Journal of Computational Physics 302 (2015) 97–113

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Time dependent scattering from a grating

Li Fan, Peter Monk *

Department of Mathematical Sciences, University of Delaware, Newark, DE 19716, USA

ARTICLE INFO

Article history:
Received 2 April 2015
Received in revised form 27 July 2015
Accepted 28 July 2015
Available online 2 September 2015

Keywords:
Diffraction grating
Time domain
Convolution quadrature
Existence
Error estimate
Finite element

ABSTRACT

Computing the electromagnetic field due to a periodic grating is critical for assessing the performance of thin film solar voltaic devices. In this paper we investigate the computation of these fields in the time domain (similar problems also arise in simulating antennas). Assuming a translation invariant periodic grating this reduces to solving the wave equation in a periodic domain. Materials used in practical devices have frequency dependent coefficients, and we provide a first proof of existence and uniqueness for a general class of such materials. Using Convolution Quadrature we can then prove time stepping error estimates. We end with some preliminary numerical results that demonstrate the convergence and stability of the scheme.

1. Introduction

We wish to approximate time domain electromagnetic scattering from a periodic grating. We shall assume that the grating is translation invariant in one direction, so that Maxwell's equations can be simplified to obtain two Helmholtz equations governing the s- and p-polarized waves. Our intended application is to modeling solar voltaic devices. Usually such devices are modeled in the frequency domain, and for descriptions of frequency domain applications in this area see [1,2]. We will consider the problem in the time domain with the potential benefit of being able to compute results at a range of frequencies in one simulation although we do not investigate that aspect here. Note that although our interest is in periodic gratings, similar problems also arise in antenna theory [3] and [2, Section 10.2.2]. We expect that the theory developed here can be extended to that case.

We start by describing the problem assuming that the grating is translation invariant parallel to the y axis, so that the permittivity of the material in the grating is independent of y (the magnetic permeability is assumed to be that of free space). Because of the reduction in dimension afforded by translation invariance, Maxwell's equations can be reduced to the wave equation in two spatial dimensions (see for example [4, Section 5.1]). So we assume that the electromagnetic wave is described by a scalar function $u = u(\mathbf{x}, t)$ depending on position $\mathbf{x} = (x, z) \in \mathbb{R}^2$ and time $t > 0$ that satisfies

$$\frac{1}{c^2} b * \frac{\partial^2 u}{\partial t^2} = \nabla \cdot (a * \nabla u) \text{ in } \mathbb{R}^2,\ t > 0. \tag{1}$$

Here $c > 0$ is the speed of light in vacuum, the symbol $*$ denotes convolution in time and the functions a and b describe the medium in which the electromagnetic field propagates. Two choices are of interest:

* Corresponding author.
E-mail addresses: fanli@udel.edu (L. Fan), monk@udel.edu (P. Monk).

http://dx.doi.org/10.1016/j.jcp.2015.07.067
0021-9991/

1. The choice

$$a = \delta(t) \text{ and } b = \epsilon_r$$

   where δ is the Dirac delta and ϵ_r is the time domain relative permittivity of the medium. In this case the wave is said to be s-polarized and u represents the y component of the electric field.
2. Alternatively

$$a = 1/\epsilon_r \text{ and } b = \delta(t)$$

   in which case the field is said to p-polarized and u represent the y component of the magnetic field.

Often, for simplicity, it is assumed that a and b are independent of frequency and are real, bounded and uniformly positive piecewise continuously differentiable functions of position. However for realistic materials both $a = a(\mathbf{x}, t)$ and $b = b(\mathbf{x}, t)$.

Since the medium is assumed to be a grating, there is a period $L > 0$ such that

$$\left.\begin{array}{rcl} a(x+L, z, t) &=& a(x, z, t) \\ b(x+L, z, t) &=& b(x, z, t) \end{array}\right\} \text{ for all } \mathbf{x} = (x, z) \in \mathbb{R}^2 \text{ and } t \in \mathbb{R}.$$

In addition the grating is assumed to have a finite height H such that

$$a = b = \delta \text{ for all } x \in \mathbb{R} \text{ and } z < 0 \text{ or } z > H. \tag{2}$$

This assumption can easily be relaxed to allow for different materials above and below the cell (one of our examples features this). We postpone further discussion of the assumptions regarding these coefficients until we have introduced sufficient notation.

Later we will reduce the problem to a bounded domain called the “unit cell” defined by

$$\Omega = (0, L) \times (0, H),$$

and we will also need the unbounded strip

$$S = (0, L) \times \mathbb{R}.$$

We assume that the total field u is due to an incident plane wave u^i propagating towards the bottom $y = 0$ of the grating. In particular

$$u^i(\mathbf{x}, t) = f(t - \mathbf{d} \cdot \mathbf{x}/c), \quad \mathbf{x} \in \mathbb{R}^2,$$

for some twice continuously differentiable function f, and unit vector

$$\mathbf{d} = (d_1, d_2) := (\cos\alpha, \sin\alpha), \quad 0 < \alpha < \pi.$$

So $\alpha = \pi/2$ gives a plane wave propagating up along the z-axis at normal incidence to the grating. In general, by linearity, the total field can be written as

$$u = u^i + u^s$$

where u^s is an unknown scattered field to be determined.

Notice that the incident field u^i is not periodic in x but instead

$$\begin{aligned} u^i(x+L, z, t) &= f(t - d_1(x+L)/c - d_2 z/c) = f(t - d_1 L/c - \mathbf{d} \cdot \mathbf{x}/c) \\ &= u^i(x, z, t - d_1 L/c) \end{aligned} \tag{3}$$

for any x, z and t. Thus we expect that the scattered field and hence the total field u should have the same translation properties so we impose

$$u(x+L, z, t) = u(x, z, t - d_1 L/c) \text{ for all } x, z \text{ and } t.$$

This is the time domain counterpart of quasi-periodicity in the frequency domain [5].

To avoid the retarded periodicity condition (3) it is common [6,7] to change variables for this problem and define

$$w(x, z, t) = u(x, z, t + (x - L)d_1/c), \text{ and } w^i(x, z, t) = u^i(x, z, t + (x - L)d_1/c).$$

With this definition it is clear that w and w^i (and hence w^s defined in the same way) is periodic in x since

$$\begin{aligned} w(x+L, z, t) &= u(x+L, z, t + x d_1/c) = u(x, z, t + (x - L)d_1/c) \\ &= w(x, z, t). \end{aligned}$$

The incident field becomes the trivially x-periodic field (independent of x)

$$w^i(x, z, t) = u^i(x, z, t + (x - L)d_1/c) = f(t - L d_1/c - d_2 z/c). \tag{4}$$