

A high-order perturbation of surfaces (HOPS) approach to Fokas integral equations: Vector electromagnetic scattering by periodic crossed gratings



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ARTICLE INFO

Article history:

Received 24 March 2015
Received in revised form 31 August 2015
Accepted 10 November 2015
Available online 19 November 2015

Keywords:

Layered media
Maxwell equations
Electromagnetic scattering
Integral equations
High-order spectral methods

ABSTRACT

The accurate simulation of linear electromagnetic scattering by diffraction gratings is crucial in many technologies of scientific and engineering interest. In this contribution we describe a High-Order Perturbation of Surfaces (HOPS) algorithm built upon a class of Integral Equations due to the analysis of Fokas and collaborators, now widely known as the Unified Transform Method. The unknowns in this formalism are boundary quantities (the electric field and current at the layer interface) which are an order of magnitude fewer than standard volumetric approaches such as Finite Differences and Finite Elements. With detailed numerical experiments we show the efficiency, fidelity, and high-order accuracy one can achieve with an implementation of this algorithm.

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1. Introduction

The scattering of linear electromagnetic waves by periodic diffraction gratings plays an important role in many applications. The robust and rapid capability of simulating these configurations numerically is of crucial importance, and in this contribution we focus upon the specific problem of vector electromagnetic radiation interacting with a periodic crossed diffraction grating (see Fig. 1). A crossed grating is usually defined as two line gratings at right angles to each other, and we model this with a biperiodic layer interface (which permits non-orthogonal line intersection).

This model arises in a wide range of applications in optics and photonics, and of particular interest to this paper, in nanoplasmonics [52,34,19]. In this field one investigates topics as diverse as extraordinary optical transmission [18], surface enhanced spectroscopy [42], and surface plasmon resonance biosensing [26,28,33,30,56,50].

Classical numerical algorithms such as Finite Elements (e.g., [59,14,27,62]) and Finite Differences (e.g., [11,58,32]) have been used to simulate these configurations. However, these volumetric approaches are clearly disadvantaged with an unnecessarily large number of unknowns for the piecewise homogeneous grating problem we consider here. In addition, for these methods the unbounded problem domain must be truncated at some finite distance from the grating structure inducing the complication and error introduced by enforcing an (approximately) “Non-Reflecting Boundary Condition” (e.g., the Perfectly Matched Layer of Berenger [6] and variants of this, e.g., [21–23]).

Consequently, methods based upon Integral Equations (IEs) [13] are a natural candidate but face several challenges. For instance, specially designed quadrature rules must be designed to deliver high-order (spectral) accuracy, and these

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rules applied to these non-local IEs generate dense, non-symmetric positive definite linear systems to be solved. However, these issues have been satisfactorily addressed (possibly with the use of iterative solution procedures accelerated by Fast Multipole Methods [25]) and they are a compelling choice [55]. However, three properties render them non-competitive for the *periodic, parametrized* problems we consider as compared with the method we advocate here. First, for *periodic* problems the relevant Green function must be periodized. This is a well-known problem [31] and the slow convergence of the periodization must be accelerated (e.g., with Ewald summation). However, even with such technology, these IE methods demand an *additional* discretization parameter: The number of terms retained in the approximation of the periodized Green function. Second, for configurations *parametrized* by the height/slope ε of the crossed interface, an IE solver must be invoked for every desired value. Finally, the dense, non-symmetric positive definite systems of linear equations which must be inverted with each simulation.

As an alternative, we advocate here for a “High-Order Perturbation of Surfaces” (HOPS) method, more specifically a Fokas Integral Equation (FIE) reformulation appropriately generalized to the fully three-dimensional vector Maxwell equations [2,43]. These schemes trace their roots to the low-order calculations of Rayleigh [54] and Rice [57]. Their high-order incarnation has been developed into the Method of Field Expansions (FE) by Bruno & Reitich [7–9], the author and Reitich [47–49], and the author and Malcolm [35,44]. A closely related algorithm, the Method of Operator Expansions, was developed in parallel by Milder and collaborators [36–41,12].

These formulations are particularly compelling as they maintain the advantageous properties of classical Integral Equations formulations (e.g., surface formulation and exact enforcement of far-field conditions) while avoiding the shortcomings listed above. First, as HOPS schemes utilize eigenfunctions of the Laplacian (suitable complex exponentials) on a *periodic* domain the quasiperiodicity of solutions is “built in” and does not need to be further approximated. Second, 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. Finally, due to the perturbative nature of the scheme, at every perturbation order one need only invert a single, sparse operator corresponding to the flat-interface approximation of the problem.

As we have shown in the context of the Helmholtz equation [2,43], the approach of Fokas [20] and collaborators (see, e.g., [1,60,61]) allows one to state simple integral relations for Dirichlet and Neumann data of elliptic boundary value problems which do *not* involve the fundamental solution. Instead they feature quite smooth kernels related to solutions of the relevant Helmholtz problem meaning that simple quadrature rules (e.g., Nyström’s Method [13]) can be brought to bear on the problem. The Fokas approach (known as the “Unified Transform Method”) does give rise to dense, poorly conditioned linear systems to be inverted, but one of the authors showed in [43] how this can be significantly ameliorated with a HOPS methodology. In particular, as we shall see, one trades a single dense and ill-conditioned matrix inversion for a sequence (one for each perturbation order retained) of fast, well-conditioned linear solves around the base (flat-interface) geometry. This matrix is of convolution-type which enables rapid solution by the FFT algorithm. Additionally, we find that, for many configurations of interest, only a small number of perturbation orders are required for a solution of high fidelity, resulting in an algorithm of remarkable speed and accuracy.

The authors have recently been made aware of the work of DeSanto and collaborators [15,17,16,3] who advanced an approach which is very close to the one presented by the author and Ambrose in [2]. A nice explanation of their approach and how it connects to the formulation of Fokas is given in [10]. In the current contribution, the authors extend this work not only in generalization to multiple layers for the full Maxwell equations, but also through the introduction of a HOPS methodology.

The rest of the paper is organized as follows: In Section 2 we briefly recall the equations which govern the interaction of vector electromagnetic waves with a three-dimensional doubly periodic diffraction grating, followed in Section 2.1 by a discussion of the classical Rayleigh expansions, efficiencies, and the Reflectivity Map. In Section 3 we describe a boundary formulation of these governing equations which allows one to simulate solutions in a rapid and robust fashion. We describe the details surrounding the interfacial boundary conditions in Section 3.1 (the tangential trace), Section 3.2 (the tangential curl), and Section 3.3 (the divergence free condition). We summarize our surface formulation in Section 3.4. In Section 4 we describe how a High-Order Perturbation of Surfaces (HOPS) approach can be utilized to perturbatively solve the equations given in Section 3.4. We present detailed numerical experiments in Section 5, including validation against a Field Expansions (FE) implementation [9,44] in Section 5.1, and results of simulations of Reflectivity Maps in Section 5.2 for configurations involving gratings composed of different metals which generate quite different plasmonic responses.

2. The governing equations

Consider a diffraction grating with crossed periodic interface located at

$$z = g(x, y),$$

where z is the vertical coordinate and x and y are the lateral coordinates, which delineates two layers

$$S^u := \{z > g(x, y)\}, \quad S^w := \{z < g(x, y)\}.$$

The layers are filled with materials having dielectric constants $\{\epsilon^u, \epsilon^w\}$, and the permeability of each is equal to μ_0 , that of the vacuum. In this contribution we consider the genuinely three-dimensional setting where the grating interface is *crossed* and *periodic*

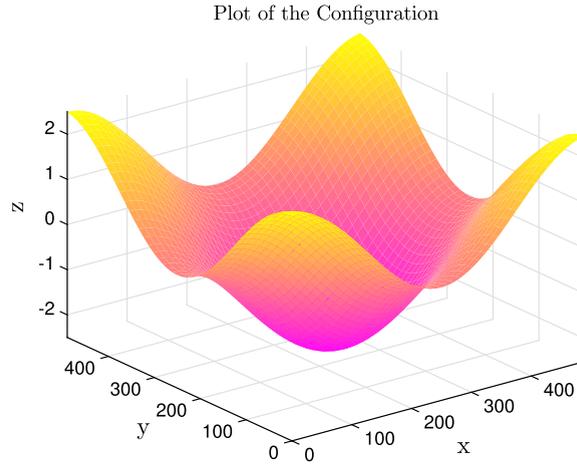


Fig. 1. Plot of the configuration with grating interface shaped by $g(x, y) = (\varepsilon/4)(\cos(2\pi x/d_1) + \cos(2\pi y/d_2))$, $d_1 = d_2 = d = 500$ nm, $\varepsilon/d = 0.01$ giving $\varepsilon = 5$ nm.

$$g(x + d_1, y + d_2) = g(x, y);$$

see Fig. 1.

