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ORIGINAL RESEARCH **Open Access**

Numerical Integration on Higher Dimensional Simplicial and Curved Finite Elements

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Abstract

We present a formula which evaluates lower degree monomials over higher dimensional simplices by means of integration of higher degree monomials over an interval, triangle or tetrahedron. Further, we show how to apply some higher order quadrature formulae on curved elements using a one-to-one mapping from the reference simplicial element to a curved element. Finally, we demonstrate that the non-zero Jacobian does not imply that this mapping is one-to-one.

Key words: numerical integration, higher dimensional finite elements, curved elements, isoparamentric elements, simplicial elements, Jacobian matrix

AMS classification: 65D30, 65D32, 65N30

1 Introduction

Numerical integration plays a very important role in practical calculations of differential and integral equations by the finite element method. In particular, when solving nonlinear problems described by partial differential equations or problems defined on domains with a curved boundary we cannot avoid a usage of certain quadrature rule, in general. The stiffness matrix, mass matrix, and the associated load vector can be computed analytically only in a few “academic" examples. That is why the question of reliability of numerical integration is very important.

Throughout the paper, we will use the standard Sobolev space notation (see e.g. [3]). Consider the following quadrature formula

$$\int_K v(x)\,\mathrm{d}x \approx \sum_{q=1}^{Q} c_q v(A_q), \tag{1}$$

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where $K \subset \mathbf{R}^d$ is a d-dimensional simplicial element, $d \in \{1,2,3,\dots\}$, $c_q \in \mathbf{R}^1$ are called coefficients (or weights), and $A_q \in K$ nodal points (or just nodes). If (1) is exact for all polynomials $p \in P_k(K)$ of degree k then under some additional assumptions (see [3, 11, 17]) the following error estimate holds

$$\left| \int_K v\,\mathrm{d}x - \sum_{q=1}^{Q} c_q v\left(A_q\right) \right| \le C h_K^{k+1} |v|_{k+1,1,K} \quad \forall v \in W_1^{k+1}(K), \tag{2}$$

where $h_K = \operatorname{diam} K$.

The application of the numerical integration formula (1) causes the so-called variational crimes which are extensively studied in the two-dimensional case, e.g., in [3, 8, 16]. For the three-dimensional case, see [1, 10, 15].

Calculation of entries of an element stiffness or mass matrix (or an element load vector) is usually transformed on the so-called reference element $\hat{K}$ (compare with (16) below). If a physical element K is straight then the transformation to the reference element $\hat{K}$ is linear affine, otherwise we have to consider a nonlinear transformation between $\hat{K}$ and K. That is why in Section 2 we will deal with nonlinear transformations defined on the reference element. This is done only in one space dimension, since first we want to introduce the basic tools described later in this paper for two or more dimensional cases.

In Section 3, we give a brief survey of several efficient higher order numerical quadrature formulae on simplices. Their nodes are always contained in the interior of the considered element. Those formulae which have at least one node on the boundary (see [3]) or even outside the element are not presented, since they usually have a lower approximation order. For instance, the seven-point integration formula on triangles from [3, p. 184] has the approximation order $\mathscr{O}(h^4)$, whereas another seven-point formula presented in this paper (see (7)) is of order $\mathscr{O}(h^6)$. Moreover, the use of numerical integration formulae with nodes on the element boundary (or outside element) brings various programming difficulties. In particular, if some material coefficient has a jump between two elements then a special care has to be taken to evaluate this “jumping" coefficient at boundary nodes.

Section 4 is devoted to isoparametric quadratic triangular elements with one curved side represented by a parabola. If only one side is curved, then the quadratic

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transformation from the reference triangle to an arbitrary triangle becomes bilinear. In this case the Jacobian is a linear function (cf. Theorem 4.1). We investigate what will happen if the Jacobian of the transformation between the reference and curved element vanishes somewhere inside the reference element. This sometimes appears when using commercial software.

Finally, in Section 5, we examine the effect of numerical integration on more general curved elements.

