Symbolic-Numerical Algorithm for Generating Interpolation Multivariate Hermite Polynomials of High-Accuracy Finite Element Method

A.A. Gusev[1(✉)], V.P. Gerdt[1,2], O. Chuluunbaatar[1,3], G. Chuluunbaatar[1], S.I. Vinitsky[1,2], V.L. Derbov[4], and A. Góźdź[5]

[1] Joint Institute for Nuclear Research, Dubna, Russia
gooseff@jinr.ru
[2] RUDN University, 6 Miklukho-Maklaya St., Moscow 117198, Russia
[3] Institute of Mathematics, National University of Mongolia, Ulaanbaatar, Mongolia
[4] N.G. Chernyshevsky Saratov National Research State University, Saratov, Russia
[5] Institute of Physics, University of M. Curie-Skłodowska, Lublin, Poland

Abstract. A symbolic-numerical algorithm implemented in Maple for constructing Hermitian finite elements is presented. The basis functions of finite elements are high-order polynomials, determined from a specially constructed set of values of the polynomials themselves, their partial derivatives, and their derivatives along the directions of the normals to the boundaries of finite elements. Such a choice of the polynomials allows us to construct a piecewise polynomial basis continuous across the boundaries of elements together with the derivatives up to a given order, which is used to solve elliptic boundary value problems using the high-accuracy finite element method. The efficiency and the accuracy order of the finite element scheme, algorithm and program are demonstrated by the example of the exactly solvable boundary-value problem for a triangular membrane, depending on the number of finite elements of the partition of the domain and the number of piecewise polynomial basis functions.

Keywords: Hermite interpolation polynomials · Boundary-value problem · High-accuracy finite element method

1 Introduction

In Refs. [9,10], the symbolic-numeric algorithms and programs for the solution of boundary-value problems for a system of second-order ordinary differential equations using the finite element method (FEM) of high accuracy order with Hermite interpolation polynomials (HIP) were developed, aimed at the calculation of spectral and optical characteristics of quantum systems.

It is known that the approximating function of the boundary-value problem solution in the entire domain can be expressed by means of its values and the values of its derivatives at the node points of the domain via the basis functions,

V.P. Gerdt et al. (Eds.): CASC 2017, LNCS 10490, pp. 134–150, 2017.
DOI: 10.1007/978-3-319-66320-3_11

referred to as Lagrange interpolation polynomials (LIP), which are nonzero only on a few elements, adjacent to the corresponding nodes. Generally, the approximating function for the entire domain is represented in terms of linear combinations of the basis functions. The coefficients of these linear combinations are the values of the approximating function and its directional derivatives on a given mesh of nodes. The basis functions themselves or their directional derivatives take a unit value at one of the nodes. In many cases, the schemes are restricted to the set of node values of the basis functions themselves. However, there are problems, in which the values of directional derivatives are also necessary. They are of particular importance when high smoothness between the elements is required, or when the gradient of solution is to be determined with increased accuracy. The construction of such basis functions, referred to as Hermite interpolation polynomials, is not possible on an arbitrary mesh of nodes. It is one of the most important and difficult problems in the finite element method and its applications in different fields, solved to date in the explicit form only for certain particular cases [1,2,4–8,11,13,14,17,19,21].

This motivation determines the aim of the present work, namely, the development of a symbolic-numerical algorithm implemented in any CAS for computing in analytical form the basis functions of Hermitian finite elements for a few variables and their application to constructing the FEM schemes with high order of accuracy.

In the paper, we present the symbolic-numeric algorithm implemented in the CAS Maple [15] for constructing the interpolation polynomials (basis functions) of Hermitian finite elements of a few variables based on a specially constructed set of values of the polynomials themselves, their partial derivatives, and derivatives along the normals to the boundaries of finite elements. The corresponding piecewise continuous basis of the high-order accuracy FEM provides the continuity not only of the approximate solution, but also of its derivatives to a given order depending on the smoothness of the variable coefficients of the equation and the domain boundary. This basis is used to construct the FEM scheme for high-accuracy solution of elliptic boundary-value problems in the bounded domain of multidimensional Euclidean space, specified as a polyhedral domain. We also used the symbolic algorithm to generate Fortran routines that allow the solution of the generalized algebraic eigenvalue problem with high-dimension matrices. The efficiency of the FEM scheme, the algorithm, and the program is demonstrated by constructing typical bases of Hermitian finite elements and their application to the benchmark exactly solvable boundary-value eigenvalue problem for a triangle membrane.

The paper is organized as follows. In Sect. 2, the setting of the boundary-value eigenvalue problem is given. In Sect. 3, we formulate the symbolic-numeric algorithm for generating the bases of Hermitian finite elements with multiple variables. In Sect. 4, we present the results of the calculations for the benchmark boundary-value problem, demonstrating the efficiency of the FEM scheme. In the Conclusion, we discuss the prospects of development of the proposed algorithm of constructing the Hermitian finite elements and its applications to high-order accuracy FEM schemes.

2 Setting of the Problem

Consider a self-adjoint boundary-value problem for the elliptic differential equation of the second order:

$$(D-E)\,\Phi(z) \equiv \left(-\frac{1}{g_0(z)}\sum_{ij=1}^{d}\frac{\partial}{\partial z_i}g_{ij}(z)\frac{\partial}{\partial z_j}+V(z)-E\right)\Phi(z)=0. \quad (1)$$

For the principal part coefficients of Eq. (1), the condition of uniform ellipticity holds in the bounded domain $z=(z_1,\ldots,z_d)\in\Omega$ of the Euclidean space $\mathcal{R}^d$, i.e., the constants $\mu>0$, $\nu>0$ exist such that $\mu\xi^2 \le \sum_{ij=1}^{d} g_{ij}(z)\xi_i\xi_j \le \nu\xi^2$, $\xi^2=\sum_{i=1}^{d}\xi_i^2$ $\forall\xi\in\mathcal{R}^d$. The left-hand side of this inequality expresses the requirement of ellipticity, while the right-hand side expresses the boundedness of the coefficients $g_{ij}(z)$. It is also assumed that $g_0(z)>0$, $g_{ji}(z)=g_{ij}(z)$ and $V(z)$ are real-valued functions, continuous together with their generalized derivatives to a given order in the domain $z\in\bar{\Omega}=\Omega\cup\partial\Omega$ with the piecewise continuous boundary $S=\partial\Omega$, which provide the existence of nontrivial solutions obeying the boundary conditions [6,12] of the first kind

$$\Phi(z)|_S=0, \quad (2)$$

or the second kind

$$\left.\frac{\partial\Phi(z)}{\partial n_D}\right|_S=0, \quad \frac{\partial\Phi(z)}{\partial n_D}=\sum_{ij=1}^{d}(\hat{n},\hat{e}_i)g_{ij}(z)\frac{\partial\Phi(z)}{\partial z_j}, \quad (3)$$

where $\frac{\partial\Phi_m(z)}{\partial n_D}$ is the derivative along the conormal direction, $\hat{n}$ is the outer normal to the boundary of the domain $S=\partial\Omega$, $\hat{e}_i$ is the unit vector of $z=\sum_{i=1}^{d}\hat{e}_i z_i$, and $(\hat{n},\hat{e}_i)$ is the scalar product in $\mathcal{R}^d$.

For a discrete spectrum problem, the functions $\Phi_m(z)$ from the Sobolev space $H_2^{s\ge1}(\Omega)$, $\Phi_m(z)\in H_2^{s\ge1}(\Omega)$, corresponding to the real eigenvalues E: $E_1\le E_2\le\ldots\le E_m\le\ldots$ satisfy the conditions of normalization and orthogonality

$$\langle\Phi_m(z)|\Phi_{m'}(z)\rangle=\int_\Omega dz g_0(z)\Phi_m(z)\Phi_{m'}(z)=\delta_{mm'}, \quad dz=dz_1\ldots dz_d. \quad (4)$$

The FEM solution of the boundary-value problems (1)–(4) is reduced to the determination of stationary points of the variational functional [3,6]

$$\Xi(\Phi_m,E_m,z)\equiv\int_\Omega dz g_0(z)\Phi_m(z)\,(D-E_m)\,\Phi(z)=\Pi(\Phi_m,E_m,z), \quad (5)$$

where $\Pi(\Phi_m,E_m,z)$ is the symmetric quadratic functional

$$\Pi(\Phi_m,E_m,z)=\int_\Omega dz\left[\sum_{ij=1}^{d}g_{ij}(z)\frac{\partial\Phi_m(z)}{\partial z_i}\frac{\partial\Phi_m(z)}{\partial z_j}+g_0(z)\Phi_m(z)(V(z)-E_m)\Phi_m(z)\right].$$

