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PI-type fully symmetric quadrature rules on the 3-, …, 6-simplexes

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ABSTRACT

We consider fully symmetric quadrature rules with positive weights, and with nodes lying inside the $3,\dots,6$ dimensional simplex (so-called PI-type). PI-type fully symmetric quadrature rules up to 20-th order on the tetrahedron, 16-th order on 4-simplex, 10-th order on 5- and 6-simplexes are presented. The number of nodes of the presented quadrature rules for the corresponding orders does not exceed the known ones, and most of them are new. In the calculation we applied the modified Levenberg-Marquardt methods for solving nonlinear equations with convex constraints. The corresponding programs are implemented in MAPLE-FORTRAN environment, and the weights and nodes are first calculated using a FORTRAN program with an accuracy of 10^{-25} and refined up to accuracy of 10^{-50} using a MAPLE program.

1. Introduction

The high-order finite element method (FEM) schemes yield highly accurate solutions of the boundary value problems due to their fast convergence. However, they are not currently used to solve multidimensional problems, since their implementation requires large resources. This obstacle is gradually being removed with the progress in computational technology.

The cornerstone hindering factor in the implementation of the FEM schemes is the calculation of integrals. It is well known [1] that, as a result of applying the p-th order FEM to the solution of the discrete spectrum problem for the elliptic (Schrödinger) equation, the eigenfunctions and the eigenvalues are determined with accuracies of the order $p+1$ and $2p$, respectively, provided that all intermediate quantities are calculated with sufficient accuracy. It follows that, for the realization of an FEM scheme of the order p, the corresponding integrals must be computed with an accuracy of the order $2p$ at least. The most economical way of calculating such integrals rests on the use of quadratures of the Gaussian type. In the one-dimensional case, these quadrature rules are known analytically. Using their Cartesian product, analytical quadrature rules may be built for rectangular hyperparallelepipeds, without being optimal, however. Such quadrature rules, which are characterized by almost minimal numbers of nodes were reported in [2]. Quadrature rules are also known for curvilinear domains [3,4].

The purpose of this work is the derivation of fully symmetric quadrature rules with positive weights and with nodes lying inside the simplex (rules of so-called PI-type). The derivation of quadrature rules (usually in barycentric coordinates) in the general case is reduced to the solution of systems of large nonlinear algebraic equations.

In the lower order cases, being expressed in terms of radicals, the weights and nodes of the quadrature rules are exact. Such solutions for quadrature rules up to the fifth order on a triangle and up to the third order on a tetrahedron were reported in [5], while quadrature rules of the second and the third orders on an arbitrary simplex were reported in [6]. The use of Gröbner bases makes it possible the derivation of general solutions of the systems of nonlinear algebraic equations for quadrature rules up to the fifth order on a simplex (for example, by using the program "PolynomialSystem" implemented in MAPLE). This approach, however, cannot provide solutions beyond the eighth order. Note that for multidimensional integrals, a variety of quadrature rules of the Grundmann-Möller and of the Newton-Cotes types are known (see, for instance, Refs. [7,8]).

Gaussian quadrature rules on a triangle have been reported in many papers (for instance [9–21]). Among them, we notice the symmetric PI-type quadrature rules up to 50-th order reported in [18], and the asymmetric quadrature rules up to 25-th order reported in [16]. In [14], Gaussian quadrature rules up to 20-th order were reported. The program presented in the article [14] allows the derivation of high-order quadrature rules in a reasonable computational time.

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Table 1
The orbits $S_{[i]} \equiv S_{m_1 \ldots m_{r_{di}}}$ with different parameters r_{di} and their numbers of permutations P_{di} for $d = 2, \ldots, 6$.

i	$d=2$			$d=3$			$d=4$			$d=5$			$d=6$		
	Orbits	r_{2i}	P_{2i}	Orbits	r_{3i}	P_{3i}	Orbits	r_{4i}	P_{4i}	Orbits	r_{5i}	P_{5i}	Orbits	r_{6i}	P_{6i}
0	S_3	1	1	S_4	1	1	S_5	1	1	S_6	1	1	S_7	1	1
1	S_{21}	2	3	S_{31}	2	4	S_{41}	2	5	S_{51}	2	6	S_{61}	2	7
2	S_{111}	3	6	S_{22}	2	6	S_{32}	2	10	S_{42}	2	15	S_{52}	2	21
3				S_{211}	3	12	S_{311}	3	20	S_{33}	2	20	S_{43}	2	35
4				S_{1111}	4	24	S_{221}	3	30	S_{411}	3	30	S_{511}	3	42
5							S_{2111}	4	60	S_{321}	3	60	S_{421}	3	105
6							S_{11111}	5	120	S_{222}	3	90	S_{331}	3	140
7										S_{3111}	4	120	S_{322}	3	210
8										S_{2211}	4	180	S_{4111}	4	210
9										S_{21111}	5	360	S_{3211}	4	420
10										S_{111111}	6	720	S_{2221}	4	630
11													S_{31111}	5	840
12													S_{22111}	5	1260
13													S_{211111}	6	2520
14													$S_{1111111}$	7	5040

In the multidimensional case, two kinds of supplementary difficulties arise in comparison with the two-dimensional case: the rapid growth of the number of independent equations with increasing dimension and the large number of different systems, which lead to the need of constructing initial estimations for the iterative process. Thus, in the case of the asymmetric p-order quadrature rules, the numbers of the independent nonlinear equations are $C^d_{p+d} = (p+d)!/(p!d!)$, where d is the dimension of the simplex. In the case of the symmetric p-order quadrature rules, the numbers of the independent equations, which can be calculated using recurrence formulas with respect to the p and d [22], are much smaller than C^d_{p+d}. At the same time, the very question of the minimal number of nodes for PI-type quadrature rules remains open. In [22] lower estimations only were inferred.

Many Gaussian quadrature rules on the 3- and 4-simplexes were reported (see, e.g., [13,15,19,20,23–29]). Among them, we notice the PI-type quadrature rules up to 20-th order on the tetrahedron [26] and up to 16-th order on the 4-simplex [29].

Finally, Gaussian PI-type quadrature rules up to 8-th order on the 5- and 6-simplexes are presented in our previous paper [23].

In this paper we report new PI-type fully symmetric quadrature rules the maximal orders p of which go up to 20 on the tetrahedron, up to 16 on the 4-simplex, and up to 10 on the 5- and 6-simplexes, under the use of almost minimal numbers of nodes. To this aim, we use modified Levenberg-Marquardt methods [30–33] to solve systems of nonlinear algebraic equations in convex domains. The boundaries of the convex domains were carefully chosen by numerical experiments. The numbers of nodes entering our high-order quadrature rules are significantly lower than the corresponding figures reported in the recent papers [26] and [29] for the $d = 3$ and $d = 4$ cases. Improvements are also reported in comparison with our previous results [23] for the 5- and 6-simplexes.

The paper is organized as follows. In Section 2, the derivation of the systems of the independent nonlinear equations is discussed. In Section 3, algorithms for solving the system of nonlinear equations are presented. In Sections 4 and 5 the calculated quadrature rules and their error estimates are analyzed. The concluding section summarizes the main features of the reported methods and discusses the applications of quadrature rules to physical problems. In Appendix A, a brief description of the program for converting quadrature rules from compact to expanded forms is presented.

2. Fully symmetric quadrature rules for the d-simplex

Let us construct the p-order quadrature rule

$$\int_{\Delta_d} V(x)dx = \frac{1}{d!}\sum_{j=1}^{N_{dp}} w_j V(x_{j1}, \ldots, x_{jd}),$$
$$x = (x_1, \ldots, x_d), \quad dx = dx_1 \ldots dx_d, \tag{1}$$

for integration over the standard unit d-simplex Δ_d with vertices $\hat{x}_j = (\hat{x}_{j1}, \ldots, \hat{x}_{jd})$, $\hat{x}_{jk} = \delta_{jk}$, $j = 0, \ldots, d$, $k = 1, \ldots, d$, which is exact for all polynomials of the variables $x_1, \ldots, x_d$ of degree not exceeding p. In Eq. (1), N_{dp} is the number of nodes, w_j are the weights, and $(x_{j1}, \ldots, x_{jd})$ are the nodes.

