Higher Order Large-Domain Hierarchical FEM Technique for Electromagnetic Modeling Using Legendre Basis Functions on Generalized Hexahedra

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Abstract: A novel higher order large-domain hierarchical finite-element technique using curl-conforming vector basis functions constructed from standard Legendre polynomials on generalized curvilinear hexahedral elements is proposed for electromagnetic modeling. The technique combines the inherent modeling flexibility of hierarchical elements with excellent orthogonality and conditioning properties of Legendre curl-conforming basis functions, comparable to those of interpolatory techniques. The numerical examples show the reduction of the condition number of several orders of magnitude for high field-approximation orders (e.g., fourteen orders of magnitude for entire-domain models) when compared to the technique using field expansions based on simple power functions and the same geometrical elements.
I. Introduction

Higher order basis functions that constitute the large-domain (entire-domain) finite element method (FEM) for modeling of three-dimensional (3-D) electromagnetic structures have significant computational advantages over traditionally used low-order (subdomain) FEM basis functions (Ilić and Notaros, 2003). Finite elements of higher geometrical orders and higher field-approximation orders enable excellent curvature modeling and excellent field-distribution modeling, as well as using as large as about $2\lambda \times 2\lambda \times 2\lambda$ curved FEM hexahedra (large domains), $\lambda$ being the wavelength in the medium, as building blocks for modeling of the electromagnetic structure, which is 20 times the traditional low-order (small-domain) modeling discretization limit of $\lambda/10$ in each dimension. This results in a considerably improved accuracy and efficiency over the traditional techniques, with a reduction in the number of unknowns of more than an order of magnitude when compared to low-order solutions.

Higher order bases designed for implementing in Galerkin-based FEM techniques automatically satisfy tangential-field continuity conditions at the interconnections of elements (curl-conforming bases) and are generally of either interpolatory or hierarchical form. Interpolatory basis functions (Graglia, Wilton, and Peterson, 1997) have excellent orthogonality properties and produce well-conditioned FEM matrices. Hierarchical basis functions enable using different orders of field approximation in different elements for efficient selective discretization of the solution domain, because each lower-order set of functions is a subset of higher-order sets. For instance, the hierarchical nature of the technique proposed by Ilić and Notaroš (2003) allows for a whole spectrum of element sizes (from a very small fraction of $\lambda$ to $2\lambda$) and the corresponding field-approximation orders to be used at the same time in a single simulation model of a complex structure. Additionally, each individual element can have drastically different sizes in different directions, enabling a whole variety of “irregular” element shapes. However, hierarchical basis functions generally have poor orthogonality properties, which results in FEM matrices with large condition numbers. This affects the overall accuracy and stability of the solution. Most importantly, if the linear equations associated with the FEM are solved using iterative solvers, the overall computation time
is much larger when the FEM matrices are badly conditioned (e.g., the number of iterations for conjugate gradient solvers is proportional to the square root of the condition number). Although problems with the ill-conditioning of the system matrices represent one of the most important issues in higher-order computational electromagnetics, only a very limited number of publications (Andersen and Volakis, 1999; Web, 1999; Djordjević and Notaroš, 2003; Jørgensen et al., 2004; Stupfel, 2004) have addressed these problems in the frame of either FEM or integral equation techniques.

This paper proposes a novel highly efficient and accurate higher order large-domain Galerkin-type hierarchical FEM technique for 3-D electromagnetics with dramatically improved orthogonality properties. The technique implements generalized curvilinear Lagrange-type hexahedra of arbitrary geometrical orders and hierarchical curl-conforming vector basis functions of arbitrary field-approximation orders constructed from standard Legendre polynomials. This work is based on our previous investigations in coping with ill-conditioning in the context of the hierarchical method of moments (MoM), where we have proposed three classes of higher order hierarchical MoM basis functions constructed from standard orthogonal polynomials (e.g., Chebyshev polynomials) yielding reductions of the condition number of MoM matrices by several orders of magnitude (Djordjević and Notaroš, 2003). The new technique represents an extension of the higher order FEM technique by Ilić and Notaros (2003), which uses curl-conforming hierarchical basis functions developed from simple power functions of local parametric coordinates and exhibits very poor orthogonality and conditioning properties. It also has similarities with the higher order hierarchical MoM technique by Jørgensen et al. (2004), where similar divergence-conforming Legendre basis functions are used.

