Hermitian Finite Elements for Hypercube

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Abstract. Algorithm for analytical construction of multivariate Hermite interpolation polynomials in a multidimensional hypercube is presented. In the case of a d-dimensional cube, the basis functions are determined by products of d Hermite interpolation polynomials depending on each of the d variables given explicitly in the analytical form. The efficiency of finite element schemes, algorithms and programs is demonstrated by benchmark calculations of the 4D Helmholtz problem.

Introduction

In this paper we present a new symbolic algorithm implemented in Maple for constructing the Hermitian finite elements or piece-wise multivariate Birkhoff interpolants in a standard d-dimensional cube that generalizes the construction and algorithm proposed for a three and four dimensional cube [1, 2, 3, 4]. Our algorithm realizes recurrence relations [5, 6] and yields explicit expressions in an analytical form for the Hermite interpolation polynomials (HIPs) in opposite the conventional constructions. The basis functions of finite elements are high-order polynomials, determined from a specially constructed set of values of the polynomials themselves and their partial derivatives up to a given order at the vertices of the hypercube. Such a choice of values allows us to construct a piecewise polynomial basis continuous at the boundaries of finite elements together with the derivatives up to a given order. In the case of a d- dimensional cube, it is shown that the basis functions are determined by products of d one-dimensional HIPs depending on each of the d variables given in the analytical form with the derivatives up to a given order continuous at the boundaries of finite elements [6].The efficiency of finite element schemes, algorithms and programs is demonstrated by benchmark calculations of the 4D Helmholtz problem.

1. Algorithm for constructing Hermitian finite elements

The HIPs $\varphi_r^{\kappa}(x) \equiv \varphi_{r_1 \ldots r_i \ldots r_d}^{\kappa_1 \ldots \kappa_i \ldots \kappa_d}(x_1, ..., x_i, ..., x_d)$ of d variables in a d-dimensional parallelepiped element $x = (x_1, ..., x_i, ..., x_d) \in [x_{1;\min}, x_{1;\max}] \times ... \times [x_{d;\min}, x_{d;\max}]$ $= \Delta_q \subset \mathbf{R}^d$ that are obtained on nodes $x_{r_1 \ldots r_i \ldots r_d} = (x_{1r_1}, ..., x_{ir_i}, ..., x_{dr_d})$, $x_{ir_i} = ((p - r_i)x_{i;\min} + r_i x_{i;\max})/p$; $r_i = 0, ..., p$, $i = 1, ..., d$ are determined by relations [1]

$$\varphi_{r_1 \ldots r_i \ldots r_d}^{\kappa_1 \ldots \kappa_i \ldots \kappa_d}(x_{1r'_1}, \ldots, x_{ir'_i}, \ldots, x_{dr'_d}) = \delta_{r_1 r'_1} \ldots \delta_{r_i r'_i} \ldots \delta_{r_d r'_d} \delta_{\kappa_1 0} \ldots \delta_{\kappa_i 0} \ldots \delta_{\kappa_d 0}, \qquad (1)$$

$$\left.\frac{\partial^{\kappa'_1+\cdots+\kappa'_d}\varphi^{\kappa_1\ldots\kappa_i\ldots\kappa_d}_{r_1\ldots r_i\ldots r_d}(x_1,\ldots,x_i,\ldots,x_d)}{\partial x_1^{\kappa'_1}\cdots\partial x_i^{\kappa'_i}\cdots x_d^{\kappa'_d}}\right|_{(x_1,\ldots,x_i,\ldots,x_d)=(x_{1r'_1},\ldots,x_{ir'_i},\ldots,x_{dr'_d})}$$
$$=\delta_{r_1r'_1}\ldots\delta_{r_ir'_i}\ldots\delta_{r_dr'_d}\delta_{\kappa_1\kappa'_1}\ldots\delta_{\kappa_i\kappa'_i}\ldots\delta_{\kappa_d\kappa'_d}.$$

These HIPs of order $p'=\prod_{s=1}^{d}p'_s$ are calculated as a product of one dimensional HIPs $\varphi^{\kappa_s}_{r_s}(x_s)$: $\varphi^{\kappa}_{r}(x)\equiv\varphi^{\kappa_1\ldots\kappa_i\ldots\kappa_d}_{r_1\ldots r_i\ldots r_d}(x_1,\ldots,x_i,\ldots,x_d)=\prod_{s=1}^{d}\varphi^{\kappa_s}_{r_s}(x_s)$, which are calculated by the following way. For each $z\equiv x_s$ as a set of basis functions, the 1D HIPs $\{\{\varphi^{\kappa}_{r}(z)\}_{r=0}^{p}\}_{\kappa=0}^{\kappa^{\max}_r-1}$ of order $p'=\sum_{r=0}^{p}\kappa^{\max}_r-1$ in a standard interval $z\in[0,1]$ at the nodes z_r, $r=0,\ldots,p$, $z_0=0$, $z_p=1$ are constructed. The values of the functions $\varphi^{\kappa}_{r}(z)\in C^{\kappa_{\max}-1}$ continuous together with their derivatives up to order $(\kappa^{\max}_r-1)$, i.e. $\kappa=0,\ldots,\kappa^{\max}_r-1$, where $\kappa^{\max}_r$ is referred to as the multiplicity [1] of the node z_r, are determined by expressions (1). These 1D HIPs are calculated analytically from the recurrence relations derived in [6]