2 A one-dimensional case

To explain the main idea of our approach we first examine a model one-dimensional problem.
Let $\hat{K} = [0,1]$ be the reference element and let a physical element K be equal, for simplicity, to $\hat{K}$. Consider the following family of one-to-one twice continuously differentiable mappings $F : \hat{K} \to K$,

$$\mathscr{F} = \{F \in C^2(\hat{K}) \quad | \quad F(0) = 0, F(1) = 1, F^{-1} \text{ exists}\},$$

i.e., $\mathscr{F}$ contains nondecreasing functions.

Theorem 2.1 It is

$$\inf_{F \in \mathscr{F}} \sup_{v \in H^2(K),\ |v|_{1,K}^2 + |v|_{2,K}^2 = 1} |v - (v(1) - v(0))F^{-1}|_{1,K} = \frac{1}{2}. \tag{3}$$

Proof: Let $F \in \mathscr{F}$ be arbitrary. Any linear shape function

$$\hat{p}(\hat{x}) = a + b\hat{x}, \quad \hat{x} \in \hat{K},$$

is mapped by F on a pull-back polynomial function

$$p(x) = a + bF^{-1}(x), \quad x \in K, \tag{4}$$

since $\hat{p}(\hat{x}) = p(x)$ for $x = F(\hat{x})$.

Let $v \in H^2(K)$ be arbitrary. Since $F \in C^2(\hat{K})$, the corresponding function $\hat{v}$, given by

$$\hat{v}(\hat{x}) = v(x) \qquad (x = F(\hat{x})),$$

is from $H^2(\hat{K})$ due to [19, p. 75]. Denote by $\hat{\Pi}\hat{v}$ the linear interpolation of $\hat{v}$, i.e., $\hat{\Pi}\hat{v} \in P_1(\hat{K})$, $(\hat{\Pi}\hat{v})(0) = \hat{v}(0)$ and $(\hat{\Pi}\hat{v})(1) = \hat{v}(1)$. These values are well defined due to the Sobolev imbedding $H^2(\hat{K}) \subset C(\hat{K})$, see [3]. According to (4), the error function $\hat{x} \mapsto \hat{v}(\hat{x}) - (\hat{\Pi}\hat{v})(\hat{x}) = \hat{v}(\hat{x}) - (\hat{v}(1) - \hat{v}(0))\hat{x} - \hat{v}(0)$ is mapped by F on the function $x \mapsto v(x) - (v(1) - v(0))F^{-1}(x) - v(0)$ (compare with (3)). It is possible to show that the infimum in (3) is attained when F is the identical mapping I, i.e., $Ix = x$. Using the standard interpolation property (see [20]), we get

$$\sup_{v \in H^2(K)} |v - (v(1) - v(0))I|_{1,K} = \frac{1}{2}|v|_{2,K},$$

which yields (3).

3 Efficient quadrature formulae on d-simplices

In this section we briefly introduce several useful numerical integration formulae which have all nodes in the interior of an element K. The choice of such formulae is advisable especially when the integrated function v has a jump on the common side (face) of two adjacent elements, i.e., we need not evaluate v on the boundary of K. This situation occurs, e.g., in problems with composite materials.

For a rough approximation in $\mathbf{R}^d$, $d = 1, 2, 3$, we can always apply the well-known centroid rule

$$\int_K v(x)\,\mathrm{d}x \approx \mathrm{meas}_d K \cdot v(G)\ , \tag{5}$$

where G is the center of gravity of the element K. It is easy to see that (5) is exact for all $v \in P_1(K)$, if K is a d-simplex.

Further we introduce some higher order quadrature formulae in two- and three-dimensional space.

Example 3.1 The numerical integration formula (see [22])

$$\int_K v(x)\,\mathrm{d}x \approx \mathrm{meas}_2 K(c_1(v(A) + v(B) + v(C)) + c_2 v(G)) \tag{6}$$

is exact for all $v \in P_3(K)$ (and thus by (2) of the order $\mathcal{O}(h_K^4)$) if we choose the triangular coordinates of the nodes as follows

$$A = (a,b,b),\ B = (b,a,b),\ C = (b,b,a),\ G = (1/3,1/3,1/3),$$

and coefficients

$$c_1 = 25/48,\ c_2 = -9/16,$$

where $a = \frac{3}{5}$ and $b = \frac{1}{5}$. (Note that the values of a and b are incorrectly cited in [22].)

