

## Numerical Integration over Pyramids

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**Abstract.** Pyramidal elements are often used to connect tetrahedral and hexahedral elements in the finite element method. In this paper we derive three new higher order numerical cubature formulae for pyramidal elements.

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## 1 Introduction

Let

$$K = \{(x, y, z) \in \mathbb{R}^3 \mid |x|, |y| \leq 1 - z, 0 \leq z \leq 1\}$$

be the reference pyramidal element. For a continuous function  $f$  of  $K$  we shall look for the numerical integration formulae

$$\int_K f(x, y, z) dx dy dz \approx \sum_{m=0}^n \omega_m f(A_m), \quad (1.1)$$

where weights  $\omega_m \in \mathbb{R}^1$  and at the same time positions of nodes  $A_m \in K$  are appropriately chosen so that Eq. (1.1) is exact for all polynomials of the highest possible degree.

Pyramidal elements are natural and useful for making face-to-face connections between tetrahedral and hexahedral elements in approximating the solutions of three-dimensional initial and boundary value problems by the finite element method (see

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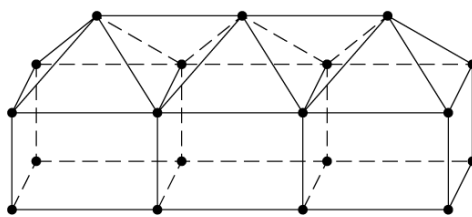


Figure 1:

Fig. 1). This often happens when one part of the solution domain is decomposed into hexahedra and the other into tetrahedra (usually near a curved boundary).

In 1997 it was independently observed in [8] and [15] that a conforming finite element method cannot be achieved with polynomial shape functions on pyramids. This surprising statement was later exactly proved in [12] Liu et al., namely, that there is no continuously differentiable function on the pyramid  $K$  that would be linear on its four triangular faces and bilinear, but not linear, on its rectangular base. Therefore, in [12] and [13] three symmetric composite finite elements with 5, 13, and 14 degrees of freedom were introduced. Their piecewise polynomial shape functions on each pyramid yield a conforming finite element space. Another way is to apply a nonconforming finite element method (see, e.g., [2]), where finite element functions are, in general, discontinuous on interior faces in a partition involving pyramidal elements. In this case we have to integrate polynomials and other smooth functions over pyramids to calculate the stiffness matrix and the corresponding right-hand side (the load vector). For instance, the famous discontinuous Galerkin method belongs to the class of nonconforming methods.

Numerical integration formulae on tetrahedra, prisms or hexahedra are very well studied in the literature (see, e.g., [5, 7, 11]). However, up to the authors's knowledge, there are only a few papers dealing with numerical integration on pyramids. For instance, nothing about this topic is mentioned in the encyclopedia [6]. Some special cubature formulae on pyramids are treated in [9, 10, 14]. In [1] a bilinear surjective vector mapping  $F$  from the unit cube to the reference pyramid  $K$  is proposed. The whole upper face of the cube is mapped onto the upper vertex of  $K$ . Numerical integration on  $K$  is then derived from the standard Gaussian formulae on the unit cube by means of the mapping  $F$ . For instance, the numerical cubature formula that is exact for all cubic polynomials has 8 nodal points inside the cube. Their images are inside of  $K$ , but the four upper integration points are somewhat unnaturally accumulated near the top vertex  $(0,0,1)$ . Moreover, the corresponding numerical cubature formula (see Eq. (4.2)) is not exact for all cubic polynomials. When solving nonlinear three-dimensional problems, numerical cubature formulae usually cannot be avoided, since the entries of the stiffness matrix and/or the right-hand side cannot be evaluated analytically.