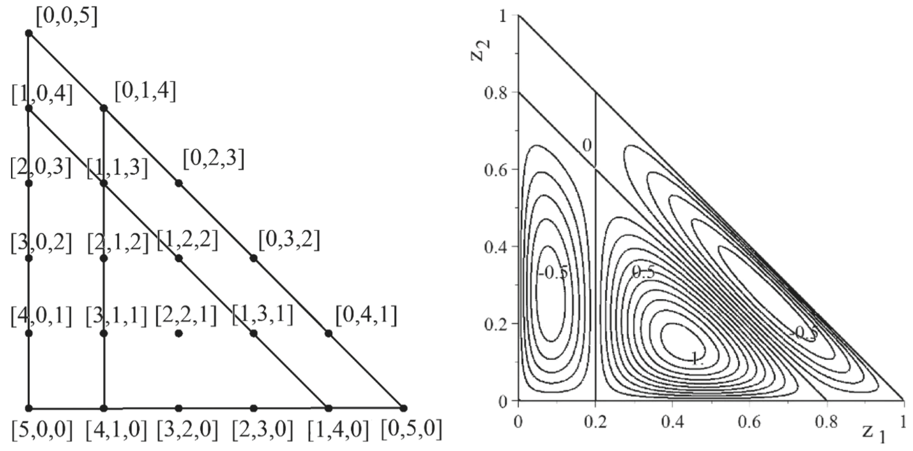

Fig. 1. (a) Enumeration of nodes A_r, $r = 1, \ldots, (p+1)(p+2)/2$ with sets of numbers $[n_0, n_1, n_2]$ for the standard (canonical) triangle element Δ in the scheme with the fifth-order LIP $p' = p = 5$ at $d = 2$. The lines (five crossing straight lines) are zeros of LIP $\varphi_{14}(z')$ from (12), equal to 1 at the point labeled with the number triple $[n_0, n_1, n_2] = [2, 2, 1]$. (b) LIP isolines of $\varphi_{14}(z')$

3 FEM Calculation Scheme

In FEM, the domain $\Omega = \Omega_h(z) = \bigcup_{q=1}^{Q} \Delta_q$, specified as a polyhedral domain, is covered with finite elements, in the present case, the simplexes Δ_q with $d+1$ vertices $\hat{z}_i = (\hat{z}_{i1}, \hat{z}_{i2}, \ldots, \hat{z}_{id})$ with $i = 0, \ldots, d$. Each edge of the simplex Δ_q is divided into p equal parts, and the families of parallel hyperplanes $H(i,k)$ are drawn, numbered with the integers $k = 0, \ldots, p$, starting from the corresponding face, e.g., as shown for $d = 2$ in Fig. 1 (see also [6]). The equation of the hyperplane is $H(i,k) : H(i;z) - k/p = 0$, where $H(i;z)$ is a linear function of z.

The node points of hyperplanes crossing A_r are enumerated with sets of integers $[n_0, \ldots, n_d]$, $n_i \geq 0$, $n_0 + \ldots + n_d = p$, where n_i, $i = 0, 1, \ldots, d$ are the numbers of hyperplanes, parallel to the simplex face, not containing the i-th vertex $\hat{z}_i = (\hat{z}_{i1}, \ldots \hat{z}_{id})$. The coordinates $\xi_r = (\xi_{r1}, \ldots, \xi_{rd})$ of the node point $A_r \in \Delta_q$ are calculated using the formula

$$(\xi_{r1}, \ldots, \xi_{rd}) = (\hat{z}_{01}, \ldots, \hat{z}_{0d}) n_0/p + (\hat{z}_{11}, \ldots, \hat{z}_{1d}) n_1/p + \ldots + (\hat{z}_{d1}, \ldots, \hat{z}_{dd}) n_d/p \quad (6)$$

from the coordinates of the vertices $\hat{z}_j = (\hat{z}_{j1}, \ldots, \hat{z}_{jd})$. Then the LIP $\varphi_r(z)$ equal to one at the point A_r with the coordinates $\xi_r = (\xi_{r1}, \ldots, \xi_{rd})$, characterized by the numbers $[n_0, n_1, \ldots, n_d]$, and equal to zero at the remaining points $\xi_{r'}$, i.e., $\varphi_r(\xi_{r'}) = \delta_{rr'}$, has the form

$$\varphi_r(z) = \left(\prod_{i=0}^{d} \prod_{n_i'=0}^{n_i - 1} \frac{H(i;z) - n_i'/p}{H(i;\xi_r) - n_i'/p} \right). \quad (7)$$

Note that the construction of the HIP $\varphi_r^\kappa(z)$, where $\kappa \equiv \kappa_1, \ldots, \kappa_d$, with the fixed values of the functions $\{\varphi_r^\kappa(\xi_{r'})\}$ and the derivatives $\{\partial^{\bullet}_{\bullet}\varphi_r^\kappa(z)|_{z=\xi_{r'}}\}$ at the nodes $\xi_{r'}$, already at $d = 2$ leads to cumbersome expressions, improper for FEM using nonuniform mesh.

The economical implementation of FEM is the following:

1. The calculations are performed in the local (reference) coordinates z', in which the coordinates of the simplex vertices are the following: $\hat{z}'_j = (\hat{z}'_{j1}, \ldots, \hat{z}'_{jd})$, $\hat{z}'_{jk} = \delta_{jk}$,
2. The HIP in the physical coordinates z in the mesh is sought in the form of linear combinations of polynomials in the local coordinates z', the transition to the physical coordinates is executed only at the stage of numerical solution of a particular boundary-value problem (1)–(5),
3. The calculation of FEM integrals is executed in the local coordinates.

Let us construct the HIP on an arbitrary d-dimensional simplex Δ_q with the $d+1$ vertices $\hat{z}_i = (\hat{z}_{i1}, \hat{z}_{i2}, \ldots, \hat{z}_{id})$, $i = 0, \ldots, d$. For this purpose, we introduce the local coordinate system $z' = (z'_1, z'_2, \ldots, z'_d) \in \mathcal{R}^d$, in which the coordinates of the simplex vertices are the following: $\hat{z}'_i = (\hat{z}'_{ik} = \delta_{ik}, k = 1, \ldots, d)$. The relation between the coordinates is given by the formula:

$$z_i = \hat{z}_{0i} + \sum_{j=1}^{d} \hat{J}_{ij} z'_j, \quad i = 1, \ldots, d, \quad \hat{J}_{ij} = \hat{z}_{ji} - \hat{z}_{0i}. \tag{8}$$

The inverse transformation and the relation between the differentiation operators are given by the formulas

$$z'_i = \sum_{j=1}^{d} (\hat{J}^{-1})_{ij}(z_j - \hat{z}_{0j}), \tag{9}$$

$$\frac{\partial}{\partial z'_i} = \sum_{j=1}^{d} \hat{J}_{ji} \frac{\partial}{\partial z_j}, \quad \frac{\partial}{\partial z_i} = \sum_{j=1}^{d} (\hat{J}^{-1})_{ji} \frac{\partial}{\partial z'_j}. \tag{10}$$

Equation (10) is used to calculate the HIP $\varphi_r^\kappa(z') = \{\check{\varphi}_r^\kappa(z'), Q_s(z')\}$ from (20) that satisfy the conditions (13), (17), and (18) of the next section, with the fixed derivatives to the given order at the nodes $\xi_{r'}$. In this case, the derivatives along the normal to the element boundary in the physical coordinate system are, generally, not those in the local coordinates z'. When constructing the HIP in the local coordinates z' one has to recalculate the fixed derivatives at the nodes $\xi_{r'}$ of the element Δ_q to the nodes $\xi'_{r'}$ of the element Δ, using the matrices $\hat{J}^{-1}$, given by cumbersome expressions. Therefore, the required recalculation is executed based on the relations (8)–(10) for each finite element Δ_q at the stage of the formation of the HIP basis $\{\varphi_r^{\bar{\kappa}'}(z')\}_{r=1}^P$ on the finite element Δ, implemented numerically using the analytical formulas, presented in the next section.

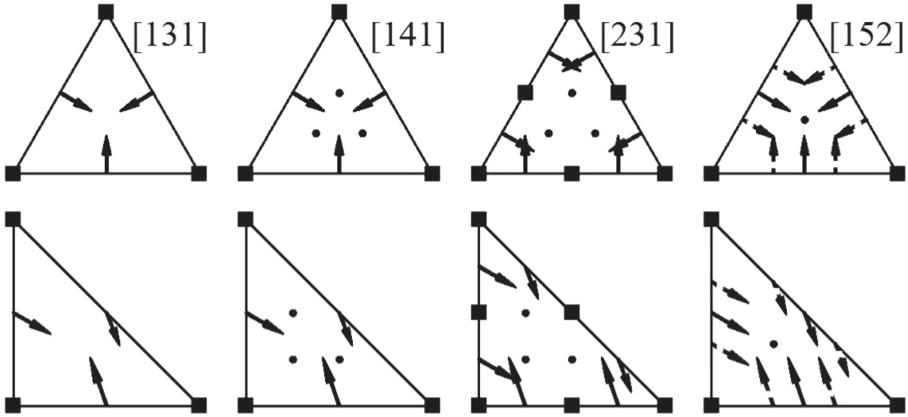

Fig. 2. Schematic diagram of the conditions on the element Δ_q (upper panel) and Δ (lower panel) for constructing the basis of HIP $[p\kappa_{\max}\kappa']$: [131], [141], [231], [152]. The squares are the points ξ'_r, where the values of the functions and their derivatives are fixed according to the conditions (13), (16); the solid (dashed) arrows begin at the points η'_s, where the values of the first (second) derivative in the direction of the normal in the physical coordinates are fixed, according to the condition (17), respectively; the circles are the points ζ'_s, where the values of the functions are fixed according to the condition (18)