The negative coefficient c_2 has almost no influence on round-off errors, since the sum $3|c_1| + |c_2|$ of absolute values of all four coefficients is approximately 2.

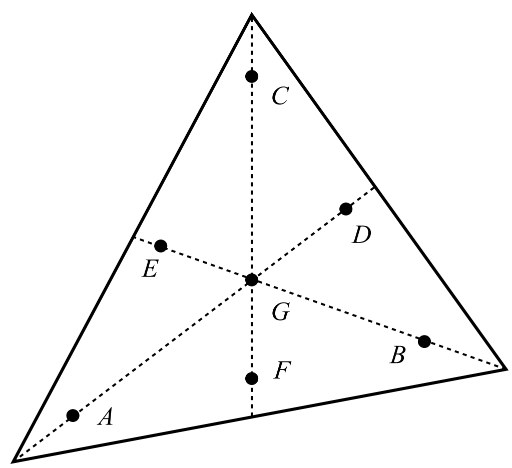

Figure 1: Integration points of quadrature formula (7).

Example 3.2 The following formula (see [17, p. 58])

$$\int_K v(x)\,\mathrm{d}x \approx \mathrm{meas}_2 K(c_1(v(A)+v(B)+v(C)) + c_2(v(D)+v(E)+v(F)) + c_3 v(G)) \quad (7)$$

is of the order $\mathcal{O}(h_K^6)$ if we choose seven the integration points $A,\ B,\ldots,G$ lying on medians as shown in Figure 1:

$$A = (a_1,b_1,b_1),\ B = (b_1,a_1,b_1),\ C = (b_1,b_1,a_1),$$

$$D = (a_2,b_2,b_2),\ E = (b_2,a_2,b_2),\ F = (b_2,b_2,a_2),\ G = (1/3,1/3,1/3),$$

and coefficients

$$c_1 = (155-\sqrt{15})/1200,\ c_2 = (155+\sqrt{15})/1200,\ c_3 = 9/40,$$

where

$$a_1 = (9+2\sqrt{15})/21\ ,\ a_2 = (9-2\sqrt{15})/21\ ,$$

$$b_1 = (6-\sqrt{15})/21\ ,\ b_2 = (6+\sqrt{15})/21\ .$$

These irrational numbers are in [22] rounded to rational numbers with several significant digits only.

The formula (7) is exact for all quintic polynomials $v \in P_5(K)$. This means that the first $1+2+\cdots+6=21$ terms! in the Taylor expansion of an integrated function are computed exactly. In this case the error of numerical integration is often smaller than round-off errors in double precision. Integration formulae on a triangle up to order of accuracy 8 are surveyed in [18].

Example 3.3 Let K be an arbitrary tetrahedron with vertices A_1, A_2, A_3, A_4 (see Figure 2). Set

$$B_q = aA_q + b\sum_{r\neq q} A_r \tag{8}$$

for every $q = 1,2,3,4$, where

$$a = (5+3\sqrt{5})/20\ ,\ b = (5-\sqrt{5})/20\ .$$

Note that the tetrahedral (barycentric) coordinates of the points $B_1,\ldots,B_4$ are $(a,b,b,b),\ldots,(b,b,b,a)$, respectively. Each node B_q lies on the spatial median passing through the vertex A_q. Now a more accurate cubature formula than (5) in $\mathbf{R}^3$ reads

$$\int_K v(x)\,\mathrm{d}x \approx \frac{1}{4}\mathrm{meas}_3 K \sum_{q=1}^{4} v(B_q)\ .$$

It is exact for all $v \in P_2(K)$.