The structure is illuminated from above by plane-wave incidence of the form

$$\mathbf{E}^{inc}(x, y, z) := e^{i\omega t} \underline{\mathbf{E}}^{inc}(x, y, z, t) = \mathbf{A}e^{i(\alpha x + \beta y - \gamma z)}$$

$$\mathbf{H}^{inc}(x, y, z) := e^{i\omega t} \underline{\mathbf{H}}^{inc}(x, y, z, t) = \mathbf{B}e^{i(\alpha x + \beta y - \gamma z)},$$

where

$$\mathbf{A} \cdot \boldsymbol{\kappa} = 0, \quad \mathbf{B} = \frac{1}{\omega\mu_0} \boldsymbol{\kappa} \times \mathbf{A}, \quad |\mathbf{A}| = |\mathbf{B}| = 1,$$

and $\boldsymbol{\kappa} := (\alpha, \beta, -\gamma)^T$.

The time-harmonic Maxwell equations [29,51] for the reduced total fields can be written (upon dropping the harmonic factor $\exp(-i\omega t)$) as

$$\nabla \times \mathbf{E} = i\omega\mu_0 \mathbf{H}, \quad \text{div}[\mathbf{E}] = 0, \tag{2.1a}$$

$$\nabla \times \mathbf{H} = -i\omega\epsilon \mathbf{E}, \quad \text{div}[\mathbf{H}] = 0. \tag{2.1b}$$

All fields satisfy the vector Helmholtz equation, e.g.,

$$\Delta \mathbf{E} + k^2 \mathbf{E} = 0, \tag{2.2}$$

with $k^2 = \omega^2 \epsilon \mu_0$ which encodes the properties of the material and the frequency of radiation into one constant.

We decompose the total fields into incident and scattered components by

$$\mathbf{E} = \begin{cases} \mathbf{E}^u + \mathbf{E}^{inc} & \text{in } S^u \\ \mathbf{E}^w & \text{in } S^w, \end{cases} \quad \mathbf{H} = \begin{cases} \mathbf{H}^u + \mathbf{H}^{inc} & \text{in } S^u \\ \mathbf{H}^w & \text{in } S^w, \end{cases}$$

and note that each of these must satisfy vector Helmholtz equations, e.g.,

$$\Delta \mathbf{E}^u + (k^u)^2 \mathbf{E}^u = 0, \quad \text{in } S^u$$

where $(k^u)^2 := \omega^2 \epsilon^u \mu_0$, and

$$\alpha^2 + \beta^2 + \gamma^2 = (k^u)^2.$$

At the material interface the fields are coupled by the transmission conditions [29,51],

$$N \times [\mathbf{E}^u - \mathbf{E}^w] = \zeta$$

$$N \times [\mathbf{H}^u - \mathbf{H}^w] = \psi,$$

where $N := (-\partial_x g, -\partial_y g, 1)^T$, and, in the present context of plane-wave illumination from above,

$$\zeta = -N \times \left[\mathbf{E}^{inc} \right]_{z=g}, \quad \psi = -N \times \left[\mathbf{H}^{inc} \right]_{z=g}.$$

In light of Maxwell's equations, (2.1a)–(2.1b), we can rewrite this in terms of the electric field as

$$N \times \left[\mathbf{E}^u - \mathbf{E}^w \right]_{z=g} = \zeta, \quad (2.3a)$$

$$N \times \left[\nabla \times \left[\mathbf{E}^u - \mathbf{E}^w \right] \right]_{z=g} = \psi, \quad (2.3b)$$

where

$$\psi = -N \times \left[\nabla \times \left[\mathbf{E}^{inc} \right] \right]_{z=g}.$$

We point out that only four of these six boundary conditions are linearly independent (the z -component of each can be written as a linear combination of the x - and y -components, for instance). Clearly it only makes sense to enforce four and we choose the x - and y -components of each. To compensate for this “defect” we recall that the electric field is divergence free in the bulk, and must also be so at the interface. Thus we enforce the two additional boundary conditions

$$\operatorname{div} \left[\mathbf{E}^u \right] = \operatorname{div} \left[\mathbf{E}^w \right] = 0, \quad z = g. \quad (2.3c)$$

Finally, the periodicity of the grating interfaces implies that the fields are quasiperiodic,

$$\mathbf{E}^m(x + d_1, y + d_2, z) = e^{i(\alpha d_1 + \beta d_2)} \mathbf{E}^m(x, y, z), \quad m = u, w,$$

and we demand that \mathbf{E}^u and \mathbf{E}^w be outgoing at positive and negative infinity, respectively.

2.1. The Rayleigh expansions, efficiencies, and the reflectivity map

Separation of variables gives the Rayleigh expansions [51] which are quasiperiodic, outgoing solutions of (2.2) that we discuss in order to introduce notation. The electric fields can be written

$$\mathbf{E}^u(x, y, z) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \mathbf{a}_{p,q} e^{i\gamma_{p,q}^u z} e^{i(\alpha_p x + \beta_q y)} \quad (2.4a)$$

and

$$\mathbf{E}^w(x, y, z) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \mathbf{d}_{p,q} e^{-i\gamma_{p,q}^w z} e^{i(\alpha_p x + \beta_q y)}, \quad (2.4b)$$

where, for $p, q \in \mathbf{Z}$,

$$\begin{aligned} \alpha_p &:= \alpha + (2\pi/d_1)p, & \beta_q &:= \beta + (2\pi/d_2)q, \\ \gamma_{p,q}^m &:= \begin{cases} \sqrt{(k^m)^2 - \alpha_p^2 - \beta_q^2} & (p, q) \in \mathcal{U}^m \\ i\sqrt{\alpha_p^2 + \beta_q^2 - (k^m)^2} & (p, q) \notin \mathcal{U}^m, \end{cases} & m &= u, w, \end{aligned}$$

and,

$$\mathcal{U}^m = \left\{ p, q \in \mathbf{Z} \mid \alpha_p^2 + \beta_q^2 < (k^m)^2 \right\}, \quad m = u, w,$$

which are the “propagating modes” in the upper and lower layers. (We point out that $\mathbf{a}_{p,q}$ and $\mathbf{d}_{p,q}$ are the upward and downward propagating Rayleigh amplitudes.) Quantities of great interest are the *efficiencies*

$$e_{p,q}^u = (\gamma_{p,q}^u / \gamma) |\mathbf{a}_{p,q}|^2, \quad (p, q) \in \mathcal{U}^u,$$

$$e_{p,q}^w = (\gamma_{p,q}^w / \gamma) |\mathbf{d}_{p,q}|^2, \quad (p, q) \in \mathcal{U}^w,$$

and the object of fundamental importance to the design of Surface Plasmon Resonance (SPR) biosensors [26,28,33,30,56,50] is the “Reflectivity Map”

$$R := \sum_{(p,q) \in \mathcal{U}^u} e_{p,q}^u. \quad (2.5)$$

If the lower layer is filled with a perfect electric conductor, and a lossless dielectric fills the upper medium, conservation of energy requires that $R = 1$. As we shall see this is *not* the case for a metal (such as gold) in the lower domain and drops in its value to a tenth or even a hundredth are the fundamental phenomenon behind the utility of Surface Plasmon Resonance (SPR) sensors [52,34,19].