Section II of the paper outlines the main numerical components of the new technique. In Section III, numerical results are presented demonstrating excellent orthogonality properties of the technique. The examples show a very slow increase of the condition number of the FEM matrix with increasing the field-approximation orders and a very dramatic reduction of the condition number for high orders as compared to the technique using field expansions based on simple power functions (Ilić and Notaros, 2003) (the
reduction is as large as fourteen orders of magnitude in some cases). To the best of our knowledge, the technique presented in this paper is the first general higher order hierarchical FEM technique with comparable orthogonality and conditioning properties as the interpolatory FEM techniques.

II. Theory and Implementation

For geometrical modeling of electromagnetic structures of arbitrary shapes and material inhomogeneities, we use generalized curved parametric hexahedra (Ilić and Notaros, 2003) of higher (theoretically arbitrary) geometrical orders. A generalized hexahedron is analytically described as

\[ r(u,v,w) = \sum_{i=1}^{M} r_i L_i^{K_{uvw}}(u,v,w) \quad -1 \leq u,v,w \leq 1, \]  

where \( r_1, r_2, \ldots, r_M \) are the position vectors of the interpolation nodes, and \( L_i^{K_{uvw}}(u,v,w) \) are the polynomials defined as

\[ L_i^{K_{uvw}}(u,v,w) = L_m^K(u)L_n^K(v)L_l^K(w), \quad i = 1 + m + n(K_u + 1) + l(K_u + 1)(K_v + 1)^2, \]

\[ 0 \leq m \leq K_u, \quad 0 \leq n \leq K_v, \quad 0 \leq l \leq K_w \quad 1 \leq i \leq M = (K_u + 1)(K_v + 1)(K_w + 1), \]  

with \( K_u, K_v, \) and \( K_w \) being the adopted geometrical orders of the element along different parametric coordinates. Functions \( L_m^K \) are Lagrange interpolating polynomials given by

\[ L_m^K(u) = \prod_{j=0}^{K} \frac{u - u_j}{u_m - u_j}, \]  

where \( u_j \) are the uniformly spaced interpolating nodes defined on an interval \(-1 \leq u \leq 1\), and similarly for \( L_n^K(v) \) and \( L_l^K(w) \). Equations (1)-(3) define a mapping from a cubical parent domain to the generalized hexahedron, as illustrated in Fig.1.

The electric fields inside the hexahedra are represented as
\[
E = \sum_{i=0}^{N_u} \sum_{j=0}^{N_v} \sum_{k=0}^{N_w} \alpha_{uijk} f_{uijk}(u,v,w) + \sum_{i=0}^{N_u} \sum_{j=0}^{N_v} \sum_{k=0}^{N_w} \alpha_{vijk} f_{vijk}(u,v,w) + \sum_{i=0}^{N_u} \sum_{j=0}^{N_v} \sum_{k=0}^{N_w} \alpha_{wijk} f_{wijk}(u,v,w)
\]

where \( f \) are curl-conforming hierarchical polynomial basis functions of coordinates \( u, v, \) and \( w \), \( N_u, N_v, \) and \( N_w \) are the adopted field approximation orders, which are entirely independent from the element geometrical orders, \( \alpha_{uijk}, \alpha_{vijk}, \) and \( \alpha_{wijk} \) are unknown field-distribution coefficients, and \( \mathbf{r} \) is given in Eq.(1). Note that the sum limits in Eq.(4) reflect a mixed-order arrangement that is in accordance with the reduced-gradient criterion.

