Hermite Interpolation Polynomials on Parallelepipeds and FEM Applications

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Introduction. The definition and properties of Hermitian interpolation polynomials (HIPs) or Birkhoff interpolants and their application in finite element method (FEM) are discussed in a number of papers, for example [1, 2]. Piecewise polynomial FEM functions constructed by matching HIPs have continuous derivatives up to a given order at the finite element boundaries, in contrast to Lagrange interpolation polynomials (LIPs). Therefore, FEM with HIPs are used in problems where continuity is required not only for the approximate solution, but also for its derivatives [3]. One constructive approach to the construction of multidimensional HIPs inside d-dimensional hypercube in the form of a polynomial of d variables of degree p' with a set of $(p'+1)^d$ unknown coefficients, which are calculated in integer arithmetic by solving the system $(p'+1)^d$ nonhomogeneous algebraic equations, was implemented as a program for $d = 3$, $p' = 3$ and $(3+1)^3 = 64$ in [3]. With an increase in d and p' and the dimension of the system, the complexity of its solution in integer arithmetic becomes difficult, therefore, in the general case, it is necessary to develop new algorithms that do not have this drawback.

In this work, we implement an algorithm in the form of a program in Maple for constructing multidimensional HIPs inside a d-dimensional hypercube in the form of product of one-dimensional HIPs of degree p' in each of d variables, in which there is no need to solve such a system of equations [4]. One-dimensional HIPs are calculated analytically using the author's recurrent relations [5]. As a result, multidimensional HIPs are also calculated in an analytical form, and satisfy all the conditions for their definition and properties. In the particular case $d = 3$, $p' = 3$, as shown in [6], they coincide with 3 dimensional HIPs in [3].

The efficiency of our finite element schemes, algorithms and program GCM-FEM implemented in Maple is demonstrated on reference calculations of the BVP for multidimensional linear and nonlinear oscillator for the Geometric Collective Model(GCM) of atomic nuclei [8].

Algorithm. The HIPs $\varphi_r^{\kappa}(x)\equiv\varphi_{r_1\cdots r_i\cdots r_d}^{\kappa_1\cdots\kappa_i\cdots\kappa_d}(x_1,\ldots,x_i,\ldots,x_d)$ variables d in an element of a d-dimensional parallelepiped

$$x=(x_1,\ldots,x_d)\in[x_{1;\min},x_{1;\max}]\otimes\cdots\otimes[x_{d;\min},x_{d;\max}]=\Delta_q\subset\mathcal{R}^d \tag{1}$$

received at nodes $x_{r_1\cdots r_i\cdots r_d}=(x_{1r_1},\ldots,x_{ir_i},\ldots,x_{dr_d})$, $x_{ir_i}=((p-r_i)x_{i;\min}+r_ix_{i;\max})/p$; $r_i=0,\ldots,p$, $i=1,\ldots,d$ are defined by the relations [1, 2]

$$\begin{aligned}&\varphi_{r_1\cdots r_i\cdots r_d}^{\kappa_1\cdots\kappa_i\cdots\kappa_d}(x_{1r_1'},\ldots,x_{ir_i'},\ldots,x_{dr_d'})=\delta_{r_1r_1'}\cdots\delta_{r_ir_i'}\cdots\delta_{r_dr_d'}\delta_{\kappa_10}\cdots\delta_{\kappa_i0}\cdots\delta_{\kappa_d0},\\&\left.\frac{\partial^{\kappa_1'+\cdots+\kappa_d'}\varphi_{r_1\cdots r_i\cdots r_d}^{\kappa_1\cdots\kappa_i\cdots\kappa_d}(x_1,\ldots,x_i,\ldots,x_d)}{\partial x_1^{\kappa_1'}\cdots\partial x_i^{\kappa_i'}\cdots x_d^{\kappa_d'}}\right|_{(x_1,\ldots,x_i,\ldots,x_d)=(x_{1r_1'},\ldots,x_{ir_i'},\ldots,x_{dr_d'})}\\&=\delta_{r_1r_1'}\ldots\delta_{r_ir_i'}\ldots\delta_{r_dr_d'}\delta_{\kappa_1\kappa_1'}\cdots\delta_{\kappa_i\kappa_i'}\cdots\delta_{\kappa_d\kappa_d'}.\end{aligned} \tag{2}$$

where $\delta_{r_1r_1'}=1(0)$ for $r_1=r_1'(r_1\neq r_1')$. These HIPs of order $p'=\prod_{s=1}^d p_s'$ are calculated as a product of one-dimensional HIPs $\varphi_{r_s}^{\kappa_s}(x_s)$,

$$\varphi_r^{\kappa}(x)\equiv\varphi_{r_1\cdots r_i\cdots r_d}^{\kappa_1\cdots\kappa_i\cdots\kappa_d}(x_1,\ldots,x_i,\ldots,x_d)=\prod_{s=1}^d\varphi_{r_s}^{\kappa_s}(x_s). \tag{3}$$

