Overview of Some Advances in Higher Order Frequency-Domain CEM Techniques

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***Abstract*—We present some advances in several major components of higher order computational electromagnetics (CEM) techniques based on the finite element method (FEM) and the method of moments (MoM) in the surface integral equation (SIE) formulation in the frequency domain. Examples include a novel singularity extraction technique for curvilinear MoM-SIE integration and novel application of adaptive FEM discretization refinement based on adjoint-informed error estimation.**

Keywords—computational electromagnetics, higher order techniques, finite element method, method of moments, surface integral equation techniques, singularity extraction, adaptive refinement, adjoint methods, direct solvers.

I. Introduction

Both the finite element method (FEM) and the method of moments (MoM) in conjunction with the surface integral equation (SIE) formulation are extremely general and powerful technologies for modeling and analysis of scattering and radiation in computational electromagnetics (CEM) in the frequency domain (FD) [1]. In spite of great recent advances in mathematics, computing hardware and software infrastructure, and numerical algorithms, there is a continuing and growing demand for FEM and MoM-SIE tools that can handle simulations of larger and more complex problems and provide efficient, accurate, and reliable solutions using given computing resources.

This paper presents some advances in several major components of FEM and MoM-SIE FD modeling and computation, within the context of higher order (also known as the large-domain or entire-domain) computational approach, which utilizes higher order basis functions. Higher order modeling enables using large curved cells and patches, which can greatly reduce the number of unknowns and enhance the accuracy and efficiency of the computation [1]. Element orders in the model, however, can also be low, so the low-order modeling approach is actually included in the higher order modeling.

II. Advances in Higher Order FEM and MoM-SIE FD Modeling and Computation

The FEM technique employs generalized curvilinear interpolatory hexahedra of arbitrary geometrical orders as volume elements for the approximation of geometry [Fig. 1(a)] and hierarchical curl-conforming polynomial vector basis functions of arbitrary orders for the approximation of fields within the elements. The FEM domain is truncated implementing a novel anisotropic locally-conformal perfectly matched layer (PML) method for electrically large curvilinear meshes based on the higher order FEM modeling paradigm and the concept of transformation electromagnetics [2]. The method uses continuously varying anisotropic material parameters, with the interpolatory parameterization of higher order curvilinear geometries providing an interface to evaluate the required Jacobian matrices.

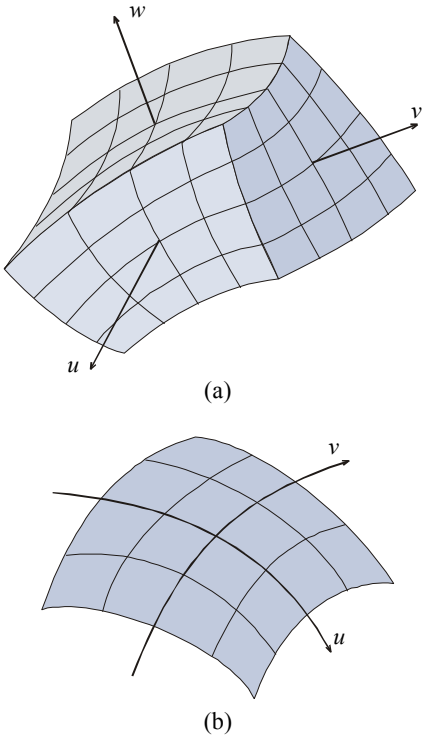


Fig. 1. Curved parametric elements for geometrical modeling in the higher order FEM and MoM-SIE techniques: (a) generalized hexahedron and (b) generalized quadrilateral.

The higher order MoM-SIE FD modeling utilizes a divergence-conforming 2-D version of FEM basis functions defined on generalized curved quadrilateral patches [Fig. 1(b)]. A key component of higher order MoM-SIE computation is accurate numerical evaluation of integrals defined on curved

patches. We focus on singularity extraction consisting of analytical integration of a principal singular part of the integrand over a parallelogram whose surface is close to the surface of the generalized curved quadrilateral near the singular point, and numerical integration of the rest [3]. The approximation function is defined using truncated Taylor's expansion over the difference between the curved quadrilateral patch and the parallelogram taking into account both the curvature of the element and the higher order of the basis function.