To solve for the coefficients \( \{ \alpha \} \), the expansion in Eq.(4) is substituted in the curl-curl electric-field vector wave equation

\[
\nabla \times \mu_r^{-1} \nabla \times E - k_0^2 \varepsilon_r E = 0,
\]

where \( \varepsilon_r \) and \( \mu_r \) are complex relative permittivity and permeability of the inhomogeneous (possibly lossy) medium, respectively, \( k_0 = \omega \sqrt{\varepsilon_0 \mu_0} \) is the free-space wave number, and \( \omega \) is the angular frequency of the implied time-harmonic variation. A standard Galerking-type weak form discretization of Eq.(8) yields

\[
\int_V \left( \frac{\mu_r^{-1}}{V} (\nabla \times f_{ijk}) \cdot (\nabla \times E) \right) dV - k_0^2 \int_S \varepsilon_r f_{ijk} \cdot E dS = -\int_S \frac{\mu_r^{-1}}{S} f_{ijk} \cdot n \times (\nabla \times E) dS,
\]

where \( V \) is the volume of a generalized hexahedron, \( f_{ijk} \) stands for any of the functions \( f_{uijk}, f_{vijk}, \) or \( f_{wijk}, S \) is the boundary surface of the hexahedron, and \( n \) is the outward unit normal \( (dS = ndS) \).
the continuity of the tangential component of the magnetic field intensity vector, $\mathbf{n} \times \mathbf{H}$, and hence the vector $\mathbf{n} \times (\nabla \times \mathbf{E})$ in Eq.(9) across the interface between any two finite elements in the FEM model, the right-hand side term in Eq.(9) contains the surface integral over the overall boundary surface of the entire FEM domain, and not over the internal boundary surfaces between the individual hexahedra in the model. The tangential component of $\mathbf{H}$ over the boundary surface of the FEM domain is determined by appropriate boundary conditions imposed at the surface, which constitute a mesh termination scheme for a particular closed or unbounded problem under consideration. In analysis of metallic cavities, for instance, these conditions reduce to the simple requirement that the tangential component of $\mathbf{E}$ vanish near the cavity walls, which is enforced by a priori setting to zero the coefficients $\{\alpha\}$ associated with the tangential $\mathbf{E}$ on the sides of elements adjacent to cavity walls.

The simplest class of hierarchical higher order basis functions on generalized hexahedra is a set of simple 3-D power functions in the $u−v−w$ coordinate system modified for curl conformity, that is, to automatically satisfy the continuity condition for the tangential component of $\mathbf{E}$ across the side shared by finite elements (Ilić and Notaros, 2003). These functions, hereafter referred to as the regular polynomials, are given by

$$f_{ijkl} (u,v,w) = u^i j = 0 \begin{cases} 1−v, & j = 0 \\ v+1, & j = 1 \\ v+1, & j ≥ 2, \text{even} \\ v^j−v, & j ≥ 3, \text{odd} \end{cases} \begin{cases} 1−w, & k = 0 \\ w+1, & k = 1 \\ w+1, & k ≥ 2, \text{even} \\ w^k−w, & k ≥ 3, \text{odd} \end{cases} \right) ,$$

with analogous expressions for $f_{ijk}$ and $f_{ijk}$ in Eq.(5). The functions $1−v$ (for $j = 0$) and $v+1$ (for $j = 1$) in an arbitrary hexahedron serve for adjusting the tangential-field continuity boundary condition (curl conformity) on the side (surface) $v = −1$ and $v = 1$, respectively, and similarly for $1−w$ and $w+1$, while the remaining (higher-order) functions (for $j ≥ 2$ and $k ≥ 2$) are zero at the hexahedron sides and serve for improving the field approximation throughout the hexahedron volume. Similar functions are used in our
higher order MoM techniques based on the volume integral equation (VIE) approach (Notaroš and Popović, 1996) and surface integral equation (SIE) approach (Djordjević and Notaroš, 2004).