3. Boundary formulation

We will now demonstrate how the governing equations (2.2) & (2.3a)–(2.3c) can be rewritten in terms of surface quantities, more specifically the Dirichlet and (exterior) Neumann traces. For this we define the surface quantities

$$\mathbf{U}(x, y) := \mathbf{E}^u(x, y, g(x, y)) \tag{3.1a}$$

$$\mathbf{W}(x, y) := \mathbf{E}^w(x, y, g(x, y)) \tag{3.1b}$$

$$\tilde{\mathbf{U}}(x, y) := [-\partial_z \mathbf{E}^u + (\partial_x g) \partial_x \mathbf{E}^u + (\partial_y g) \partial_y \mathbf{E}^u](x, y, g(x, y)) \tag{3.1c}$$

$$\tilde{\mathbf{W}}(x, y) := [\partial_z \mathbf{E}^w - (\partial_x g) \partial_x \mathbf{E}^w - (\partial_y g) \partial_y \mathbf{E}^w](x, y, g(x, y)), \tag{3.1d}$$

where

$$\mathbf{U} = \begin{pmatrix} U^x \\ U^y \\ U^z \end{pmatrix}, \quad \mathbf{W} = \begin{pmatrix} W^x \\ W^y \\ W^z \end{pmatrix}, \quad \tilde{\mathbf{U}} = \begin{pmatrix} \tilde{U}^x \\ \tilde{U}^y \\ \tilde{U}^z \end{pmatrix}, \quad \tilde{\mathbf{W}} = \begin{pmatrix} \tilde{W}^x \\ \tilde{W}^y \\ \tilde{W}^z \end{pmatrix},$$

so

$$\begin{aligned} \{\mathbf{U}, \mathbf{W}, \tilde{\mathbf{U}}, \tilde{\mathbf{W}}\} : \mathbf{R}^2 &\rightarrow \mathbf{R}^3, \\ \{U^j, W^j, \tilde{U}^j, \tilde{W}^j\} : \mathbf{R}^2 &\rightarrow \mathbf{R}, \quad j = x, y, z. \end{aligned}$$

As each of the components of $\{\mathbf{E}^u, \mathbf{E}^w\}$ is an outgoing, quasiperiodic solution of the Helmholtz equation, (2.2), the Dirichlet and Neumann traces are related by the Fokas Integral Equations (FIE) [2,43]

$$A^u[\tilde{U}^j] - R^u[U^j] = 0, \quad A^w[\tilde{W}^j] - R^w[W^j] = 0, \quad j = x, y, z. \tag{3.2}$$

The operators are defined (for $j = x, y, z$) by

$$A^u[\tilde{U}^j] := \frac{1}{d_1 d_2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \hat{A}_{p,q}^u[\tilde{U}^j] e^{i(\alpha_p x + \beta_q y)},$$

$$R^u[U^j] := \frac{1}{d_1 d_2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \hat{R}_{p,q}^u[U^j] e^{i(\alpha_p x + \beta_q y)},$$

and

$$A^w[\tilde{W}^j] := \frac{1}{d_1 d_2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \hat{A}_{p,q}^w[\tilde{W}^j] e^{i(\alpha_p x + \beta_q y)},$$

$$R^w[W^j] := \frac{1}{d_1 d_2} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \hat{R}_{p,q}^w[W^j] e^{i(\alpha_p x + \beta_q y)}.$$

In these

$$\hat{A}_{p,q}^u[\tilde{U}] := \int_0^{d_1} \int_0^{d_2} e^{i\gamma_{p,q}^u g(x,y)} e^{-i(\alpha_p x + \beta_q y)} \tilde{U}(x, y) \, dx \, dy$$

$$\hat{R}_{p,q}^u[U] := \int_0^{d_1} \int_0^{d_2} e^{i\gamma_{p,q}^u g(x,y)} e^{-i(\alpha_p x + \beta_q y)} \left\{ \frac{i\alpha_p \partial_x + i\beta_q \partial_y + (k^u)^2}{i\gamma_{p,q}^u} \right\} U(x, y) \, dx \, dy$$

$$\hat{A}_{p,q}^w[\tilde{W}] := \int_0^{d_1} \int_0^{d_2} e^{-i\gamma_{p,q}^w g(x,y)} e^{-i(\alpha_p x + \beta_q y)} \tilde{W}(x, y) \, dx \, dy$$

$$\hat{R}_{p,q}^w[W] := \int_0^{d_1} \int_0^{d_2} e^{-i\gamma_{p,q}^w g(x,y)} e^{-i(\alpha_p x + \beta_q y)} \left\{ \frac{i\alpha_p \partial_x + i\beta_q \partial_y + (k^w)^2}{i\gamma_{p,q}^w} \right\} W(x, y) \, dx \, dy.$$

3.1. Tangential trace

Regarding the boundary conditions, we begin with the trace of the tangential component of a vector field. For this we have

$$N \times \mathbf{U} = S\mathbf{U},$$

where

$$S := \begin{pmatrix} 0 & -1 & -(\partial_y g) \\ 1 & 0 & (\partial_x g) \\ (\partial_y g) & -(\partial_x g) & 0 \end{pmatrix}.$$

We further require the (x, y) -projection operator

$$P_{x,y}\mathbf{U} = P_{x,y} \begin{pmatrix} U^x \\ U^y \\ U^z \end{pmatrix} = \begin{pmatrix} U^x \\ U^y \end{pmatrix},$$

so that

$$P_{x,y} := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

This gives

$$S_{x,y} := P_{x,y}S = \begin{pmatrix} S^{xx} & S^{xy} & S^{xz} \\ S^{yx} & S^{yy} & S^{yz} \end{pmatrix},$$

where

$$S^{xx} = 0, \quad S^{xy} = -1, \quad S^{xz} = -(\partial_y g), \quad S^{yx} = 1, \quad S^{yy} = 0, \quad S^{yz} = (\partial_x g). \quad (3.3)$$

Thus, the two x - and y -components of the Dirichlet boundary conditions, (2.3a), read

$$S_{x,y}\mathbf{U} - S_{x,y}\mathbf{W} = P_{x,y}\zeta. \quad (3.4)$$

3.2. Tangential curl

We recall that the curl of \mathbf{E}^m is given by

$$\nabla \times \mathbf{E}^m = \begin{pmatrix} \partial_y E^{m,z} - \partial_z E^{m,y} \\ \partial_z E^{m,x} - \partial_x E^{m,z} \\ \partial_x E^{m,y} - \partial_y E^{m,x} \end{pmatrix}, \quad m = u, w.$$

We now change to the surface variables $\{\mathbf{U}, \mathbf{W}\}$ with tangential derivatives $\{(\partial_x \mathbf{U}, \partial_y \mathbf{U}), (\partial_x \mathbf{W}, \partial_y \mathbf{W})\}$, and normal derivatives, $\{\tilde{\mathbf{U}}, \tilde{\mathbf{W}}\}$. The chain rule gives

$$\begin{aligned} \partial_x \mathbf{U}(x, y) &= [\partial_x \mathbf{E}^u + (\partial_x g) \partial_z \mathbf{E}^u](x, y, g(x, y)), \\ \partial_y \mathbf{U}(x, y) &= [\partial_y \mathbf{E}^u + (\partial_y g) \partial_z \mathbf{E}^u](x, y, g(x, y)), \\ \partial_x \mathbf{W}(x, y) &= [\partial_x \mathbf{E}^w + (\partial_x g) \partial_z \mathbf{E}^w](x, y, g(x, y)), \\ \partial_y \mathbf{W}(x, y) &= [\partial_y \mathbf{E}^w + (\partial_y g) \partial_z \mathbf{E}^w](x, y, g(x, y)), \end{aligned}$$

while (3.1a)–(3.1d) gives formulas for $\tilde{\mathbf{U}}$ and $\tilde{\mathbf{W}}$. It is not difficult to see that

$$\begin{aligned} |N|^2 \partial_x \mathbf{E}^u &= \left(|N|^2 - (\partial_x g)^2 \right) \partial_x \mathbf{U} - (\partial_x g)(\partial_y g) \partial_y \mathbf{U} + (\partial_x g) \tilde{\mathbf{U}} \\ |N|^2 \partial_y \mathbf{E}^u &= -(\partial_x g)(\partial_y g) \partial_x \mathbf{U} + \left(|N|^2 - (\partial_y g)^2 \right) \partial_y \mathbf{U} + (\partial_y g) \tilde{\mathbf{U}} \\ |N|^2 \partial_z \mathbf{E}^u &= (\partial_x g) \partial_x \mathbf{U} + (\partial_y g) \partial_y \mathbf{U} - \tilde{\mathbf{U}}, \end{aligned}$$

and

$$\begin{aligned} |N|^2 \partial_x \mathbf{E}^w &= \left(|N|^2 - (\partial_x g)^2 \right) \partial_x \mathbf{W} - (\partial_x g)(\partial_y g) \partial_y \mathbf{W} - (\partial_x g) \tilde{\mathbf{W}} \\ |N|^2 \partial_y \mathbf{E}^w &= -(\partial_x g)(\partial_y g) \partial_x \mathbf{W} + \left(|N|^2 - (\partial_y g)^2 \right) \partial_y \mathbf{W} - (\partial_y g) \tilde{\mathbf{W}} \\ |N|^2 \partial_z \mathbf{E}^w &= (\partial_x g) \partial_x \mathbf{W} + (\partial_y g) \partial_y \mathbf{W} + \tilde{\mathbf{W}}, \end{aligned}$$

where

$$|N|^2 = (\partial_x g)^2 + (\partial_y g)^2 + 1.$$

In light of this inconvenient pre-factor, regarding the tangential curl boundary condition, (2.3b), we premultiply by $|N|^2$ and enforce the equivalent equation

$$N \times \left[|N|^2 \nabla \times [\mathbf{E}^u - \mathbf{E}^w] \right]_{z=g} = |N|^2 \psi. \quad (3.5)$$