To building up PI-type fully symmetric quadrature rules, we use the barycentric coordinates (BC) $(y_1, \ldots, y_{d+1})$ of nodes:

$$\sum_{k=1}^{d+1} y_k = 1. \tag{2}$$

Using the invariance of the symmetric quadrature rules, Eq. (1) can be represented in the symmetric expanded form,

$$\int_{\Delta_d} V(x)dx = \frac{1}{d!}\sum_{j=1} w_j \sum_{k_1,\ldots,k_{d+1}} V(y_{jk_1}, \ldots, y_{jk_d}|y_{jk_{d+1}}), \tag{3}$$

where the internal summation over $k_1, \ldots, k_{d+1}$ is carried out over the different permutations of the BC $(y_{j1}, \ldots, y_{jd+1})$, while $V(y_{jk_1}, \ldots, y_{jk_d}|y_{jk_{d+1}})$ means that the d-dimensional integrand function $V(x)$ is calculated for the set $y_{jk_1}, \ldots, y_{jk_d}$.

In Table 1 we present the different ordered orbits $S_{[i]}$, $i = 0, \ldots, M_d$, for $d = 2, \ldots, 6$ that have been used in [22], where $M_2 = 2$, $M_3 = 4$, $M_4 = 6$, $M_5 = 10$, $M_6 = 14$. The orbit $S_{[i]} \equiv S_{m_1 \ldots m_{r_{di}}}$ contains the BC

$$(y_1, \ldots, y_{d+1}) = (\overbrace{\lambda_1, \ldots, \lambda_1}^{m_1 \text{ times}}, \ldots, \overbrace{\lambda_{m_{r_{di}}}, \ldots, \lambda_{m_{r_{di}}}}^{m_{r_{di}} \text{ times}}), \tag{4}$$

with

$$\sum_{j=1}^{r_{di}} m_j = d+1, \quad \sum_{j=1}^{r_{di}} m_j \lambda_j = 1, \quad m_1 \geq \ldots \geq m_{r_{di}}. \tag{5}$$

The number of different permutations of the BC (4) is expressed by permutations of multisets

$$P_{di} = \frac{(d+1)!}{m_1! \ldots m_{r_{di}}!}. \tag{6}$$

The following formula holds for any permutations $(l_1, \ldots, l_{d+1})$ of $(k_1, \ldots, k_{d+1})$:

$$\int_{\Delta_d} x_1^{l_1} \cdots x_{d+1}^{l_{d+1}} dx = \frac{\prod_{i=1}^{d+1} k_i!}{\left(d + \sum_{i=1}^{d+1} k_i\right)!}, \quad x_{d+1} = 1 - \sum_{i=1}^{d} x_i. \tag{7}$$

Substituting symmetric polynomials with respect to the variables $x_1, \ldots, x_{d+1}$ of degree not exceeding p in (3) instead of $V(x)$, and taking into account (7), we obtain the system of nonlinear algebraic equations:

Table 2
The numbers E_{dp} of independent equations for fully symmetric p-order quadrature rules.

p	E_{dp}				
	$d=2$	$d=3$	$d=4$	$d=5$	$d=6$
4	4	5	5	5	5
5	5	6	7	7	7
6	7	9	10	11	11
7	8	11	13	14	15
8	10	15	18	20	21
9	12	18	23	26	28
10	14	23	30	35	38
11	16	27	37	44	49
12	19	34	47	58	65
13	21	39	57	71	82
14	24	47	70	90	105
15	27	54	84	110	131
16	30	64	101	136	164
17	33	72	119	163	201
18	37	84	141	199	248
19	40	94	164	235	300
20	44	108	192	282	364

Table 3
The minimal numbers $\hat{N}_{dp}$ of nodes for fully symmetric p-order quadrature rules. The numbers in the second, third, fourth, fifth and seventh columns are taken from [22]. The numbers in the right columns at $d=5$ and $d=6$ are the new recalculated results.

p	$\hat{N}_{dp}$						
	$d=2$	$d=3$	$d=4$	$d=5$		$d=6$	
4	6	11	16	22	22	29	29
5	7	14	21	28	28	36	36
6	12	24	41	68	63	98	84
7	13	30	55	84	79	140	127
8	16	43	90	164	164	267	259
9	19	52	120	210	210	351	344
10	24	68	171	325	325	644	623
11	27	81	206	470	466	848	827
12	33	117	306	736	706	1456	1330
13	36	133	381	917	882	1911	1772
14	42	163	485	1272	1267	2870	2786
15	46	190	616	1662	1623	3816	3613
16	52	233	766	2218	2188		5019
17	58	266	931	2734	2734		
18	66	318	1161	3649	3609		
19	70	355	1396				
20	78	415	1750				

$$\int_{\Delta_d} s_2^{l_2} \times \cdots \times s_{d+1}^{l_{d+1}} dx = \frac{1}{d!} \sum_{i=0}^{M_d} P_{di} \sum_{j=1}^{K_{di}} W_{i,j} s_{i,j2}^{l_2} \times \cdots \times s_{i,jd+1}^{l_{d+1}}, \quad (8)$$

$$2l_2 + \cdots + (d+1)l_{d+1} \le p, \quad (9)$$

where, for each orbit $S_{[i]}$, a set of K_{di} different BC is used. In (8), $K_{d0}=0$ or 1 and $K_{di} \ge 0$, $i \ne 0$; $W_{i,j}$ is the j-th weight of the orbit $S_{[i]}$;

$$s_k = \sum_{l=1}^{d+1} x_l^k, \quad k = 2, \dots, d+1, \quad (10)$$

is the symmetric polynomial of degree k. Finally,

$$s_{i,jk} = \sum_{l=1}^{r_{di}} m_l \lambda_{i,jl}^k \quad (11)$$

denotes the j-th value of (10) on the components $\lambda_{i,jl}$ of the BC of the orbit $S_{[i]}$.

The count of all the solutions of Eq. (9) characterized by $l_k \ge 0$ provides the number E_{dp} of the independent nonlinear equations for the p-ordered quadrature rule. The value of E_{dp} can be calculated by recurrence for arbitrary d and p [22]:

$$E_{dp} = \begin{cases} 1 + \left\lfloor \frac{p}{2} \right\rfloor, & d = 1, \quad p \ge 0 \\ E_{d-1p}, & d \ge 2, \quad 0 \le p \le d, \\ E_{d-1p} + E_{dp-d-1}, & d \ge 2, \quad p \ge d+1, \end{cases} \quad (12)$$

where $\lfloor x \rfloor$ denotes the integer part of x. Table 2 presents the E_{dp} values for $d = 2, \dots, 6$ and $p = 4, \dots, 20$.

The number of the unknowns U_{dp} in Eq. (8) and the number N_{dp} of nodes are given respectively by

$$U_{dp} = \sum_{i=0}^{M_d} r_{di} K_{di}, \quad N_{dp} = \sum_{i=0}^{M_d} P_{di} K_{di}. \quad (13)$$

A necessary condition for the existence of a solution of the nonlinear system (8) is

$$E_{dp} \le U_{dp}. \quad (14)$$

From Eq. (13) it follows that the number K_{di} is bounded from above,

$$K_{di} \le \min \left(\left\lfloor \frac{U_{dp}}{r_{di}} \right\rfloor, \left\lfloor \frac{N_{dp}}{P_{di}} \right\rfloor \right). \quad (15)$$

The additional consistency conditions described in [22,27] have also been used. These consistency conditions help to find the combinations of orbits for which the nonlinear system (8) can have solutions, thereby significantly reducing the total computational time. In particular, for the orbits with $r_{dj} = 1, 2$ and $d = 3, \dots, 6$, six sets of simple conditions follow from [22,27]:

$$K_{d0} + 2K_{dj} \le U_{dp} - E_{dp} + p, \quad (16)$$

where $j = 1$ for $d = 2, 3$, $j = 1, 2$ for $d = 4, 5$ and $j = 1, 2, 3$ for $d = 6$;

$$K_{d0} + 2K_{dj} \le U_{dp} - E_{dp} + \left\lfloor \frac{p}{2} \right\rfloor + 1, \quad (17)$$

where $j = 2$ for $d = 3$ and $j = 3$ for $d = 5$;

$$K_{d0} + 2K_{di} + 2K_{dj} \le U_{dp} - E_{dp} + \max(p, 2p-3), \quad (18)$$

where $i = 1$, $j = 2$ for $d = 5$ and $(i, j) \in (1, 2, 3)$, $i < j$ for $d = 6$;

$$K_{d0} + 2K_{di} + 2K_{dj} \le U_{dp} - E_{dp} + p + \left\lfloor \frac{p}{2} \right\rfloor - 1, \quad (19)$$

where $i = 1$, $j = 2$ for $d = 3$ and $i = 1, 2$, $j = 3$ for $d = 5$;

$$K_{d0} + 2K_{d1} + 2K_{d2} + 2K_{d3} \le U_{dp} - E_{dp} + \max\left(E_{dp}, 3p - 8\right), \quad (20)$$

where $d = 6$;

$$K_{d0} + 2K_{d1} + 2K_{d2} + 2K_{d3} \le U_{dp} - E_{dp} + \max\left(E_{dp}, 2p + \left\lfloor \frac{p}{2} \right\rfloor - 5\right), \quad (21)$$

where $d = 5$.