We note that, as the polynomial degrees \( N_u, N_v, \) and \( N_w \) in Eq.(4) increase, the basis functions in Eq.(10) become increasingly similar to one another, and consequently the condition number of the FEM matrix built from them deteriorates. The ill-conditioning is principally caused by a strong mutual coupling between the pairs of higher-order functions defined on the same (electrically large) generalized hexahedron. In order to reduce this coupling (and thus improve the condition number of the resulting FEM matrix), basis functions with better orthogonality properties have to be utilized. Due to their simplicity and flexibility, standard orthogonal polynomials (Abramowitz and Stegun, 1996) (and their modifications) are adopted as candidate basis functions in this paper. In MoM solutions to SIE, we have been using Chebyshev polynomials as a basis for constructing surface-current divergence-conforming higher order expansions with improved orthogonality over quadrilateral patches (Djordjević and Notaroš, 2003), because, out of all weighting functions with respect to which individual standard polynomials are orthogonal, the one with Chebyshev polynomials of the first kind, \( w(x) = (1 - x^2)^{-1/2} \), most closely resembles the 1-D version of the Green’s function in the SIE for combined metallic and dielectric structures \[ g = e^{-\gamma R} / (4\pi R) \], where \( \gamma \) is the complex propagation constant and \( R \) is the distance between the source and field points. In FEM, the kernels of Galerkin integrals based on Eq.(9) contain no Green’s functions as “weighting functions” in the inner product, and therefore Legendre polynomials, which also contain no weighting function in the orthogonality relationship, appear to be the most attractive choice for constructing FEM basis functions with improved orthogonality. Hence, we propose the implementation of the following class of Legendre basis functions on generalized hexahedral finite elements:

\[
 f_{uijk}(u,v,w) = C_i \hat{C}_j \hat{C}_k L_i(u) \begin{cases} 
 1 - v, & j = 0 \\
 v + 1, & j = 1 \\
 L_j(v) - L_{j-2}(v), & j \geq 2
 \end{cases} \begin{cases} 
 1 - w, & k = 0 \\
 w + 1, & k = 1 \\
 L_k(w) - L_{k-2}(w), & k \geq 2
 \end{cases}, \tag{11}
\]
\[ C_i = \sqrt{i + \frac{1}{2}} \quad \hat{C}_j = \begin{cases} \frac{\sqrt{3}}{4}, & j = 0,1 \\ \frac{1}{2} \sqrt{\frac{2j-3)(2j+1)}{2j-1}}, & j \geq 2 \end{cases} \]

as a higher-order generalization of traditionally used rooftop functions, with analogous expressions for \( f_{vijk} \) and \( f_{wijk} \) in Eq.(5), where standard Legendre polynomials \( L \) (Abramowitz and Stegun, 1996, 771–802) defined on the interval \([-1, 1]\), which have nonzero values at the interval boundaries, are combined for \( j \geq 2 \) and \( k \geq 2 \) in a way similar to that in (Djordjević and Notaroš, 2003) and (Jørgensen et al., 2004) to ensure the curl-conformity of the expansions. Note that using the difference of the polynomials of orders \( j \) and \( j - 2 \) and \( k \) and \( k - 2 \) as the basis function of order \( j \) and \( k \) in approximating the variation of the \( u \) component of the electric field intensity vector \( \mathbf{E} \) in Eq.(4) along the \( v \) and \( w \) coordinate, respectively, and analogously for \( v \) and \( w \) components of \( \mathbf{E} \), makes the higher-order expansions for the tangential field zero across boundary surfaces shared by adjacent generalized hexahedra and allows for the maximum number of basis functions to be mutually orthogonal within the solution procedure. The scaling factors \( C \) and \( \hat{C} \) are adopted to further reduce the condition number by ensuring that the Euclidean norm of basis functions is unity on a cube of unit side length (Jørgensen et al., 2004).