Regarding the curl of \mathbf{E}^u we now proceed deliberately, beginning with the x -component

$$\begin{aligned} |N|^2 (\partial_y E^{u,z} - \partial_z E^{u,y}) &= \left\{ -(\partial_x g)(\partial_y g) \partial_x U^z + \left(|N|^2 - (\partial_y g)^2 \right) \partial_y U^z + (\partial_y g) \tilde{U}^z \right\} \\ &\quad - \left\{ (\partial_x g) \partial_x U^y + (\partial_y g) \partial_x U^y - \tilde{U}^y \right\} \\ &= \tilde{C}^{u,xx} \tilde{U}^x + \tilde{C}^{u,xy} \tilde{U}^y + \tilde{C}^{u,xz} \tilde{U}^z + C^{u,xx} U^x + C^{u,xy} U^y + C^{u,xz} U^z, \end{aligned}$$

where

$$\tilde{C}^{u,xx} = 0, \quad (3.6a)$$

$$\tilde{C}^{u,xy} = 1, \quad (3.6b)$$

$$\tilde{C}^{u,xz} = (\partial_y g), \quad (3.6c)$$

$$C^{u,xx} = 0, \quad (3.6d)$$

$$C^{u,xy} = -(\partial_x g) \partial_x - (\partial_y g) \partial_y, \quad (3.6e)$$

$$C^{u,xz} = -(\partial_x g)(\partial_y g) \partial_x + \left(|N|^2 - (\partial_y g)^2 \right) \partial_y. \quad (3.6f)$$

Continuing, for the y -component,

$$\begin{aligned} |N|^2 (\partial_z E^{u,x} - \partial_x E^{u,z}) &= \left\{ (\partial_x g) \partial_x U^x + (\partial_y g) \partial_y U^x - \tilde{U}^x \right\} \\ &\quad - \left\{ \left(|N|^2 - (\partial_x g)^2 \right) \partial_x U^z - (\partial_x g)(\partial_y g) \partial_y U^z + (\partial_x g) \tilde{U}^z \right\} \\ &= \tilde{C}^{u,yx} \tilde{U}^x + \tilde{C}^{u,yy} \tilde{U}^y + \tilde{C}^{u,yz} \tilde{U}^z + C^{u,yx} U^x + C^{u,yy} U^y + C^{u,yz} U^z, \end{aligned}$$

where

$$\tilde{C}^{u,yx} = -1, \quad (3.7a)$$

$$\tilde{C}^{u,yy} = 0, \quad (3.7b)$$

$$\tilde{C}^{u,yz} = -(\partial_x g), \quad (3.7c)$$

$$C^{u,yx} = (\partial_x g) \partial_x + (\partial_y g) \partial_y, \quad (3.7d)$$

$$C^{u,yy} = 0, \quad (3.7e)$$

$$C^{u,yz} = -\left(|N|^2 - (\partial_x g)^2 \right) \partial_x + (\partial_x g)(\partial_y g) \partial_y. \quad (3.7f)$$

Finally, for the z -component,

$$\begin{aligned} |N|^2 (\partial_x E^{u,y} - \partial_y E^{u,x}) &= \left\{ \left(|N|^2 - (\partial_x g)^2 \right) \partial_x U^y - (\partial_x g)(\partial_y g) \partial_y U^y + (\partial_x g) \tilde{U}^y \right\} \\ &\quad - \left\{ -(\partial_x g)(\partial_y g) \partial_x U^x + \left(|N|^2 - (\partial_y g)^2 \right) \partial_y U^x + (\partial_y g) \tilde{U}^x \right\} \\ &= \tilde{C}^{u,zx} \tilde{U}^x + \tilde{C}^{u,zy} \tilde{U}^y + \tilde{C}^{u,zz} \tilde{U}^z + C^{u,zx} U^x + C^{u,zy} U^y + C^{u,zz} U^z, \end{aligned}$$

where

$$\tilde{C}^{u,zx} = -(\partial_y g), \quad (3.8a)$$

$$\tilde{C}^{u,zy} = (\partial_x g), \quad (3.8b)$$

$$\tilde{C}^{u,zz} = 0, \quad (3.8c)$$

$$C^{u,zx} = (\partial_x g)(\partial_y g) \partial_x - \left(|N|^2 - (\partial_y g)^2 \right) \partial_y, \quad (3.8d)$$

$$C^{u,zy} = \left(|N|^2 - (\partial_x g)^2 \right) \partial_x - (\partial_x g)(\partial_y g) \partial_y, \quad (3.8e)$$

$$C^{u,zz} = 0. \quad (3.8f)$$

Defining

$$\tilde{C}^u = \begin{pmatrix} \tilde{C}^{u,xx} & \tilde{C}^{u,xy} & \tilde{C}^{u,xz} \\ \tilde{C}^{u,yx} & \tilde{C}^{u,yy} & \tilde{C}^{u,yz} \\ \tilde{C}^{u,zx} & \tilde{C}^{u,zy} & \tilde{C}^{u,zz} \end{pmatrix}, \quad C^u = \begin{pmatrix} C^{u,xx} & C^{u,xy} & C^{u,xz} \\ C^{u,yx} & C^{u,yy} & C^{u,yz} \\ C^{u,zx} & C^{u,zy} & C^{u,zz} \end{pmatrix},$$

we have

$$|N|^2 \nabla \times \mathbf{E}^u = \begin{pmatrix} \tilde{C}^u & C^u \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{U}} \\ \mathbf{U} \end{pmatrix}.$$

Again considering that we only wish to enforce these for the x - and y -components, we define

$$C_{x,y}^u := S_{x,y} C^u = \begin{pmatrix} -C^{u,yx} - (\partial_y g) C^{u,zx} & -C^{u,yy} - (\partial_y g) C^{u,zy} & -C^{u,yz} - (\partial_y g) C^{u,zz} \\ C^{u,xx} + (\partial_x g) C^{u,zx} & C^{u,xy} + (\partial_x g) C^{u,zy} & C^{u,xz} + (\partial_x g) C^{u,zz} \end{pmatrix}$$

$$\tilde{C}_{x,y}^u := S_{x,y} \tilde{C}^u = \begin{pmatrix} -\tilde{C}^{u,yx} - (\partial_y g) \tilde{C}^{u,zx} & -\tilde{C}^{u,yy} - (\partial_y g) \tilde{C}^{u,zy} & -\tilde{C}^{u,yz} - (\partial_y g) \tilde{C}^{u,zz} \\ \tilde{C}^{u,xx} + (\partial_x g) \tilde{C}^{u,zx} & \tilde{C}^{u,xy} + (\partial_x g) \tilde{C}^{u,zy} & \tilde{C}^{u,xz} + (\partial_x g) \tilde{C}^{u,zz} \end{pmatrix}.$$

In an analogous manner one can derive for the curl of \mathbf{E}^w that

$$|N|^2 \nabla \times \mathbf{E}^w = \begin{pmatrix} \tilde{C}^w & C^w \end{pmatrix} \begin{pmatrix} \tilde{\mathbf{U}} \\ \mathbf{U} \end{pmatrix}.$$

where

$$\tilde{C}^w = \begin{pmatrix} \tilde{C}^{w,xx} & \tilde{C}^{w,xy} & \tilde{C}^{w,xz} \\ \tilde{C}^{w,yx} & \tilde{C}^{w,yy} & \tilde{C}^{w,yz} \\ \tilde{C}^{w,zx} & \tilde{C}^{w,zy} & \tilde{C}^{w,zz} \end{pmatrix}, \quad C^w = \begin{pmatrix} C^{w,xx} & C^{w,xy} & C^{w,xz} \\ C^{w,yx} & C^{w,yy} & C^{w,yz} \\ C^{w,zx} & C^{w,zy} & C^{w,zz} \end{pmatrix}.$$

