The spectral element method for the solution of Maxwell’s equations

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Abstract. Among the numerical methods of solving Maxwell’s equations for structures with complex geometry and incorporating various materials, the method of spectral elements is one of the most accurate. Compared with other methods of computation, such as finite-difference method and the finite-element method, this method appeared relatively recently, in the mid-80s. It is not so popular as global spectral methods, such as the Fourier Modal Method (FMM, RCWA). One of the main reasons for this lies in much more complicated programming. To date, various approaches have emerged to simplify the application of this method. In this paper we discuss some of them, including the implementation of the method by utilizing the Dirichlet-to-Neumann (DtN) map in complex geometry modelling, when within each element a local coordinate transformation is used. The application of the DtN mapping allows to naturally divide the problem into a set of subtasks for finding DtN operator for each element, which is convenient for parallel computations. From this point of view, the method is promising for simulation of large complex structures on distributed computing systems.

1. Introduction

The methods subsequently called “spectral methods” were widely used in solving partial differential equations long before the appearance of the first digital computers. According to these methods the solution of the problem was written as expansion by known basis functions with subsequent calculation of expansion coefficients. These are, for example, the Ritz method [1], the Galerkin method and its varieties [2], which appeared at the beginning of the last century. This is the well-known Rayleigh method [3] in optics. Spectral methods provided sufficient accuracy with a minimum of handmade computations. With the advent of the first digital computers, finite difference methods (FDM) became widespread due to their simplicity and universality. In numerical electrodynamics this is the FDTD (Finite Difference Time Domain) [4] method. Starting from the mid-60s with the development of more powerful computer systems and the advancement in computer programming the finite-element methods (FEM) [5] began to progress rapidly. They made possible to conveniently carry out calculations in complex geometry with dissimilar material properties. And at present FDM and FEM are the dominant approaches to problems of computational physics and to engineering calculations. However, where the geometry of the problem was relatively simple and increased accuracy with a minimum of computation time was required, spectral methods [2] remained relevant. In computational nanooptics and nanophotonics spectral methods are presented, for example, by such
well-known methods based on eigenmodes decomposition technique like FMM [6], C-method [7], where eigenmodes are represented by Fourier series.

In 1984 the spectral elements method (SEM) was proposed [8]. It combined geometric flexibility of finite elements with the high accuracy of spectral methods. Speaking about the spectral elements, we shall adhere to the terminology of the book [9]. SEM also was implemented as an integral part of modal methods, when the physical domain is divided into sections with continuous dielectric constant, in which the eigenmodes are represented as polynomial series [10, 11], thereby avoiding the appearance of the Gibbs phenomenon and the solution turns out to be more accurate than in case of global spectral methods. The main obstacle to the widespread use of SEM lies in much more complicated programming. To date, various approaches have emerged to simplify the application of this method. In this paper we consider SEM based on the Dirichlet-to-Neumann (DtN) map. It can be used both to solve scattering problems and to search for eigenmodes. In the next part of the paper we shall demonstrate the application of the method to the two-dimensional periodic structures such as diffraction gratings; however, this approach can be extended to arbitrary three-dimensional calculations.

2. Method description

The general solution of Maxwell’s equations for nonconical diffraction in the 2-D case can be represented as a linear combination of two fundamental polarizations: the transverse electric polarization (TE) and the transverse magnetic one (TM). In this paper, we devote attention to TM-case due to its higher complexity. Results for TE case are very similar.

In the case of TM polarization the magnetic field \( H_y(x, z) \) satisfies the following equation:

\[
\partial_x \left( \varepsilon \partial_x H_y \right) + \partial_y \left( \varepsilon^{-1} \partial_y H_y \right) + k_0^2 H_y = 0, \quad H_x = H_z = 0,
\]

where \( \partial_x, \partial_y \) denote partial derivatives by \( x \) and \( y \), respectively, \( \epsilon = \epsilon(x, z) \) is the relative dielectric constant, \( k_0 = 2\pi / \lambda \), and \( \lambda \) is the wavelength of the incident radiation. The relative permeability is set equal to unity. The incident wave is described by \( H_y^{inc} = \exp[i k_0 n_0 (x \sin \theta + z \cos \theta)] \), where \( \theta \) is the angle of incidence of the radiation with respect to the normal to the device plane (Fig. 1) and \( n_0 \) is the refractive index of the superstrate. Along the axis \( x \) the quasiperiodic Floquet boundary conditions are applied: \( H_y(x + p, z) = \exp(i k_0 n_0 p \sin \theta) H_y(x, z) \), where \( p \) is the period of grating. We consider the