For such sets, the rank of the corresponding matrix [22] is calculated in the Maple without loss of accuracy. Table 3 summarizes the minimal number $\hat{N}_{dp}$ of nodes at which a consistency set of orbits can exist for fully symmetric quadrature rules of p-order. Our obtained minimal numbers $\hat{N}_{dp}$ of nodes coincides with the results of [22] at $d = 2, 3, 4$, while some of our obtained minimal numbers $\hat{N}_{dp}$ of nodes at $d = 5, 6$ are smaller than those reported in [22].

Note that, for $d = 2$ the condition (16) is equivalent to

$$3K_{22} \ge E_{2p} - p, \quad (22)$$

and it coincides with the condition derived in [10]. Our calculations show that the symmetric quadrature rules must include the last orbit S_{111} for $d = 2$ at $p \ge 6$ (in agreement with [10,22]); the last orbit S_{1111} for $d = 3$ at $p \ge 12$ (in agreement with [22]); the last orbit S_{11111} for $d = 4$ at $p \ge 20$ (in agreement with [22]). Finally, at $p \ge 30$ the last orbit S_{111111} for $d = 5$ and at least one of the last two orbits $S_{2111111}$, $S_{1111111}$ for $d = 6$ are to enter the symmetric quadrature rules.

Table 4
The approximated minimal numbers $\bar{N}_{dp}$ of nodes for asymmetric and the approximated maximal numbers $\check{N}_{dp}$ of nodes for fully symmetric p-order quadrature rules.

p	$d=2$		$d=3$	$d=4$		$d=5$	$d=6$	
	$\bar{N}_{dp}$	$\check{N}_{dp}$	$\bar{N}_{dp}=\check{N}_{dp}$	$\bar{N}_{dp}$	$\check{N}_{dp}$	$\bar{N}_{dp}=\check{N}_{dp}$	$\bar{N}_{dp}$	$\check{N}_{dp}$
4	5	6	9	14	15	21	30	35
5	7	7	14	26	26	42	66	70
6	10	12	21	42	45	77	132	133
7	12	12	30	66	66	132	246	246
8	15	15	42	99	100	215	429	434
9	19	19	55	143	145	334	715	715
10	22	22	72	201	201	501	1144	1148
11	26	27	91	273	275	728	1768	1771
12	31	31	114	364	365	1032	2652	2653
13	35	36	140	476	476	1428	3876	3878
14	40	40	170	612	615	1938	5538	5538
15	46	48	204	776	776	2584	7752	7756
16	51	51	243	969	970	3392	10659	10661
17	57	57	285	1197	1200	4389	14421	14421
18	64	64	333	1463	1465	5609	19228	19229
19	70	70	385	1771	1771	7084	25300	25305
20	77	78	443	2126	2126	8855	32890	32893

On the other hand, the minimal numbers $\bar{E}_{dp}$ of the independent nonlinear equations for asymmetric p-order quadrature rules are found from the formula

$$\bar{E}_{dp} = C^d_{p+d} \equiv \frac{(p+d)!}{p!d!}, \tag{23}$$

and the corresponding minimal numbers $\bar{N}_{dp}$ of nodes (see Table 4) are found from

$$\bar{N}_{dp} = \left\lceil \frac{\bar{E}_{dp}}{d+1} \right\rceil, \tag{24}$$

where $\lceil x \rceil$ denotes the smallest integer that is greater than or equal to x. From here, we defined the approximated maximal numbers $\check{N}_{dp}$ of nodes for fully symmetric p-order quadrature rules (see Table 4),

$$\check{N}_{dp} = \begin{cases} \bar{N}_{dp}, & \\ \quad \text{for } d=3,5 \text{ or } d=2,4,6 \text{ and } \mathrm{mod}(\bar{N}_{dp}, d+1) = 0, 1, & \\ \bar{N}_{dp} + d + 1 - \mathrm{mod}(\bar{N}_{dp}, d+1), & \\ \quad \text{for } d = 2,4,6 \text{ and } \mathrm{mod}(\bar{N}_{dp}, d+1) \neq 0, 1. \end{cases} \tag{25}$$

In addition, taking into account the conditions (8) at $l_2 = \ldots = l_{d+1} = 0$ and (5), the j-th weight $W_{i,j}$ and components $\lambda_{i,jl}$ of the BC of the orbit $S_{[i]}$, must obey the simple bounds and the linear constraints respectively,

$$0 \le W_{i,j} \le \frac{1}{P_{di}}, \quad 0 \le \lambda_{i,jl} \le \frac{1}{m_l}, \quad 0 \le \sum_{l=1}^{r_{di}-1} m_l \lambda_{i,jl} \le 1. \tag{26}$$

Using a coordinate transformation in the integral (1), one obtains the following quadrature rule for an arbitrary simplex Δ_q:

$$\int_{\Delta_q} V(x)dx = |\Delta_q| \sum_{j=1}^{N_{dp}} w_j V(x_{j1}(y_{j1}, \ldots, y_{jd+1}), \ldots, x_{jd}(y_{j1}, \ldots, y_{jd+1})), \tag{27}$$

where $|\Delta_q|$ denotes the volume of the simplex Δ_q. It equals $1/d!$ for the standard unit d-simplex.

3. Solving system of nonlinear equations with convex constraints

Below we discuss a modified Levenberg-Marquardt (LM) method [30–33] for the solution of a system of nonlinear equations with convex constraints, instead of the quasi-Newtonian method used in our previous article [23], because the LM method is more robust to the initial guess, and it can be more stable in the cases when the inverse problem becomes ill-posed.

Consider the problem of solving the constrained system of nonlinear equations

$$f_i(\mathbf{x}) = 0, \quad i = 1, \ldots, m, \quad \mathbf{x} = (x_1, \ldots, x_n) \in \mathcal{X}, \tag{28}$$

and the corresponding minimization problem

$$\min_{\mathbf{x}\in\mathcal{X}} \|\mathbf{F}(\mathbf{x})\|^2, \quad \mathbf{F}(\mathbf{x}) = (f_1(\mathbf{x}), \ldots, f_m(\mathbf{x}))^T, \tag{29}$$

where $\mathcal{X} \subseteq R^n$ is a nonempty, closed and convex set.

