \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{1}{2} + \frac{1}{2}r, \frac{-1}{2} + \frac{1}{2}s, \frac{-1}{2} + \frac{1}{2}t\right) dr ds dt$$

$$+ \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{-1}{2} + \frac{1}{2}r, \frac{1}{2} + \frac{1}{2}s, \frac{1}{2} + \frac{1}{2}t\right) dr ds dt$$

$$+ \frac{1}{8} \int_{-1}^1 \int_{-1}^1 \int_{-1}^1 F\left(\frac{1}{2} + \frac{1}{2}r, \frac{1}{2} + \frac{1}{2}s, \frac{1}{2} + \frac{1}{2}t\right) dr ds dt$$

.....(12d)

Now referring to eqn(12), we can compute the new coordinate transformations $(x^{i,j}, y^{i,j}, z^{i,j})$, and the corresponding Jacobians $J^{i,j}$ over the hexahedron $\Omega_{i,j}$ ($i=1,2,3,4; j=1,2,3,4,5,6,7,8$), which refers to j th division of the i th hexahedron Ω_i . We may now mention that the integration over an arbitrary linear tetrahedron can be now computed as a sum of thirty two integrals over the 2-cube: $-1 \leq r, s, t \leq 1$ which is shown in Fig.4. These integrals can be computed numerically by applying Gaussian rules and it will be explained later.

4. NUMERICAL INTEGRATION OVER A LINEAR POLYHEDRON

Numerical integration over a n arbitrary linear hexahedron will be very tedious and complicated if trilinear transformations are

directly used. However, the alternative is to divide the hexahedron into an assemblage of tetrahedrons and then sum the contributions to get the desired accuracy. This procedure can also be applied to the numerical integration over a linear polyhedron.

Let P denote the linear polyhedron. We can write $P = \cup_{i=1}^M T_{a^e, b^e, c^e, d^e}^e$, where T_{a^e, b^e, c^e, d^e}^e is a linear tetrahedron element 'e' with nodal addresses a^e, b^e, c^e, d^e and M is the total number of tetrahedral elements made in P.

Let us consider the volume integral over an arbitrary linear polyhedron $P = \cup_{i=1}^M T_{a^e, b^e, c^e, d^e}^e$, defined as

$$III_P(f) = \iiint_{P = \cup_{i=1}^M T_{a^e, b^e, c^e, d^e}^e} f(X, Y, Z) dX dY dZ$$

$$= \sum_{e=1}^M \iiint_{T_{a^e, b^e, c^e, d^e}^e} f(X, Y, Z) dX dY dZ \dots(13)$$

We illustrate this procedure to integrate over a unit cube. We first consider a unit cube. We first choose to divide the unit cube into six linear tetrahedra which is shown in Fig.6. We have next shown the division of a unit cube into 24 tetrahedra which can be applied to integrate a linear convex polyhedron. This is done by partitioning the unit cube first into six pyramids and then divides each of these pyramids further into four unique tetrahedra. Base of the pyramid is a square which is divide into four isoscles right triangles. Then join the corner nodal points of these triangles to the centroid of the unit cube. This division is shown in Fig.7. We may note that the procedure applied is equivalent to first triangulating the six faces of unit cube, We then select an interior point in the unit cube. By joining the three corner nodes of a triangle to this interior point creates a tetrahedron. We repeat this process for all the triangles of triangulated faces of the unit cube

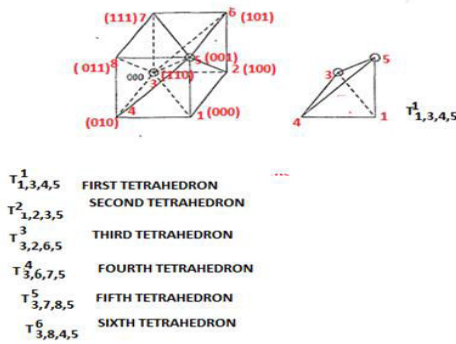


Fig.6 DIVISION OF A CUBE INTO SIX TETRAHEDRA

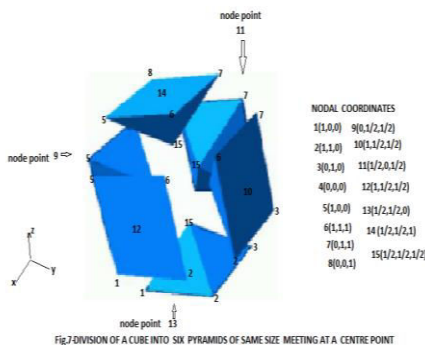


Fig.7 DIVISION OF A CUBE INTO SIX PYRAMIDS OF SAME SIZE MEETING AT A CENTRE POINT

NUMERICAL EXAMPLES

We now consider some integrals on the regions described above in Figs.6-7 The integral are:

$$III_j^i = \int \int \int_{V_i} f_j(x, y, z) dx dy dz, i=0,1; j=1,2,3,4$$

Where V_0 a unit is cube and V_1 is a irregular heptahedron; and the integrands $f_j(x, y, z), j = 1,2,3,4$ are defined as

$$f_1(x, y, z) = x^3 \sin(\pi y) \sin(\pi z)$$

$$f_2(x, y, z) = \sin(\pi x) \sin(\pi y) \sin(\pi z)$$

$$f_3(x, y, z) = e^{-((x-0.5)^2 + (y-0.5)^2 + (z-0.5)^2)}$$

$$f_4(x, y, z) =$$

$$= \frac{27}{8} \sqrt{(1 - |2x - 1|)} \sqrt{(1 - |2y - 1|)} \sqrt{(1 - |2z - 1|)}$$