In Sections 2 and 3, we derive new numerical cubature formulae which are exact for all quadratic and cubic polynomials and they have only 5 and 6 integration points, respectively. Our formulae are different from those presented in [1, 9, 10, 14]. Section

4 is devoted to numerical tests, concluding remarks, and another higher order cubature formula on pyramids. Our formulae have fewer integration points than the formulae of a pyramid decomposed into two tetrahedra with the same approximation order applied to each tetrahedron. For instance, our formula which is exact for all quadratic polynomials on a pyramid has 5 integration points, whereas the use of the same order formula for two tetrahedra (see, e.g., [11, p. 59]) requires evaluation at  $2 \times 4 = 8$  points.

Now we introduce quite common formulae for the exact integration of monomial functions over the reference pyramidal element  $K$ . For nonnegative integers  $i, j, k$  define

$$I_{ijk} = \int_K x^i y^j z^k dx dy dz.$$

We observe that

$$I_{ijk} = 0 \quad \text{if } i \text{ or } j \text{ is odd.} \quad (1.2)$$

So let us calculate the integral of the monomial function  $x^i y^j z^k$  when both  $i$  and  $j$  are even. In this case

$$\begin{aligned} I_{ijk} &= \int_0^1 \left( \int_{|x|, |y| \leq 1-z} x^i y^j z^k dx dy \right) dz \\ &= \frac{4}{(i+1)(j+1)} \int_0^1 (1-z)^{i+j+2} z^k dz = \frac{4(i+j+2)!k!}{(i+1)(j+1)(i+j+k+3)}, \end{aligned} \quad (1.3)$$

where the last equality was evaluated by means of the Bernoulli numbers.

To show the main idea of our approach in Sections 2-4, we first derive a very simple numerical integration formula (1.1) which will be exact for all polynomials from the five-dimensional space

$$Q^{(1)} = \text{span}\{1, x, y, z, xy\}.$$

From Eq. (1.2) we see that it is enough to examine only two polynomial basis functions from the set

$$\mathcal{P} = \{1, z\}.$$

We shall choose only one integration point  $A_0 = (0, 0, z_0)$  and solve the following equation with two unknowns  $\omega_0 > 0$  and  $z_0 \in [0, 1]$ ,

$$\int_K p(x, y, z) dx dy dz = \omega_0 p(A_0), \quad p \in \mathcal{P}.$$

From this and Eq. (1.3) we get the system

$$\omega_0 = I_{0,0,0} = \frac{4}{3}, \quad \omega_0 z_0 = I_{0,0,1} = \frac{1}{3}, \quad (1.4)$$

yielding  $z_0 = \frac{1}{4}$ . Therefore, the resulting one-point numerical integration formula is

$$\int_K p(x, y, z) dx dy dz = \frac{4}{3} p(A_0), \quad \forall p \in Q^{(1)},$$

where  $A_0 = (0, 0, \frac{1}{4})$  is at the centre of gravity of  $K$ .

## 2 Second order five-point numerical integration formula

Now we shall find numerical integration points and the corresponding weights so that Eq. (1.1) is exact for all polynomials from the space

$$Q^{(2)} = \text{span}\{1, x, y, z, x^2, y^2, z^2, xy, xz, yz, xyz, x^2y, xy^2, x^2y^2\}.$$

Note that the dimension of  $Q^{(2)}$  is the pyramidal number  $14=1+4+9$  which is the sum of square numbers. In practice, shape functions of several kinds of often used pyramidal finite elements are contained in this space. From Eq. (1.2) we observe that it is enough to examine only the following 6 basis functions

$$\mathcal{P} = \{1, z, x^2, y^2, z^2, x^2y^2\}.$$

As the pyramid  $K$  is symmetric with respect to the planes  $y=\pm x$ , we shall consider the following five integration points  $A_0=(0,0,z_0)\in K$  and  $A_m=(\pm a, \pm a, z_1)\in K$  for  $m=1,2,3,4$  with  $a>0$  and the formula

$$\int_K p(x,y,z) dx dy dz = \omega_0 p(A_0) + \omega_1 \sum_{m=1}^4 p(A_m), \quad p \in \mathcal{P}. \quad (2.1)$$