As before we define

$$C_{x,y}^w := S_{x,y} C^w = \begin{pmatrix} -C^{w,yx} - (\partial_y g) C^{w,zx} & -C^{w,yy} - (\partial_y g) C^{w,zy} & -C^{w,yz} - (\partial_y g) C^{w,zz} \\ C^{w,xx} + (\partial_x g) C^{w,zx} & C^{w,xy} + (\partial_x g) C^{w,zy} & C^{w,xz} + (\partial_x g) C^{w,zz} \end{pmatrix}$$

$$\tilde{C}_{x,y}^w := S_{x,y} \tilde{C}^w = \begin{pmatrix} -\tilde{C}^{w,yx} - (\partial_y g) \tilde{C}^{w,zx} & -\tilde{C}^{w,yy} - (\partial_y g) \tilde{C}^{w,zy} & -\tilde{C}^{w,yz} - (\partial_y g) \tilde{C}^{w,zz} \\ \tilde{C}^{w,xx} + (\partial_x g) \tilde{C}^{w,zx} & \tilde{C}^{w,xy} + (\partial_x g) \tilde{C}^{w,zy} & \tilde{C}^{w,xz} + (\partial_x g) \tilde{C}^{w,zz} \end{pmatrix},$$

so that the (x - and y -components of the) two Neumann boundary conditions, (3.5), read

$$\tilde{C}_{x,y}^u \tilde{\mathbf{U}} + C_{x,y}^u \mathbf{U} - \tilde{C}_{x,y}^w \tilde{\mathbf{W}} - C_{x,y}^w \mathbf{W} = P_{x,y} |N|^2 \psi. \quad (3.9)$$

The entries of these operators can be shown to be

$$\tilde{C}^{w,xx} = 0, \quad (3.10a)$$

$$\tilde{C}^{w,xy} = -1, \quad (3.10b)$$

$$\tilde{C}^{w,xz} = -(\partial_y g), \quad (3.10c)$$

$$C^{w,xx} = 0, \quad (3.10d)$$

$$C^{w,xy} = -(\partial_x g) \partial_x - (\partial_y g) \partial_y, \quad (3.10e)$$

$$C^{w,xz} = -(\partial_x g)(\partial_y g) \partial_x + \left(|N|^2 - (\partial_y g)^2 \right) \partial_y, \quad (3.10f)$$

and

$$\tilde{C}^{w,yx} = 1, \quad (3.11a)$$

$$\tilde{C}^{w,yy} = 0, \quad (3.11b)$$

$$\tilde{C}^{w,yz} = (\partial_x g), \quad (3.11c)$$

$$C^{w,yx} = (\partial_x g) \partial_x + (\partial_y g) \partial_y, \quad (3.11d)$$

$$C^{w,yy} = 0, \quad (3.11e)$$

$$C^{w,yz} = -\left(|N|^2 - (\partial_y g)^2 \right) \partial_x + (\partial_x g)(\partial_y g) \partial_y, \quad (3.11f)$$

and

$$\tilde{C}^{w,zx} = (\partial_y \mathbf{g}), \tag{3.12a}$$

$$\tilde{C}^{w,zy} = -(\partial_x \mathbf{g}), \tag{3.12b}$$

$$\tilde{C}^{w,zz} = 0, \tag{3.12c}$$

$$C^{w,zx} = (\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_x - (|N|^2 - (\partial_y \mathbf{g})^2)\partial_y, \tag{3.12d}$$

$$C^{w,zy} = (|N|^2 - (\partial_x \mathbf{g})^2)\partial_x - (\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_y, \tag{3.12e}$$

$$C^{w,zz} = 0. \tag{3.12f}$$

3.3. Divergence-free conditions

Finally, we enforce the divergence-free condition (again premultiplied by the factor $|N|^2$) in the new variables

$$\begin{aligned} |N|^2 \operatorname{div}[\mathbf{E}^u] &= |N|^2 (\partial_x E^{u,x} + \partial_y E^{u,y} + \partial_z E^{u,z}) \\ &= (|N|^2 - (\partial_x \mathbf{g})^2)\partial_x U^x - (\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_y U^x + (\partial_x \mathbf{g})\tilde{U}^x \\ &\quad - (\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_x U^y + (|N|^2 - (\partial_y \mathbf{g})^2)\partial_y U^y + (\partial_y \mathbf{g})\tilde{U}^y \\ &\quad + (\partial_x \mathbf{g})\partial_x U^z + (\partial_y \mathbf{g})\partial_y U^z - \tilde{U}^z \\ &= \tilde{D}^{u,x}\tilde{U}^x + \tilde{D}^{u,y}\tilde{U}^y + \tilde{D}^{u,z}\tilde{U}^z + D^{u,x}U^x + D^{u,y}U^y + D^{u,z}U^z, \end{aligned}$$

where,

$$\tilde{D}^{u,x} = (\partial_x \mathbf{g}), \tag{3.13a}$$

$$\tilde{D}^{u,y} = (\partial_y \mathbf{g}), \tag{3.13b}$$

$$\tilde{D}^{u,z} = -1, \tag{3.13c}$$

$$D^{u,x} = (|N|^2 - (\partial_x \mathbf{g})^2)\partial_x - (\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_y, \tag{3.13d}$$

$$D^{u,y} = -(\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_x + (|N|^2 - (\partial_y \mathbf{g})^2)\partial_y, \tag{3.13e}$$

$$D^{u,z} = (\partial_x \mathbf{g})\partial_x + (\partial_y \mathbf{g})\partial_y. \tag{3.13f}$$

In a similar manner,

$$\begin{aligned} |N|^2 \operatorname{div}[\mathbf{E}^w] &= |N|^2 (\partial_x E^{w,x} + \partial_y E^{w,y} + \partial_z E^{w,z}) \\ &= \tilde{D}^{w,x}\tilde{W}^x + \tilde{D}^{w,y}\tilde{W}^y + \tilde{D}^{w,z}\tilde{W}^z + D^{w,x}W^x + D^{w,y}W^y + D^{w,z}W^z, \end{aligned}$$

where

$$\tilde{D}^{w,x} = -(\partial_x \mathbf{g}), \tag{3.14a}$$

$$\tilde{D}^{w,y} = -(\partial_y \mathbf{g}), \tag{3.14b}$$

$$\tilde{D}^{w,z} = 1, \tag{3.14c}$$

$$D^{w,x} = (|N|^2 - (\partial_x \mathbf{g})^2)\partial_x - (\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_y, \tag{3.14d}$$

$$D^{w,y} = -(\partial_x \mathbf{g})(\partial_y \mathbf{g})\partial_x + (|N|^2 - (\partial_y \mathbf{g})^2)\partial_y, \tag{3.14e}$$

$$D^{w,z} = (\partial_x \mathbf{g})\partial_x + (\partial_y \mathbf{g})\partial_y. \tag{3.14f}$$

If we define

$$\begin{aligned} \tilde{D}^u &:= (\tilde{D}^{u,x} \quad \tilde{D}^{u,y} \quad \tilde{D}^{u,z}), \quad D^u := (D^{u,x} \quad D^{u,y} \quad D^{u,z}), \\ \tilde{D}^w &:= (\tilde{D}^{w,x} \quad \tilde{D}^{w,y} \quad \tilde{D}^{w,z}), \quad D^w := (D^{w,x} \quad D^{w,y} \quad D^{w,z}), \end{aligned}$$

then the two divergence-free conditions read

$$(\tilde{D}^u \quad D^u) \begin{pmatrix} \tilde{\mathbf{U}} \\ \mathbf{U} \end{pmatrix} = 0, \quad (\tilde{D}^w \quad D^w) \begin{pmatrix} \tilde{\mathbf{W}} \\ \mathbf{W} \end{pmatrix} = 0. \tag{3.15}$$

3.4. Surface equations

Summarizing all of these developments, we find that we must solve (3.2), (3.4), (3.9), and (3.15) which we state abstractly as

$$Mv = b \tag{3.16}$$

where

$$M = \begin{pmatrix} \tilde{M}_{BC} & M_{BC} \\ \tilde{M}_{DN} & M_{DN} \end{pmatrix}, \quad v = \begin{pmatrix} \tilde{\mathbf{U}} \\ \tilde{\mathbf{W}} \\ \mathbf{U} \\ \mathbf{W} \end{pmatrix}, \quad b = \begin{pmatrix} b_{BC} \\ b_{DN} \end{pmatrix}. \tag{3.17}$$

