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Interpolation Hermite Polynomials For Finite Element Method

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Abstract. We describe a new algorithm for analytic calculation of high-order Hermite interpolation polynomials of the simplex and give their classification. A typical example of triangle element, to be built in high accuracy finite element schemes, is given.

1 Introduction

For more than half a century, the finite element method (FEM) has won universal recognition as an efficient method for solving the most diverse problems of mathematical physics and engineering. In the multidimensional case the finite element grids of various shapes are used. The problem of constructing high-order interpolation polynomials for FEM has a simple solution only for simplex finite elements, such as the well known Lagrange interpolation polynomials (LIPs) [1]. Meanwhile, in the case of a d-dimensional simplex domain, the LIPs of the order $p' \geq 1$ are often sought by compiling and solving systems of $(d+p')!/d!/p'!$ linear algebraic equations [2].

However, there are problems in which values of directional derivatives of the solutions are also necessary. They are of particular importance when high smoothness between the elements is required, or when highly accurate values of the gradient of the solution are necessary. The construction of such basis functions, referred to as Hermite interpolation polynomials (HIPs), is not possible on arbitrary meshes. This is one of the most important and difficult problems in the FEM and its applications in different fields, solved to date explicitly only for certain particular cases [2, 3].

In this paper we report a new algorithm for the calculation of HIPs of the order $p' = \kappa_{\max}(p+1)-1$ providing continuity of the approximating piecewise polynomial functions and of their directional derivatives up to an order κ' along the normals to the boundaries of the simplex finite elements in the Euclidean space $\mathcal{R}^d$, which reduces to solving systems consisting of

$$\frac{(d+p')!}{d!\,p'!} - \frac{(d+p)!}{d!\,p!} \cdot \frac{(d+\kappa^{\max}-1)!}{d!\,(\kappa^{\max}-1)!}$$

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linear algebraic equations, where p and $\kappa^{\max}$ will be specified below.

2 Algorithm for Calculating the Hermite Interpolating Polynomials

The conventional FEM implementation for a problem defined in terms of the set of coordinates $z = (z_1, \ldots, z_d) \in \mathcal{R}^d$ performs all calculations in local (reference) coordinates $z' = (z'_1, \ldots, z'_d) \in \mathcal{R}^d$, in which the $d + 1$ coordinates of the *simplex vertices* are [3]: $\hat{z}'_j{=}(\hat{z}'_{j1}, \ldots, \hat{z}'_{jd})$, $\hat{z}'_{jk}{=}\delta_{jk}$, $j = 0, \ldots, d$,

$$z_i = \hat{z}_{0i} + \sum_{j=1}^{d} \hat{J}_{ij} z'_j, \quad z'_i = \sum_{j=1}^{d} (\hat{J}^{-1})_{ij}(z_j - \hat{z}_{0j}), \quad \frac{\partial}{\partial z'_i} {=} \sum_{j=1}^{d} \hat{J}_{ji} \frac{\partial}{\partial z_j}, \quad \frac{\partial}{\partial z_i} {=} \sum_{j=1}^{d} (\hat{J}^{-1})_{ji} \frac{\partial}{\partial z'_j}, \tag{1}$$

where $\hat{J}_{ij} = \hat{z}_{ji} - \hat{z}_{0i}$, $i, j = 1, \ldots, d$, given by the corresponding $d + 1$ physical coordinates $\hat{z}_j{=}(\hat{z}_{j1}, \ldots, \hat{z}_{jd})$.

In the local coordinates of the d-dimensional simplex Δ, the LIP $\varphi_r(z')$ of the order $p' = p$ which equates one at the node points $\xi'_r = (n_1/p, \ldots, n_d/p)$, $n_i \geq 0$, $n_1 + \cdots + n_d \leq p$, $r = 1, \ldots, (d+p)!/d!/p!$ and zero at the remaining node points $\xi'_{r'}$, i.e., $\varphi_r(\xi'_{r'}) = \delta_{rr'}$, is determined by the formula:

$$\varphi_r(z') {=} \left(\prod_{i=1}^{d} \prod_{n'_i=0}^{n_i-1} \frac{z'_i - n'_i/p}{n_i/p - n'_i/p} \right) \left(\prod_{n'_0=0}^{n_0-1} \frac{1 - z'_1 - \ldots - z'_d - n'_0/p}{n_0/p - n'_0/p} \right), \qquad n_0 = p - n_1 - \cdots - n_d. \tag{2}$$