Substituting all  $p \in \mathcal{P}$  into Eq. (2.1) we get from Eq. (1.3) altogether six equations. Since two of them (corresponding to  $x^2$  and  $y^2$ ) are the same, we obtain the following nonlinear system of five algebraic equations for 5 unknowns

$$\begin{aligned} \omega_0 + 4\omega_1 &= I_{0,0,0} = \frac{4}{3}, & \omega_0 z_0 + 4\omega_1 z_1 &= I_{0,0,1} = \frac{1}{3}, & 4\omega_1 a^2 &= I_{2,0,0} = \frac{4}{15}, \\ \omega_0 z_0^2 + 4\omega_1 z_1^2 &= I_{0,0,2} = \frac{2}{15}, & 4\omega_1 a^4 &= I_{2,2,0} = \frac{4}{63}. \end{aligned}$$

From the third and fifth equation above we find that

$$a^2 = \frac{15}{63}, \quad a = \sqrt{\frac{5}{21}}, \quad \omega_1 = \frac{7}{25},$$

and from the first equation

$$\omega_0 = \frac{4}{3} - 4 \cdot \frac{7}{25} = \frac{16}{75}.$$

From this, the second and fourth equation we obtain the following system

$$16z_0 + 84z_1 = 25, \quad 16z_0^2 + 84z_1^2 = 10,$$

whose solution is  $z_0 = (25 - 84z_1)/16$ , where

$$z_1 = \frac{35 \pm 2\sqrt{35}}{140}.$$

In fact, we have got exactly two distinct solutions for  $z_1$ , but the larger one yields a negative value of  $z_0$ , so this case will be excluded. Thus, we get the following theorem about the resulting five-point numerical integration formula.

**Theorem 2.1.** *Let  $K$  be the reference pyramid. Then*

$$\int_K p(x,y,z) dx dy dz = \frac{16}{75} p(A_0) + \frac{7}{25} \sum_{m=1}^4 p(A_m), \quad \forall p \in Q^{(2)}, \quad (2.2)$$

where  $A_0 = (0,0,z_0)$ ,  $A_m = (\pm\sqrt{5/21}, \pm\sqrt{5/21}, z_1)$ ,

$$z_0 = \frac{70+21\sqrt{35}}{280} = 0.693705983732\dots \quad \text{and} \quad z_1 = \frac{35-2\sqrt{35}}{140} = 0.165484574527\dots \quad (2.3)$$

We see that  $A_m \in K$  for  $m=1, \dots, 4$ , since  $a < 1 - z_1$ . Moreover, note that Eq. (2.2) is exact particularly for all quadratic polynomials.

### 3 Third order six-point numerical integration formula

Finally, we propose numerical integration points and the corresponding weights so that Eq. (1.1) is exact for all cubic polynomials from the space  $P_3$ . This space is suitable for the use of the famous Bramble-Hilbert Lemma (cf. [4]). Let us point out that the dimension of  $P_3$  is the tetrahedral number  $20 = 1 + 3 + 6 + 10$  which is the sum of triangular numbers. In practice, shape functions of several kinds of often used pyramidal finite elements are contained in this space. According to Eq. (1.2), it is enough to examine only the following 8 basis functions

$$\mathcal{P} = \{1, z, x^2, y^2, z^2, x^2z, y^2z, z^3\}.$$

The pyramidal element  $K$  does not possess so many symmetries like the regular tetrahedron or cube. Therefore, our choice of integration points will be a bit artificial to avoid an overdetermined or underdetermined nonlinear system of algebraic equations. We shall consider similarly as in the previous sections the following integration points  $A_0 = (0,0,z_0) \in K$ ,  $A_m = (\pm a, \pm a, z_1) \in K$  for  $m=1,2,3,4$  with  $a > 0$ , and the center of gravity  $A_5 = G = (0,0,1/4)$  of  $K$ . We shall look for appropriate weights  $\omega_0, \omega_1, \omega_2$  and coordinates  $a, z_0, z_1$  so that

$$\int_K p(x,y,z) dx dy dz = \omega_0 p(A_0) + \omega_1 \sum_{m=1}^4 p(A_m) + \omega_2 p(G), \quad p \in P_3. \quad (3.1)$$