Singular and hypersingular 4-D integrals, computed over the testing and basis elements, are building blocks of the matrix entries in the MoM-SIE FD technique. Their calculation needs to be accurate and efficient in order to solve for unknown coefficients in the current expansion. A novel singularity extraction method has been developed for 2-D integrals (over basis elements) to overcome the (hyper)singular behavior of the integrand as well take into account higher order properties of the current expansion and geometry of the element. We are solving integrals of the following forms:

$$I_{ij}^{\mathrm{s}} = \int_{-1}^{1}\int_{-1}^{1} u^i v^j \frac{e^{-\gamma R}}{4\pi R}\mathrm{d}u\mathrm{d}v, \tag{2}$$

$$I_{ij}^{\mathrm{hs}} = \int_{-1}^{1}\int_{-1}^{1} u^i v^j \frac{(1+\gamma R)e^{-\gamma R}}{4\pi R^3}\mathrm{d}u\mathrm{d}v\ , \tag{3}$$

where 's" and 'hs" stand for 'singular' and 'hypersingular' respectively, u and v are local parametric coordinates, i and j represent arbitrary polynomial orders of the basis functions, γ is the propagation coefficient in the medium on either side of the element, and R is the distance from the source point on the basis element to the field point (on the testing element).

The extraction methods traditionally remove or mitigate the (hyper)singularity by approximating the integrand by an analytically integrable function. The difference between the (hyper)singular function and the approximation can then numerically be evaluated using Gauss-Legendre quadrature formulas. In the new method, the approximated function is computed through Taylor's expansion series of the (hyper)singular function and is defined over a parallelogram that is tangential to the quadrilateral basis element at the so-called closest projection point (CPP) with u_0 and v_0 being coordinates in the u-v domain. CPP is the point on the infinite parametric surface containing the basis element that is closest to the field point. Analytically evaluated integral is computed over four triangles forming the parallelogram, similarly to the method developed in [4].

With increasing the size/complexity of CEM problems, the need for quantitative error estimation and sensitivity analysis techniques for FEM-PML and MoM-SIE has become apparent. Such techniques allow for optimal remeshing [5], adaptive discretization refinement, and many other such improvements over the base FEM-PML or MoM-SIE method that allow for decreased computation time and increased accuracy. Toward this goal, we derive and formulate adjoint problems [6] for variants of the FEM and SIE problem. We furthermore demonstrate how these adjoint problems and their solutions can be applied to modern, large-scale CEM problems to obtain more-accurate results more quickly.

The adjoint problem is the dual of the forward problem. In general, the adjoint operator is the operator which satisfies the following identity:

$$\langle L\mathbf{u}, \mathbf{v}\rangle = \langle \mathbf{u}, L^*\mathbf{v}\rangle, \tag{1}$$

where $\langle\cdot,\cdot\rangle$ denotes the L^2 inner product. The adjoint problem is solved with respect to linear (or linearized) functional defining a relevant quantity of interest (QoI) from the forward solution. We use the higher-order parameter sampling (HOPS) and dual-weighted residual techniques to generate important gradient and sensitivity information, and error estimates throughout the discretization, including those localized to elements or direction.

By applying adjoint-based error estimates towards refinement, computational resources can be allocated optimally. Indicators of the error in the QoI are used in adaptive *p*- and *h*-refinement schemes, to determine how the adaption is done, namely, how and where the new basis function orders and/or new element sizes are assigned in a new, refined FD higher order FEM or SIE model. This can lead to an ability to control the quality of a solution, in terms of the discretization of the mesh, both geometrically (*h*-refinement) and with respect to basis functions (*p*-refinement).