$$\varphi^{\kappa}_{r}(z)=w_r(z)\sum_{\kappa'=0}^{\kappa^{\max}_r-1}a^{\kappa,\kappa'}_{r}(z-z_r)^{\kappa'},\quad w_r(z)=\prod_{r'=0,r'\neq r}^{p}\left(\frac{z-z_{r'}}{z_r-z_{r'}}\right)^{\kappa^{\max}_{r'}},\qquad(2)$$

$$a^{\kappa,\kappa'}_{r}=\begin{cases}0, & \kappa'<\kappa,\\ 1/\kappa'!, & \kappa'=\kappa,\\ -\sum\limits_{\kappa''=\kappa}^{\kappa'-1}\frac{a^{\kappa,\kappa''}_{r}}{(\kappa'-\kappa'')!}g_r^{\kappa'-\kappa''}(z_r), & \kappa'>\kappa,\end{cases}\qquad g^{\kappa}_{r}(z)=\frac{\frac{d^{\kappa}w_r(z)}{dz^{\kappa}}}{w_r(z)}.$$

Below we consider only the HIPs with the nodes of identical multiplicity, $\kappa^{\max}_r=\kappa^{\max}$, $r=0,...,p$, then $p'=\kappa^{\max}(p+1)-1$. For example, at $\kappa_{\max}=2$, $p'=2p+1$ the 1D HIPs take the form:

$$\varphi^{\kappa_s=0}_{r}(z)=\left(1-(z-z_r)\sum_{r'=0,r'\neq r}^{p}\frac{2}{z_r-z'_r}\right)\prod_{r'=0,r'\neq r}^{p}\left(\frac{z-z_{r'}}{z_r-z_{r'}}\right)^2,$$
$$\phi^{\kappa_s=1}_{r}(z)=(z-z_r)\prod_{r'=0,r'\neq r}^{p}\left(\frac{z-z_{r'}}{z_r-z_{r'}}\right)^2,$$

for polynomials $\phi^{\kappa_s=0}_{r}(z)$ or $\phi^{\kappa_s=1}_{r}(z)$ whose value or value of first derivative is equal to 1, respectively.

2. Benchmark Calculations with Hermitian Finite Elements

As benchmark calculations we solve the 4D Helmholtz problem with the edge length π and Neumann boundary conditions. This problem has exact degenerate spectrum: E_m =0 [1] 1 [4] 2 [6] 3 [4] 4 [5] 5 [12]6 [12] 7 [4] 8 [6] 9 [16] 10 [18] 11 [12] 12 [8] 13 [16] 14 [24] 15 [12] ... , where the multiplicity of degeneracy is given in square brackets. The results were calculated on uniform grids using FEM with hypercube LIPs and HIPs of the third order that are obtained by product of four

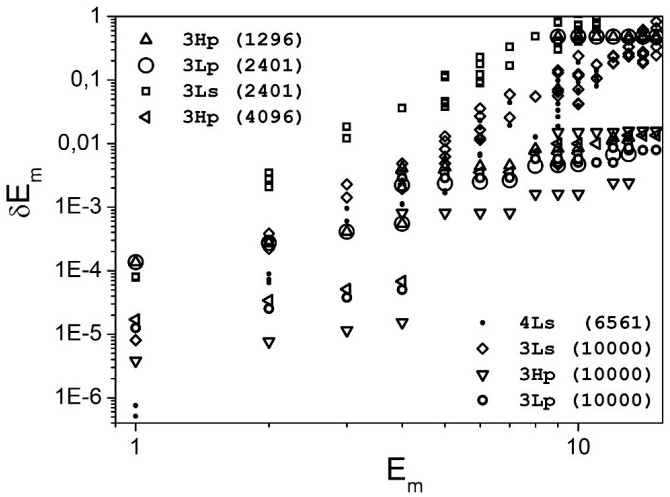

FIGURE 1. The discrepancy $\delta E_m = E_m^h - E_m$ of calculated eigenvalue E_m^h of the Helmholtz problem for a four-dimensional cube with the edge length π. Calculations were performed using FEM with 3rd-order (3Ls) and 4th-order (4Ls) simplex Lagrange elements, and 3rd-order parallelepiped Lagrange (3Lp) and Hermite (3Hp) elements. The dimension of the algebraic problem is given in parentheses.

1D LIPs or four 1D HIPs, respectively. They are compared with simplex LIPs of the third and the fourth order [7].

Figure 1 shows the discrepancy $\delta E_m = E_m^h - E_m$ between the numerical eigenvalues E_m^h and the exact ones E_m. There is a stepwise structure of the discrepancy δE_m calculated with 4D hypercubic LIPs and HIPs, with the steps appearing at the values $E_m = 1, 4, 9, ...$ The structure is also due to the prevalence of approximation errors of eigenfunctions caused by the pure partial derivatives. For the simplex LIPs the oscillating structure of the discrepancy δE_m is due to different contributions the approximation errors caused by the different mixed partial derivatives. The calculation is performed using MAPLE with 12-digit precision. As a consequence, the FEM scheme with the hypercubic LIPs and a large length of the eigenvectors equal to 10000 demonstrates poorer performance than the one with a smaller length due to rounding errors. The above analysis shows the agreement the numerical and theoretical estimations of discrepancy for eigenvalues, $\left|E_m - E_m^h\right| \leq c_m h^{2p'}$, with respect to order p' of FEM schemes with LIPs or HIPs, where h is the step of the uniform grid and $c_m > 0$ are constants independent from h.

Conclusion

The proposed algorithm allows one to construct in analytical form a piecewise polynomial basis continuous on the boundaries of finite elements together with the derivatives up to the given order. It can be used to solve elliptic BVPs as well as other problems with partial derivatives of a high order by means of the high-accuracy finite element method.

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