The LM-type algorithm is an iterate method which, basically, solves at each iteration a linearization subproblem of the form

$$\min_{\mathbf{x}^k+\mathbf{h}\in\mathcal{X}} G_k(\mathbf{h}), \tag{30}$$

with the objective function

$$G_k(\mathbf{h}) = \frac{1}{2}\|\mathbf{F}(\mathbf{x}^k) + \mathbf{J}_k \mathbf{h}\|^2 + \frac{1}{2}\mu_k(\mathbf{h}, \mathbf{D}_k \mathbf{h}), \tag{31}$$

where $\mathbf{x}^k$ is the current iterate, $\mathbf{J}_k \in R^{m\times n}$ is a Jacobian of $\mathbf{F}(\mathbf{x})$ at $\mathbf{x} = \mathbf{x}^k$, $\mathbf{D}_k \in R^{n\times n}$ is a positive diagonal matrix and in most cases $\mathbf{D}_k = \mathrm{diag}(\mathbf{J}_k^T \mathbf{J}_k)$ or a unit matrix, and μ_k is a positive parameter. Note that $G_k(\mathbf{h})$ is a strictly convex quadratic function. Hence the solution $G_k(\mathbf{h})$ of the subproblem (30) always exists and is unique, in particular for the unconstrained case

$$\mathbf{h}^k = -(\mathbf{J}_k^T \mathbf{J}_k + \mu_k \mathbf{D}_k)^{-1} \mathbf{J}_k^T \mathbf{F}(\mathbf{x}^k). \tag{32}$$

In [32] the following two algorithms (with unit matrix D_k) have been proposed:

Algorithm 1. (local version)

1. Choose $\mathbf{x}^0 \in \mathcal{X}$, $\nu > 0$, $\epsilon > 0$, and set $k = 0$.
2. If $\|\mathbf{F}(\mathbf{x}^k)\| \le \epsilon$, stop.
3. Calculate $\mathbf{J}_k$ and set $\mu_k = \nu \|\mathbf{F}(\mathbf{x}^k)\|^2$, and compute $\mathbf{h}^k$ as the solution of (30).
4. $\mathbf{x}^{k+1} = \mathbf{x}^k + \mathbf{h}^k$, $k = k+1$, and go to 2.

Algorithm 2. (global version)

1. Choose $\mathbf{x}^0 \in \mathcal{X}$, $\nu > 0$, $\beta, \sigma, \gamma \in (0,1)$, $\epsilon > 0$, and set $k = 0$.
2. If $\|\mathbf{F}(\mathbf{x}^k)\| \le \epsilon$, stop.
3. Calculate $\mathbf{J}_k$ and set $\mu_k = \nu \|\mathbf{F}(\mathbf{x}^k)\|^2$, and compute $\mathbf{h}^k$ as the solution of (30).

Table 5
The minimal numbers N_{dp} of nodes for PI-type fully symmetric p-order quadrature rules and comparison with the known numbers N_{dp}.

p	N_{dp}													
	$d=2$		$d=3$					$d=4$			$d=5$		$d=6$	
	cur., [18,20]	[15]	cur.	[23]	[20]	[15]	[26]	cur.	[23]	[29]	cur.	[23]	cur.	[23]
4	6	6	14	14	14	14	14	20	20	20	27	27	43	43
5	7	7	14	14	14	14	14	30	30	30	37	37	64	64
6	12	12	24	24	24	24	24	56	56	56	102	102	175	175
7	15	15	35	35	35	36	35	70	76	70	137	137	252	266
8	16	16	46	46	46	46	46	105	110	105	228	257	448	553
9	19	19	59		59	61	59	151		151	338		700	
10	25	25	79		81	81	81	210		210	479		1078	
11	28	28	98			109	110	275		281				
12	33	33	123			140	168	370		445				
13	37	37	145			171	172	470		555				
14	42	46	175			236	204	601		725				
15	49	52	209				264	781		905				
16	55	55	248				304	956		1055				
17	60	61	284				364							
18	67	72	343				436							
19	73	73	383				487							
20	79	88	441				552							

4. If

$$\|\mathbf{F}(\mathbf{x}^k+\mathbf{h}^k)\| \le \gamma \|\mathbf{F}(\mathbf{x}^k)\|,$$

then set $\mathbf{x}^{k+1}=\mathbf{x}^k+\mathbf{h}^k$, $k=k+1$, and go to 1; otherwise go to 5.
5. Compute a stepsize $t=\max(\beta^l \,|\, l=0,1,2,\ldots)$, such that

$$\|\mathbf{F}(\mathbf{x}^k(t))\|^2 \le \|\mathbf{F}(\mathbf{x}^k)\|^2 + 2\sigma \mathbf{F}^T(\mathbf{x}^k)\mathbf{J}_k(\mathbf{x}^k(t)-\mathbf{x}^k),$$

where $\mathbf{x}^k(t)=P_{\mathcal{X}}(\mathbf{x}^k-2t\mathbf{J}_k^T\mathbf{F}(\mathbf{x}^k))$. Set $\mathbf{x}^{k+1}=\mathbf{x}^k(t)$, $k=k+1$, and go to 2.

Here $P_{\mathcal{X}}(\mathbf{x})$ denotes the projection of $\mathbf{x}$ onto the feasible set $\mathcal{X}$. The local convergences of the above algorithms are proved.

We used $\nu \equiv \nu_k = \|\mathrm{diag}(\mathbf{J}_k^T\mathbf{J}_k)\|^{-1}$ in all the following calculations.

4. Numerical results

The existence of the solution of the constrained system of nonlinear equations (8), (26) strongly depends on the number U_{dp} of unknowns and the number N_{dp} of nodes, and on the combinations of the corresponding orbits $S_{[i]}$. The number of the iteration processes for finding the solution depends on the initial estimates of the weights $W_{i,j}$ and the components $\lambda_{i,jl}$ of the BC. Also the weights $W_{i,j}$ depend on the location of the components $\lambda_{i,jl}$ of the BC. We choose uniform initial estimates of the weights $W_{i,j}$ for all N_{dp} nodes, namely

$$W_{i,j}=\frac{1}{N_{dp}}. \tag{33}$$

The initial estimates of the components $\lambda_{i,jl}$ of the BC into the simplex for each orbit $S_{[i]}$ are chosen randomly using different algorithms. For our calculations, the most efficient was found to be provided by the multivariate extreme value distribution algorithm [34]:

$$\lambda_{i,jl}=\frac{z_{i,jl}}{m_l}, \quad z_{i,jl}=\frac{\log(q_{i,jl})}{\sum_{n=1}^{r_{di}}\log(q_{i,jn})}, \tag{34}$$

where $q_{i,jn}\in(0,1)$ are sequences of standard quasi-random numbers. Note that this algorithm is used to generate the Grundmann-Möller quadrature rules for the simplexes [7,35]. In [26,29], to calculate higher order quadrature rules ($p>10$), the calculated weights and nodes in the previous orders were used as initial estimates.

With the increase of the order p, the number N_{dp} of nodes also increases, while decreasing the minimum and maximum values of the weights. Therefore, to reduce the search domain for the weights $W_{i,j}$ and the components $\lambda_{i,jl}$ of the BC of the orbit $S_{[i]}$, we used the following simple bound and linear constraints instead of (26)

$$\frac{W^{\min}}{10} \le W_{i,j} \le W^{\max}, \quad \lambda^{\min} \le \lambda_{i,jl} \le \lambda_l^{\max}, \quad \sum_{l=1}^{r_{di}-1} m_l\lambda_{i,jl} \le 1-m_{r_{di}}\lambda^{\min}. \tag{35}$$

Here $W^{\min}$ and $W^{\max}$ are the minimum and maximum values of the weights of the quadrature rules of the orders $p-2$ and $p-1$, and

$$\lambda_l^{\max}=\frac{1-(d+1-m_l)\lambda^{\min}}{m_l}. \tag{36}$$

In the calculation, we used $\lambda^{\min}=10^{-t}$, $t=4,\ldots,8$. This helps finding nodes that are not very close to the vertices, edges, and faces of the d-simplex.

To find the minimal number N_{dp} of nodes for high-order quadrature rules using the minimal number N_{dp-1} previously found at the order $p-1$, we start the search with the number

$$\max\left(\hat{N}_{dp}, \left\lfloor \frac{N_{dp-1}}{E_{dp-1}} \right\rfloor E_{dp}\right). \tag{37}$$

While the necessary condition (14) for the nonlinear system (8) to have a solution yields a bound to the minimal number of unknowns U_{dp}, their maximal number is, in principle, unknown. The larger the number of unknowns, the higher the probability that the system of nonlinear equation (8) will have a solution. This leads, however, to the increase of the total number of orbits or of the number of orbits with large numbers of permutations. Because of this, the number N_{dp} of nodes (see Eq. (13)) can be unnecessarily increased. To put an upper bound to this trend, all the quadrature rules are calculated with the additional constraint

$$U_{dp} \le E_{dp}+d-1. \tag{38}$$

The corresponding programs are implemented in Maple-Fortran environment. The weights and nodes are first calculated using a Fortran program with an accuracy $\epsilon_f=10^{-25}$. The Jacobian matrix is calculated analytically. To solve the subproblem (30), (31) with simple bound and linear constraints (26), we used a modification of the routine VE17AD [36] in quadruple precision. The calculated results are refined on Maple system by the Newton-type method for the unconstrained minimization with analytic Jacobian and Hessian of the function $\|\mathbf{F}(\mathbf{x})\|^2$ (see the Eq. (29)) up to an accuracy $\epsilon_m=10^{-50}$.