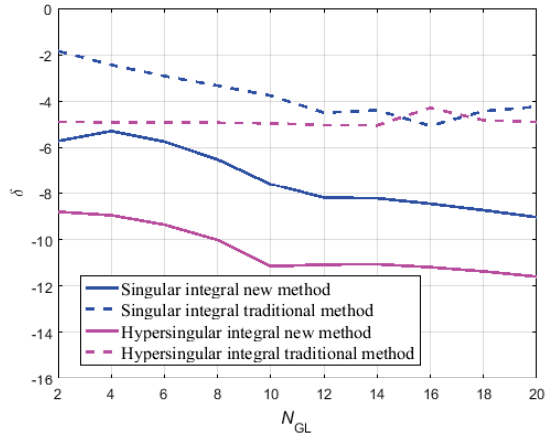
The adjoint solutions can also be applied in computing QoI gradients with respect to input parameters and in large-scale optimization problems. Traditional methods for computing gradients of a quantity of interest with respect to multiple parameters are extremely costly. Instead of introducing small perturbation in input parameters and resolving for a desired QoI, this information can be generated simply and effectively using the adjoint problem. Additionally, while Monte-Carlo methods are simple to implement and effective, they require significant computational resources and are impractical for large problems. Adjoint based approaches, on the other hand, are much more efficient; using HOPS, accurate sensitivity information can be generated with just a handful of solves.

Adjoint based methods have so far found little use in CEM, and particularly in FD higher order FEM and SIE modeling. A goal of this paper is to promote the use of such methods in FD CEM.

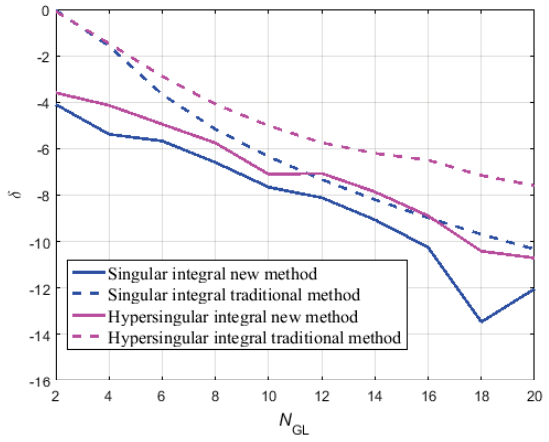
We discuss hierarchically semiseparable structures (HSS) and analysis of large scattering problems using a fast scalable parallel direct HSS solver combined with the rank-revealing QR decomposition for memory compression and higher order MoM-SIE modeling [7]. In addition, we discuss the higher order fast multipole method (FMM) MoM-SIE technique, and its multilevel (MLFMM) version, and explore the advantages, shortcomings, and commonalities of all approaches. We discuss combining MLFMM concepts with fast direct solvers, in order to accelerate matrix compression and reduce the computation cost but still maintain some benefits of direct over iterative solvers.

III. Illustrative Results and Discussion

As an illustration of the results using the novel singularity extraction SIE integration technique, one out of the six second-order SIE elements modeling a sphere of unit radius is tested for $\gamma \approx j0.7755$ rad/m, for the distance between the field point and the CPP point of $d = 10^{-5}$ m, and different values of projection point coordinates and i and j degrees. A corrected new method is used for cases where the CPP point is outside of the basis element domain. It creates a parallelogram at the most singular point on the basis element rather than on the whole parametric surface. The integration results are shown in Figs. 2 and 3, where it can be observed that the new extraction method shows higher accuracy for small numbers of integration points, which is especially pronounced for higher order polynomial basis functions.