In these

$$\tilde{M}_{BC} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \tilde{C}^{u,xx} & \tilde{C}^{u,xy} & \tilde{C}^{u,xz} & -\tilde{C}^{w,xx} & -\tilde{C}^{w,xy} & -\tilde{C}^{w,xz} \\ \tilde{C}^{u,yx} & \tilde{C}^{u,yy} & \tilde{C}^{u,yz} & -\tilde{C}^{w,yx} & -\tilde{C}^{w,yy} & -\tilde{C}^{w,yz} \\ \tilde{D}^{u,x} & \tilde{D}^{u,y} & \tilde{D}^{u,z} & 0 & 0 & 0 \\ 0 & 0 & 0 & \tilde{D}^{w,x} & \tilde{D}^{w,y} & \tilde{D}^{w,z} \end{pmatrix}, \tag{3.18a}$$

and

$$M_{BC} = \begin{pmatrix} S^{xx} & S^{xy} & S^{xz} & -S^{xx} & -S^{xy} & -S^{xz} \\ S^{yx} & S^{yy} & S^{yz} & -S^{yx} & -S^{yy} & -S^{yz} \\ C^{u,xx} & C^{u,xy} & C^{u,xz} & -C^{w,xx} & -C^{w,xy} & -C^{w,xz} \\ C^{u,yx} & C^{u,yy} & C^{u,yz} & -C^{w,yx} & -C^{w,yy} & -C^{w,yz} \\ D^{u,x} & D^{u,y} & D^{u,z} & 0 & 0 & 0 \\ 0 & 0 & 0 & D^{w,x} & D^{w,y} & D^{w,z} \end{pmatrix}, \tag{3.18b}$$

and

$$\tilde{M}_{DN} = \begin{pmatrix} A^u & 0 & 0 & 0 & 0 & 0 \\ 0 & A^u & 0 & 0 & 0 & 0 \\ 0 & 0 & A^u & 0 & 0 & 0 \\ 0 & 0 & 0 & A^w & 0 & 0 \\ 0 & 0 & 0 & 0 & A^w & 0 \\ 0 & 0 & 0 & 0 & 0 & A^w \end{pmatrix}, \tag{3.18c}$$

and

$$M_{DN} = \begin{pmatrix} -R^u & 0 & 0 & 0 & 0 & 0 \\ 0 & -R^u & 0 & 0 & 0 & 0 \\ 0 & 0 & -R^u & 0 & 0 & 0 \\ 0 & 0 & 0 & -R^w & 0 & 0 \\ 0 & 0 & 0 & 0 & -R^w & 0 \\ 0 & 0 & 0 & 0 & 0 & -R^w \end{pmatrix}, \tag{3.18d}$$

and

$$b_{BC} = \begin{pmatrix} -\zeta^y - (\partial_y g)\zeta^z \\ \zeta^x + (\partial_x g)\zeta^z \\ -\psi^y - (\partial_y g)\psi^z \\ \psi^x + (\partial_x g)\psi^z \\ 0 \\ 0 \end{pmatrix}, \quad b_{DN} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{3.18e}$$

4. A high-order perturbation of surfaces (HOPS) approach

Our High-Order Perturbation of Surfaces (HOPS) methodology for solving (3.16) is a straightforward application of regular perturbation theory under the assumption $g(x) = \varepsilon f(x)$. It can be shown that not only are the (known) linear operator $M = M(g) = M(\varepsilon f)$ and inhomogeneity $b = b(g) = b(\varepsilon f)$ analytic functions of ε for f sufficiently smooth (e.g., C^2 , $C^{1+\alpha}$, or even Lipschitz), so is our unknown $v = v(g) = v(\varepsilon f)$ [45,46,48]. Therefore we can make the strongly convergent expansions

$$\{M, v, b\} = \{M, v, b\}(g) = \{M, v, b\}(\varepsilon f) = \sum_{n=0}^{\infty} \{M_n, v_n, b_n\}(f)\varepsilon^n. \tag{4.1}$$

Insertion of these into (3.16) followed by equating at order ε^n yields

$$M_0 v_n = b_n - \sum_{\ell=0}^{n-1} M_{n-\ell} v_\ell. \tag{4.2}$$

Note that at each perturbation order, while one must apply the operators $M_{n-\ell}$, one need only invert the flat-interface operator M_0 (repeatedly). Once this has been accomplished for a range of orders $0 \leq n \leq N$ (delivering v_n) one can form an approximate solution

$$v^N(x, y; \varepsilon) := \sum_{n=0}^N v_n(x, y)\varepsilon^n. \tag{4.3}$$

All that remains is to specify M_n and b_n . These come from (3.17) and it is clear that this will mandate expansions

$$\begin{aligned} & \left\{ \tilde{M}_{BC}, M_{BC}, \tilde{M}_{DN}, M_{DN}, b_{BC}, b_{DN} \right\}(\varepsilon f) \\ &= \sum_{n=0}^{\infty} \left\{ \tilde{M}_{BC,n}, M_{BC,n}, \tilde{M}_{DN,n}, M_{DN,n}, b_{BC,n}, b_{DN,n} \right\}(f)\varepsilon^n. \end{aligned}$$

This, in turn, requires forms for

$$\begin{aligned} & \left\{ S^{rs}, \tilde{C}^{m,rs}, C^{m,rs}, \tilde{D}^{m,r}, D^{m,r}, A^u, A^w, R^u, R^w, \zeta^r, \psi^r \right\} \\ &= \sum_{n=0}^{\infty} \left\{ S_n^{rs}, \tilde{C}_n^{m,rs}, C_n^{m,rs}, \tilde{D}_n^{m,r}, D_n^{m,r}, A_n^u, A_n^w, R_n^u, R_n^w, \zeta_n^r, \psi_n^r \right\}(f)\varepsilon^n, \end{aligned}$$

for $m \in \{u, w\}$ and $r, s \in \{x, y, z\}$. All of these are easily derived, and forms for $\{A_n^u, A_n^w, R_n^u, R_n^w, \zeta_n, \psi_n\}$ appear in one of the author’s previous work [43]. We presently specify the remainder.

From (3.3) we have the non-zero components

$$S_0^{xy} = -1, \quad S_1^{xz} = -(\partial_y f), \quad S_0^{yx} = 1, \quad S_1^{yz} = (\partial_x f).$$

Equations (3.6a)–(3.6f), (3.7a)–(3.7f), and (3.8a)–(3.8f) give the non-zero members

$$\begin{aligned} & \tilde{C}_0^{u,xy} = 1, \quad \tilde{C}_1^{u,xz} = (\partial_y f), \\ & C_1^{u,xy} = -(\partial_x f)\partial_x - (\partial_y f)\partial_y, \quad C_0^{u,xz} = \partial_y, \quad C_2^{u,xz} = -(\partial_x f)(\partial_y f)\partial_x + (\partial_x f)^2\partial_y, \end{aligned}$$

and

$$\begin{aligned} & \tilde{C}_0^{u,yx} = -1, \quad \tilde{C}_1^{u,yz} = -(\partial_x f), \\ & C_1^{u,yx} = (\partial_x f)\partial_x + (\partial_y f)\partial_y, \quad C_0^{u,yz} = -\partial_x, \quad C_2^{u,yz} = -(\partial_y f)^2\partial_x + (\partial_x f)(\partial_y f)\partial_y, \end{aligned}$$

and

$$\begin{aligned} & \tilde{C}_1^{u,zx} = -(\partial_y f), \quad \tilde{C}_1^{u,zy} = (\partial_x f), \\ & C_0^{u,zx} = -\partial_y, \quad C_2^{u,zx} = (\partial_x f)(\partial_y f)\partial_x - (\partial_x f)^2\partial_y, \\ & C_0^{u,zy} = \partial_x, \quad C_2^{u,zy} = (\partial_y f)^2\partial_x - (\partial_x f)(\partial_y f)\partial_y. \end{aligned}$$

Similarly, (3.10a)–(3.10f), (3.11a)–(3.11f), and (3.12a)–(3.12f) deliver

$$\begin{aligned} & \tilde{C}_0^{w,xy} = -1, \quad \tilde{C}_1^{w,xz} = -(\partial_y f), \\ & C_1^{w,xy} = -(\partial_x f)\partial_x - (\partial_y f)\partial_y, \quad C_0^{w,xz} = \partial_y, \quad C_2^{w,xz} = -(\partial_x f)(\partial_y f)\partial_x + (\partial_x f)^2\partial_y, \end{aligned}$$

and

$$\begin{aligned} & \tilde{C}_0^{w,yx} = 1, \quad \tilde{C}_1^{w,yz} = (\partial_x f), \\ & C_1^{w,yx} = (\partial_x f)\partial_x + (\partial_y f)\partial_y, \quad C_0^{w,yz} = -\partial_x, \quad C_2^{w,yz} = -(\partial_y f)^2\partial_x + (\partial_x f)(\partial_y f)\partial_y, \end{aligned}$$

and

$$\begin{aligned} \tilde{C}_1^{w,zx} &= (\partial_y f), & \tilde{C}_1^{w,zy} &= -(\partial_x f), \\ C_0^{w,zx} &= -\partial_y, & C_2^{w,zx} &= (\partial_x f)(\partial_y f)\partial_x - (\partial_x f)^2\partial_y, \\ C_0^{w,zy} &= \partial_x, & C_2^{w,zy} &= (\partial_y f)^2\partial_x - (\partial_x f)(\partial_y f)\partial_y. \end{aligned}$$