Table 6
The list of quadrature rules on triangle with the corresponding combination of orbits and their error estimates.

p	N_{dp}	S_3	S_{21}	S_{111}	$\max \epsilon_{i_1,i_2}$	$\sum \epsilon_{i_1,i_2}$	$\sqrt{\sum \epsilon^2_{i_1,i_2}}$
4	6		2		$2.62 \cdot 10^{-6}$	$4.71 \cdot 10^{-6}$	$3.00 \cdot 10^{-6}$
5	7	1	2		$1.27 \cdot 10^{-6}$	$2.64 \cdot 10^{-6}$	$1.61 \cdot 10^{-6}$
6	12		2	1	$2.46 \cdot 10^{-9}$	$6.28 \cdot 10^{-9}$	$3.44 \cdot 10^{-9}$
7	15		1	2	$3.82 \cdot 10^{-9}$	$8.96 \cdot 10^{-9}$	$5.15 \cdot 10^{-9}$
8	16	1	3	1	$3.89 \cdot 10^{-11}$	$9.01 \cdot 10^{-11}$	$5.00 \cdot 10^{-11}$
9	19	1	4	1	$6.30 \cdot 10^{-12}$	$2.10 \cdot 10^{-11}$	$1.16 \cdot 10^{-11}$
10	25	1	2	3	$9.39 \cdot 10^{-15}$	$3.00 \cdot 10^{-14}$	$1.48 \cdot 10^{-14}$
11	28	1	5	2	$3.08 \cdot 10^{-15}$	$6.69 \cdot 10^{-15}$	$3.99 \cdot 10^{-15}$
12	33		5	3	$1.02 \cdot 10^{-17}$	$3.57 \cdot 10^{-17}$	$1.66 \cdot 10^{-17}$
13	37	1	4	4	$1.28 \cdot 10^{-17}$	$3.56 \cdot 10^{-17}$	$1.87 \cdot 10^{-17}$
14	42		6	4	$7.09 \cdot 10^{-20}$	$2.29 \cdot 10^{-19}$	$1.12 \cdot 10^{-19}$
15	49	1	4	6	$2.95 \cdot 10^{-21}$	$7.51 \cdot 10^{-21}$	$4.11 \cdot 10^{-21}$
16	55	1	4	7	$5.31 \cdot 10^{-23}$	$1.92 \cdot 10^{-22}$	$8.71 \cdot 10^{-23}$
17	60		6	7	$8.27 \cdot 10^{-24}$	$2.66 \cdot 10^{-23}$	$1.29 \cdot 10^{-23}$
18	67	1	6	8	$1.24 \cdot 10^{-26}$	$3.92 \cdot 10^{-26}$	$1.94 \cdot 10^{-26}$
19	73	1	6	9	$3.73 \cdot 10^{-28}$	$1.13 \cdot 10^{-27}$	$5.14 \cdot 10^{-28}$
20	79	1	8	9	$5.92 \cdot 10^{-30}$	$2.09 \cdot 10^{-29}$	$9.65 \cdot 10^{-30}$

Note that the Algorithm 1 was more efficient than the Algorithm 2, and it was faster in solving the constrained system of nonlinear equations (8), (35), (36), for most cases of the random generations of the components $\lambda_{i,jl}$ of the BC smaller than $5 \times U_{dp}$. This may be due to the fact that, within the Algorithm 2, $\|\mathbf{F}(\mathbf{x}^k)\|$ decreases at each iteration, and this results in the search of solutions over narrower regions than in Algorithm 1. As a consequence, in most cases, the iterative process of the **Algorithm 2** converges to a local minimum $\|\mathbf{F}(\mathbf{x}^k)\| \gg \epsilon_f$, $\|\mathbf{J}_k^T\mathbf{F}(\mathbf{x}^k)\| \le \epsilon_f$ instead of a global minimum $\|\mathbf{F}(\mathbf{x}^k)\| \le \epsilon_f$.

Our calculated minimal numbers N_{dp} of the nodes for PI-type fully symmetric p-order quadrature rules are presented in Table 5. For comparison, similar previously reported the numbers N_{dp} are also shown.

To assess the reliability of the present quadrature rules, we compared our calculated results for 2-simplex (triangle) with known quadrature rules [14,15,18,20]. In [15,18,20] the presented fully symmetric quadrature rules are PI-type, while in [14] only some quadrature rules are of PI-type. Our minimal numbers N_{2p} up to 20-orders are exactly the same as in [18,20], also some quadrature rules are the same as presented in the Supplementary material of [20].

Unlike our results, in [20,29] the constructed 59 points 9-order rule for $d = 3$ and the 210 points 10-order rule for $d = 4$ contain nodes which are very close to the vertices, or edges, or faces ($\sim 5 \cdot 10^{-17} - 4 \cdot 10^{-7}$).

Moreover, the comparison of the numbers N_{dp} of nodes of the present PI-type fully symmetric quadrature rules with those reported in previous publications ([26] at $d = 3$ and [29] at $d = 4$) showed equal to each other values at lower order p values, thresholds $p(d)$ have been found ($p(3) = 9$ and $p(4) = 10$) beyond which the present algorithms show less nodes. The difference generally increases with the order p (from 2 at $p = 10$ to 111 at $p = 20$ in the $d = 3$ case, and from 6 at $p = 11$ to 124 at $p = 15$ in the $d = 4$ case). Similar trends have been noticed in the cases $d = 5$ and $d = 6$, where comparisons are available with our previous results [23].

The quadrature rules themselves in compact form including programs for converting in expanded form, and examples of their application are provided in the JINRLIB Program Library [37] (for details see Appendix A). Note that [37] contains some additional high-order quadrature rules with close to the minimal number of nodes that the users may choose for the solution of further practical problems.

5. Estimates of the errors of the quadrature rules

To estimate the error of the quadrature rules (1), we decompose the integrand $V(x)$ into a Taylor series in the vicinity of the point $x_t = (x_{1t}, \dots, x_{dt})$ inside the simplex

$$V(x) = V^t(x) + O(x^{p+2}), \quad V^t(x)$$

$$= \sum_{i_1+\ldots+i_d \le p+1} V^{(i_1,\ldots,i_d)}(x_t) \frac{(x_1 - x_{1t})^{i_1} \times \ldots \times (x_d - x_{dt})^{i_d}}{i_1! \times \ldots \times i_d!}, \tag{39}$$

where $V^{(i_1,\ldots,i_d)}(x_t)$ is a mixed derivative at $x = x_t$ and consider the auxiliary function

$$\varepsilon(V(x)) = \left| \int_{\Delta_d} V(x)dx - \frac{1}{d!} \sum_{j=1}^{N_{dp}} w_j V(x_{j1}, \ldots, x_{jd}) \right|. \tag{40}$$

Taking into account that the quadrature is exact for polynomials of degree less than p, one has

$$\begin{aligned} \varepsilon(V^t(x)) &= \left| \int_{\Delta_d} V^t(x)dx - \frac{1}{d!} \sum_{j=1}^{N_{dp}} w_j V^t(x_{j1}, \ldots, x_{jd}) \right| \\ &= \Bigg| \sum_{i_1+\ldots+i_d=p+1} V^{(i_1,\ldots,i_d)}(x_t) \Bigg(\int_{\Delta_d} \frac{x_1^{i_1} \times \ldots \times x_d^{i_d}}{i_1! \times \ldots \times i_d!} dx \\ &\qquad - \frac{1}{d!} \sum_{j=1}^{N_{dp}} w_j \frac{x_{j1}^{i_1} \times \ldots \times x_{jd}^{i_d}}{i_1! \times \ldots \times i_d!} \Bigg) \Bigg| \\ &\le \sum_{i_1+\ldots+i_d=p+1} |V^{(i_1,\ldots,i_d)}| \, \varepsilon_{i_1,\ldots,i_d}, \quad \varepsilon_{i_1,\ldots,i_d} \equiv \varepsilon \left(\frac{x_1^{i_1} \times \ldots \times x_d^{i_d}}{i_1! \times \ldots \times i_d!} \right), \end{aligned} \tag{41}$$

where $|V^{(i_1,\ldots,i_d)}|$ is the absolute maximum value of the mixed derivative on the simplex. As it can be seen from (41), to estimate the errors of quadrature rules, it is enough to calculate the coefficients $\varepsilon_{i_1,\ldots,i_d}$ for the corresponding derivatives. However, there are quite a lot of such coefficients, so to compare the quadrature rules found, we limited ourselves to the largest of the coefficients, $\max \varepsilon_{i_1,\ldots,i_d}$, their sum $\sum \varepsilon_{i_1,\ldots,i_d}$ and the root of the sum of their squares $\sqrt{\sum \varepsilon^2_{i_1,\ldots,i_d}}$, where summation was carried out over sets of numbers $i_1, \ldots, i_d$ at $i_1 + \ldots + i_d = p + 1$ and only one permutation $i_1, \ldots, i_d$ was taken into account. The results obtained are presented in the Tables 6–10.

