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A stable high-order perturbation of surfaces method for numerical simulation of diffraction problems in triply layered media

Youngjoon Hong, David P. Nicholls *

Department of Mathematics, Statistics, and Computer Science, University of Illinois at Chicago, Chicago, IL, 60607, USA

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ABSTRACT

The accurate numerical simulation of linear waves interacting with periodic layered media is a crucial capability in engineering applications. In this contribution we study the stable and high-order accurate numerical simulation of the interaction of linear, time-harmonic waves with a periodic, triply layered medium with irregular interfaces. In contrast with volumetric approaches, High-Order Perturbation of Surfaces (HOPS) algorithms are inexpensive interfacial methods which rapidly and recursively estimate scattering returns by perturbation of the interface shape. In comparison with Boundary Integral/Element Methods, the stable HOPS algorithm we describe here does not require specialized quadrature rules, periodization strategies, or the solution of dense non-symmetric positive definite linear systems. In addition, the algorithm is provably stable as opposed to other classical HOPS approaches. With numerical experiments we show the remarkable efficiency, fidelity, and accuracy one can achieve with an implementation of this algorithm.

1. Introduction

The accurate numerical simulation of linear waves interacting with periodic layered media is a crucial capability in many areas of scientific and industrial interest. Examples exist in areas such as geophysics [1,2], materials science [3], imaging [4], oceanography [5], and nanoplasmonics [6–8]. The latter includes topics as diverse as extraordinary optical transmission [9], surface enhanced spectroscopy [10], and surface plasmon resonance biosensing [11–16]. For each application, it is necessary to approximate the scattering returns of such models in a fast, highly accurate, and reliable fashion.

While all of the classical numerical algorithms (e.g., Finite Differences and Finite/Spectral Element methods) have been brought to bear upon this problem (see, particularly, the work of Dobson [17,18] and Bao [19–21] on Finite Element solution of the doubly layered problem), we have recently argued [22–25] that such *volumetric* approaches are greatly disadvantaged with an unnecessarily large number of unknowns for the layered media problems we consider here. Interfacial methods based upon Integral Equations (IEs) [26], for instance [27–32], are a natural candidate but, as we have pointed out [22–25], these also face difficulties. Most of these have been addressed in recent years through (i.) the use of sophisticated quadrature rules to deliver High-Order Spectral accuracy, (ii.) the design of preconditioned iterative solvers with suitable acceleration [33], and (iii.) new strategies to avoid periodizing the Green function [27–32]. Consequently, they are a compelling alternative (see, e.g., the survey article of [34] for more details), however, two properties render them non-competitive for the

* Corresponding author.
E-mail addresses: hongy@uic.edu (Y. Hong), davidn@uic.edu (D.P. Nicholls).

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parameterized problems we consider as compared with the methods we advocate here. First, for configurations characterized by the real value ε (for us the heights/slopes of the irregular interfaces), an IE solver will return the scattering returns only for a *particular* value of ε. If this value is changed then the solver must be run again. Second, the dense, non-symmetric positive definite systems of linear equations generated by IEs which must be inverted with each simulation. We note that the "Rigorous Coupled Wave Analysis" (RCWA) [35,36] is very popular amongst practitioners for the problem we consider here. While it is very convenient to code and can be very fast if implemented with care, non-trivial interface shapes are modeled as thin layers using a staircase approximation which is, necessarily, a low-order approximation.

A "High Order Perturbation of Surfaces" (HOPS) approach can effectively address these concerns. More specifically, in [23–25] we put forth the method of Field Expansions (FE) which traces its roots to the low-order calculations of Rayleigh [37] and Rice [38]. This was extended to a high-order algorithm by Bruno & Reitich [39–41] and later enhanced and stabilized by Nicholls and Reitich [42–44], and Nicholls and Malcolm [45,23,25]. These formulations are particularly compelling as they maintain the advantageous properties of classical IE formulations (e.g., surface formulation and exact enforcement of far-field and quasiperiodicity conditions) while avoiding the shortcomings listed above. First, since the methods are built upon expansions in the boundary parameter, ε, once the Taylor coefficients are known for the scattering quantities, it is simply a matter of summing these (rather than beginning a new simulation) for any given choice of ε to recover the returns. Second, due to the nature of the scheme, at every perturbation order one need only invert a single, sparse operator corresponding to the flat-interface, order-zero approximation of the problem.

However, Nicholls and Reitich [46] showed that, like other classical HOPS schemes, the FE method depends upon strong *cancellations* for its convergence which can result in quite ill-conditioned simulations. We refer the interested reader to [46–48,42,43] for the initial description of this phenomena, and the additional exhaustive and illuminating simulations of Wilkening and Vasan [49].

In response to these observations, Nicholls and Reitich described an alternative HOPS scheme, the method of Transformed Field Expansions (TFE), which does *not* possess strong cancellations [46–48,42,43]. In fact, the resulting recursions can be used in a *rigorous* proof of the strong convergence of the perturbation expansions in a Sobolev space [46,48], which was later extended to Lipschitz profiles in [50]. In addition, the TFE recursions were implemented to reveal a stable and highly accurate numerical scheme for the simulation of scattering returns by singly layered periodic gratings [47,43].

This work was generalized by Nicholls and Shen to the case of irregular bounded obstacles in two [51] and three dimensions [52], who later delivered a rigorous numerical analysis of the method [53]. Subsequently, He, Nicholls, and Shen [54] devised a highly non-trivial extension to the case of periodic gratings separating *two* materials of different dielectric constants. Here, of course, one must be concerned not only with a reflected field and its far-field boundary condition (upward propagating) at positive infinity, but also with a transmitted field which satisfies a different condition (downward propagating) at negative infinity. In this contribution we make the further extension to the case of *three* layers which introduces the added complication of waves propagating both "up" and "down" in a vertically bounded layer in between. This difficulty manifests itself in the governing equations (and our numerical algorithm) through the complication of a *coupled* system of three boundary value problems (at each wavenumber in the spatial variable).

More specifically, to begin we introduce artificial boundaries above and below the interfaces of the structure, which truncate the unbounded domain. We use Dirichlet–Neumann operators at each of these artificial boundaries to enforce the outgoing wave conditions *transparently* and without reflection [55–64]. Our spectrally accurate method involves the novelty of a modified Legendre–Galerkin approach where the standard basis is supplemented with additional connecting basis functions across the layer boundaries in the spirit of the work by He, Nicholls, and Shen [54] for two layers. However, our contribution is more subtle than what appears in the aforementioned publication; for more details we refer the reader to Section 5.

The organization of the paper is as follows: In Section 2 we recall the governing equations of an electromagnetic field incident upon a periodic, two-dimensional, triply layered irregular grating structure. In Section 3 we derive the TFE recursions in this triply layered context, and discuss a Legendre–Galerkin method to solve the resulting *coupled* boundary value problems in Sections 4 and 5. Extensive numerical results are provided in Section 6, followed by concluding remarks in Section 7.

2. Governing equations

The geometry we consider is displayed in Fig. 1: A z-invariant, triply layered structure. Dielectrics occupy all three domains, the upper (with refractive index n^u) fills the region

$$S_g^u := \left\{ y > \overline{g} + g(x) \right\},$$

the middle (with refractive index n^v) occupies

$$S_{g,h}^v := \left\{ \overline{h} + h(x) < y < \overline{g} + g(x) \right\},$$

while the lower (with index of refraction n^w) fills

$$S_h^w := \left\{ z < \overline{h} + h(x) \right\}.$$