The integrals that enter the variational functional (5) on the domain $\Omega_h(z) = \bigcup_{q=1}^{Q} \Delta_q$, are expressed via the integrals, calculated on the element Δ_q, and recalculated to the local coordinates z' on the element Δ,

$$\int\limits_{\Delta_q} dz g_0(z)\varphi_r^{\kappa}(z)\varphi_{r'}^{\kappa''}(z)U(z) = J\int\limits_{\Delta} dz' g_0(z(z'))\varphi_r^{\kappa}(z')\varphi_{r'}^{\kappa''}(z')U(z(z')), \tag{11}$$

$$\int\limits_{\Delta_q} dz g_{s_1 s_2}(z)\frac{\partial\varphi_r^{\kappa}(z)}{\partial z_{s_1}}\frac{\partial\varphi_{r'}^{\kappa''}(z)}{\partial z_{s_2}} = J\sum_{t_1,t_2=1}^{d}\hat{J}^{-1}_{s_1 s_2;t_1 t_2}\int\limits_{\Delta} dz' g_{s_1 s_2}(z(z'))\frac{\partial\varphi_r^{\kappa}(z')}{\partial z'_{t_1}}\frac{\partial\varphi_{r'}^{\kappa''}(z')}{\partial z'_{t_2}},$$

where $J = \det\hat{J} > 0$ is the determinant of the matrix $\hat{J}$ from Eq. (8), $\hat{J}^{-1}_{s_1 s_2;t_1 t_2} = (\hat{J}^{-1})_{t_1 s_1}(\hat{J}^{-1})_{t_2 s_2}$, $dz' = dz'_1 \ldots dz'_d$, and $\varphi_r^{\kappa}(z') = \{\check{\varphi}_r^{\kappa}(z'), Q_s(z')\}$ from Eq. (20).

3.1 Lagrange Interpolation Polynomials

In the local coordinates, the LIP $\varphi_r(z')$ is equal to one at the node point ξ'_r characterized by the numbers $[n_0, n_1, \ldots, n_d]$, and zero at the remaining node points $\xi'_{r'}$, i.e., $\varphi_r(\xi'_{r'}) = \delta_{rr'}$, are determined by Eq. (7) at $H(0; z') = 1 - z'_1 - \ldots - z'_d$, $H(i; z') = z'_i$, $i = 1, \ldots, d$:

Table 1. Characteristics of the HIP bases (20) at $d = 2$

	$[p\kappa_{\max}\kappa']$	[131]	[141]	[231]	[152]	[162]	[241]	[173]
p'	$\kappa_{\max}(p+1)-1$	5	7	8	9	11	11	13
$N_{\kappa_{\max}p'}$	$(p+1)(p+2)\kappa_{\max}(\kappa_{\max}+1)/4$	18	30	36	45	63	60	84
$N_{1p'}$	$(p'+1)(p'+2)/2$	21	36	45	55	78	78	105
K	$p(p+1)\kappa_{\max}(\kappa_{\max}-1)/4$	3	6	9	10	15	9	21
$T_1(1)$	$3p$	3	3	6	3	3	6	3
$T_1(2)$	$9p$	9	9	18	9	9	18	9
N(AP1)	$N_{\kappa_{\max}p'}$	18	30	36	45	63	60	84
N(AP2)	$T_1(\kappa')$	3	3	6	9	9	6	18
N(AP3)	$K - T_1(\kappa')$	0	3	3	1	6	12	3
Restriction of derivative order κ' :	$3p\kappa'(\kappa'+1)/2 \le K$							

$$\varphi_r(z') = \left(\prod_{i=1}^{d}\prod_{n_i'=0}^{n_i-1}\frac{z_i'-n_i'/p}{n_i/p-n_i'/p}\right)\left(\prod_{n_0'=0}^{n_0-1}\frac{1-z_1'-\ldots-z_d'-n_0'/p}{n_0/p-n_0'/p}\right). \quad (12)$$

Setting the numerators in Eq. (12) equal to zero yields the families of equations for the straight lines, directed "horizontally", "vertically", and "diagonally" in the local coordinate system of the element Δ, which is related by the affine transformation with the "oblique" family of straight lines of the element Δ_q. In Fig. 1, an example is presented that illustrates the construction of the LIP at $d = 2$, $r, r' = 1, \ldots, (p+1)(p+2)/2$, $p = 5$ on the element Δ in the form of a rectangular triangle with the vertices $\hat{z}_0' = (\hat{z}_{01}', \hat{z}_{02}') = (0, 0)$, $\hat{z}_1' = (\hat{z}_{11}', \hat{z}_{12}') = (1, 0)$, $\hat{z}_2' = (\hat{z}_{21}', \hat{z}_{22}') = (0, 1)$.

The piecewise polynomial functions $P_{\bar{l}}(z)$ forming the finite-element basis $\{P_{\bar{l}}(z)\}_{\bar{l}=1}^{P}$, which are constructed by joining the LIP $\varphi_r(z)$ of Eq. (7), obtained from Eq. (12) by means of the transformation (9), on the finite elements Δ_q:

$$P_l(z) = \{\varphi_l(z),\ A_l \in \Delta_q;\ 0, A_l \notin \Delta_q\},$$

are continuous, but their derivatives are discontinuous at the boundaries of the elements Δ_q.

3.2 Algorithm for Calculating the Basis of Hermite Interpolating Polynomials

Let us construct the HIP of the order p' by joining of which the piecewise polynomial functions (27) with the continuous derivatives up to the given order κ' can be obtained.

Step 1. Auxiliary Polynomials (AP1). To construct HIP in the local coordinates z', let us introduce the set of auxiliary polynomials (AP1)

$$\varphi_r^{\kappa_1\ldots\kappa_d}(\xi'_r) = \delta_{rr'}\delta_{\kappa_1 0}\ldots\delta_{\kappa_d 0}, \quad \left.\frac{\partial^{\mu_1\ldots\mu_d}\varphi_r^{\kappa_1\ldots\kappa_d}(z')}{\partial z_1'^{\mu_1}\ldots\partial z_d'^{\mu_d}}\right|_{z'=\xi'_{r'}} = \delta_{rr'}\delta_{\kappa_1\mu_1}\ldots\delta_{\kappa_d\mu_d}, \quad (13)$$

$$0 \le \kappa_1+\kappa_2+\ldots+\kappa_d \le \kappa_{\max}-1, \quad 0 \le \mu_1+\mu_2+\ldots+\mu_d \le \kappa_{\max}-1.$$

Here at the node points ξ'_r, defined according to (6), in contrast to LIP, the values of not only the functions themselves, but of their derivatives to the order $\kappa_{\max}-1$ are specified. AP1 are given by the expressions

$$\varphi_r^{\kappa_1\kappa_2\ldots\kappa_d}(z') = w_r(z')\sum_{\mu\in\Delta_\kappa} a_r^{\kappa_1\ldots\kappa_d,\mu_1\ldots\mu_d}(z'_1-\xi'_{r1})^{\mu_1}\times\ldots\times(z'_d-\xi'_{rd})^{\mu_d}, \quad (14)$$

$$w_r(z') = \left(\prod_{i=1}^{d}\prod_{n'_i=0}^{n_i-1}\frac{(z'_i-n'_i/p)^{\kappa^{\max}}}{(n_i/p-n'_i/p)^{\kappa^{\max}}}\right)\left(\prod_{n'_0=0}^{n_0-1}\frac{(1-z'_1-\ldots-z'_d-n'_0/p)^{\kappa^{\max}}}{(n_0/p-n'_0/p)^{\kappa^{\max}}}\right),$$

$$w_r(\xi'_r) = 1,$$

where the coefficients $a_r^{\kappa_1\ldots\kappa_d,\mu_1\ldots\mu_d}$ are calculated from recurrence relations obtained by substitution of Eq. (14) into conditions (13),

$$a_r^{\kappa_1\ldots\kappa_d,\mu_1\ldots\mu_d} = \begin{cases} 0, \quad \mu_1+\ldots+\mu_d \le \kappa_1+\ldots+\kappa_d, (\mu_1,\ldots,\mu_d)\ne(\kappa_1,\ldots,\kappa_d), \\ \prod_{i=1}^{d}\frac{1}{\mu_i!}, \qquad (\mu_1,\ldots,\mu_d)=(\kappa_1,\ldots,\kappa_d); \\ -\sum_{\nu\in\Delta_\nu}\left(\prod_{i=1}^{d}\frac{1}{(\mu_i-\nu_i)!}\right) g_r^{\mu_1-\nu_1,\ldots,\mu_d-\nu_d}(\xi'_r)a_r^{\kappa_1\ldots\kappa_d,\nu_1\ldots\nu_d}, \\ \qquad \mu_1+\ldots+\mu_d > \kappa_1+\ldots+\kappa_d; \end{cases} \quad (15)$$

$$g^{\kappa_1\kappa_2\ldots\kappa_d}(z') = \frac{1}{w_r(z')}\frac{\partial^{\kappa_1\kappa_2\ldots\kappa_d}w_r(z')}{\partial z_1'^{\kappa_1}\partial z_2'^{\kappa_2}\ldots\partial z_d'^{\kappa_d}}.$$

For $d>1$ and $\kappa_{\max}>1$, the number $N_{\kappa_{\max}p'}$ of HIP of the order p' and the multiplicity of nodes $\kappa_{\max}$ are smaller than the number $N_{1p'}$ of the polynomials that form the basis in the space of polynomials of the order p' (e.g., the LIP from (12)), i.e., the polynomials satisfying Eq. (13) are determined not uniquely.