Step 1. To construct the HIPs in the local coordinates z', we define the set of auxiliary polynomials $\varphi_r^{\kappa_1 \ldots \kappa_d}(z')$ referred to as AP1

$$\varphi_r^{\kappa_1 \ldots \kappa_d}(\xi'_r) {=} \delta_{rr'} \delta_{\kappa_1 0} \ldots \delta_{\kappa_d 0}, \quad \left. \frac{\partial^{\mu_1 \ldots \mu_d} \varphi_r^{\kappa_1 \ldots \kappa_d}(z')}{\partial z_1'^{\mu_1} \ldots \partial z_d'^{\mu_d}} \right|_{z'=\xi'_{r'}} = \delta_{rr'} \delta_{\kappa_1 \mu_1} \ldots \delta_{\kappa_d \mu_d}, \tag{3}$$
$$0 \leq \kappa_1 + \kappa_2 + \cdots + \kappa_d \leq \kappa_{\max}{-}1, \quad 0 \leq \mu_1 + \mu_2 + \cdots + \mu_d \leq \kappa_{\max}{-}1.$$

Here in contrast to the LIPs, the values of the functions themselves, and of their derivatives up to the order $\kappa_{\max}{-}1$ are specified at the node points ξ'_r. The explicit expressions of AP1 are given by

$$\varphi_r^{\kappa_1 \kappa_2 \ldots \kappa_d}(z') = w_r(z') \sum_{\mu_1 + \cdots + \mu_d = 0,1,\ldots,\kappa^{\max}-1} a_r^{\kappa_1 \ldots \kappa_d, \mu_1 \ldots \mu_d} (z'_1 - \xi'_{r1})^{\mu_1} \times \cdots \times (z'_d - \xi'_{rd})^{\mu_d}, \tag{4}$$
$$w_r(z') {=} \left(\prod_{i=1}^{d} \prod_{n'_i=0}^{n_i-1} \frac{(z'_i - n'_i/p)^{\kappa^{\max}}}{(n_i/p - n'_i/p)^{\kappa^{\max}}} \right) \left(\prod_{n'_0=0}^{n_0-1} \frac{(1 - z'_1 - \ldots - z'_d - n'_0/p)^{\kappa^{\max}}}{(n_0/p - n'_0/p)^{\kappa^{\max}}} \right), \quad w_r(\xi'_r) = 1,$$

where the coefficients $a_r^{\kappa_1 \ldots \kappa_d, \mu_1 \ldots \mu_d}$ are calculated from recurrence relations obtained by the substitution of Eq. (4) into the conditions (3).

Step 2. To enforce a uniquely defined polynomial basis, two types of auxiliary polynomials $Q_s(z)$ denoted respectively AP2 and AP3 are defined. AP2 and AP3 are linearly independent of AP1 from Eq. (4) and satisfy the following conditions at the node points $\xi'_{r'}$ of AP1:

$$Q_s(\xi'_{r'}){=}0, \quad \left. \frac{\partial^{\kappa'_1 \kappa'_2 \ldots \kappa'_d} Q_s(z')}{\partial z_1'^{\mu_1} \partial z_2'^{\mu_2} \ldots \partial z_d'^{\mu_d}} \right|_{z'=\xi'_{r'}} {=}0, \quad s{=}1, \ldots, K, \quad K = \frac{(d{+}p')!}{d!p'!} - \frac{(d{+}p)!}{d!p!} \frac{(d{+}\kappa^{\max}{-}1)!}{d!(\kappa^{\max}{-}1)!}. \tag{5}$$

To provide the continuity of derivatives, the polynomials referred to as AP2 are asked to satisfy the condition

$$\left. \frac{\partial^k Q_s(z')}{\partial n_{i(s)}^k} \right|_{z'=\eta'_{s'}} {=} \delta_{ss'}, \quad s, s'{=}1, \ldots, T_1(\kappa'), \quad k = k(s'), \tag{6}$$