The one-dimensional HIPs $\varphi_{r_s}^{\kappa_s}(x_s)$, are calculated as follows. For each $x\equiv x_s$, a set of basis functions, one-dimensional HIPs $\{\{\varphi_r^{\kappa}(x)\}_{r=0}^p\}_{\kappa=0}^{\kappa_r^{\max}-1}$ order $p's\equiv p'=\sum_{r=0}^p\kappa_r^{\max}-1$ on the standard interval $x\in[0,1]$ at the nodes x_r, $r=0,\ldots,p$, $x_0=0$, $x_p=1$ are built. The values of functions $\varphi_r^{\kappa}(x)\in C^{\kappa_{\max}-1}$ are continuous together with their derivatives up to order $(\kappa_r^{\max}-1)$, i.e. $\kappa=0,\ldots,\kappa_r^{\max}-1$, where $\kappa_r^{\max}$ is denoted as the multiplicity [1] of the node x_r, determined by equations (2). Note that for $\kappa_{\max}=1$, the HIPs correspond to LIPs that do not have continuous derivatives at the boundaries of finite elements. These one-dimensional HIPs are calculated analytically based on the recurrence relations[5]

$$\varphi_r^{\kappa}(x)=w_r(x)\sum_{\kappa'=0}^{\kappa_r^{\max}-1}a_r^{\kappa,\kappa'}(x-x_r)^{\kappa'},\quad w_r(x)=\prod_{r'=0,r'\neq r}^{p}\left(\frac{x-x_{r'}}{x_r-x_{r'}}\right)^{\kappa_{r'}^{\max}}, \tag{4}$$

$$a_r^{\kappa,\kappa'}=\begin{cases}0, & \kappa'<\kappa,\\ 1/\kappa'!, & \kappa'=\kappa,\\ -\sum\limits_{\kappa''=\kappa}^{\kappa'-1}\frac{1}{(\kappa'-\kappa'')!}g_r^{\kappa'-\kappa''}(x_r)a_r^{\kappa,\kappa''}, & \kappa'>\kappa,\end{cases}\qquad g_r^{\kappa}(x)=(w_r(x))^{-1}\frac{d^{\kappa}w_r(x)}{dx^{\kappa}}.$$

Below we consider only HIPs with nodes of the same multiplicity, $\kappa_r^{\max}=\kappa^{\max}$, $r=0,\ldots,p$, then $p'=\kappa^{\max}(p+1)-1$.

Examples. As an example of the application of the algorithms described above, we present the results of solving the BVP in $x=(x_1,...,x_d)\in R^d$

$$(H-E_m)\,\Phi_m(x)\equiv\left(-\frac{1}{g_0(x)}\sum_{i,j=1}^d\frac{\partial}{\partial x_i}g_{ij}(x)\frac{\partial}{\partial x_j}+V(x)-E_m\right)\Phi_m(x)=0. \tag{5}$$

Assumed that $g_0(x)>0$, $g_{ji}(x)=g_{ij}(x)$ and $V(x)$ are real-valued functions, continuous together with their generalized derivatives up to a given order in the

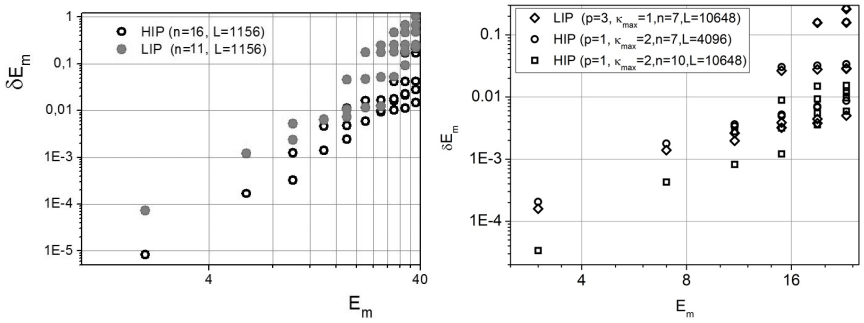


Fig. 1. The discrepancy $\delta E_m{=}E_m^h{-}E_m$, $m{=}0,1,...$ (along the y-axis) of the computed eigenvalue E_m^h oscillator problem from their exact values of E_m (at R_+): $E_m{=}2[1],6[2],10[3],...$ for $d{=}2$ (left panel) and $E_m{=}3[1],7[3],11[6],...$ for $d{=}3$ (right panel), where the degeneracy multiplicity is indicated in square brackets. The results of the FEM for cubic elements are noted — product one-dimensional LIPs ($p{=}3$, $\kappa_{\max}{=}1$) and HIPs ($p{=}1$, $\kappa_{\max}{=}2$) of the third order, while the quadrat or cube was divided into n^d equal quadrates or cubes. The dimension of the matrix of the algebraic problem is $L{\times}L{=}1156{\times}1156$ for $d{=}2$, $L{\times}L{=}4096{\times}4096$ and $L{\times}L{=}10648{\times}10648$ for $d{=}3$.

domain $x \in \bar{\Omega} = \Omega \cup \partial\Omega \in \mathcal{R}^d$ with the piecewise continuous boundary $S = \partial\Omega$, which provides the existence of nontrivial solutions $\Phi(x)$ obeying the Neumann or Dirichlet boundary conditions (BCs) [4].