Table 2. The HIP $p=1$, $\kappa_{\max}=3$, $\kappa'=1$, $p'=5$ (the Argyris element [5,6,14])

AP1 : $\xi_1=(0,1),\ \xi_2=(1,0),\xi_3=(0,0)$		
$\varphi_1^{0,0}=z_2^3(6z_2^2-15z_2+10)$	$\varphi_2^{0,0}=z_1^3(6z_1^2-15z_1+10)$	$\varphi_3^{0,0}=z_0^3(6z_0^2-15z_0+10)$
$\varphi_1^{0,1}=-z_2^3(z_2-1)(3z_2-4)$	$\varphi_2^{0,1}=-z_1^3z_2(3z_1-4)$	$\varphi_3^{0,1}=-z_0^3z_2(3z_0-4)$
$\varphi_1^{1,0}=-z_1z_2^3(3z_2-4)$	$\varphi_2^{1,0}=-z_1^3(z_1-1)(3z_1-4)$	$\varphi_3^{1,0}=-z_0^3z_1(3z_0-4)$
$\varphi_1^{0,2}=z_2^3(z_2-1)^2/2$	$\varphi_2^{0,2}=z_1^3z_2^2/2$	$\varphi_3^{0,2}=z_0^3z_2^2/2$
$\varphi_1^{1,1}=z_1z_2^3(z_2-1)$	$\varphi_2^{1,1}=(z_1-1)z_1^3z_2$	$\varphi_3^{1,1}=z_0^3z_1z_2$
$\varphi_1^{2,0}=z_1^2z_2^3/2$	$\varphi_2^{2,0}=z_1^3(z_1-1)^2/2$	$\varphi_3^{2,0}=z_0^3z_1^2/2$
AP2 : $\eta_1=(0,1/2),\eta_2=(1/2,0),\eta_3=(1/2,1/2)$		
$Q_1=16z_0^2z_1z_2^2/f_{11}$	$Q_2=16z_0^2z_1^2z_2/f_{22}$	$Q_3=-8z_0z_1^2z_2^2/f_{01}$

Step 2. Auxiliary Polynomials (AP2 and AP3). For unique determination of the polynomial basis let us introduce $K = N_{1p'} - N_{\kappa_{\max}p'}$ auxiliary polynomials $Q_s(z)$ of two types: AP2 and AP3, linearly independent of AP1 from (14) and satisfying the following conditions at the node points $\xi'_{r'}$ of AP1:

$$Q_s(\xi'_{r'}) = 0, \quad \left.\frac{\partial^{\kappa'_1\kappa'_2\ldots\kappa'_d} Q_s(z')}{\partial {z'_1}^{\mu_1}\partial {z'_2}^{\mu_2}\ldots\partial {z'_d}^{\mu_d}}\right|_{z'=\xi'_{r'}} = 0, \quad s = 1,\ldots,K, \quad (16)$$

$$0 \le \kappa_1 + \kappa_2 + \ldots + \kappa_d \le \kappa_{\max} - 1, \quad 0 \le \mu_1 + \mu_2 + \ldots + \mu_d \le \kappa_{\max} - 1.$$

Note that to provide the continuity of derivatives the part of polynomials referred to as AP2 must satisfy the condition

$$\left.\frac{\partial^k Q_s(z')}{\partial n^k_{i(s)}}\right|_{z'=\eta'_{s'}} = \delta_{ss'}, \quad s, s' = 1,\ldots,T_1(\kappa'), \quad k = k(s'), \quad (17)$$

where $\eta'_{s'} = (\eta'_{s'1},\ldots,\eta'_{s'd})$ are the chosen points lying on the faces of various dimensionalities (from 1 to $d-1$) of the d-dimensional simplex Δ and not coincident with the nodal points of HIP ξ'_r, where (13) is valid, $\partial/\partial n_{i(s)}$ is the directional derivative along the vector n_i, normal to the corresponding ith face of the d-dimensional simplex Δ_q at the point $\eta_{s'}$ in the physical coordinate system, which is recalculated to the point $\eta'_{s'}$ of the face of the simplex Δ in the local coordinate system using relations (8)–(10), e.g., for $d = 2$ see Eq. (25). Calculating the number $T_1(\kappa)$ of independent parameters required to provide the continuity of derivatives to the order κ, we determine its maximal value κ' that can be obtained for the schemes with given p and $\kappa_{\max}$ and, correspondingly, the additional conditions (17).

$T_2 = K - T_1(\kappa')$ parameters remain independent and, correspondingly, T_2 additional conditions are added, necessary for the unique determination of the polynomials referred to as AP3,

$$Q_s(\zeta'_{s'}) = \delta_{ss'}, \quad s, s' = T_1(\kappa') + 1,\ldots,K, \quad (18)$$

where $\zeta'_{s'} = (\zeta'_{s'1},\ldots,\zeta'_{s'd}) \in \Delta$ are the chosen points belonging to the simplex without the boundary, but not coincident with the node points of AP1 ξ'_r.

The auxiliary polynomials AP2 are given by the expression

$$Q_s(z') = \left(\prod_{t=0}^{d} {z'_t}^{k_t}\right) \sum_{j_1,\ldots,j_d} b_{j_1,\ldots,j_d;s} {z'_1}^{j_1}\ldots{z'_d}^{j_d}, \quad z'_0 = 1 - z'_1 - \ldots - z'_d, \quad (19)$$

where $k_t = 1$, if the point η_s, in which the additional conditions (17) are specified, lies on the corresponding face of the simplex Δ, i.e., $H(t, \eta_s) = 0$, and $k_t = \kappa'$, if $H(t, \eta_s) \ne 0$. The auxiliary polynomials AP3 are given by the expression (19) at $k_t = \kappa'$. The coefficients $b_{j_1,\ldots,j_d;s}$ are determined from the uniquely solvable system of linear equations, obtained as a result of the substitution of the expression (19) into conditions (16)–(18).

Table 3. The HIP $p=1$, $\kappa_{\max}=4$, $\kappa'=1$, $p'=7$

AP1 : $\xi_1=(0,1),\ \xi_2=(1,0),\xi_3=(0,0)$		
$\varphi_1^{0,0}=-z_2^4P_0(z_3)$	$\varphi_2^{0,0}=-z_1^4P_0(z_1)$	$\varphi_3^{0,0}=-z_0^4P_0(z_0)$
$\varphi_1^{0,1}=z_2^4(z_2-1)P_1(z_2)$	$\varphi_2^{0,1}=z_1^4z_2P_1(z_1)$	$\varphi_3^{0,1}=z_0^4z_2P_1(z_0)$
$\varphi_1^{1,0}=z_1z_2^4P_1(z_2)$	$\varphi_2^{1,0}=z_1^4(z_1-1)P_1(z_1)$	$\varphi_3^{1,0}=z_0^4z_1P_1(z_0)$
$\varphi_1^{0,2}=-z_2^4(z_2-1)^2(4z_2-5)/2$	$\varphi_2^{0,2}=-(1/2)z_1^4z_2^2(4z_1-5)$	$\varphi_3^{0,2}=-z_0^4z_2^2(4z_0-5)/2$
$\varphi_1^{1,1}=-z_1z_2^4(z_2-1)(4z_2-5)$	$\varphi_2^{1,1}=-z_1^4z_2(z_1-1)(4z_1-5)$	$\varphi_3^{1,1}=-z_0^4z_1z_2(4z_0-5)$
$\varphi_1^{2,0}=-z_1^2z_2^4(4z_2-5)/2$	$\varphi_2^{2,0}=-z_1^4(z_1-1)^2(4z_1-5)/2$	$\varphi_3^{2,0}=-z_0^4z_1^2(4z_0-5)/2$
$\varphi_1^{0,3}=z_2^4(z_2-1)^3/6$	$\varphi_2^{0,3}=z_1^4z_2^3/6$	$\varphi_3^{0,3}=z_0^4z_2^3/6$
$\varphi_1^{1,2}=z_1z_2^4(z_2-1)^2/2$	$\varphi_2^{1,2}=z_1^4z_2^2(z_1-1)/2$	$\varphi_3^{1,2}=z_0^4z_1z_2^2/2$
$\varphi_1^{2,1}=z_1^2z_2^4(z_2-1)/2$	$\varphi_2^{2,1}=z_1^4z_2(z_1-1)^2/2$	$\varphi_3^{2,1}=z_0^4z_1^2z_2/2$
$\varphi_1^{3,0}=z_1^3z_2^4/6$	$\varphi_2^{3,0}=z_1^4(z_1-1)^3/6$	$\varphi_3^{3,0}=z_0^4z_1^3/6$
AP2 : $\eta_1=(0,1/2),\eta_2=(1/2,0),\eta_3=(1/2,1/2)$		
$Q_1=8z_1z_2^2z_0^2(12z_1^2-7z_1-8z_1z_2-8z_2^2+8z_2)/f_{11}$		
$Q_2=-8z_1^2z_2z_0^2(8z_1^2+8z_1z_2-8z_1+7z_2-12z_2^2)/f_{22}$		
$Q_3=4z_1^2z_2^2z_0(12z_2^2-17z_2+5-17z_1+32z_1z_2+12z_1^2)/f_{01}$		
AP3 : $\zeta_4=(1/4,1/2),\zeta_5=(1/2,1/4),\zeta_6=(1/4,1/4)$		
$Q_4=1024z_0^2z_1^2z_2^2(4z_2-1)$	$Q_5=1024z_0^2z_1^2z_2^2(4z_1-1)$	$Q_6=1024z_0^2z_1^2z_2^2(4z_0-1)$
$P_0(z_j)=(20z_j^3-70z_j^2+84z_j-35)$, $P_1(z_j)=(10z_j^2-24z_j+15)$		