Substituting all  $p \in \mathcal{P}$  into Eq. (3.1) we get from Eq. (1.3) altogether eight equations. Since two equations corresponding to  $x^2$  and  $y^2$  and another two equations corresponding to  $x^2z$  and  $y^2z$  are the same, we obtain the following nonlinear system of six algebraic equations for 6 unknowns

$$\begin{aligned} \omega_0 + 4\omega_1 + \omega_2 &= I_{0,0,0} = \frac{4}{3}, & \omega_0 z_0 + 4\omega_1 z_1 + \frac{1}{4}\omega_2 &= I_{0,0,1} = \frac{1}{3}, \\ 4\omega_1 a^2 &= I_{2,0,0} = \frac{4}{15}, & \omega_0 z_0^2 + 4\omega_1 z_1^2 + \frac{1}{16}\omega_2 &= I_{0,0,2} = \frac{2}{15}, \\ 4\omega_1 a^2 z_1 &= I_{2,0,1} = \frac{2}{45}, & \omega_0 z_0^3 + 4\omega_1 z_1^3 + \frac{1}{64}\omega_2 &= I_{0,0,3} = \frac{1}{15}. \end{aligned}$$

From the third and the fifth equation above, we find that

$$z_1 = \frac{1}{6}. \tag{3.2}$$

Hence, our system reduces to

$$\omega_0 + 4\omega_1 + \omega_2 = \frac{4}{3}, \quad \omega_0 z_0 + \frac{2}{3}\omega_1 + \frac{1}{4}\omega_2 = \frac{1}{3}, \quad 4\omega_1 a^2 = \frac{4}{15}, \tag{3.3a}$$

$$\omega_0 z_0^2 + \frac{1}{9}\omega_1 + \frac{1}{16}\omega_2 = \frac{2}{15}, \quad \omega_0 z_0^3 + \frac{1}{54}\omega_1 + \frac{1}{64}\omega_2 = \frac{1}{15}. \tag{3.3b}$$

Substituting  $\omega_2$  from the first equation into the second, fourth, and fifth equation, we get the following nonlinear system of three equations

$$3\omega_0 z_0 - \frac{3}{4}\omega_0 - \omega_1 = 0, \tag{3.4a}$$

$$\omega_0 z_0^2 - \frac{1}{16}\omega_0 - \frac{5}{36}\omega_1 = \frac{1}{20}, \tag{3.4b}$$

$$\omega_0 z_0^3 - \frac{1}{64}\omega_0 - \frac{19}{432}\omega_1 = \frac{11}{240}. \tag{3.4c}$$

Now we substitute  $\omega_1$  from the first equation into the second and third one to obtain

$$\omega_0 \left( z_0^2 - \frac{5}{12}z_0 + \frac{1}{24} \right) = \frac{1}{20}, \quad \omega_0 \left( z_0^3 - \frac{19}{144}z_0 + \frac{5}{288} \right) = \frac{11}{240}. \tag{3.5}$$

From this we get the cubic equation for  $z_0$

$$20 \left( z_0^2 - \frac{5}{12}z_0 + \frac{1}{24} \right) = \frac{240}{11} \left( z_0^3 - \frac{19}{144}z_0 + \frac{5}{288} \right),$$

which can be rewritten as

$$z_0^3 - \frac{11}{12}z_0^2 + \frac{1}{4}z_0 - \frac{1}{48} = \left( z_0 - \frac{1}{6} \right) \left( z_0 - \frac{1}{4} \right) \left( z_0 - \frac{1}{2} \right) = 0,$$

i.e., all its roots are rational numbers.

By Eq. (3.5) the choice  $z_0 = 1/6$  or  $z_0 = 1/4$  yields an infinite value of  $\omega_0$ . The last value  $z_0 = 1/2$  gives by Eq. (3.2)-Eq. (3.5) that  $\omega_0 = 3/5$ ,  $\omega_1 = 9/20$ ,  $\omega_2 = -16/15$ , and  $a = \sqrt{4/27}$ . Thus, we get the following theorem about the resulting six-point numerical integration formula which is exact for all cubic polynomials.