As a numerical experiment, we consider the class of integrals

$$I_d = \int_{\Delta_d} (x_1 + \ldots + x_d) \exp(-x_1 - \ldots - x_d) dx_1 \ldots dx_d \tag{42}$$

that for $d = 2, \ldots, 6$ are equal to:

$$\begin{aligned} &I_2 = 2 - \frac{5}{e}, \quad I_3 = 3 - \frac{8}{e}, \quad I_4 = 4 - \frac{65}{6e}, \\ &I_5 = 5 - \frac{163}{12e}, \quad I_6 = 6 - \frac{1957}{120e}. \end{aligned} \tag{43}$$

In particular, we calculated the Runge coefficient

$$\beta = \log_2 \left| \frac{\epsilon^q_{\text{test}} - \epsilon^{2q}_{\text{test}}}{\epsilon^{2q}_{\text{test}} - \epsilon^{4q}_{\text{test}}} \right|, \tag{44}$$

on three twice condensed grids with the discrepancies $\epsilon^q_{\text{test}} = I^q_d - I_d$, where I^q_d are the numerical results obtained by splitting the simplex Δ_d into q^d equal simplexes with integration on each of them. The discrepancies ϵ^q_{test} and the Runge coefficient β are presented in Tables 11–15. One can see that for the above quadrature rules, the numerical estimates of the Runge coefficients correspond to the theoretical error estimates.

6. Conclusions

We presented PI-type fully symmetric quadrature rules up to 20-th order on the tetrahedron, 16-th order on 4-simplex, 10-th order on 5- and 6-simplexes with almost minimal numbers of nodes.

We have briefly explained the application of the versions of the LM-type algorithm, adapted to solve different systems of the nonlinear algebraic equations (8) with convex constraints, as well as the corresponding choice of the convex domain for the initial estimations of

Table 7
The same as in Table 6, but for the tetrahedron.

p	N_{dp}	S_4	S_{31}	S_{22}	S_{211}	S_{1111}	$\max \varepsilon_{i_1,i_2,i_3}$	$\sum \varepsilon_{i_1,i_2,i_3}$	$\sqrt{\sum \varepsilon^2_{i_1,i_2,i_3}}$
4	14		2	1			$4.73 \cdot 10^{-8}$	$1.42 \cdot 10^{-7}$	$6.95 \cdot 10^{-8}$
5	14		2	1			$1.43 \cdot 10^{-7}$	$3.98 \cdot 10^{-7}$	$1.96 \cdot 10^{-7}$
6	24		3		1		$4.82 \cdot 10^{-9}$	$1.60 \cdot 10^{-8}$	$6.92 \cdot 10^{-9}$
7	35	1	1	1	2		$1.86 \cdot 10^{-10}$	$9.95 \cdot 10^{-10}$	$3.71 \cdot 10^{-10}$
8	46		4	1	2		$2.80 \cdot 10^{-11}$	$6.09 \cdot 10^{-11}$	$3.24 \cdot 10^{-11}$
9	59	1	4	1	3		$6.19 \cdot 10^{-13}$	$2.03 \cdot 10^{-12}$	$8.83 \cdot 10^{-13}$
10	79	1	3	1	5		$1.47 \cdot 10^{-14}$	$8.40 \cdot 10^{-14}$	$2.68 \cdot 10^{-14}$
11	98		5	1	4	1	$8.59 \cdot 10^{-16}$	$3.39 \cdot 10^{-15}$	$1.21 \cdot 10^{-15}$
12	123	1	5	1	6	1	$8.73 \cdot 10^{-18}$	$6.79 \cdot 10^{-17}$	$2.00 \cdot 10^{-17}$
13	145	1	3	2	8	1	$8.01 \cdot 10^{-19}$	$3.27 \cdot 10^{-18}$	$1.21 \cdot 10^{-18}$
14	175	1	6	1	10	1	$2.23 \cdot 10^{-20}$	$1.11 \cdot 10^{-19}$	$3.49 \cdot 10^{-20}$
15	209	1	4	2	11	2	$5.92 \cdot 10^{-22}$	$4.32 \cdot 10^{-21}$	$1.14 \cdot 10^{-21}$
16	248		8	2	11	3	$1.04 \cdot 10^{-23}$	$9.06 \cdot 10^{-23}$	$2.25 \cdot 10^{-23}$
17	284		8	2	14	3	$5.29 \cdot 10^{-25}$	$3.30 \cdot 10^{-24}$	$8.96 \cdot 10^{-25}$
18	343	1	6	1	18	4	$2.02 \cdot 10^{-27}$	$1.93 \cdot 10^{-26}$	$4.58 \cdot 10^{-27}$
19	383	1	7	3	18	5	$1.37 \cdot 10^{-28}$	$1.50 \cdot 10^{-27}$	$3.39 \cdot 10^{-28}$
20	441	1	8	4	20	6	$8.94 \cdot 10^{-30}$	$4.32 \cdot 10^{-29}$	$1.32 \cdot 10^{-29}$

Table 8
The same as in Table 6, but for the 4-simplex.

p	N_{dp}	S_5	S_{41}	S_{32}	S_{311}	S_{221}	S_{2111}	$\max \varepsilon_{i_1,\dots,i_4}$	$\sum \varepsilon_{i_1,\dots,i_4}$	$\sqrt{\sum \varepsilon^2_{i_1,\dots,i_4}}$
4	20		2	1				$6.23 \cdot 10^{-8}$	$2.88 \cdot 10^{-7}$	$1.20 \cdot 10^{-7}$
5	30		2	2				$1.97 \cdot 10^{-8}$	$6.70 \cdot 10^{-8}$	$2.76 \cdot 10^{-8}$
6	56	1	1	1	2			$2.63 \cdot 10^{-10}$	$1.23 \cdot 10^{-9}$	$4.28 \cdot 10^{-10}$
7	70		2	2	2			$1.03 \cdot 10^{-10}$	$1.95 \cdot 10^{-10}$	$1.08 \cdot 10^{-10}$
8	105		3	2	2	1		$2.15 \cdot 10^{-12}$	$5.70 \cdot 10^{-12}$	$2.49 \cdot 10^{-12}$
9	151	1	2	2	3	2		$4.03 \cdot 10^{-14}$	$2.26 \cdot 10^{-13}$	$6.73 \cdot 10^{-14}$
10	210		4	2	4	3		$1.59 \cdot 10^{-15}$	$9.73 \cdot 10^{-15}$	$2.79 \cdot 10^{-15}$
11	275		3	3	4	3	1	$4.12 \cdot 10^{-17}$	$3.61 \cdot 10^{-16}$	$8.71 \cdot 10^{-17}$
12	370		4	4	5	3	2	$1.06 \cdot 10^{-18}$	$9.59 \cdot 10^{-18}$	$1.97 \cdot 10^{-18}$
13	470		4	5	5	4	3	$4.66 \cdot 10^{-20}$	$3.91 \cdot 10^{-19}$	$9.38 \cdot 10^{-20}$
14	601	1	4	2	10	6	3	$1.42 \cdot 10^{-21}$	$1.36 \cdot 10^{-20}$	$2.89 \cdot 10^{-21}$
15	781	1	4	2	10	8	5	$7.88 \cdot 10^{-23}$	$3.35 \cdot 10^{-22}$	$9.21 \cdot 10^{-23}$
16	956	1	5	4	10	9	7	$2.79 \cdot 10^{-25}$	$4.29 \cdot 10^{-24}$	$7.67 \cdot 10^{-25}$