Step 3. As a result, we get the required set of basis HIP

$$\varphi_r^{\kappa}(z')=\{\check{\varphi}_r^{\kappa}(z'),Q_s(z')\},\quad \kappa=\kappa_1,\ldots,\kappa_d, \tag{20}$$

composed of the polynomials $Q_s(z')$ of the type AP2 and AP3, and the polynomials $\check{\varphi}_r^{\kappa}(z')$ of the type AP1 that satisfy the conditions

$$\check{\varphi}_r^{\kappa_1\ldots\kappa_d}(\xi'_r)=\delta_{rr'}\delta_{\kappa_1 0}\ldots\delta_{\kappa_d 0},\quad \left.\frac{\partial^{\mu_1\ldots\mu_d}\check{\varphi}_r^{\kappa_1\ldots\kappa_d}(z')}{\partial z_1'^{\mu_1}\ldots\partial z_d'^{\mu_d}}\right|_{z'=\xi'_{r'}}=\delta_{rr'}\delta_{\kappa_1\mu_1}\ldots\delta_{\kappa_d\mu_d}, \tag{21}$$

$$0\le\kappa_1+\kappa_2+\ldots+\kappa_d\le\kappa_{\max}-1,\quad 0\le\mu_1+\mu_2+\ldots+\mu_d\le\kappa_{\max}-1;$$

$$\left.\frac{\partial^k\check{\varphi}_r^{\kappa_1\ldots\kappa_d}(z')}{\partial n_{i(s)}^k}\right|_{z'=\eta'_{s'}}=0,\quad s'=1,\ldots,T_1(\kappa'),\quad k=k(s'), \tag{22}$$

$$\check{\varphi}_r^{\kappa_1\ldots\kappa_d}(\zeta'_{s'})=0,\quad s'=T_1(\kappa')+1,\ldots,K, \tag{23}$$

and are calculated using the formulas

$$\check{\varphi}_r^{\kappa}(z')=\varphi_r^{\kappa}(z')-\sum_{s=1}^{K}c_{\kappa;r;s}Q_s(z'),\ c_{\kappa;r;s}=\left\{\begin{array}{ll}\left.\frac{\partial^k\varphi_r^{\kappa}(z')}{\partial n_{i(s)}^k}\right|_{z'=\eta'_s}, & Q_s(z')\in\text{AP2},\\ \varphi_r^{\kappa}(\zeta_s), & Q_s(z')\in\text{AP3}.\end{array}\right. \tag{24}$$

Step 4. The AP1 $\check{\varphi}_r^{\kappa}(z')$ from (20), where κ denotes the directional derivatives along the local coordinate axes, are recalculated using formulas (10) into $\check{\varphi}_r^{\kappa}(z')$, specified in the local coordinates, but now κ denotes already the directional derivatives along the physical coordinate axes.

Table 4. The HIP $p = 2$, $\kappa_{\max} = 3$, $\kappa' = 1$, $p' = 8$

AP1 : $\xi_1 = (0,1), \xi_2 = (1/2,1/2), \xi_3 = (1,0), \xi_4 = (0,1/2), \xi_5 = (1/2,0), \xi_6 = (0,0)$		
$\varphi_1^{0,0} = z_2^3(2z_2-1)^3 S_0(z_2)$	$\varphi_3^{0,0} = z_1^3(2z_1-1)^3 S_0(z_1)$	$\varphi_6^{0,0} = z_0^3(2z_0-1)^3 S_0(z_0)$
$\varphi_1^{0,1} = -z_2^3(z_2-1)S_1(z_2)$	$\varphi_3^{0,1} = -z_1^3 z_2 S_1(z_1)$	$\varphi_6^{0,1} = -z_0^3 z_2 S_1(z_0)$
$\varphi_1^{1,0} = -z_1 z_2^3 S_1(z_2)$	$\varphi_3^{1,0} = -z_1^3(z_1-1)S_1(z_1)$	$\varphi_6^{1,0} = -z_0^3 z_1 S_1(z_0)$
$\varphi_1^{0,2} = z_2^3(z_2-1)^2(2z_2-1)^3/2$	$\varphi_3^{0,2} = z_1^3(2z_1-1)^3 z_2^2/2$	$\varphi_6^{0,2} = z_0^3 z_2^2(2z_0-1)^3/2$
$\varphi_1^{1,1} = z_2^3(2z_2-1)^3 z_1(z_2-1)$	$\varphi_3^{1,1} = z_1^3 z_2(z_1-1)(2z_1-1)^3$	$\varphi_6^{1,1} = z_0^3 z_1 z_2(2z_0-1)^3$
$\varphi_1^{2,0} = z_2^3(2z_2-1)^3 z_1^2/2$	$\varphi_3^{2,0} = z_1^3(z_1-1)^2(2z_1-1)^3/2$	$\varphi_6^{2,0} = z_0^3 z_1^2(2z_0-1)^3/2$
$\varphi_2^{0,0} = 64 z_1^3 z_2^3 S_2(z_0)$	$\varphi_4^{0,0} = 64 z_0^3 z_2^3 S_2(z_1)$	$\varphi_5^{0,0} = 64 z_0^3 z_1^3 S_2(z_2)$
$\varphi_2^{0,1} = 32 z_1^3 z_2^3 S_3(z_2,z_0)$	$\varphi_4^{0,1} = 32 z_0^3 z_2^3 S_3(z_2,z_1)$	$\varphi_5^{0,1} = 64 z_0^3 z_1^3 z_2(6z_2+1)$
$\varphi_2^{1,0} = 32 z_1^3 z_2^3 S_3(z_1,z_0)$	$\varphi_4^{1,0} = 64 z_0^3 z_1 z_2^3(6z_1+1)$	$\varphi_5^{1,0} = 32 z_0^3 z_1^3 S_3(z_1,z_2)$
$\varphi_2^{0,2} = 8 z_1^3 z_2^3(2z_2-1)^2$	$\varphi_4^{0,2} = 8 z_0^3 z_2^3(2z_2-1)^2$	$\varphi_5^{0,2} = 32 z_0^3 z_1^3 z_2^2$
$\varphi_2^{1,1} = 16 z_1^3 z_2^3(2z_1-1)(2z_2-1)$	$\varphi_4^{1,1} = 32 z_0^3 z_1 z_2^3(2z_2-1)$	$\varphi_5^{1,1} = 32 z_0^3 z_1^3 z_2(2z_1-1)$
$\varphi_2^{2,0} = 8 z_1^3 z_2^3(2z_1-1)^2$	$\varphi_4^{2,0} = 32 z_0^3 z_1^2 z_2^3$	$\varphi_5^{2,0} = 8 z_0^3 z_1^3(2z_1-1)^2$
AP2 : $\eta_1 = (0,1/4), \eta_2 = (0,3/4), \eta_3 = (1/4,0), \eta_4 = (3/4,0), \eta_5 = (1/4,3/4), \eta_6 = (3/4,1/4)$		
$Q_1 = \quad (512/9) z_0^2 z_1 z_2^2(2z_0-1)(2z_2-1)(4z_0-1)/f_{11}$		
$Q_2 = -(512/9) z_0^2 z_1 z_2^2(2z_0-1)(2z_2-1)(4z_2-1)/f_{11}$		
$Q_3 = -(512/9) z_0^2 z_1^2 z_2(2z_0-1)(2z_1-1)(4z_0-1)/f_{22}$		
$Q_4 = -(512/9) z_0^2 z_1^2 z_2(2z_0-1)(2z_1-1)(4z_1-1)/f_{22}$		
$Q_5 = \quad (256/9) z_0 z_1^2 z_2^2(2z_1-1)(2z_2-1)(4z_2-1)/f_{01}$		
$Q_6 = \quad (256/9) z_0 z_1^2 z_2^2(2z_1-1)(2z_2-1)(4z_1-1)/f_{01}$		
AP3 : $\zeta_7 = (1/4,1/2), \zeta_8 = (1/2,1/4), \zeta_9 = (1/4,1/4)$		
$Q_7 = 4096 z_0^2 z_1^2 z_2^2(2z_0-1)(2z_1-1)$ $Q_8 = 4096 z_0^2 z_1^2 z_2^2(2z_0-1)(2z_2-1)$ $Q_9 = 4096 z_0^2 z_1^2 z_2^2(2z_1-1)(2z_2-1)$		
$S_0(z_j) = (48z_2^2 - 105z_2 + 58)$, $S_1(z_j) = (2z_j-1)^3(9z_j-10)$, $S_2(z_j) = (24z_j^2 - 12z_0z_1z_2/z_j + 4)$, $S_3(z_i,z_j) = (2z_i-1)(6z_j+1)$		

Step 5. The final transition to the physical coordinates is implemented by means of transformation (9).