Finally, from (3.13a)–(3.13f) and (3.14a)–(3.14f) we find, respectively, the non-zero contributions

$$\begin{aligned} \tilde{D}_1^{u,x} &= (\partial_x f), & \tilde{D}_1^{u,y} &= (\partial_y f), & \tilde{D}_0^{u,z} &= -1, \\ D_0^{u,x} &= \partial_x, & D_2^{u,x} &= (\partial_y f)^2\partial_x - (\partial_x f)(\partial_y f)\partial_y, \\ D_0^{u,y} &= \partial_y, & D_2^{u,y} &= -(\partial_x f)(\partial_y f)\partial_x + (\partial_x f)^2\partial_y, \\ D_1^{u,z} &= (\partial_x f)\partial_x + (\partial_y f)\partial_y, \end{aligned}$$

and

$$\begin{aligned} \tilde{D}_1^{w,x} &= -(\partial_x f), & \tilde{D}_1^{w,y} &= -(\partial_y f), & \tilde{D}_0^{w,z} &= 1, \\ D_0^{w,x} &= \partial_x, & D_2^{w,x} &= (\partial_y f)^2\partial_x - (\partial_x f)(\partial_y f)\partial_y, \\ D_0^{w,y} &= \partial_y, & D_2^{w,y} &= -(\partial_x f)(\partial_y f)\partial_x + (\partial_x f)^2\partial_y, \\ D_1^{w,z} &= (\partial_x f)\partial_x + (\partial_y f)\partial_y. \end{aligned}$$

5. Numerical results

We now point out that a numerical implementation of this algorithm is immediate. Indeed, we consider a HOPS approach to the solution of (3.16) which amounts to a numerical approximation of solutions to (4.2),

$$v_n = M_0^{-1} \left[b_n - \sum_{\ell=0}^{n-1} M_{n-\ell} v_\ell \right].$$

We approximate the members of the truncated Taylor series (4.3),

$$v_n(x, y) = \begin{pmatrix} \tilde{\mathbf{U}}_n(x, y) \\ \tilde{\mathbf{W}}_n(x, y) \\ \mathbf{U}_n(x, y) \\ \mathbf{W}_n(x, y) \end{pmatrix},$$

by

$$v_n^{N_x, N_y}(x, y) := \sum_{p=-N_x/2}^{N_x/2-1} \sum_{q=-N_y/2}^{N_y/2-1} \begin{pmatrix} \tilde{\mathbf{U}}_{n,p,q} \\ \tilde{\mathbf{W}}_{n,p,q} \\ \mathbf{U}_{n,p,q} \\ \mathbf{W}_{n,p,q} \end{pmatrix} e^{i\alpha_p x + i\beta_q y},$$

where $\{\tilde{\mathbf{U}}_{n,p,q}, \tilde{\mathbf{W}}_{n,p,q}, \mathbf{U}_{n,p,q}, \mathbf{W}_{n,p,q}\}$ are the Fourier coefficients of $\{\tilde{\mathbf{U}}_n, \tilde{\mathbf{W}}_n, \mathbf{U}_n, \mathbf{W}_n\}$, respectively. The unknown coefficients are recovered upon demanding that (4.2) be true for these forms. Convolution products are computed using the FFT algorithm [24] and the only “discretization” is that we restrict to $-N_x/2 \leq p \leq N_x/2 - 1$ and $-N_y/2 \leq q \leq N_y/2 - 1$.

Of great importance is how the Taylor series in ε , (4.3), is to be summed. To be specific, to approximate v we have just considered the truncation

$$v^{N_x, N_y, N}(x, y; \varepsilon) := \sum_{p=-N_x/2}^{N_x/2-1} \sum_{q=-N_y/2}^{N_y/2-1} \left(\sum_{n=0}^N \hat{v}_{p,q,n} \varepsilon^n \right) e^{i\alpha_p x + i\beta_q y},$$

which generates the Taylor polynomials

$$\hat{v}_{p,q}^N(\varepsilon) := \sum_{n=0}^N \hat{v}_{p,q,n} \varepsilon^n.$$

The classical numerical analytic continuation technique of Padé approximation [4] has been successfully used with HOPS methods on many occasions (see, e.g., [8,46]), and we recommend its use here. Padé approximation seeks to simulate the truncated Taylor series $\hat{v}_{p,q}^N(\varepsilon)$ by the rational function

$$[L/M](\varepsilon) := \frac{a^L(\varepsilon)}{b^M(\varepsilon)} = \frac{\sum_{\ell=0}^L a_\ell \varepsilon^\ell}{1 + \sum_{m=1}^M b_m \varepsilon^m} \tag{5.1}$$

where $L + M = N$ and

$$[L/M](\varepsilon) = \hat{v}_{p,q}^N(\varepsilon) + \mathcal{O}(\varepsilon^{L+M+1});$$

well-known formulas for the coefficients $\{a_\ell, b_m\}$ can be found in [4]. This approximant has remarkable properties of enhanced convergence, and we refer the interested reader to Section 2.2 of Baker & Graves-Morris [4] and the insightful calculations of Section 8.3 of Bender & Orszag [5] for a thorough discussion of the capabilities and limitations of Padé approximants.

5.1. Validation

For the problem of plane-wave scattering by a (non-flat) diffraction grating there are, of course, no exact solutions. Therefore, in order to validate our code, we compare results of our simulations with those generated from Field Expansions (FE) simulations described and previously verified in the work of the author [44]. Among the myriad choices of quantities to measure we have selected the zeroth (“specular”) reflected efficiency, $e_{0,0}^u$, as it is the precipitous drop in this quantity which signals the onset of a Surface Plasmon Resonance [52,34,19]. This efficiency is computed by an approach outlined in our previous work [43]. The method amounts to introducing additional “artificial boundaries” strictly above and below the uppermost and lowermost interfaces where the Rayleigh expansions (2.4a)–(2.4b) are valid so that the efficiencies can be trivially recovered.

With this in mind we chose a particular physical configuration which is motivated by the seminal work of Bruno & Reitich [9] on the FE scheme for simulating the vector Maxwell equations for a doubly layered medium. We consider the sinusoidal biperiodic grating shape specified by

$$f(x, y) = \frac{1}{4} \left[\cos\left(\frac{2\pi x}{d}\right) + \cos\left(\frac{2\pi y}{d}\right) \right], \tag{5.2a}$$

so that $d_1 = d_2 = d$. We chose their wavelength-to-period ratio $\lambda/d = 0.83$, but did not restrict to normally incident radiation. Indeed, if we express

$$\alpha = (2\pi/\lambda)v^u \sin(\theta) \cos(\phi), \quad \beta = (2\pi/\lambda)v^u \sin(\theta) \sin(\phi), \tag{5.2b}$$

$$k^u = (2\pi/\lambda)v^u, \quad k^w = (2\pi/\lambda)v^w, \tag{5.2c}$$

$$\gamma^u = \sqrt{(k^u)^2 - \alpha^2 - \beta^2}, \quad \gamma^w = \sqrt{(k^w)^2 - \alpha^2 - \beta^2}, \tag{5.2d}$$

where v^m is the index of refraction of layer m , then we chose

$$\theta = 10(2\pi/360), \quad \phi = 5(2\pi/360), \quad v^u = 1, \quad v^w = 2. \tag{5.2e}$$

To conclude the specification of the configuration, we selected

$$\varepsilon/d = 0.003, 0.01, 0.03, 0.1, \quad d = 0.500. \tag{5.2f}$$

For numerical parameters we chose

$$N_x = N_y = 16, \quad N = 10,$$

and computed the relative error between our new approach (denoted “FIE”) and the FE algorithm:

$$\text{Error} = \frac{|e_{0,0}^{u,\text{FIE}} - e_{0,0}^{u,\text{FE}}|}{|e_{0,0}^{u,\text{FE}}|}.$$

In Fig. 2 we study the convergence of our new methodology for various perturbation orders N utilizing Padé approximation as the profile height ε is varied. In Fig. 3 we display results of our convergence study for different values of the height ε as N is refined. In each of these figures we note the rapid and robust convergence of our new approach to the results of the validated, high-order accurate FE methodology [44].