Table 1. Characteristics of the HIP bases

$[p\kappa_{\max}\kappa']$	[120]	[131]	[141]	[231]	[152]	[162]	[241]	[173]
$p' = \kappa_{\max}(p+1) - 1$	3	5	7	8	9	11	11	13
$N_{1p'} = (p'+1)(p'+2)/2$	10	21	36	45	55	78	78	105
$K = p(p+1)\kappa_{\max}(\kappa_{\max}-1)/4$	1	3	6	9	10	15	9	21
$N(\text{AP1}) = N_{\kappa_{\max}p'}$	9	18	30	36	45	63	60	84
$N(\text{AP2}) = T_1(\kappa')$	0	3	3	6	9	9	6	18
$N(\text{AP3}) = K - T_1(\kappa')$	1	0	3	3	1	6	12	3
$N_{\kappa_{\max}p'} = (p+1)(p+2)\kappa_{\max}(\kappa_{\max}+1)/4$								
Restriction of derivative order κ': $3p\kappa'(\kappa'+1)/2 \le K$								

where $\eta'_{s'} = (\eta'_{s'1}, \ldots, \eta'_{s'd})$ are conveniently chosen points lying on the faces of various dimensionalities (from 1 to $d-1$) of the d-dimensional simplex Δ and do not coincide with the nodal points of HIP ξ'_r, where Eq. (3) is valid, $\partial/\partial n_{i(s)}$ is the directional derivative along the vector n_i, normal to the corresponding i-th face of the d-dimensional simplex Δ_q at the point $\eta_{s'}$ in the physical frame, which is recalculated to the point $\eta'_{s'}$ of the face of the simplex Δ in the local frame using the relations (1). 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 (6).

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

$$Q_s(\zeta'_{s'}){=}\delta_{ss'}, \quad s, s'{=}T_1(\kappa'){+}1, \ldots, K, \tag{7}$$

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 and AP3 are given by the expression

$$Q_s(z') = \left(\prod_{t=0}^{d} z'^{k_t}_t\right) \sum_{j_1,\ldots,j_d} b_{j_1,\ldots,j_d;s} z'^{j_1}_1 \ldots z'^{j_d}_d, \qquad z'_0 = 1 - z'_1 - \cdots - z'_d. \tag{8}$$

For AP2 $k_t = 1$ if the point η_s, at which the additional conditions (6) are specified, lies on the corresponding face of the simplex Δ, and $k_t = \kappa'$, otherwise, $t = 0, \ldots, d$. For AP3 $k_t = \kappa'$, $t = 0, \ldots, d$. 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 Eq. (8) into the conditions (5)–(7).

Step 3. As a result, we get the required set of basis HIPs $\varphi^\kappa_r(z') = \{\check{\varphi}^\kappa_r(z'), Q_s(z')\}$, $\kappa = \kappa_1, \ldots, \kappa_d$, composed of the polynomials $Q_s(z')$ of the type AP2 and AP3, and the polynomials $\check{\varphi}^\kappa_r(z')$

$$\check{\varphi}^\kappa_r(z'){=}\varphi^\kappa_r(z'){-}\sum_{s=1}^{K} c_{\kappa;r;s} Q_s(z'), \qquad c_{\kappa;r;s}{=}\left\{\begin{array}{ll} \left.\dfrac{\partial^\kappa \varphi^\kappa_r(z')}{\partial n^\kappa_{i(s)}}\right|_{z'=\eta'_s}, & Q_s(z') \in \text{AP2}, \\ \varphi^\kappa_r(\zeta_s), & Q_s(z') \in \text{AP3}. \end{array}\right. \tag{9}$$

Step 4. The AP1 $\check{\varphi}^\kappa_r(z')$ from (9), where κ denotes the directional derivatives along the local coordinate axes, are recalculated using Eqs. (1) into $\check{\varphi}^{\check{\kappa}}_r(z')$ specified in the local coordinates, but now $\check{\kappa} = \check{\kappa}_1, \ldots, \check{\kappa}_d$ denotes the directional derivatives along the physical coordinate axes.

For example, at $d = 2$ the derivatives $\partial/\partial n_i$ along the direction n_i, perpendicular to the appropriate face $i = 0, 1, 2$ in the physical frame are expressed in terms of the partial derivatives $\partial/\partial z'_j$, $j = 1, 2$ in

Table 2. The 20 HIPs p=1, $\kappa_{\max}$=4, κ'=1, p'=7, remaining 16 HIPs are obtained by permutation $z_1 \leftrightarrow z_2$.