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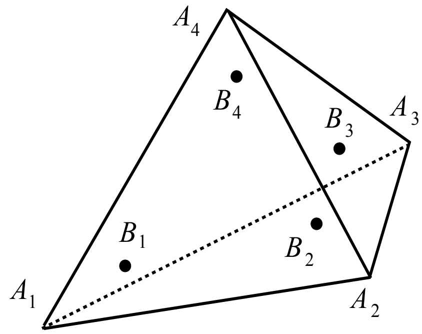

Figure 2: Integration points of cubature formula (8)

Example 3.4 Another formula which is exact for all $v \in P_3(K)$ reads

$$\int_K v(x)\,\mathrm{d}x \approx \mathrm{meas}_3 K\Big(\frac{9}{20}\sum_{q=1}^{4} v(C_q) - \frac{4}{5}v(G)\Big), \tag{9}$$

where

$$C_q = aA_q + b\sum_{r\neq q} A_r, \quad q = 1,2,3,4,$$

$a = 1/2$, $b = 1/6$ and the tetrahedral coordinates of G are $(\frac{1}{4},\frac{1}{4},\frac{1}{4},\frac{1}{4})$.

For higher order cubature formulae with 11 and 24 integration points inside tetrahedra we refer to [12]. They are exact for all polynomials of the fourth and sixth degree, respectively.

Example 3.5 Consider now a 4-simplex K with vertices A_1, A_2, A_3, A_4, and A_5. The following quadrature formula is exact for all cubic polynomials $v \in P_3(K)$,

$$\int_K v(x)\,\mathrm{d}x \approx \mathrm{meas}_4 K\Big(\frac{49}{120}\sum_{q=1}^{5} v(D_q) - \frac{25}{24}v(G)\Big), \tag{10}$$

where

$$D_q = aA_q + b\sum_{r\neq q} A_r, \quad q = 1,2,3,4,5,$$

$a = \frac{3}{7}$, $b = \frac{1}{7}$, and the simplicial (barycentric) coordinates of the center of gravity G are $(\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5},\frac{1}{5})$.

Further numerical integration formulae for d-simplices can be found in [6] and [9].

Now we will show how to evaluate integrals of monomial functions over d-dimensional simplices.

Theorem 3.6 Suppose that $A_0 = (0,0,\dots,0)$, $A_1 = (1,0,\dots,0)$,..., $A_d = (0,0,\dots,1)$ are vertices of a generalized cube-corner d-simplex K_d. Let $\mathbf{x} = (x,y,z,\dots) \in K_d$ and let $e \in \{1,2,3,\dots\}$ be an arbitrary exponent. Then

$$\left(d!\int_{K_d} x^e \mathrm{d}\mathbf{x}\right)_{d,e=1}^{\infty} = \begin{pmatrix} \frac{1}{2} & \frac{1}{3} & \frac{1}{4} & \frac{1}{5} & \frac{1}{6} & \cdots \\ \frac{1}{3} & \frac{1}{6} & \frac{1}{10} & \frac{1}{15} & \frac{1}{21} & \cdots \\ \frac{1}{4} & \frac{1}{10} & \frac{1}{20} & \frac{1}{35} & \frac{1}{56} & \cdots \\ \frac{1}{5} & \frac{1}{15} & \frac{1}{35} & \frac{1}{70} & \frac{1}{126} & \cdots \\ \frac{1}{6} & \frac{1}{21} & \frac{1}{56} & \frac{1}{126} & \frac{1}{252} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \quad (11)$$

Proof: The volume of the d-simplex K_d is equal to $1/d!$. Now the proof follows easily by induction and the Fubini theorem (or formulae (5), (6), (9), (10), etc).

We see that the second row of formula (11) contains the triangular numbers $(d+1)(d+2)/2$ in denominators, the third row contains the tetrahedral numbers $(d+1)(d+2)(d+3)/6$ in denominators, etc. Moreover, this infinite matrix is symmetric, i.e.,

$$d!\int_{K_d} x^e \mathrm{d}\mathbf{x} = e!\int_{K_e} x^d \mathrm{d}\mathbf{x}. \quad (12)$$

Formula (12) has several useful applications. It enables us to evaluate easily integrals of a lower degree monomials over higher dimensional simplices. For instance, if $d = 100$ and $e = 1$ then we can integrate a higher degree monomial over interval $[0,1]$ only instead of integration of x over 100-dimensional cube-corner simplex, namely,

$$\int_{K_{100}} x\,\mathrm{d}\mathbf{x} = \frac{1}{100!}\int_0^1 x^{100}\mathrm{d}x = \frac{1}{101!}.$$

Similarly, for $d=5$ and $e=2$ we get by (12) that

$$\int_{K_5} x^2\mathrm{d}\mathbf{x} = \frac{2!}{5!}\int_{K_2} x^5\mathrm{d}x\mathrm{d}y = \frac{1}{60}\int_0^1\int_0^{1-y} x^5\mathrm{d}x\mathrm{d}y =$$

$$= \frac{1}{360}\int_0^1 (1-y)^6\mathrm{d}y = \frac{1}{2520},$$

where K_2 is the reference triangle with vertices $(0,0)$, $(1,0)$, and $(0,1)$.