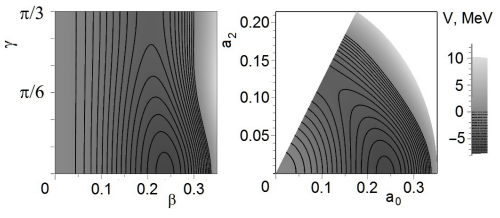
This problem with oscillator potential $V(x){=}x_1^2{+}...{+}x_d^2$ has the degenerate pure discrete spectrum $E_m \equiv E_{k_1...k_d}{=}\sum_{i=1}^d(2k_i{+}1)$ with degeneracy $D(E_m){=}(k_1{+}...{+}k_d)!/(k_1!...k_d!)$ and corresponding set of eigenfunctions $\Phi_m(x){\equiv}\Phi_{k_1...k_d}(x) {=}\prod_{i=1}^d \phi_{k_i}(x_i)$, where $\phi_{k_i}(x_i){=}(\sqrt{\pi}2^{k_i}k_i!)^{-1/2}H_{k_i}(x_i)\exp(-x_i^2)$ are the orthonormalized eigenfunctions of the 1D oscillator, $H_{k_i}(x_i)$ are Hermite polynomials [7]. The problem in R_+^d with Neumann boundary conditions in origin $x_i{=}0$ has the same spectrum but with even k_i and normalization coefficient divided by $\sqrt{2}^d$.

The 2D ($d{=}2$) and 3D ($d{=}3$) oscillator problems were solved on quadrat or cube $[0,7]^d$ with Neumann boundary conditions. The discrepancy $\delta E_m{=}E_m^h - E_m$, $m{=}0,1,...$ numerical eigenvalues E_m^h of these problem from their exact values are shown in Fig. 1. As can be seen from the figure, the accuracy of the approximate FEM solution of the algebraic eigenvalue problems with the same dimension L, calculated using the HIPs is higher than the accuracy of the approximate FEM solution calculated using the LIPs.

In paper [8] the GCM FORTRAN program for solving the BVP for 5-dimensional nonlinear oscillator of GCM Model of atomic nuclei with a pure discrete degenerated spectrum of eigenvalues of energy $E_n^L{=}E_1^L{<}E_2^L$, $<E_3^L,<...$ has been created. It was done in irreducible representations of the rotational group $\overline{\mathrm{O(3)}}$ parameterized by the Euler angles x_3, x_4, x_5 in the intrinsic frame (IF). They are specify by a set of quantum numbers of the integer angular momentum $L{=}0,2,3,4,...$, and its projections $-L{\le}M{\le}L$ and $0 \le K \le L$ on the third axes of laboratory and intrinsic frames and basis functions $\Phi_K^L(x_1,x_2)$,

Table 1. The eigenenergies E_n^L (B) and E_n^L (F) (in MeV) of nucleus ^{186}Os at the parameter P_3=0 (see [8]) calculated by expansion over a basis and by FEM with HIPs p=1, $\kappa_{\max}$=2, p'=3 in grid $[\beta=0.08, 0.107, ..., 0.35]\otimes[\gamma=0., \pi/30, ..., \pi/3]$ and potential energy surface $V(x_1, x_2)$ vs variables a_0 and a_2 (in fm), and β (in fm) and angle γ.

L	n	E_n^L (B)	E_n^L (F)
0	1	−5.491	−5.493
2	1	−5.378	−5.381
2	2	−4.411	−4.414
3	1	−4.221	−4.222
4	1	−5.139	−5.157
4	2	−4.092	−4.109
4	3	−3.439	−3.453
5	1	−3.837	−3.857



x_1=a_0=$\beta\cos\gamma$, x_2=a_2=$\beta/\sqrt{2}\sin\gamma$ in IF. This problem at any fixed L and M is reduced to a set of $L/2$+1 for even L, or $(L-1)/2$ for odd L, of 2D BVP coupling by a three-diagonal matrix[9]. In Table 1 we compare our FEM results for a low part of the spectrum of energy E_n^L of nucleus ^{186}Os calculated by FEM using HIPs with one calculated by expansion of desired solution over the basis functions implemented in the GCM FORTRAN code [8]. There is a good agreement results obtained by GCMFEM and the expansion over the basis functions. Moreover, GCMFEM is applicable to a more wide class of BVP (5) like Ref. [9].

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