AP1 : $\xi_0=(0,0)$, $\xi_1=(1,0)$, $\xi_2=(0,1)$, $P_0(z_j)=(20z_j^3-70z_j^2+84z_j-35)$, $P_1(z_j)=(10z_j^2-24z_j+15)$			
$\varphi_2^{0,0}=-z_2^4P_0(z_2)$	$\varphi_2^{0,1}=z_2^4(z_2-1)P_1(z_2)$	$\varphi_2^{1,0}=z_1z_2^4P_1(z_2)$	$\varphi_0^{0,0}=-z_0^4P_0(z_0)$
$\varphi_2^{0,2}=-z_2^4(z_2-1)^2(4z_2-5)/2$	$\varphi_2^{1,1}=-z_1z_2^4(z_2-1)(4z_2-5)$	$\varphi_2^{2,0}=-z_1^2z_2^4(4z_2-5)/2$	$\varphi_0^{0,1}=z_0^4z_2P_1(z_0)$
$\varphi_2^{0,3}=z_2^4(z_2-1)^3/6$	$\varphi_2^{1,2}=z_1z_2^4(z_2-1)^2/2$	$\varphi_2^{2,1}=z_1^2z_2^4(z_2-1)/2$	$\varphi_2^{3,0}=z_1^3z_2^4/6$
$\varphi_0^{2,0}=-z_0^4z_1^2(4z_0-5)/2$	$\varphi_0^{1,1}=-z_0^4z_1z_2(4z_0-5)$	$\varphi_0^{0,3}=z_0^4z_2^3/6$	$\varphi_0^{1,2}=z_0^4z_1z_2^2/2$
AP2 : $\eta_1=(0,1/2), \eta_2=(1/2,0), \eta_3=(1/2,1/2)$		AP3 : $\zeta_4=(1/4,1/2), \zeta_5=(1/2,1/4), \zeta_6=(1/4,1/4)$	
$Q_1=8z_1z_2^2z_0^2(12z_1^2-7z_1-8z_1z_2-8z_2^2+8z_2)/f_{11}$		$Q_4=1024z_0^2z_1^2z_2^2(4z_2-1)$	
$Q_3=4z_1^2z_2^2z_0(12z_2^2-17z_2+5-17z_1+32z_1z_2+12z_1^2)/f_{01}$		$Q_6=1024z_0^2z_1^2z_2^2(4z_0-1)$	

the local frame of the triangle Δ, using the relations (1), as

$$\frac{\partial}{\partial n_i}=f_{i1}\frac{\partial}{\partial z'_1}+f_{i2}\frac{\partial}{\partial z'_2},\quad i=1,2,\quad \frac{\partial}{\partial n_0}=(f_{01}+f_{02})\frac{\partial}{\partial z'_1}+(f_{01}-f_{02})\frac{\partial}{\partial z'_2}, \tag{10}$$

where $f_{ij}=f_{ij}(\hat{z}_0,\hat{z}_1,\hat{z}_2)$ are functions of the coordinates of the vertices $\hat{z}_0,\hat{z}_1,\hat{z}_2$ of the triangle Δ_q in the physical frame. The characteristics of the polynomial basis of HIPs on the *triangle element* Δ at $d=2$, including known Argyris triangle [131] (see [3]), are presented in Table 1. Table 2 presents the results of executing the Algorithm for calculating the HIPs in the case (p=1, $\kappa_{\max}$=4, κ'=1, p'=7), AP1: $\varphi_r^k(z')$, AP2 and AP3: $Q_s(z')$, and the corresponding coefficients $c_{\kappa;r;s}$ are calculated using Eqs. (9). The notations are as follows: ξ_r, η_s, ζ_s are the coordinates of the nodes, which are specified in the conditions (3), (6) or (7), respectively, $z_0=1-z_1-z_2$, the arguments of functions and the primes in the notations of independent variables are omitted. The explicit expressions for the HIPs from Table 1 were calculated too, but are not presented here because of the paper size limitations (they can be obtained under request to the authors or using the program TRIAHP implemented in Maple, which will be published in the library JINRLIB). The calculations were carried out using the Intel Pentium CPU 987, x64, 4 GB RAM, the Maple 16, during 6 seconds.

3 Conclusion

We presented a symbolic-numeric algorithm, implementable in any computer algebra system, in particular, the Maple system, for analytical calculation of the basis of Hermite interpolation polynomials of several variables of the simplex, which can be used to construct a FEM computational scheme of high-order accuracy. The efficiency of the FEM computational schemes using high-order accuracy LIPs and HIPs for benchmark calculations of exactly solvable problems for the triangle membrane and hypercube is shown in the forthcoming paper of this issue.

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