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A high-order perturbation of surfaces method for vector electromagnetic scattering by doubly layered periodic crossed gratings

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ABSTRACT

The accurate simulation of scattering of electromagnetic waves in three dimensions by a diffraction grating is crucial in many applications of engineering and scientific interest. In this contribution we present a novel High-Order Perturbation of Surfaces method for the numerical approximation of vector electromagnetic scattering by a doubly periodic layered medium. For this we restate the governing time harmonic Maxwell equations as vector Helmholtz equations which are coupled by transmission boundary conditions at the layer interface. We then apply the method of Transformed Field Expansions which delivers a Fourier collocation, Legendre–Galerkin, Boundary Perturbation approach to solve the problem in transformed coordinates. A sequence of numerical simulations demonstrate the efficient and robust spectral convergence which can be achieved with the proposed algorithm.

1. Introduction

The accurate simulation of scattering of electromagnetic waves in three dimensions by a diffraction grating is crucial in many applications of engineering and scientific interest. Examples include surface enhanced Raman scattering [72], extraordinary optical transmission [28], surface enhanced spectroscopy [50], photovoltaic devices [1], and surface plasmon resonance biosensing [38,47]. Clearly, the ability to numerically simulate such configurations with speed, accuracy, and robustness is of the utmost importance to many disciplines. In this contribution we present a novel High-Order Perturbation of Surfaces (HOPS) method for the numerical approximation of vector electromagnetic scattering by a periodic doubly layered medium.

Volumetric approaches to these problems are pervasive in the engineering literature. More specifically Finite Difference [46], Finite Element [42], Discontinuous Galerkin [40], Spectral Element [27], and Spectral [32,71] methods are all widely used by practitioners. However, such methods are clearly disadvantaged with an unnecessarily large number of unknowns for the piecewise homogeneous problems we consider here. In addition, the faithful enforcement of outgoing wave conditions is problematic for these approaches typically necessitating approximations such as the Perfectly Matched Layer [4,5] or exact, non-reflecting boundary conditions [41,39,44,30,54,12] which spoil the sparseness properties of the relevant linear systems.

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For these reasons, surface methods are an ideal choice as they are orders of magnitude faster when compared to volumetric approaches due to the greatly reduced number of degrees of freedom required to resolve a computation. In addition, far-field boundary conditions are enforced exactly through the choice of the Green function. Consequently, these methods are a very appealing alternative which are gaining favor with practitioners. The most prevalent among these interfacial algorithms are those based upon Boundary Integral Equations (BIEs) [24,69], but these face difficulties. Most have been resolved in recent years through (i.) the use of sophisticated quadrature rules to deliver High-Order Spectral (HOS) accuracy; (ii.) the design of preconditioned iterative solvers with suitable acceleration [33]; (iii) new strategies to accelerate the convergence of the periodized Green function [13,11] (or avoiding its periodization entirely [9,22]); and (iv.) new approaches to deal with the Rayleigh singularities (widely known in the literature as "Wood's anomalies") [3,7,21]. As a result they are a compelling alternative for many problems of applied interest, however, two properties render them disadvantaged for the *parameterized* problems we consider as compared with the methods we advocate here: (i.) For geometries specified by the real value, ε, (here the deviation of the interface shapes from trivial), a BIE solver will provide a solution for a single value of ε. If this is changed then the solver must be initiated again; (ii.) the dense, non-symmetric positive definite systems of linear equations that must be solved with each simulation. As specific examples where such considerations arise, we point the interested reader to the work of the second author, F. Reitich, T. Johnson, and S.-H. Oh. on (i.) simulating "reflectivity maps" associated to multilayer plasmonic devices [61] and (ii.) determining the minimal configuration required to excite surface plasmons with shallow gratings [55]. In the former, the parameterized nature of the configuration and the associated reflectivity map would require a BIE to be restarted with each new data point (unlike the scheme we advocate here). In the latter, the geometry shape was, by design, a *very* small perturbation of a flat-interface configuration. For a BIE method the cost of simulating this is the same as that of approximating a grating with a large deformation, while a perturbative algorithm (such as the one we discuss in this paper) can run much more quickly.