The values of integrals are

$$III_1^0 = \frac{1}{\pi^2} = 0.10132118364233778397171412865964$$

$$III_2^0 = \frac{8}{\pi^3} = 0.258012275465595961328179939373$$

$$III_3^0 = 0.78521159617436901020962024602291$$

$$III_j^0 = 1$$

We have compared the computed values of the integrals ($III_j^1, j=1, 2, 3, 4$) which are in agreement. The computed numerical values of the above integrals are presented in tables.

7. CONCLUSION

In this paper, a method to discretize the physical domain in the shape of a linear polyhedron into an assemblage of all

hexahedral finite elements is discussed. Each of these hexahedra can be divided into 2^3 and $[(2^3)]^2$ hexahedra. This generates an all hexahedral finite element mesh which can be used for various applications. Numerical schemes which decompose a arbitrary linear tetrahedron into 4, $4(2^3)$ hexahedra are considered. These numerical schemes are applied to solve typical integrals over a unit cube using Gauss Legendre Quadrature Rules.

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TABLE 1

DOMAIN IS A UNIT CUBE DISCRITISED BY SIX TETRA HEDRONS (EACH TETRAHEDRON IS DECOMPOSED INTO FOUR HEXAHEDRA)
OGLR=ORDER OF GAUSS LEGENDRE RULE

OGLR	III_1^0	III_2^0	III_3^0	III_4^0
5	1.013211806444221e-001	2.580122959339014e-001	7.852115963588021e-001	1.001478584900792e+000
10	1.013211836423378e-001	2.580122754655960e-001	7.852115961743690e-001	1.000227646249210e+000
15	1.013211836423378e-001	2.580122754655954e-001	7.852115961743692e-001	1.000061678153538e+000
20	1.013211836423378e-001	2.580122754655963e-001	7.852115961743685e-001	1.000025804554168e+000
25	1.013211836423379e-001	2.580122754655957e-001	7.852115961743715e-001	1.000016478982331e+000
30	1.013211836423380e-001	2.580122754655955e-001	7.852115961743695e-001	1.000007373245699e+000
35	1.013211836423377e-001	2.580122754655954e-001	7.852115961743712e-001	1.000006273893386e+000
40	1.013211836423377e-001	2.580122754655946e-001	7.852115961743718e-001	1.000004744754559e+000

TABLE 2

DOMAIN IS A UNIT CUBE DISCRITISED BY SIX PYRAMIDS (=24 TETRAHEDRA) (EACH TETRAHEDRON IS DECOMPOSED INTO FOUR HEXAHEDRA) OGLR=ORDER OF GAUSS LEGENDRE RULE

OGLR	III_1^0	III_2^0	III_3^0	III_4^0
5	1.013211836443502e-001	2.580122754044406e-001	7.852115961737480e-001	1.002158759290186e+000
10	1.013211836423378e-001	2.580122754655962e-001	7.852115961743691e-001	1.000509125714392e+000
15	1.013211836423376e-001	2.580122754655944e-001	7.852115961743688e-001	1.000220551380930e+000
20	1.013211836423378e-001	2.580122754655957e-001	7.852115961743686e-001	1.000122286256523e+000
25	1.013211836423376e-001	2.580122754655948e-001	7.852115961743690e-001	1.000077545110675e+000
30	1.013211836423374e-001	2.580122754655982e-001	7.852115961743688e-001	1.000053507040659e+000
35	1.013211836423377e-001	2.580122754655942e-001	7.852115961743681e-001	1.000039126709146e+000
40	1.013211836423389e-001	2.580122754655933e-001	7.852115961743797e-001	1.000029848591206e+000

TABLE 3

DISCRITISED BY SIX PYRAMIDS (=24 TETRAHEDRA) (EACH TETRAHEDRON IS DECOMPOSED INTO TWO HUNDRED FIFTY SIX HEXAHEDRA) OGLR=ORDER OF GAUSS LEGENDRE RULE

OGLR	III_1^0	III_2^0	III_3^0	III_4^0
2	1.013208334385053e-001	2.580140862513543e-001	7.852119020811539e-001	1.001418294412512e+000
3	1.013211837125683e-001	2.580122744592550e-001	7.852115961249017e-001	1.000566005640103e+000
4	1.013211836423264e-001	2.580122754658746e-001	7.852115961743749e-001	1.000297938031433e+000
5	1.013211836423378e-001	2.580122754655975e-001	7.852115961743655e-001	1.000181368230410e+000
10	1.013211836423384e-001	2.580122754655989e-001	7.852115961743788e-001	1.000039539963383e+000