**Theorem 3.1.** *Let  $K$  be the reference pyramid. Then*

$$\int_K p(x,y,z) dx dy dz = \frac{3}{5}p(A_0) + \frac{9}{20} \sum_{m=1}^4 p(A_m) - \frac{16}{15}p(G), \quad \forall p \in P_3, \tag{3.6}$$

where  $A_0 = (0,0,\frac{1}{2})$ ,  $A_m = (\pm\sqrt{4/27}, \pm\sqrt{4/27}, \frac{1}{6})$  and  $G = (0,0,\frac{1}{4})$ .

We again see that  $A_m \in K$  for  $m = 1, \dots, 4$ , as  $a < 1 - z_1 = \frac{5}{6}$ .

A certain drawback is the negative value of  $\omega_2 = -\frac{16}{15}$  which may cause that the six-point formula is sensitive to rounding errors in very large scale computations. On the other hand,  $z$ -coordinates of all nodes are rational numbers, whereas in formula (2.2) all  $z$ -coordinates are irrational numbers, see Eq. (2.3).

**Remark 3.1.** Numerical integration formulae on an arbitrary pyramidal element  $K'$  can be derived from Eqs. (1.4), (2.2) and (3.6) by means of an invertible affine mapping from the reference pyramid  $K$  to  $K'$ .

**Remark 3.2.** To derive a numerical integration formula which would be exact for all polynomial of the fourth degree, we should consider the set

$$\mathcal{P} = \{1, z, x^2, y^2, z^2, x^2z, y^2z, z^3, x^4, y^4, z^4, x^2y^2, x^2z^2, y^2z^2\}$$

yielding a nonlinear system of 10 equations. For the time being, it is an open problem how to choose an appropriate position of integration points in this case.

### 4 Numerical examples and concluding remarks

Numerical example. Let  $\Omega = [0,1] \times [0,1] \times [0,1]$  be partitioned into  $N \times N \times N$  small subcubes and let  $h = 1/N$ . We decompose each subcube into six pyramidal elements containing a common vertex in the centre of each subcube (see Fig. 2). In this way we get the partition  $\mathcal{T}_h$  of  $\Omega$  into pyramids.



Figure 2:

For

$$f(x,y,z) = x^3 \sin(\pi y) \sin(\pi z) \quad \text{on } \Omega,$$

define

$$E(h) = \int_{\Omega} f(x,y,z) dx dy dz - \sum_{K' \in \mathcal{T}_h} \sum_{m=0}^n \omega_m f(A_m^{K'}),$$

where  $\int_{\Omega} f(x,y,z) dx dy dz = \pi^{-2}$ . By the Bramble-Hilbert Lemma (see [4,11]) we can establish that the error is of order  $E(h) = \mathcal{O}(h^{d+1})$ , where  $d$  is the maximal polynomial degree for which the used numerical integration formula is exact.

Table 1:

| $h^{-1}$ | (1.4)     | Ratio | (2.2)     | Ratio  | (3.6)     | Ratio  | (4.1)     | Ratio  |
|----------|-----------|-------|-----------|--------|-----------|--------|-----------|--------|
| 4        | -9.472e-4 | None  | 4.595e-6  | None   | 8.393e-7  | None   | 5.238e-6  | None   |
| 8        | -2.266e-4 | 4.180 | 2.765e-7  | 16.621 | 2.331e-8  | 36.002 | 3.213e-7  | 16.303 |
| 16       | -5.604e-5 | 4.044 | 1.712e-8  | 16.153 | 1.019e-9  | 22.881 | 1.999e-8  | 16.075 |
| 32       | -1.397e-5 | 4.011 | 1.067e-9  | 16.038 | 5.690e-11 | 17.907 | 1.128e-9  | 16.019 |
| 64       | -3.491e-6 | 4.002 | 6.666e-11 | 16.009 | 3.450e-12 | 16.490 | 7.796e-11 | 16.005 |
| 128      | -8.725e-7 | 4.001 | 4.166e-12 | 16.002 | 2.140e-13 | 16.125 | 4.872e-12 | 16.001 |

From Table 1, we observe that the practical rate of convergence of the proposed Eqs. (1.4), (2.2), and (3.6) seems to be  $\mathcal{O}(h^2)$ ,  $\mathcal{O}(h^4)$ , and  $\mathcal{O}(h^4)$ .