3.3 Example: HIP for $d = 2$

For $d = 2$, the order p' of the polynomial with respect to the tangential variable t at the boundary of the triangle $\frac{\partial^{\kappa'+1}}{\partial n^{\kappa'}\partial t}, \ldots, \frac{\partial^{\kappa_{\max}}}{\partial n^{\kappa'}\partial t^{\kappa_{\max}-\kappa'-1}}$. Thus, since the triangle has three sides, the unique determination of the derivatives to the order of κ' at the boundary requires $T_1(\kappa') = 3p + \ldots + 3\kappa' p = 3p\kappa'(\kappa'+1)/2$ parameters and, correspondingly, the additional conditions (17).

For example, if $p = 1$ and $\kappa_{\max} = 4$, then there are $K = 6$ additional conditions for the determination of AP2 and AP3. The order $p' = 7$ of the polynomial in the tangential variable t at the boundary of the triangle coincides with the order of the polynomial of two variables, and its unique determination requires $p' + 1 = 8$ parameters. The first-order derivative $\kappa' = 1$ in the variable

Table 5. The HIP $p = 1$, $\kappa_{\max} = 5$, $\kappa' = 2$, $p' = 9$

AP1 : $\xi_1 = (0,1),\ \xi_2 = (1,0), \xi_3 = (0,0)$		
$\varphi_1^{0,0} = z_2^5 T_0(z_2)$	$\varphi_2^{0,0} = z_1^5 T_0(z_1)$	$\varphi_3^{0,0} = z_0^5 T_0(z_0)$
$\varphi_1^{0,1} = -z_2^5(z_2-1)T_1(z_2)$	$\varphi_2^{0,1} = -z_1^5 z_2 T_1(z_1)$	$\varphi_3^{0,1} = -z_0^5 z_2 T_1(z_0)$
$\varphi_1^{1,0} = -z_1 z_2^5 T_1(z_2)$	$\varphi_2^{1,0} = -z_1^5(z_1-1)T_1(z_1)$	$\varphi_3^{1,0} = -z_0^5 z_1 T_1(z_0)$
$\varphi_1^{0,2} = z_2^5(z_2-1)^2 T_2(z_2)/2$	$\varphi_2^{0,2} = z_1^5 z_2^2 T_2(z_1)/2$	$\varphi_3^{0,2} = z_0^5 z_2^2 T_2(z_0)/2$
$\varphi_1^{1,1} = z_1 z_2^5(z_2-1)T_2(z_2)$	$\varphi_2^{1,1} = z_1^5 z_2(z_1-1)T_2(z_1)$	$\varphi_3^{1,1} = z_0^5 z_1 z_2 T_2(z_0)$
$\varphi_1^{2,0} = z_1^2 z_2^5 T_2(z_2)/2$	$\varphi_2^{2,0} = z_1^5(z_1-1)^2 T_2(z_1)/2$	$\varphi_3^{2,0} = z_0^5 z_1^2 T_2(z_0)/2$
$\varphi_1^{0,3} = -z_2^5(z_2-1)^3(5z_2-6)/6$	$\varphi_2^{0,3} = -z_1^5 z_2^3(5z_1-6)/6$	$\varphi_3^{0,3} = -z_0^5 z_2^3(5z_0-6)/6$
$\varphi_1^{1,2} = -z_1 z_2^5(z_2-1)^2(5z_2-6)/2$	$\varphi_2^{1,2} = -z_1^5 z_2^2(z_1-1)(5z_1-6)/2$	$\varphi_3^{1,2} = -z_0^5 z_1 z_2^2(5z_0-6)/2$
$\varphi_1^{2,1} = -z_1^2 z_2^5(z_2-1)(5z_2-6)/2$	$\varphi_2^{2,1} = -z_1^5 z_2(z_1-1)^2(5z_1-6)/2$	$\varphi_3^{2,1} = -z_0^5 z_1^2 z_2(5z_0-6)/2$
$\varphi_1^{3,0} = -z_1^3 z_2^5(5z_2-6)/6$	$\varphi_2^{3,0} = -z_1^5(z_1-1)^3(5z_1-6)/6$	$\varphi_3^{3,0} = -z_0^5 z_1^3(5z_0-6)/6$
$\varphi_1^{0,4} = z_2^5(z_2-1)^4/24$	$\varphi_2^{0,4} = z_1^5 z_2^4/24$	$\varphi_3^{0,4} = z_0^5 z_2^4/24$
$\varphi_1^{1,3} = z_1 z_2^5(z_2-1)^3/6$	$\varphi_2^{1,3} = z_1^5 z_2^3(z_1-1)/6$	$\varphi_3^{1,3} = z_0^5 z_1 z_2^3/6$
$\varphi_1^{2,2} = z_1^2 z_2^5(z_2-1)^2/4$	$\varphi_2^{2,2} = z_1^5 z_2^2(z_1-1)^2/4$	$\varphi_3^{2,2} = z_0^5 z_1^2 z_2^2/4$
$\varphi_1^{3,1} = z_1^3 z_2^5(z_2-1)/6$	$\varphi_2^{3,1} = z_1^5 z_2(z_1-1)^3/6$	$\varphi_3^{3,1} = z_0^5 z_1^3 z_2/6$
$\varphi_1^{4,0} = z_1^4 z_2^5/24$	$\varphi_2^{4,0} = z_1^5(z_1-1)^4/24$	$\varphi_3^{4,0} = z_0^5 z_1^4/24$
AP2 : $\eta_1 = (0,1/2), \eta_2 = (1/2,0), \eta_3 = (1/2,1/2), \eta_4 = (0,1/3), \eta_5 = (0,2/3),$		
$\eta_6 = (1/3,0), \eta_7 = (2/3,0), \eta_8 = (1/3,2/3), \eta_9 = (2/3,1/3)$		
$Q_1 = 256 z_0^3 z_1 z_2^3((3z_1 z_2 - 5z_1^2 - z_2^2 + z_2)f_{11} - 4z_1(z_2 - z_0)f_{12})/f_{11}^2$		
$Q_2 = 256 z_0^3 z_1^3 z_2((3z_1 z_2 - 5z_2^2 - z_1^2 + z_1)f_{22} + 4z_2(z_1 - z_0)f_{21})/f_{22}^2$		
$Q_3 = 128 z_0 z_1^3 z_2^3((7z_0^2 - 2z_0 - z_1 z_2)f_{01} + 2z_0(z_1 - z_2)f_{02})/f_{01}^2$		
$Q_4 = (729/16)z_0^3 z_1^2 z_2^3(3z_0 - 1)/f_{11}^2$		
$Q_5 = (729/16)z_0^3 z_1^2 z_2^3(3z_2 - 1)/f_{11}^2$		
$Q_6 = (729/16)z_0^3 z_1^3 z_2^2(3z_0 - 1)/f_{22}^2$		
$Q_7 = (729/16)z_0^3 z_1^3 z_2^2(3z_1 - 1)/f_{22}^2$		
$Q_8 = (729/64)z_0^2 z_1^3 z_2^3(3z_2 - 1)/f_{01}^2$		
$Q_9 = (729/64)z_0^2 z_1^3 z_2^3(3z_1 - 1)/f_{01}^2$		
AP3 : $\zeta_{10} = (1/3,1/3)$	$Q_{10} = 19683 z_0^3 z_1^3 z_2^3$	
$T_0(z_j) = (70z_j^4 - 315z_j^3 + 540z_j^2 - 420z_j + 126)$		
$T_1(z_j) = (35z_2^3 - 120z_2^2 + 140z_2 - 56), T_2(z_j) = (15z_j^2 - 35z_j + 21)$		

normal to the boundary will be a polynomial of the order $p' - \kappa' = 6$, and its unique determination will require $p' - \kappa' + 1 = 7$ parameters. However, it is determined by only $p' - \kappa'(p+1) = 6$ parameters: the mixed derivatives $\frac{\partial}{\partial n}$, $\frac{\partial^2}{\partial n \partial t}$ and $\frac{\partial^3}{\partial n \partial t^2}$, specified at two vertices. The missing parameter can be determined by specifying the directional derivative along the direction, non-parallel to the triangle boundary, at one of the points on its side (e.g., in the middle of the side). Thus, for $p = 1$ and $\kappa_{\max} = 4$, one can construct HIP with the fixed values of the first derivative on the boundary of the triangle, and $6 - 3 = 3$ parameters remain free.

