Efficient numerical solvers for frequency- and time-domain electromagnetic simulation, optimization and design

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Abstract

We present a family of numerical methods for the solution of the acoustic and electromagnetic wave equations, with application to simulation, optimization, and design. In particular, a novel rectangular-polar integral equation solver will be described which can produce solutions to the time harmonic Helmholtz and Maxwell's equations, with high order accuracy, for general 2D and 3D structures, with an extension to time domain problems on the basis of a time re-centering synthesis technique. An effective integral equation acceleration method, the IFGF method (Interpolated Factored Green Function) will be presented which, without recourse to the FFT, and, thus, lending itself to effective distributed memory parallelization, evaluates the action of Green function-based integral operators for an N-point surface discretization at a computational cost of N log(N) operations. A number of computational illustrations, including applications to photonic optimization and design problems, will be presented.

Keywords: Fast Integral Equation Solvers, Frequency and Time Computational Electromagnetics, Photonic Device Simulation and Optimization

1 Scattering solvers and applications

We present a range of methodologies developed recently for the solution of the frequency domain and time domain Maxwell and acoustic wave equations, with application to the simulation of wave propagation and scattering by a variety of structures and media, as well as analysis, optimization, and design of photonic structures. In particular, a novel rectangular-polar high-order integral-equation solver will be discussed which can produce accurate solutions to the Helmholtz and Maxwell's equations, with high order accuracy, for general two- and three-dimensional structures in the frequency domain [4,8] and, by additionally exploiting a time windowing-andrecentering Fourier-time synthesis technique [1], in the time domain as well. Associated optimization and design methods [7,9] will be demonstrated, including mention of the fabricated and tested grating demultiplexer device introduced in [10]. An enabling technique underlying these design applications, the Windowed Green Function method (WGF) [5–7], will be mentioned.

An effective integral acceleration technique, the IFGF (Interpolated Factored Green Function) [2] will be presented which, without recourse to the Fast Fourier Transform (FFT), evaluates the action of Green function-based integral operators for surface discretization containing N points at an $\mathcal{O}(N \log N)$ computing cost, instead of the $\mathcal{O}(N^2)$ cost associated with unaccelerated methods. The IFGF algorithm, which is well suited for treatment of extremely large scattering problems, exploits the slow variations of certain "factored Green functions" and thus enables the fast evaluation of fields generated by groups of sources on the basis of a recursive interpolation scheme. Owing in part to its independence from the FFT, the IFGF is amenable to efficient parallelization on massively parallel computers. But the parallel IFGF approach is effective on small computers as well: a recent IFGF-accelerated parallel implementation [8] of the combined IFGF and rectangularpolar method [4] will be presented, which, based on the OpenMP programming interface can be used to tackle problems of scattering by large engineering structures on small parallel computer nodes. For example, on the basis of a 28-core computing node, full scattering solutions with several digits of accuracy can be obtained for realistic engineering structures of the order of one hundred wavelengths in size in computing times of the order of a few minutes per iteration and a few tens of iterations of the GMRES iterative solver; see e.g. Figure 1.

A massively parallel implementation of the IFGF algorithm [3], in turn, will also be presented which relies on both the Message Passing Interface (MPI) and OpenMP. This hybrid parallel IFGF implementation, which is suitable for implementation in modern high-performance computing (HPC) systems, provides excellent parallel efficiency without limitations in the size of the computer system used. In recent test cases, for example, an ellipsoid 4.096 wavelengths in diameter (resp. a sphere 1,389 wavelengths in diameter) containing approximately 400 million discretization points (resp. 1.610 billion points) was considered, for which the discrete forward operator was evaluated with an error of $1.5 \cdot 10^{-2}$ (resp. $4.0 \cdot 10^{-3}$), requiring, in both cases, a computing time of under one hour in a 30-node, 1,680-core parallel cluster, with a memory requirement of 30 GB per node (resp. 125 GB per node).

In all, the Green function methods presented, which are based on a small set of basic underlying ideas, span a wide range of applications, problem complexity, computer architectures and varied capabilities



Figure 1: Upper left image group: High-order rectangular-polar integral solver [4] on a patch geometry (upper left), IFGF acceleration boxand-cone octree [2] (upper right), nacelle geometry (lower left) and nacelle patch description (Lower right). Lower left, center and right images: Total field magnitude $|u(x)| = |u^i(x) + u^s(x)|$ under point source incidence (lower left and center) and 82-wavelength plane-wave incidence (right) [8]. Details can be appreciated by enlarged pdf viewing.

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