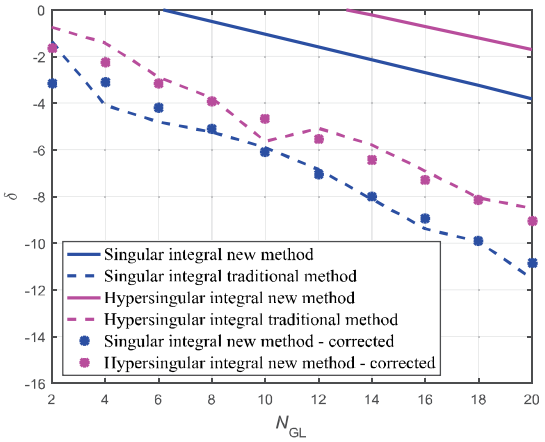


(a)

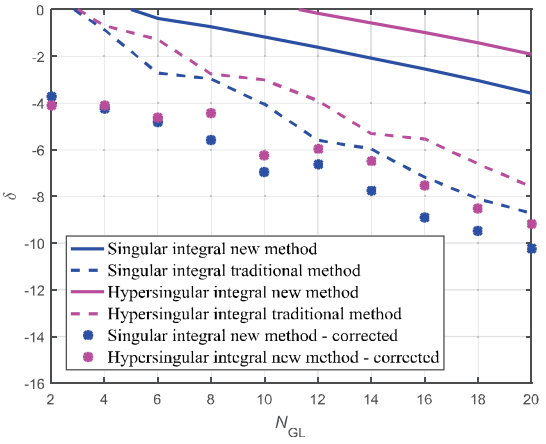


(b)

Fig. 2. Convergence results for the geometrically second-order element modeling a sixth of a sphere and $u_0 = 0.1$, $v_0 = -0.1$ (inside the parametric domain): (a) $i = 0, j = 0$; (b) $i = 6, j = 6$.



(a)



(b)

Fig. 3. Convergence results for the geometrically second-order element (sixth of a sphere) and $u_0 = 1.2$, $v_0 = 1.2$ (outside the parametric domain): (a) $i = 0, j = 0$; (b) $i = 6, j = 6$.

By intelligently targeting error in the discretization using adjoint-based error estimation, the accuracy can be improved very effectively, even for very poor initial discretizations. Traditional element selection schemes typically apply a magnitude-based refinement, in which elements with the largest QoI error estimates are prioritized for refinement. However, the magnitude refinement scheme fails to consider the interaction and error cancellation between elements in the discretization. We have developed a minimum sum grouping (MSG) strategy which provides a computational inexpensive method to relate the error between elements for refinement and groups them accordingly. Figure 4 shows an example of this technique, for adaptive p-refinement for spherical scatterers of various material parameters.

As seen in Fig. 4, for all three cases of spherical scatterers of various material parameters, both the magnitude and MSG approaches quickly reduce the error in the solution with respect to the Mie Series computation of the bistatic RCS across a wide-range of reception directions. In each case, the initial discretization is extremely poor. Both the magnitude

and MSG selection schemes are hybridized with a genetic algorithm (GA) optimizer for choosing expansion orders between 3 and 5 for each element based on the QoI error estimates. At each iteration, the maximum number of unknowns is increased incrementally. MSG achieves much greater stability, reducing the error near monotonically.

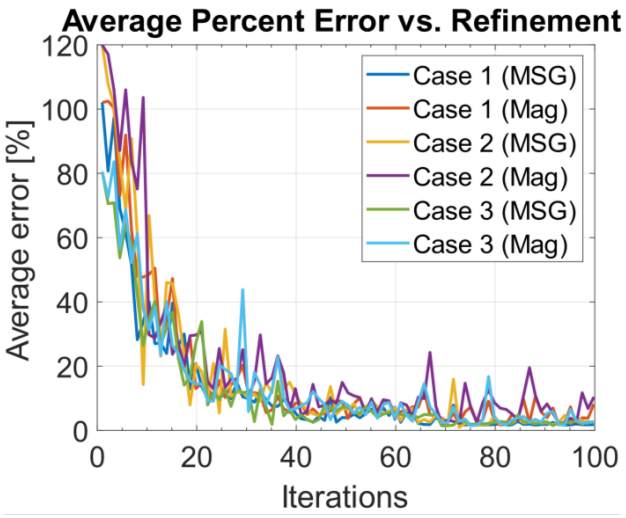


Fig. 4. Average percent error w.r.t. Mie Series for adaptive *p*-refinement for spherical scatterers of various material parameters.

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