The second-order derivative $\kappa' = 2$ in the variable normal to the boundary is a polynomial of the order $p' - \kappa' = 5$, and its unique determination requires $p' - \kappa' + 1 = 6$ parameters. However, it is determined by only $p' - \kappa'(p+1) = 4$ parameters: the mixed derivatives $\frac{\partial^2}{\partial n^2}$ and $\frac{\partial^3}{\partial n^2 \partial t}$ specified at two vertices of the triangle. Thus, the unique determination of the second derivative will require 6 parameters. This fact means that using this algorithm for $p = 1$ and $\kappa_{\max} = 4$, it is impossible to construct the FEM scheme with continuous second derivative. In this case, one should use the scheme with $\kappa_{\max} > 4$, e.g., denoted as [152] in Table 1 and Fig. 2. Then the three remaining free parameters are used to construct AP3. Note that it is possible to construct the schemes providing the continuity of the second derivatives at some boundaries of the finite elements. This case is not considered in the present paper.

For $d = 2$, the derivatives $\partial/\partial n_i$ along the direction n_i, perpendicular to the appropriate face $i = 0, 1, 2$ in the physical coordinate system are given in terms of the partial derivatives $\partial/\partial z'_j$, $j = 1, 2$ in the local coordinate system Δ, using (8)–(10), by the expressions

$$\frac{\partial}{\partial n_i} = f_{i1}\frac{\partial}{\partial z'_1} + f_{i2}\frac{\partial}{\partial z'_2}, \quad i = 1, 2, \quad \frac{\partial}{\partial n_0} = (f_{01} + f_{02})\frac{\partial}{\partial z'_1} + (f_{01} - f_{02})\frac{\partial}{\partial z'_2}, \quad (25)$$

where $f_{ij} = f_{ij}(\hat{z}_0, \hat{z}_1, \hat{z}_2)$ are the functions of the coordinates of vertices $\hat{z}_0, \hat{z}_1, \hat{z}_2$ of the triangle Δ_q in the physical coordinate system

$$\begin{aligned}
&f_{11} = J^{-1}R(\hat{z}_2, \hat{z}_0), \quad f_{12} = -\frac{(\hat{z}_{12} - \hat{z}_{02})(\hat{z}_{22} - \hat{z}_{02}) + (\hat{z}_{21} - \hat{z}_{01})(\hat{z}_{11} - \hat{z}_{01})}{JR(\hat{z}_2, \hat{z}_0)},\\
&f_{22} = J^{-1}R(\hat{z}_1, \hat{z}_0), \quad f_{21} = -\frac{(\hat{z}_{12} - \hat{z}_{02})(\hat{z}_{22} - \hat{z}_{02}) + (\hat{z}_{21} - \hat{z}_{01})(\hat{z}_{11} - \hat{z}_{01})}{JR(\hat{z}_1, \hat{z}_0)},\\
&f_{01} = -(2J)^{-1}R(\hat{z}_2, \hat{z}_1), \; f_{02} = \frac{(\hat{z}_{11} - \hat{z}_{01})^2 + (\hat{z}_{12} - \hat{z}_{02})^2 - (\hat{z}_{22} - \hat{z}_{02})^2 - (\hat{z}_{21} - \hat{z}_{01})^2}{2JR(\hat{z}_2, \hat{z}_1)},\\
&J = (\hat{z}_{11} - \hat{z}_{01})(\hat{z}_{22} - \hat{z}_{02}) - (\hat{z}_{12} - \hat{z}_{02})(\hat{z}_{21} - \hat{z}_{01}), \qquad (26)\\
&R(\hat{z}_j, \hat{z}_{j'}) = ((\hat{z}_{1j} - \hat{z}_{1j'})^2 + (\hat{z}_{2j} - \hat{z}_{2j'})^2)^{1/2}.
\end{aligned}$$

The implementation of conditions (13), (16), (17), and (18), using which the basis HIP were constructed, is schematically shown for $d = 2$ in Fig. 2. The characteristics of the polynomial basis of HIP on the element Δ at $d = 2$ are presented in Table 1.

Tables 2, 3, 4 and 5 present the results of executing the Algorithm from Sect. 3.2 for the HIP ($p = 1$, $\kappa_{\max} = 3$, $\kappa' = 1$, $p' = 5$), ($p = 1$, $\kappa_{\max} = 4$, $\kappa' = 1$, $p' = 7$), ($p = 2$, $\kappa_{\max} = 3$, $\kappa' = 1$, $p' = 8$) and ($p = 1$, $\kappa_{\max} = 5$, $\kappa' = 2$, $p' = 9$): AP1 $\varphi_r^k(z')$, AP2 and AP3 $Q_s^k(z')$, and the corresponding coefficients $c_{\kappa;r;s}$ are calculated using Eq. (24). The notations are as follows: ξ_r, η_s, ζ_s are the coordinates of the nodes, in which the right-hand side of Eqs. (21), (17) or (18) equals one, $z_0 = 1 - z_1 - z_2$, f_{ij} is found from formulas (26), the arguments of functions and the primes at the notations of independent variables are omitted. The explicit expressions for the HIPs ($p = 1$, $\kappa_{\max} = 6$, $\kappa' = 2$, $p' = 11$), ($p = 2$, $\kappa_{\max} = 4$, $\kappa' = 1$, $p' = 11$), and ($p = 1$, $\kappa_{\max} = 7$, $\kappa' = 3$, $p' = 13$) were calculated too, but are not presented here because of the paper size limitations (one can receive it with request to authors or using program TRIAHP implemented in Maple which will be published in the library JINRLIB). The calculations were carried out using the computer Intel Pentium CPU 987, ×64, 4 GB RAM, the Maple 16. The computing time for the considered examples did not exceed 6 s.

Remark 1. At $\kappa' = 1$ on uniform grids, one can make use of the basis with continuous first derivative consisting of the reduced HIP $\check{\varphi}_r^k(z')$ and $Q_s(z')$ for $f_{01} = f_{11} = f_{22} = 1$. In this case, the derivatives of such polynomials along the direction normal to the boundary generally do not satisfy conditions (17).

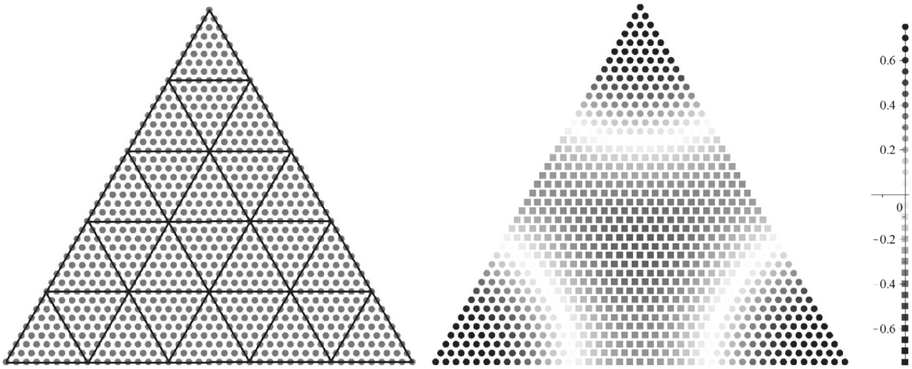

Fig. 3. (a) The mesh on the domain $\Omega_h(z) = \bigcup_{q=1}^{Q} \Delta_q$ of the triangle membrane composed of triangle elements Δ_q (b) the profiles of the fourth eigenfunction $\Phi_4^h(z)$ with $E_4^h = 3 + 1.90 \cdot 10^{-17}$ obtained using the LIP of the order $p' = p = 8$

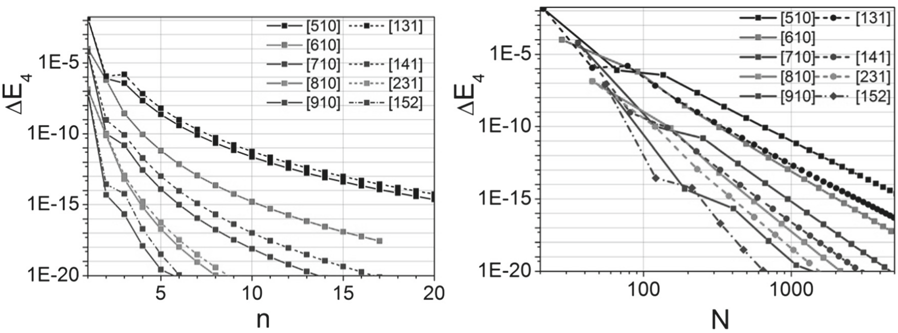

Fig. 4. The error ΔE_4^h of the eigenvalue E_4^h versus the number of elements n and the length of the vector N

3.4 Piecewise Polynomial Functions

The piecewise polynomial functions $P_l(z)$ with continuous derivatives to the order κ' are constructed by joining the polynomials $\varphi_r^{\kappa}(z) = \{\check{\varphi}_r^{\kappa}(z), Q_s(z)\}$ from (20), obtained using the Algorithm on the finite elements $\Delta_q \in \Omega_h(z) = \bigcup_{q=1}^{Q} \Delta_q$:

$$P_{l'}(z) = \left\{ \pm\varphi^{\kappa}_{l(l')}(z), A_{l(l')} \in \Delta_q; 0, A_{l(l')} \notin \Delta_q \right\}, \quad (27)$$

where the sign "−" can appear only for AP2, when it is necessary to join the normal derivatives of the odd order.