Why is the practical rate of convergence  $\mathcal{O}(h^4)$  of formula (2.2) one order higher than its theoretical rate  $\mathcal{O}(h^3)$ ? This remarkable superconvergence phenomenon can be explained as follows. The formula (2.2) integrates exactly not only all polynomials up to the second degree, but also all cubic monomials  $x^i y^j z^k$  when  $i$  or  $j$  is odd, i.e.,  $x^3$ ,  $x^2 y$ ,  $x y^2$ ,  $y^3$ ,  $x y z$ ,  $x z^2$ ,  $y z^2$ . However, it integrates unexpectedly well also the cubic monomials  $x^2 z$  and  $y^2 z$  that do not belong to  $Q^{(2)}$ . Namely, for  $\omega_1 = \frac{7}{25}$ ,  $a^2 = \frac{5}{21}$ , and  $z_1$  given in Eq. (2.3) we have

$$4\omega_1 a^2 z_1 = 0.04411 \dots,$$

which is surprisingly very close to the value  $I_{2,0,1} = \frac{2}{45} = 0.04444 \dots$  with the relative error less than 1%. For the remaining cubic monomial  $z^3$ , we have by Eq. (2.3)

$$\omega_0 z_0^3 + 4\omega_1 z_1^3 = 0.07629 \dots \approx I_{0,0,3} = \frac{1}{15} = 0.06666 \dots.$$

The difference between these two constants is again relatively small. Moreover, formula (2.2) integrates exactly also the fourth order term  $x^2 y^2$ . A further reason may be the symmetry of the domain, of the partition, and of the function  $f$ , which may lead to cancellations of some numerical integration errors.

A further reason may be the symmetry of the partition, which leads to cancellations of some numerical integration errors. In particular, we found that the monomials  $x^2 z$ ,  $y^2 z$ , and  $z^3$  are integrated exactly by Eq. (2.2) over the partition of Fig. 2. Note that formula (2.2) does not have this superconvergence property on a single pyramidal element.

**Remark 4.1.** It seems from the numerical results of Eq. (3.6) in Table 1 that the error practically behaves like  $E(h) \approx c_1 h^4 + c_2 h^6$  with  $c_1 \ll c_2$ , since the ratio  $E(2h)/E(h)$  is relatively large for  $h = 1/8$  and  $h = 1/16$ .

**Remark 4.2.** The space  $Q^{(2)}$  from Section 2 can be expressed as follows

$$Q^{(2)} = \text{span}\{Q^{(1)}, x^2, x^2 y, x^2 y^2, x y^2, y^2, x z, y z, x y z, z^2\},$$



where  $Q^{(1)} = \text{span}\{Q^{(0)}, x, xy, y, z\}$  with  $Q^{(0)} = \text{span}\{1\}$ . Similarly, we can define the space

$$Q^{(3)} = \text{span}\{Q^{(2)}, x^3, x^3y, x^3y^2, x^3y^3, x^2y^3, xy^3, y^3, x^2z, x^2yz, x^2y^2z, xy^2z, y^2z, xz^2, yz^2, xyz^2, z^3\},$$

which is more natural for the pyramidal element  $K$  than the space  $P_3$ . Note that the dimension of  $Q^{(3)}$  is again equal to the pyramidal number  $30 = 1 + 4 + 9 + 16$ .