More details on numerical quadrature can be found in [2, 4, 5, 7, 12, 18, 21, 22], for example.

4 Isoparametric quadratic triangular elements

Let $\hat{K}$ be the reference triangle with vertices $\hat{A}_0=(0,0)$, $\hat{A}_1=(1,0)$, $\hat{A}_2=(0,1)$ and the midpoints $\hat{A}_3=(1/2,1/2)$, $\hat{A}_4=(1/2,0)$, and $\hat{A}_5=(0,1/2)$.

Assume that A_i, $i=0,\dots,5$, are such that A_0, A_1 and A_2 do not lie on the same straight line, A_4 and A_5 are the midpoints of the straight line segment A_0A_1 and A_0A_2, respectively. If A_3 lies in the shadow area of Figure 3, then the transformation

$$x = F(\hat{x}) = \sum_{i=0}^{5}\hat{p}_i(\hat{x})A_i, \quad \hat{x}\in\hat{K}, \tag{13}$$

where $\hat{p}_i$, $i=0,\dots,5$, are the standard quadratic basis functions on the reference element ($\hat{p}_i(\hat{A}_j)=\delta_{ij}$), is a one-to-one mapping (see [11, p. 242]) from the reference triangle onto a curved triangle

$$K = F(\hat{K}) = \{x\in\mathbf{R}^2 \mid x = F(\hat{x}),\ \hat{x}\in\hat{K}\} \tag{14}$$

such that $F(\hat{A}_i)=A_i$ for $i=0,1,\dots,5$. The curved side A_1A_2 of K is a parabolic arc. The function space

$$P_K = \{p \mid p(x) = \hat{p}(F^{-1}(x)),\ x\in K,\ \hat{p}\in P_2(\hat{K})\}$$

contains pull-back quadratic polynomials.

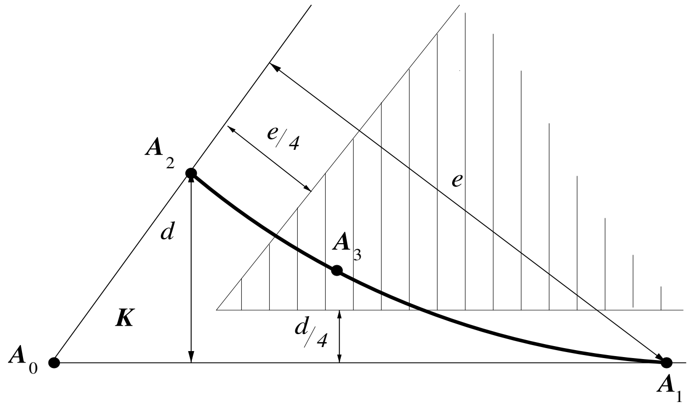

Figure 3: The curved triangle K with vertices A_0, A_1, A_2, and A_3. The point $A_3 = F_K(\hat{A}_3)$ should be in the shaded area, which is uniquely defined by the distances d and e.

Let $S = \frac{1}{2}(A_1 + A_2)$. Setting $s = A_3 - S$ and $w = 4s$, transformation (13) can be rewritten as the bilinear function

$$x = F(\hat{x}) = (A_1 - A_0, A_2 - A_0)\hat{x} + A_0 + \hat{x}_1\hat{x}_2 w, \tag{15}$$

where $(A_1 - A_0, A_2 - A_0)$ is a nonsingular matrix and $\hat{x} = (\hat{x}_1, \hat{x}_2)$. The Jacobian matrix of bilinear transformation (15) is

$$J_K(\hat{x}) = \frac{\partial F}{\partial \hat{x}} = \left(\frac{\partial F}{\partial \hat{x}_1}, \frac{\partial F}{\partial \hat{x}_2}\right) = (A_1 - A_0 + \hat{x}_2 w, A_2 - A_0 + \hat{x}_1 w),$$

and its Jacobian

$$\det J_K(\hat{x}) = \det(A_1 - A_0, A_2 - A_0) + \hat{x}_1 \det(A_1 - A_0, w) + \hat{x}_2 \det(w, A_2 - A_0)$$

is a linear function in $\hat{x}_1$ and $\hat{x}_2$. Therefore, the following statement holds.