Table 9
The same as in Table 6, but for the 5-simplex.

p	N_{dp}	S_6	S_{51}	S_{42}	S_{33}	S_{411}	S_{321}	S_{222}	$\max \varepsilon_{i_1,\dots,i_5}$	$\sum \varepsilon_{i_1,\dots,i_5}$	$\sqrt{\sum \varepsilon^2_{i_1,\dots,i_5}}$
4	27	1	1		1				$6.89 \cdot 10^{-8}$	$1.11 \cdot 10^{-7}$	$7.24 \cdot 10^{-8}$
5	37	1	1	2					$1.39 \cdot 10^{-9}$	$4.79 \cdot 10^{-9}$	$2.10 \cdot 10^{-9}$
6	102		2	2			1		$6.31 \cdot 10^{-11}$	$2.22 \cdot 10^{-10}$	$8.12 \cdot 10^{-11}$
7	137		2	1	1	1	1		$1.23 \cdot 10^{-12}$	$9.20 \cdot 10^{-12}$	$2.76 \cdot 10^{-12}$
8	228	1	2	1	1	2	2		$1.34 \cdot 10^{-13}$	$4.92 \cdot 10^{-13}$	$1.68 \cdot 10^{-13}$
9	338		3	2	1	1	4		$1.42 \cdot 10^{-14}$	$2.72 \cdot 10^{-14}$	$1.50 \cdot 10^{-14}$
10	479		4	1	1	3	4	1	$8.36 \cdot 10^{-17}$	$6.05 \cdot 10^{-16}$	$1.51 \cdot 10^{-16}$

Table 10
The same as in Table 6, but for the 6-simplex.

p	N_{dp}	S_7	S_{61}	S_{52}	S_{43}	S_{511}	S_{421}	S_{331}	S_{322}	$\max \varepsilon_{i_1,\dots,i_6}$	$\sum \varepsilon_{i_1,\dots,i_6}$	$\sqrt{\sum \varepsilon^2_{i_1,\dots,i_6}}$
4	43	1	1		1					$2.23 \cdot 10^{-9}$	$4.88 \cdot 10^{-9}$	$-4.03 \cdot 10^{-10}$
5	64	1	1	1	1					$2.45 \cdot 10^{-10}$	$5.89 \cdot 10^{-10}$	$+5.58 \cdot 10^{-11}$
6	175		2	1	1		1			$2.41 \cdot 10^{-12}$	$1.43 \cdot 10^{-11}$	$-2.65 \cdot 10^{-12}$
7	252		2	1	2	1	1			$3.01 \cdot 10^{-13}$	$8.26 \cdot 10^{-13}$	$-1.97 \cdot 10^{-14}$
8	448		3		2	1	3			$7.08 \cdot 10^{-15}$	$3.30 \cdot 10^{-14}$	$+5.80 \cdot 10^{-16}$
9	700		2	2	3	2	1	1	1	$6.48 \cdot 10^{-16}$	$2.05 \cdot 10^{-15}$	$+6.50 \cdot 10^{-18}$
10	1078		2	3	2	3	3	2	1	$3.99 \cdot 10^{-18}$	$3.30 \cdot 10^{-17}$	$-1.59 \cdot 10^{-20}$

Table 11
The differences ϵ^q_{test}, between the numerical and exact values, and the corresponding Runge coefficient β in the numerical experiments (42).

p	ϵ^2_{test}	ϵ^4_{test}	ϵ^8_{test}	β
4	$-3.75\cdot10^{-8}$	$-5.96\cdot10^{-10}$	$-9.35\cdot10^{-12}$	5.97
5	$+5.21\cdot10^{-9}$	$+7.97\cdot10^{-11}$	$+1.24\cdot10^{-12}$	6.03
6	$-6.38\cdot10^{-12}$	$-2.54\cdot10^{-14}$	$-9.98\cdot10^{-17}$	7.97
7	$+1.72\cdot10^{-12}$	$+6.58\cdot10^{-15}$	$+2.55\cdot10^{-17}$	8.03
8	$+7.50\cdot10^{-15}$	$+7.39\cdot10^{-18}$	$+7.23\cdot10^{-21}$	9.99
9	$+3.16\cdot10^{-16}$	$+3.02\cdot10^{-19}$	$+2.93\cdot10^{-22}$	10.03
10	$-4.85\cdot10^{-19}$	$-1.20\cdot10^{-22}$	$-2.94\cdot10^{-26}$	11.98
11	$+1.94\cdot10^{-21}$	$+4.45\cdot10^{-25}$	$+1.07\cdot10^{-28}$	12.09
12	$-7.23\cdot10^{-23}$	$-4.47\cdot10^{-27}$	$-2.73\cdot10^{-31}$	13.98
13	$+2.73\cdot10^{-24}$	$+1.62\cdot10^{-28}$	$+9.84\cdot10^{-33}$	14.04
14	$+3.38\cdot10^{-27}$	$+5.20\cdot10^{-32}$	$+7.95\cdot10^{-37}$	15.99
15	$+3.54\cdot10^{-28}$	$+5.26\cdot10^{-33}$	$+7.98\cdot10^{-38}$	16.04
16	$-1.98\cdot10^{-30}$	$-7.63\cdot10^{-36}$	$-2.92\cdot10^{-41}$	17.99
17	$+1.71\cdot10^{-32}$	$+6.36\cdot10^{-38}$	$+2.41\cdot10^{-43}$	18.03
18	$+5.06\cdot10^{-35}$	$+4.87\cdot10^{-41}$	$+4.65\cdot10^{-47}$	19.99
19	$+8.55\cdot10^{-37}$	$+7.96\cdot10^{-43}$	$+7.53\cdot10^{-49}$	20.04
20	$-2.04\cdot10^{-39}$	$-4.90\cdot10^{-46}$	$+1.06\cdot10^{-52}$	21.99

Table 12
The same as in Table 11, but for the tetrahedron.

p	ϵ^2_{test}	ϵ^4_{test}	ϵ^8_{test}	β
4	$+1.56\cdot10^{-10}$	$+2.20\cdot10^{-12}$	$+3.34\cdot10^{-14}$	6.15
5	$+7.33\cdot10^{-10}$	$+1.09\cdot10^{-11}$	$+1.68\cdot10^{-13}$	6.07
6	$-7.84\cdot10^{-12}$	$-2.98\cdot10^{-14}$	$-1.15\cdot10^{-16}$	8.04
7	$+1.53\cdot10^{-13}$	$+4.90\cdot10^{-16}$	$+1.81\cdot10^{-18}$	8.28
8	$-5.82\cdot10^{-16}$	$-5.56\cdot10^{-19}$	$-5.40\cdot10^{-22}$	10.03
9	$+3.50\cdot10^{-17}$	$+3.59\cdot10^{-20}$	$+3.55\cdot10^{-23}$	9.93
10	$-2.65\cdot10^{-19}$	$-6.27\cdot10^{-23}$	$-1.52\cdot10^{-26}$	12.04
11	$+3.94\cdot10^{-21}$	$+8.32\cdot10^{-25}$	$+1.95\cdot10^{-28}$	12.21
12	$-3.83\cdot10^{-23}$	$-2.28\cdot10^{-27}$	$-1.38\cdot10^{-31}$	14.04
13	$+3.27\cdot10^{-25}$	$+2.18\cdot10^{-29}$	$+1.36\cdot10^{-33}$	13.87
14	$+1.37\cdot10^{-28}$	$+2.02\cdot10^{-33}$	$+3.06\cdot10^{-38}$	16.05
15	$+5.31\cdot10^{-29}$	$+7.87\cdot10^{-34}$	$+1.19\cdot10^{-38}$	16.04
16	$-6.11\cdot10^{-32}$	$-2.27\cdot10^{-37}$	$-8.58\cdot10^{-43}$	18.04
17	$+7.27\cdot10^{-35}$	$-4.62\cdot10^{-40}$	$-2.48\cdot10^{-45}$	17.26
18	$-6.96\cdot10^{-37}$	$-6.36\cdot10^{-43}$	$-6.00\cdot10^{-49}$	20.06
19	$+3.15\cdot10^{-38}$	$+2.06\cdot10^{-44}$	$+1.74\cdot10^{-50}$	20.54
20	$-6.93\cdot10^{-41}$	$-1.61\cdot10^{-47}$	$-9.86\cdot10^{-53}$	22.04