Let  $A_0 = (0, 0, z_0)$  with  $z_0 \in [0, 1]$ ,  $A_m = (\pm a, \pm a, z_1) \in K$  for  $m = 1, 2, 3, 4$  with  $a > 0$  and  $z_1 > 0$ , and let  $A_m = (\pm b, \pm b, z_2) \in K$  for  $m = 5, 6, 7, 8$  with  $b > 0$  and  $z_2 > 0$ . Now consider a nine-point integration formula so that

$$\int_K p(x, y, z) dx dy dz = \omega_0 p(A_0) + \omega_1 \sum_{m=1}^4 p(A_m) + \omega_2 \sum_{m=5}^8 p(A_m), \quad \forall p \in Q^{(3)}. \quad (4.1)$$

In this case the corresponding set

$$\mathcal{P} = \{1, z, x^2, y^2, z^2, x^2z, y^2z, z^3, x^2y^2, x^2y^2z\}$$

contains 10 functions. However, the monomials  $x^2$  and  $y^2$  and also  $x^2z$  and  $y^2z$  produce the same equations. So altogether we get a nonlinear system of 8 equations for 8 unknowns  $a, b, z_0, z_1, z_2, \omega_0, \omega_1, \omega_2$ :

$$\begin{aligned} \omega_0 + 4\omega_1 + 4\omega_2 &= I_{0,0,0} = \frac{4}{3}, & \omega_0 z_0 + 4\omega_1 z_1 + 4\omega_2 z_2 &= I_{0,0,1} = \frac{1}{3}, \\ 4\omega_1 a^2 + 4\omega_2 b^2 &= I_{2,0,0} = \frac{4}{15}, & \omega_0 z_0^2 + 4\omega_1 z_1^2 + 4\omega_2 z_2^2 &= I_{0,0,2} = \frac{2}{15}, \\ 4\omega_1 a^2 z_1 + 4\omega_2 b^2 z_2 &= I_{2,0,1} = \frac{2}{45}, & \omega_0 z_0^3 + 4\omega_1 z_1^3 + 4\omega_2 z_2^3 &= I_{0,0,3} = \frac{1}{15}, \\ 4\omega_1 a^4 + 4\omega_2 b^4 &= I_{2,2,0} = \frac{4}{63}, & 4\omega_1 a^4 z_1 + 4\omega_2 b^4 z_2 &= I_{2,2,1} = \frac{1}{126}. \end{aligned}$$

Using substitutions  $r = a^2$ ,  $s = b^2$ , and  $t = \omega_0/4$ , this nonlinear system can be simplified. However, we were not able to solve it analytically like in Sections 1-3.

By means of a fixed-point based Homotopy Algorithm (see [3, p. 332]) we have got the solution with accuracy  $10^{-17}$  (see Table 2).

Table 2:

| $j$ | $\pm x_j, \pm y_j$       | $z_j$                 | $\omega_j$            |
|-----|--------------------------|-----------------------|-----------------------|
| 0   | 0                        | 0.8602 7273 0595 7032 | 0.0381 9738 9067 2464 |
| 1   | $a = 0.3358853513951881$ | 0.4208 8174 7524 4836 | 0.1403 5406 0818 8171 |
| 2   | $b = 0.5264217043960195$ | 0.0874 7660 9247 1387 | 0.1834 2992 5247 7046 |

Notice that all weights are positive and the points  $A_m$  are inside  $K$ . Since  $P_3 \subset Q^{(3)}$ , the theoretical convergence rate of formula (4.1) is  $\mathcal{O}(h^4)$  which perfectly fits with the numerical tests given in Table 1. We could, of course, consider another choice of integration

points, e.g.,  $A_5 = (c, 0, z_2)$ ,  $A_6 = (-c, 0, z_2)$ ,  $A_7 = (0, c, z_2)$  and  $A_8 = (0, -c, z_2)$ . But this will require a further research.