III. Numerical Results

The first two examples are air-filled metallic electromagnetic cavities of cubical and spherical shapes. In both cases, the computation is performed on entire-domain FEM models (the entire computational domain is represented by a single element): the cubical cavity is modeled by a single hexahedral element of the first geometrical orders \( (K_u = K_v = K_w = 1) \), and a single curved hexahedron of the 2\(^{nd} \) geometrical orders \( (K_u = K_v = K_w = 2) \) is used to model the spherical cavity, as shown in Fig.2. Note that the volume of the hexahedron in Fig.2 is 2.67% smaller than the volume of the sphere it approximates. The field-expansion polynomial orders are varied from \( N_u = N_v = N_w = 2 \) to \( N_u = N_v = N_w = 8 \) (\( p \)-refinement) for both
geometries. The results for $k_0$ for several modes for each of the cavities obtained using the two types of basis functions (regular and Legendre polynomials) appear to be practically identical, and agree very well with the analytical solution. Shown in Fig.3 is the relative error $|k_0 - k_0^{exact}| / k_0^{exact}$ for the dominant mode against the field-approximation order. We observe that the convergence of $p$-refined results for the cubical cavity is excellent, with the error as small as $10^{-13}$ for $N_u = N_v = N_w = 8$. On the other side, while the error in calculating $k_0$ for the spherical cavity quickly drops to about 1%, further $p$-refinement is not possible because of the inherent geometrical error of the model in Fig.2. This can be improved by further increasing the geometrical order $K_u = K_v = K_w$ of the model and/or using $hp$-refinement (Ilić and Notaros, 2003). Fig.4 shows the condition number of the FEM mass matrix for each of the cavities, as a function of the field approximation order in one dimension ($N_u = N_v = N_w$), obtained using the two types of basis functions. We observe that the use of regular polynomial basis functions, Eq.(10), yields a severely ill-conditioned FEM matrix, with the condition number rapidly increasing as the field approximation order increases. On the other hand, with using Legendre basis functions, Eq.(11), the increase of the condition number caused by the increase of the approximation order is much slower, and the reduction of the condition number for higher orders is indeed dramatic (the reduction is approximately $10^{14}$ times when compared to the regular polynomials for the highest order used). We note that, while the condition numbers of the cubical and spherical cavities are practically the same if regular polynomials of the same orders are used, the condition number with Legendre functions for the spherical cavity is slightly larger than that for the cubical cavity for a given approximation order, which is attributed to the Jacobian in Eq.(6) in the spherical case being a function of parametric coordinates $u$, $v$, and $w$, and not a constant, so that the orthogonality of basis functions within FEM integrals is slightly reduced. We also note that the condition number for the cubical cavity with Legendre functions of even the highest order used ($N_u = N_v = N_w = 8$) is comparable to (actually smaller than) that reported by Andersen and Volakis (1999) for a similar rectangular cavity analyzed using 130 interpolatory mixed-order tetrahedral elements developed by Graglia, Wilton, and Peterson (1997) of order 1.5 (reported condition number of the global mass
matrix for the rectangular cavity with the electric-field FEM formulation and normalized interpolatory vector basis functions by Graglia et al. is 99).

Fig. 5 shows the condition number as a function of the total number of unknowns for the cubical cavity modeled by 1, 8, and 27 hexahedral elements (h-refinement), with the field-approximation polynomial orders being varied from 2 to 8, from 1 to 4, and from 1 to 3, respectively, in all directions. The models with 8 and 27 elements correspond to the combined hp-refinement of the solution. We again observe dramatic reductions in the condition number using Legendre FEM basis functions as compared to the regular polynomials. We also note that, somewhat surprisingly, the condition number for hp-refined solutions with Legendre polynomials is larger than in the case of the pure p-refinement, which is another confirmation of excellent orthogonality properties of Legendre basis functions in the context of our higher order Galerkin FEM modeling, especially for rectangular elements.