Theorem 4.1 Under the above assumptions

$$\det J_K(\hat{x}) \neq 0 \quad \forall \hat{x} \in \hat{K}$$

if and only if its values at the vertices of $\hat{K}$:

$$\det J_K(\hat{A}_0), \quad \det J_K(\hat{A}_1), \quad \det J_K(\hat{A}_2)$$

are simultaneously all positive or all negative.

By the substitution theorem we have

$$\int_K v\,\mathrm{d}x = \int_{\hat{K}} \hat{v}|\det J_K|\,\mathrm{d}\hat{x}.$$

This formula is employed to calculate the element mass matrix or the element load vector corresponding to the curved element K on the straight reference element $\hat{K}$.

Let us show how to calculate the stiffness matrix, for instance, in the case of the Laplace operator. The entries of the corresponding element stiffness matrix are

$$a_{ij}^K = (\operatorname{grad} v^i, \operatorname{grad} v^j)_{0,K},$$

where v^i and v^j are pull-back polynomial finite element basis functions. This scalar product is again computed by the substitution theorem on the reference triangle $\hat{K}$ as follows

$$a_{ij}^K = ((J_K^{-1})^\top \operatorname{grad} \hat{v}^i, (J_K^{-1})^\top \operatorname{grad} \hat{v}^j |\det J_K|)_{0,\hat{K}}, \qquad (16)$$

where $\operatorname{grad} v^i = (J_K^{-1})^\top \operatorname{grad} \hat{v}^i$. Inserting

$$J_K^{-1} = \frac{1}{\det J_K} J_K^*,$$

where J_K^* is the matrix of algebraic adjoints, into (16), we see that we have to integrate numerically a rational function over $\hat{K}$ (see Section 3 for efficient quadrature rules in this respect). The corresponding error estimates can be found in [3, pp. 251–259].

Remark 4.2 To avoid the calculation of the ratio $\frac{0}{0}$ at integration points, one should employ another numerical quadrature formula.

5 More general cases

If A_4 and A_5 are not the midpoints of sides of the straight line segment A_0A_1 and A_0A_2, respectively, then the transformation

$$x = F(\hat{x}) = \sum_{i=0}^{5} \hat{p}_i(\hat{x})A_i \quad \hat{x} \in \hat{K},$$

is not bilinear but quadratic, i.e., $F \in (P_2(\hat{K}))^2$. In this case the element $K = F(\hat{K})$ has, in general, three curved sides.

Example 5.1 Let $\hat{K}$ be the triangle with vertices $\hat{A}_0 = (1,0)$, $\hat{A}_1 = (2,0)$, and $\hat{A}_0 = (2,2\pi)$. Consider the mapping $F : \hat{K} \to K$ such that

$$F(\hat{x}_1,\hat{x}_2) = (\hat{x}_1 \cos\hat{x}_2, \hat{x}_1 \sin\hat{x}_2)$$

and $K = F(\hat{K})$. Then the Jacobian

$$\det\frac{\partial F}{\partial \hat{x}} = (\cos\hat{x}_2)(\hat{x}_1 \cos\hat{x}_2) + (\sin\hat{x}_2)(\hat{x}_1 \sin\hat{x}_2) = \hat{x}_1$$

is continuous and non-zero over $\hat{K}$. However, we observe that the mapping F is not one-to-one, since $F(\hat{A}_1) = F(\hat{A}_2)$. This example shows that the condition that the Jacobian is non-zero is not sufficient to guarantee that a mapping is one-to-one.

A general nonlinear transformation F to an “ideal" element is investigated in the pioneering paper [23]. For a generalization to the three-dimensional case see [2, 4, 5, 12, 13, 14, 15].

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