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A high-order perturbation of surfaces method for scattering of linear waves by periodic multiply layered gratings in two and three dimensions

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ABSTRACT

The capability to rapidly and robustly simulate the scattering of linear waves by periodic, multiply layered media in two and three dimensions is crucial in many engineering applications. In this regard, we present a High-Order Perturbation of Surfaces method for linear wave scattering in a multiply layered periodic medium to find an accurate numerical solution of the governing Helmholtz equations. For this we truncate the bi-infinite computational domain to a finite one with artificial boundaries, above and below the structure, and enforce transparent boundary conditions there via Dirichlet–Neumann Operators. This is followed by a Transformed Field Expansion resulting in a Fourier collocation, Legendre–Galerkin, Taylor series method for solving the problem in a transformed set of coordinates. Assorted numerical simulations display the spectral convergence of the proposed algorithm.

1. Introduction

The scattering of linear waves by periodic, multiply layered media in two and three dimensions arises in many engineering and physics applications. Examples exist in materials science [1], geophysics [2,3], imaging [4], oceanography [5], and nanoplasmonics [6–8]. It is clear that the capability to rapidly and robustly simulate such interactions with high accuracy is of fundamental importance to practical applications. The most popular approaches to these problems are volumetric in nature and include the Finite Difference Method [9,10], the Finite Element Method [11,12], the Discontinuous Galerkin Method [13], the Spectral Element Method [14], and Spectral Methods [15–17]. However, these methods are greatly disadvantaged with an unnecessarily large number of unknowns for layered media problems (see, e.g., the discussion in [18,19]). Interfacial methods based on Integral Equations (IEs) [20–24] are a natural alternative but these also face several challenges. First, for the parameterized problems we consider here (characterized by the interface height/slope ε) a new simulation must be run for every configuration in the family of interest. Additionally, for every invocation there is a dense, non-symmetric positive definite system of linear equations generated by the IEs which must be inverted.

High-Order Perturbation of Surfaces (HOPS) methods can avoid these concerns. These highly accurate algorithms, based upon the low-order theories of Rayleigh [25] and Rice [26], were first developed by Bruno and Reitich [27] and later enhanced and stabilized by Nicholls and Reitich [28], and Nicholls and Malcolm [29]. HOPS approaches are compelling as they maintain the advantageous properties of classical IE formulations (e.g., surface formulation, exact enforcement of

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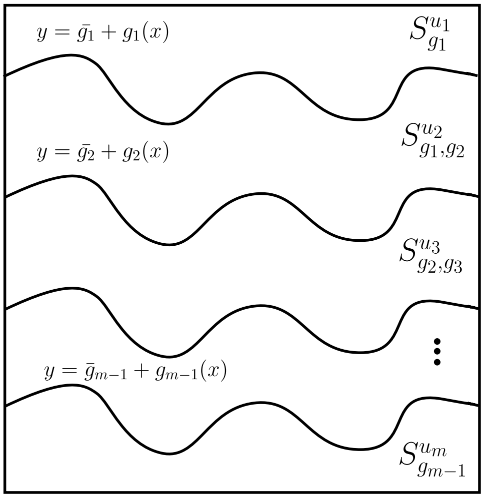

Fig. 1. A depiction of a multiply layered grating structure.

far-field boundary conditions, and quasiperiodic boundary conditions) while avoiding their shortcomings. For instance, in the setting of parameterized interfaces, scattering returns from an entire family of such configurations can be obtained with negligible additional cost beyond a single simulation. In addition, the perturbative nature of the algorithm allows one to invert, at every perturbation order, the *same* sparse (after Fast Fourier Transformation) operator corresponding to the flat-interface, order-zero approximation of the problem.

The method we present here is a generalization of the work of Nicholls and Shen on irregular, bounded obstacles in two [30] and three dimensions [31]. (Nicholls and Shen then gave a rigorous numerical analysis of a wide class of HOPS schemes in [32].) Subsequent to this He, Nicholls, and Shen [33] devised a non-trivial extension to the case of periodic gratings separating two materials of different dielectric constants. In [34] the authors made the further extension to the case of three layers. This work addressed the additional complication of waves propagating both up and down in a vertically bounded layer in between. The novelties of the current contribution include the highly non-trivial extension to three dimensions and an arbitrary number of layers. In addition, we not only demonstrate its applicability to *large* deformations with the use of Padé summation [35], but we also state and briefly prove the existence, uniqueness, and analyticity of solutions to our governing equations. A careful numerical analysis of the convergence of our scheme to these solutions we save for a forthcoming publication.

When considering real-world applications such as seismic imaging, underwater acoustics, and the modeling of plasmonic nanostructures, the multiply layered nature of the structure is essential. In the current contribution, we study linear waves interacting with periodic gratings separating several layers of materials with different dielectric constants; see, e.g., Fig. 1. The first step of our method is to equivalently reformulate the governing equations on a *bounded* domain with artificial boundaries and transparent boundary conditions (implemented via Dirichlet–Neumann Operators) above and below the interfaces of the structure. With a nonlinear change of variables, the computational domain can be transformed to one with flat interfaces between material layers, at the cost of nonlinear terms in the governing equations. Using boundary perturbations, we express the scattered field in a Taylor series and write a sequence of linear problems to be solved at each perturbation order for higher order corrections; this is the essence of the Transformed Field Expansions (TFE) algorithm. Due to inhomogeneities in the governing Helmholtz equations arising from the change of variables, a vertical discretization is required which we implement with a spectrally accurate Legendre–Galerkin method [36,37]. This Legendre–Galerkin algorithm is slightly unorthodox in that the standard basis is supplemented with additional connecting basis functions across the layer boundaries [34].

The article is organized as follows: In Section 2 the governing equations for linear waves interacting with a periodic multiply layered structure are given. The TFE method in this setting is described in Section 3, together with a discussion of the Legendre–Galerkin scheme we implemented for the vertical discretization in Sections 4 and 5. An assortment of numerical experiments are presented in Section 6 including simulations of smooth and rough interfaces, of small and large size, in two and three dimensions.

2. Governing equations

In this section, we describe the governing equations of linear waves scattered by a multiply layered medium. The geometry is depicted in Fig. 1. Dielectrics occupy each of the m-many domains: The upper material fills the region

$$S^{u_1}_{g_1} := \{y > \bar{g}_1 + g_1(x)\},$$