The expansion of the sought solution $\Phi_m(z)$ in the basis of piecewise polynomial functions $P_{l'}(z)$, $\Phi^h_m(z) = \sum_{l'=1}^{N} P_{l'}(z)\Phi^h_{l'm}$ and its substitution into the variational functional (5) leads to the generalized algebraic eigenvalue problem, $(A - BE^h_m)\Phi^h_m = 0$, solved using the standard method (see, e.g., [3]). The elements of the symmetric matrices of stiffness A and mass B comprise the integrals like Eq. (5), which are calculated on the elements in the domain $\Delta_q \in \Omega_h(z) = \bigcup_{q=1}^{Q} \Delta_q$, recalculated into the local coordinates on the element Δ.

The deviation of the approximate solution $E^h_m, \Phi^h_m(z) \in \mathcal{H}_2^{\kappa'+1\geq 1}(\Omega_h)$ from the exact one $E_m, \Phi_m(z) \in \mathcal{H}^2_2(\Omega)$ is theoretically estimated as [6,20]

$$\left|E_m - E^h_m\right| \leq c_1 h^{2p'}, \quad \left\|\Phi_m(z) - \Phi^h_m(z)\right\|_0 \leq c_2 h^{p'+1}, \quad (28)$$

where $\|\Phi_i(z)\|^2_0 = \int_\Omega g_0(z)dz\overline{\Phi_i}(z)\Phi_i(z)$, h is the maximal size of the finite element Δ_q, p' is the order of the FEM scheme, m is the number of the eigenvalue, c_1 and c_2 are coefficients independent of h.

4 Results and Discussion

As an example, let us consider the solution of the discrete-spectrum problem (1)–(4) at $d = 2$, $g_0(z) = g_{ij}(z) = 1$, and $V(z) = 0$ in the domain $\Omega_h(z) = \cup_{q=1}^{Q}\Delta_q$ in the form of an equilateral triangle with the side $4\pi/3$ under the boundary conditions of the second kind (3) partitioned into $Q = n^2$ equilateral triangles Δ_q with the side $h = 4\pi/3n$. The eigenvalues of this problem having the degenerate spectrum [16,18] are the integers $E_m = m_1^2 + m_2^2 + m_1 m_2 = 0, 1, 1, 3, 4, 4, 7, 7, \ldots$, $m_1, m_2 = 0, 1, 2, \ldots$. Figure 3 presents the finite-element mesh with the LIP of the eighth order and the profile of the fourth eigenfunction $\Phi^h_4(z)$. Figure 4 shows the errors $\Delta E_m = E^h_m - E_m$ of the eigenvalue $E^h_4(z)$ depending on the number n (the number of elements being n^2) and on the length N of the vector Φ^h_m of the algebraic eigenvalue problem for the FEM schemes from the fifth to the ninth order of accuracy: using LIP with the labels $[p\kappa_{\max}\kappa'] = [510], \ldots, [910]$, and using HIP with the labels [131], [141], [231] and [152] from Table 1, conserving the continuity of the first and the second derivative of the approximate solution, respectively.

As seen from Fig. 4, the errors of the eigenvalue $\Delta E^h_4(z)$ of the FEM schemes of the same order are nearly similar and correspond to the theoretical estimates (28), but in the FEM schemes conserving the continuity of the first and the second derivatives of the approximate solution, the matrices of smaller dimension are used that correspond to the length of the vector N smaller by 1.5–2 times than in the schemes with LIP that conserve only the continuity of the functions themselves at the boundaries of the finite elements. The calculations were carried out using the computer 2× Xeon 3.2 GHz, 4 GB RAM, the Intel Fortran 77 with quadruple precision real*16, with 32 significant digits. The computing time for the considered examples did not exceed 3 min.

5 Conclusion

We presented a symbolic-numeric algorithm, implemented in the Maple system for analytical calculation of the basis of Hermite interpolation polynomials of several variables, which is used to construct a FEM computational scheme of high-order accuracy. The scheme is intended for solving the eigenvalue problem for the elliptic partial differential equation in a bounded domain of multidimensional Euclidean space. The procedure provides the continuity not only of the approximate solution itself, but also of its derivatives to a given order. By the example of the exactly solvable problem for the triangle membrane it is shown that the errors for the eigenvalue are nearly the same for the FEM schemes of the same order and correspond to the theoretical estimates. To achieve the given accuracy of the approximate solution the FEM schemes with HIP, providing the continuity of the first and the second derivatives of the approximate solutions the required matrices have smaller dimension, corresponding to the length of the vector N smaller by 1.5–2 times than for the schemes with LIP, providing only the continuity of the approximate solution itself at the boundaries of the finite elements.

The FEM computational schemes are oriented at the calculations of the spectral and optical characteristics of quantum dots and other quantum mechanical systems. The implementation of FEM with HIP in the space with $d \geq 2$ and the domains different from a polyhedral domain will be presented elsewhere.

The work was partially supported by the Russian Foundation for Basic Research (grants Nos. 16-01-00080 and 17-51-44003 Mong_a) and the Bogoliubov-Infeld program. The reported study was partially funded within the Agreement N 02.03.21.0008 dated 24.04.2016 between the MES RF and RUDN University.

References

1. Ames, W.F.: Numerical Methods for Partial Differential Equations. Academic Press, London (1992)
2. Argyris, J.H., Buck, K.E., Scharpf, D.W., Hilber, H.M., Mareczek, G.: Some new elements for the matrix displacement method. In: Proceedings of the Conference on Matrix Methods in Structural Mechanics (2nd), Wright-Patterson Air Force Base, Ohio, 15–17 October 1968
3. Bathe, K.J.: Finite Element Procedures in Engineering Analysis. Prentice Hall, Englewood Cliffs/New York (1982)
4. Bell, K.: A refined triangular plate bending element. Int. J. Numer. Methods Eng. **1**, 101–122 (1969)

5. Brenner, S.C., Scott, L.R.: The Mathematical Theory of Finite Element Methods. Texts in Applied Mathematics, vol. 15, 3rd edn. Springer, New York (2008). doi:10.1007/978-0-387-75934-0
6. Ciarlet, P.: The Finite Element Method for Elliptic Problems. North-Holland Publishing Company, Amsterdam (1978)
7. Dhatt, G., Touzot, G., Lefrançois, E.: Finite Element Method. Wiley, Hoboken (2012)
8. Gasca, M., Sauer, T.: On the history of multivariate polynomial interpolation. J. Comp. Appl. Math. **122**, 23–35 (2000)
9. Gusev, A.A., Chuluunbaatar, O., Vinitsky, S.I., Derbov, V.L., Góźdź, A., Le Hai, L., Rostovtsev, V.A.: Symbolic-numerical solution of boundary-value problems with self-adjoint second-order differential equation using the finite element method with interpolation hermite polynomials. In: Gerdt, V.P., Koepf, W., Seiler, W.M., Vorozhtsov, E.V. (eds.) CASC 2014. LNCS, vol. 8660, pp. 138–154. Springer, Cham (2014). doi:10.1007/978-3-319-10515-4_11
10. Gusev, A.A., Hai, L.L., Chuluunbaatar, O., Vinitsky, S.I.: KANTBP 4M: Program for Solving Boundary Problems of the System of Ordinary Second Order Differential Equations. http://wwwinfo.jinr.ru/programs/jinrlib/indexe.html
11. Habib, A.W., Goldman, R.N., Lyche, T.: A recursive algorithm for Hermite interpolation over a triangular grid. J. Comput. Appl. Math. **73**, 95–118 (1996)
12. Ladyzhenskaya, O.A.: The Boundary Value Problems of Mathematical Physics. Applied Mathematical Sciences, vol. 49. Springer, New York (1985). doi:10.1007/978-1-4757-4317-3
13. Lekien, F., Marsden, J.: Tricubic interpolation in three dimensions. Int. J. Numer. Meth. Eng. **63**, 455–471 (2005)
14. Logg, A., Mardal, K.-A., Wells, G.N. (eds.): Automated Solution of Differential Equations by the Finite Element Method (The FEniCS Book). Springer, Heidelberg (2012). doi:10.1007/978-3-642-23099-8
15. www.maplesoft.com
16. McCartin, B.J.: Laplacian Eigenstructure of the Equilateral Triangle. Hikari Ltd., Ruse, Bulgaria (2011)
17. Mitchell, A.R., Wait, R.: The Finite Element Method in Partial Differential Equations. Wiley, Chichester (1977)
18. Pockels, F.: Über die Partielle Differential-Gleichung $\Delta u + k^2 u = 0$ und deren Auftreten in der Mathematischen Physik. B.G. Teubner, Leipzig (1891)
19. Ramdas Ram-Mohan, L.: Finite Element and Boundary Element Aplications in Quantum Mechanics. Oxford University Press, New York (2002)
20. Strang, G., Fix, G.J.: An Analysis of the Finite Element Method. Prentice-Hall, Englewood Cliffs/New York (1973)
21. Zienkiewicz, O.C.: Finite elements. The background story. In: Whiteman, J.R. (ed.) The Mathematics of Finite Elements and Applications, p. 1. Academic Press, London (1973)