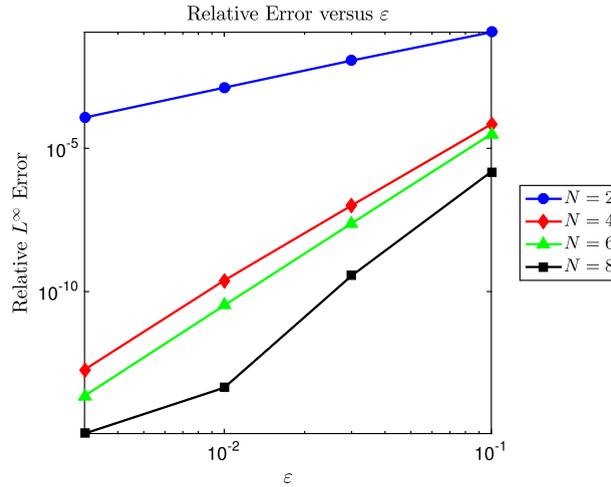


Fig. 2. Relative error versus perturbation parameter ε for various perturbation orders N (with $[N/2, N/2]$ Padé approximation). Results for the cosine–cosine configuration, (5.2a)–(5.2f), with $N_x = N_y = 16$.

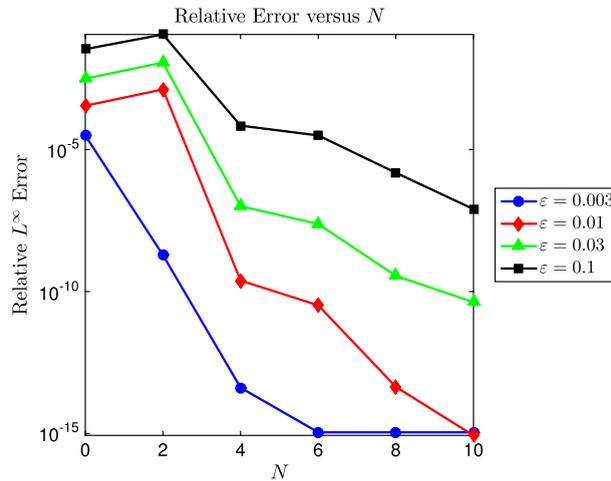


Fig. 3. Relative error versus perturbation order N (with $[N/2, N/2]$ Padé approximation) for various perturbation parameters ε . Results for the cosine–cosine configuration, (5.2a)–(5.2f), with $N_x = N_y = 16$.

5.2. Simulation of reflectivity maps

To conclude, we considered configurations inspired by the simulations of the laboratory of S.-H. Oh (Minnesota), particularly the Surface Plasmon Resonance (SPR) sensing devices studied in [33,50]. In these a two-dimensional sensor was studied featuring a corrugated insulator/conductor interface. While we are unable at present to study the third insulator layer featured there, we are able to add three-dimensional effects and, with very little trouble, change the types of the insulator and/or conductor.

We retained the grating interface shape f defined in (5.2a), chose vacuum as the insulator above the interface so that $\nu^u = 1$, and filled the lower layer with either gold or silver. The indices of refraction of these metals are the subject of current research, and for these we selected Lorentz models

$$\epsilon^\sigma = \epsilon_\infty^\sigma + \sum_{j=1}^6 \frac{\Delta_j^\sigma}{-a_j^\sigma \omega^2 - ib_j^\sigma \omega + c_j^\sigma}, \quad \sigma \in \{\text{Au}, \text{Ag}\},$$

where $\omega = 2\pi/\lambda$, and the parameters ϵ_∞^σ , Δ_j^σ , a_j^σ , b_j^σ , c_j^σ can be found in [53]. For physical and numerical parameters we chose

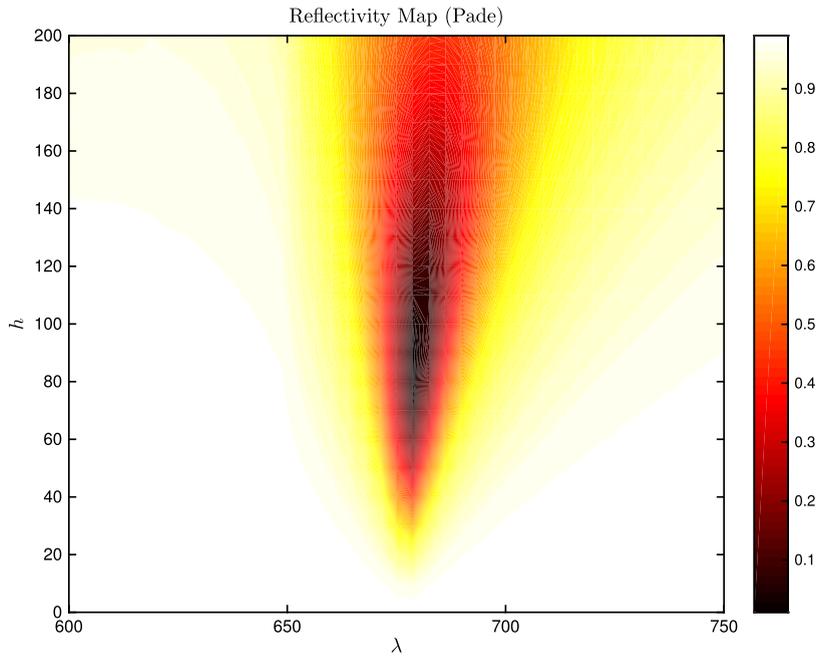


Fig. 4. Reflectivity Map for the two-layer vacuum/gold configuration, $R(\lambda, h)$, versus incident wavelength, λ , and deformation height $h = \varepsilon$. Results for the sinusoidal shape (5.2a) with $N_x = N_y = 12$, [4/4] Padé approximant.

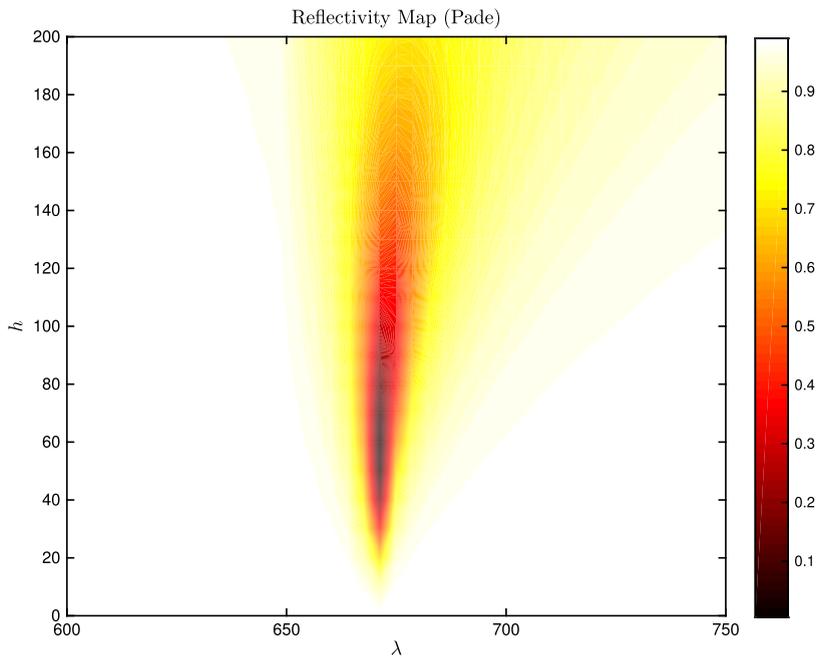


Fig. 5. Reflectivity Map for the two-layer vacuum/silver configuration, $R(\lambda, h)$, versus incident wavelength, λ , and deformation height $h = \varepsilon$. Results for the sinusoidal shape (5.2a) with $N_x = N_y = 12$, [4/4] Padé approximant.

$$\theta = 0, \quad \phi = 0,$$

$$h = \varepsilon = 0, \dots, 0.200, \quad d_1 = d_2 = 0.650,$$

$$N_x = N_y = 12, \quad N = 0, \dots, 8.$$

In Fig. 4 we display the Reflectivity Map, $R(\lambda, h)$, (2.5), for this configuration which shows a strong resonance around $\lambda = 670$ nm and $h = 90$ nm.

By contrast, in Fig. 5 we display R , (2.5), where we have replaced gold with silver. This shows a much more sensitive (narrower in λ) resonance at the new values $\lambda = 665$ nm and $h = 60$ nm.

Acknowledgements

DPN gratefully acknowledges support from the National Science Foundation through grant No. DMS-1115333.

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