In contrast, a High-Order Perturbation of Surfaces (HOPS) methodology effectively addresses these concerns. These formulations have the advantageous properties of BIE formulations (e.g., surface formulation, reduced numbers of degrees of freedom, and exact enforcement of far-field boundary conditions) while being immune to the shortcomings listed above: (i.) Since HOPS approaches are built upon expansions in the deformation parameter, ε, once the Taylor coefficients are known for the problem unknowns, one simply sums these for any choice of ε to recover the solution rather than beginning a new simulation; (ii.) the perturbative nature of the scheme is built upon the flat-interface solution which is trivially solved in Fourier space by inverting a sparse operator at each wavenumber. We point out that the initial smallness assumption on the deformation parameter, ε, can be dropped in light of the analytic continuation results in [58,34] which demonstrate that the domain of analyticity contains a neighborhood of the *entire* real axis. Therefore, with appropriate numerical analytic continuation methodologies (e.g., Padé approximation [10]) to access this region of analyticity, quite large and irregular perturbations can be simulated. We direct the interested reader to [15,17,20,57,60] for numerical demonstrations.

There are several approaches to HOPS simulation of partial differential equations posed on irregular domains, but they all trace their beginnings to low-order calculations such as those of Rayleigh [67] and Rice [68]. The first high-order incarnations appeared in the early 1990s with the introduction of the methods of Operator Expansions (OE) by Milder [48,49,51,52] and Field Expansions (FE) by Bruno and Reitich [14–16]. Each has been enhanced by various authors, but the most significant was the stabilization of these methods by one of the authors and Reitich with the Transformed Field Expansions (TFE) algorithm [56–60]. Beyond this, these HOPS schemes have been extended in a number of directions. Of particular interest to this contribution we mention bounded obstacle configurations [19,62,29], the full vector Maxwell equations [18,53,64] and a rigorous numerical analysis [63].

In addition to these, the authors have initiated a comprehensive study of the TFE recursions for linear wave scattering and their extension to multiple (three) layers in two dimensions [36] and multiple (arbitrary numbers of) layers in three dimensions [35]. However, these investigations fixed upon the scalar Helmholtz equations which only govern electromagnetic wave propagation in two dimensions under Transverse Electric or Transverse Magnetic polarization [65]. In this contribution we examine the much more difficult problem of simulating electromagnetic radiation scattered by a crossed grating in three dimensions in general polarization. This demands that we not only solve the vector Helmholtz equations in three dimensions, but also accommodate the more subtle interfacial boundary conditions of continuity of tangential fields with appropriate jumps in the normal direction. To this one must also add divergence-free constraints while imposing appropriate outgoing wave conditions to avoid pollution of solutions. We demonstrate how this can be achieved in the doubly layered scenario for which the TFE recursions have yet to be derived and implemented. Of particular note, we describe a novel, spectrally accurate, modified Legendre–Galerkin approach to the vertical discretization where the standard basis is enriched with additional connecting basis functions across the layer boundary.

In addition to the novelty of our new algorithm for this model, we also point out that our approach will be the method of choice for simulating the technologically relevant case of homogeneous layers separated by an interface which is a slight to moderate deviation of flat. In this case volumetric approaches will not be competitive due to their onerous operation counts and memory requirements, while BIE approaches (which have the same memory constraints as our TFE method) will take longer as their computational cost in this setting will be significantly greater. The combination of (i.) dense, non-symmetric positive-definite matrix inversion, and (ii.) the algorithmic and operational complications of evaluating the Green function (both its periodization and accounting for the Rayleigh singularities) render such approaches non-competitive for the problems we consider here.