### Comparison of (2.2) with other cubature formulae

Consider the Gaussian integration points  $G_m = (\pm\sqrt{3}/3, \pm\sqrt{3}/3, \pm\sqrt{3}/3)$ ,  $m=0, \dots, 7$ , inside the cube  $C = [-1, 1]^3$ . It is known that the corresponding numerical cubature formula on  $C$  is exact for all cubic polynomials (cf. [11, p. 59]). However, this positive property will be negated by the surjective mapping  $F: C \rightarrow K$  (proposed in [1]),

$$F(x, y, z) = \left( \frac{x}{2}(1-z), \frac{y}{2}(1-z), \frac{1}{2}(1+z) \right),$$

which maps the whole upper face of  $C$  onto the upper vertex of the reference pyramid  $K$ . The associated numerical cubature formula on  $K$  is given by

$$\int_K f(x, y, z) dx dy dz \approx \omega_0 \sum_{m=0}^3 f(A_m) + \omega_1 \sum_{m=4}^7 f(A_m), \quad (4.2)$$

where  $A_m = F(G_m)$ , for  $m=0, \dots, 7$ , the  $z$ -coordinate of  $A_0, A_1, A_2, A_3$  and  $A_4, A_5, A_6, A_7$  is equal to  $z_0 = 1/2 - \sqrt{3}/6$  and  $z_1 = 1/2 + \sqrt{3}/6$ , respectively. Solving the system

$$4\omega_0 + 4\omega_1 = \frac{4}{3}, \quad 4\omega_0 z_0 + 4\omega_1 z_1 = \frac{1}{3},$$

we find that  $\omega_0 = (2 + \sqrt{3})/12$  and  $\omega_1 = (2 - \sqrt{3})/12$  are such that Eq. (4.2) is exact for all linear polynomials (but not quadratic).

In Table 3 we observe a quadratic rate of convergence of Eq. (4.2) for

$$f(x, y, z) = e^x y^2 z \quad \text{on } \Omega = [0, 1]^3 \quad (4.3)$$

and the same families of decompositions as in the previous examples (see Fig. 2).

The exact value of the integral of  $f$  over  $\Omega$  is  $(e-1)/6$ .

Table 3:

| $h^{-1}$ | (4.2)    | Ratio | (4.4)      | Ratio  | (2.2)     | Ratio  |
|----------|----------|-------|------------|--------|-----------|--------|
| 4        | 1.354e-3 | None  | -4.701e-7  | None   | 3.434e-7  | None   |
| 8        | 3.390e-4 | 3.996 | -2.953e-8  | 15.919 | 2.145e-8  | 16.013 |
| 16       | 8.477e-5 | 3.999 | -1.848e-9  | 15.980 | 1.340e-9  | 16.003 |
| 32       | 2.119e-5 | 4.000 | -1.155e-10 | 15.995 | 8.376e-11 | 16.001 |
| 64       | 5.299e-6 | 4.000 | -7.221e-12 | 15.999 | 5.235e-12 | 16.000 |
| 128      | 1.325e-6 | 4.000 | -4.513e-13 | 15.999 | 3.272e-13 | 16.000 |

Each pyramid can be bisected into two tetrahedra (even though it represents a certain asymmetry of the resulting tetrahedralization). Let  $T$  be an arbitrary tetrahedron with vertices  $V_0, V_1, V_2, V_3$ . Set

$$A_m = \alpha V_m + \beta \sum_{k \neq m} V_k$$

for every  $m=0,1,2,3$ , where

$$\alpha = (5+3\sqrt{5})/20, \quad \beta = (5-\sqrt{5})/20.$$

According to [11, p. 59], the following cubature formula

$$\int_T f(x,y,z) dx dy dz \approx \frac{1}{4} \text{meas} T \sum_{m=0}^3 f(A_m) \quad (4.4)$$

is exact for all  $f \in P_2(K)$ . However, numerical results corresponding to Eq. (4.3) in Table 3 indicate that the rate of convergence seems to be  $\mathcal{O}(h^4)$  as for formula (2.2). The reason for this high convergence rate is again a special structure of the partition of Fig. 2 which leads to cancellations of some errors. Note that formula (2.2) requires only 5 function evaluations on each pyramid, whereas Eq. (4.4) requires 8 evaluations.

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