Fig. 6(a) shows a 90° bend with rounded outer corner in a WR75 rectangular waveguide with dimensions $a = 19.05$ mm and $b = 9.525$ mm. In Fig. 7, the results for scattering parameters of an H-plane bend (with radius $r = a$) and an $E$-plane bend (with radius $r = b$) over a wide range of frequencies obtained using higher order Legendre FEM basis functions are compared with the modal analysis and a low-order FEM solution using HFSS and about 9000 small tetrahedra (MacPhie and Wu, 2001). The higher order FEM model is composed of three large elements of the first and second geometrical orders, with field-approximation orders ranging from 2 to 6 in different directions as shown in Fig. 6(b) (second- and fourth-order approximations are used in the direction perpendicular to the plane of drawing for the $H$- and $E$-plane bends, respectively), which results in a total of 286 unknowns and 29 seconds of CPU time for the $H$-plane bend and 362 unknowns and 46 seconds of CPU time for the $E$-plane bend on a 1.7 GHz Pentium III CPU with 1 GB of RAM for 80 frequencies (note an effective single-element model of the rounded corners). We observe from Fig. 7 a very good agreement of the three sets of results for both bends. Fig. 8 shows the condition number of the FEM matrix for the $H$-plane bend against the number of unknowns, obtained for four different $hp$-refined higher order FEM models, with 3, 9, 18, and 34
elements shown in Fig.6(b)-(e) and the field approximation orders being varied from 2 to 6, 1 to 5, 1 to 4, and 1 to 3, along the sides of elements in different directions in models (b), (c), (d), and (e), respectively. The approximation orders in models with more than three elements are chosen such that the same accuracy of the results is achieved as the optimal, three-element, model, throughout the considered frequency range. It can be observed from the figure that the condition number with Legendre functions is not only dramatically reduced when compared to the regular polynomials, but also that, within that reduced range of values, it is much less dependent on the field approximation orders than on the total number of unknowns, which is a much desired property for higher order hierarchical bases in FEM modeling.

IV. Conclusions

This paper has proposed a novel higher order large-domain hierarchical FEM technique for 3-D electromagnetic modeling using curl-conforming vector basis functions constructed from standard Legendre polynomials on electrically large generalized curvilinear Lagrange-type hexahedral elements (large domains). The numerical examples have shown excellent orthogonality properties of the technique and a much slower increase of the condition number of the FEM matrices with increasing the field-approximation orders as compared to the technique using field expansions based on simple power functions (regular polynomials), in both pure $p$- and combined $hp$-refined models. The reduction of the condition number using Legendre FEM basis functions is by several orders of magnitude for high field-approximation orders (e.g., fourteen orders of magnitude for entire-domain models) when compared to regular polynomials. The new technique combines, for the first time, the inherent modeling flexibility of hierarchical higher order curved finite elements with orthogonality and conditioning properties of Legendre curl-conforming basis functions comparable to those of interpolatory FEM techniques.
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References


Fig. 1. Cube to hexahedron mapping defined by Eqs. (1)-(3).
Fig. 2. Geometrical model of a spherical electromagnetic cavity using a single hexahedral element of the 2nd geometrical order ($K_u = K_v = K_w = 2$).
Fig. 3. Relative error (with respect to the exact analytical solutions) in calculating the free-space wavenumber for the dominant mode of cubical and spherical electromagnetic cavities using Legendre basis functions of different orders ($N_u = N_v = N_w$).
Fig. 4. Condition number of FEM mass matrices against the field approximation orders in the eigenvalue analysis of cubical and spherical cavities for two classes of higher order hierarchical basis functions.
Fig. 5. Condition number of the FEM mass matrix of a cubical cavity against the total number of unknowns for three different $hp$-refined FEM models and two classes of higher order hierarchical basis functions (see the text for details on the $p$-refinement of the elements).
Fig. 6. FEM computation of scattering parameters of a 90° bend with rounded outer corner in a rectangular waveguide ($a = 19.05$ mm, $b = 9.525$ mm)—H-plane bend ($r = a$) and E-plane bend ($r = b$) geometry (a) and four higher order FEM models composed of 3, 9, 18, and 34 elements (b)-(e).
Fig. 7. Magnitude of scattering parameters of the 90° waveguide bend in Fig. 6(a) over a wide range of frequencies: comparison of the higher order FEM solution with Legendre basis functions, low-order FEM solution (MacPhie and Wu, 2001), and modal analysis (MacPhie and Wu, 2001) for (a) $H$-plane bend and (b) $E$-plane bend.
Fig. 8. Condition number of the FEM matrix of the $H$-plane waveguide bend in Fig.6(a) ($r = a$) against the total number of unknowns for four $hp$-refined FEM models in Fig.6(b)-(e) and two classes of higher order hierarchical basis functions.