Table 13
The same as in Table 11, but for the 4-simplex.

p	ϵ^2_{test}	ϵ^4_{test}	ϵ^8_{test}	β
4	$-1.46\cdot10^{-9}$	$-2.33\cdot10^{-11}$	$-3.66\cdot10^{-13}$	5.97
5	$+3.62\cdot10^{-11}$	$+3.20\cdot10^{-13}$	$+4.08\cdot10^{-15}$	6.83
6	$-9.17\cdot10^{-13}$	$-3.71\cdot10^{-15}$	$-1.46\cdot10^{-17}$	7.95
7	$-1.57\cdot10^{-14}$	$-6.13\cdot10^{-17}$	$-2.40\cdot10^{-19}$	8.00
8	$-3.88\cdot10^{-17}$	$-2.33\cdot10^{-20}$	$-1.92\cdot10^{-23}$	10.70
9	$-1.69\cdot10^{-18}$	$-1.49\cdot10^{-21}$	$-1.42\cdot10^{-24}$	10.15
10	$-4.05\cdot10^{-20}$	$-9.80\cdot10^{-24}$	$-2.39\cdot10^{-27}$	12.01
11	$+2.28\cdot10^{-22}$	$+4.58\cdot10^{-26}$	$+1.06\cdot10^{-29}$	12.28
12	$-2.88\cdot10^{-24}$	$-1.57\cdot10^{-28}$	$-9.28\cdot10^{-33}$	14.16
13	$+3.51\cdot10^{-26}$	$+1.94\cdot10^{-30}$	$+1.16\cdot10^{-34}$	14.14
14	$+4.83\cdot10^{-29}$	$+9.35\cdot10^{-34}$	$+1.50\cdot10^{-38}$	15.66
15	$+9.87\cdot10^{-31}$	$+1.24\cdot10^{-35}$	$+1.80\cdot10^{-40}$	16.28
16	$+7.13\cdot10^{-33}$	$+2.92\cdot10^{-38}$	$+1.13\cdot10^{-43}$	17.90

Table 14
The same as in Table 11, but for the 5-simplex.

p	ϵ^2_{test}	ϵ^4_{test}	ϵ^8_{test}	β
4	$+2.22\cdot10^{-10}$	$+3.96\cdot10^{-12}$	$+6.38\cdot10^{-14}$	5.80
5	$+1.12\cdot10^{-11}$	$+1.97\cdot10^{-13}$	$+3.17\cdot10^{-15}$	5.83
6	$-8.27\cdot10^{-14}$	$-2.79\cdot10^{-16}$	$-1.05\cdot10^{-18}$	8.21
7	$+1.37\cdot10^{-15}$	$+5.75\cdot10^{-18}$	$+2.30\cdot10^{-20}$	7.90
8	$+1.25\cdot10^{-18}$	$+3.03\cdot10^{-21}$	$+3.39\cdot10^{-24}$	8.69
9	$+6.69\cdot10^{-20}$	$+2.73\cdot10^{-23}$	$+1.62\cdot10^{-26}$	11.26
10	$-2.69\cdot10^{-21}$	$-6.45\cdot10^{-25}$	$-1.57\cdot10^{-28}$	12.02

Table 15
The same as in Table 11, but for the 6-simplex.

p	ϵ^2_{test}	ϵ^4_{test}	ϵ^8_{test}	β
4	$+7.91\cdot10^{-12}$	$+1.73\cdot10^{-13}$	$+2.90\cdot10^{-15}$	5.50
5	$+1.06\cdot10^{-12}$	$+1.81\cdot10^{-14}$	$+2.90\cdot10^{-16}$	5.87
6	$-1.73\cdot10^{-14}$	$-7.35\cdot10^{-17}$	$-2.93\cdot10^{-19}$	7.88
7	$-1.81\cdot10^{-16}$	$-8.02\cdot10^{-19}$	$-3.22\cdot10^{-21}$	7.82
8	$+2.09\cdot10^{-18}$	$+2.34\cdot10^{-21}$	$+2.35\cdot10^{-24}$	9.80
9	$-3.86\cdot10^{-20}$	$-5.12\cdot10^{-23}$	$-5.34\cdot10^{-26}$	9.56
10	$-1.18\cdot10^{-22}$	$-3.63\cdot10^{-26}$	$-9.35\cdot10^{-30}$	11.66

the weights and nodes (35), (36). Table 5, which compares the minimal number of nodes for PI-type fully symmetric p-order quadrature rules with known ones, points to an increased efficiency of the present quadrature rules, especially in the higher order cases. We presented error estimates of the obtained quadrature rules. The quadrature rules are given in compact form. Programs for converting in expanded form are presented in the JINRLIB Program Library [37].

For high dimensional cases the rapid growth of the number of independent equations with increasing order of the quadrature rule, and a large number of different systems, depending on the combinations of the orbits, which lead to the problem of constructing initial estimations for the iterative process. We have already encountered this problem at $p = 10$ and $d = 6$ and we expect it at $p = 8$ and $d > 6$. To construct a quadrature formula of the 6-th order, the system to be solved contains 11 equations, and at the present time fast solution is obtained by the considered computational methods.

It should be noted, that we have already used the obtained quadrature rules for the FEM solution of 2 and 3 dimensional boundary value problems in the calculation of the spectral and optical characteristics of the helium atom [38], the axially symmetric quantum dots [39] and the collective nuclear model with tetrahedral symmetry [40]. We plan to use the obtained quadrature rules in solving multidimensional (up to 6-dimensional) boundary value problems by the FEM method for the quadrupole-octupole collective nuclear models [41,42] and for the models of complex physical systems considered in [43].

CRediT authorship contribution statement

G. Chuluunbaatar: Software, Visualization, Conceptualization. **O. Chuluunbaatar:** Software, Visualization, Conceptualization, Supervision, Writing–original draft, Writing–review, editing. **A.A. Gusev:** Software, Visualization, Conceptualization, Supervision, Writing–original draft, Writing–review, editing. **S.I. Vinitsky:** Conceptualization, Writing–original draft.

Data availability

Data will be made available on request.

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Appendix A. INQSIM: A program for converting PI-type fully symmetric quadrature rules on 2-, ..., 6-simplexes from compact form to expanded form

The *.mw and *.f files contain the Maple and Fortran programs for converting quadrature formulas up to the 20-th order on a triangle and a tetrahedron, the 16-th order on a 4-simplex, the 10-th order on 5- and 6-simplexes from compact form to expanded form [37], and examples of their application:

- on INPUT
  - 'ddxoy_z.dat' file,
- on OUTPUT
  - wg is an array of weights with a dimension of gnodes,
  - xg is an array of BC of nodes with a dimension of $(\dim+1)\times$ gnodes.

The "ddxoy_z.dat" files contain the dimension of the simplex, the order of the quadrature rule, the number of nodes, the information about orbits, and PI-type fully symmetric quadrature rules in BC $(y_1, \ldots, y_{d+1})$ in compact form, where

- x = dim means the dimension of the simplex,
- y = p means the order of the quadrature rule,
- z = gnodes means the number of nodes.

As test examples, we consider the integrals (42). Convergence of quadrature rules of order p to exact values is given in the output files [37].

Appendix B. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.camwa.2022.08.016. It contains "ddxoy_z.dat" files with the PI-type fully symmetric quadrature rules in compact form (50 digits of precision):

- second line: the dimension of the simplex, the order of the quadrature rule, the number of nodes;
- fourth line: the number of orbits of each type, in the same order as in Table 1;
- next lines: for each orbit: first weights of the quadrature formula, then different BCs λ_i of the nodes from (4), ordered by the numbers m_i from (5), the last λ_i can be found from (5) and is not printed.

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