![Figure 1](image_url)

**Figure 1.** a) Sketch of the grating configuration. One period is depicted. Here the entire domain is divided into 4×3=12 spectral elements; b) The absolute value of the magnetic field for the right-angle triangular grating a), left base angle= 30°, \( \varepsilon_1 = 1 \), \( \varepsilon_2 = 1.5 + 5i \), \( \lambda / p = 3 / 4 \), \( \theta = 30^\circ \), TM polarization.
application of the method for the example of a simple diffraction grating Fig. 1. The lower boundary of the domain \( \Omega_1 \) is specified by a function \( a_x(x) \), and the upper one by \( a_z(x) \), so that the solution is found inside the region: \([0, \rho] \times [a_1(x), a_2(x)]\). To switch to rectangular geometry we introduce new variables:

\[
x = u, \quad z = \left[ a_2(u) - a_1(u) \right] v/2 + \left[ a_2(u) + a_1(u) \right]/2 = b(u) v + a(u).
\]

The derivatives are related by:

\[
\partial_z = \left( \partial_z \right)^{-1} \partial_v = b^{-1} \partial_u, \quad \partial_v = \partial_u - \left( \partial_z \right)^{-1} \partial_v = \partial_u - \left( \partial_z \right)^{-1} \partial_v,
\]

where the dots mark the derivatives by variable \( u \). The domain \( \Omega_2 \) is divided into \( M = M_a \times M_v \) elements with coordinates \([u_i : u_i + \Delta u_i; v_j : v_j + \Delta v_j] \), \( i = 1..M_a, j = 1..M_v \), so that the boundaries of different material (if any) coincide with the borders of the elements. Within each element with constant permittivity the equation (1) is rewritten:

\[
\frac{\partial^2}{\partial x^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial z^2} - b^2 \frac{\partial^2}{\partial u^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial v^2} - \frac{2}{\rho^2} \left( \frac{\partial}{\partial u} + \rho \frac{\partial}{\partial v} \right) - \frac{2}{\rho^2} \left( \frac{\partial}{\partial v} + \rho \frac{\partial}{\partial u} \right)H_\rho = 0
\]

For each rectangular element \( M_i \times M_v \) a local coordinate system \((\xi, \zeta)\), \(-1 \leq \xi \leq 1, -1 \leq \zeta \leq 1\) is defined: \( \xi = -1 + 2 \cdot (u - u_i)/\Delta u_i \), \( \zeta = -1 + 2 \cdot (v - v_j)/\Delta v_j \). Then, for each element, the matrix of the DtN map operator of problem (1) is obtained. To do this, a rectangular grid of \((N_x + 1) \times (N_z + 1)\) Chebyshev-Gauss-Lobato nodes is defined inside the element:

\[
\xi_k = -\cos(\pi k / N_x), \quad k = 0..N_x; \quad \zeta_l = -\cos(\pi l / N_z), \quad l = 0..N_z.
\]

Following the influence matrix method \([9,12]\), which is completely identical to the Schur complement method \([12,13]\), a set of \(N = 2(N_x - 1) + 2(N_z - 1)\) linearly independent boundary conditions is defined. At the same time, \( N \) is equal to the number of nodes on the boundary, excluding corner nodes. Thus, any arbitrary boundary condition at these nodes can be decomposed into such a basis set. Replacing the differentiation operators in (5) with the Chebyshev differentiation matrices \([12,13]\), the Dirichlet problem for each of the boundary conditions is solved sequentially, producing two square matrices \( N \times N \) : in the first matrix \( \mathbf{F} \) there will be \( N \) boundary conditions as columns, and in the second matrix \( \partial_v \mathbf{F} \) there will be columns of corresponding normal derivatives at the boundary. So, for an arbitrary boundary condition \( \mathbf{f}_r \), the normal derivative \( \partial_v \mathbf{f}_r \) can be easily calculated:

\[
\partial_v \mathbf{f}_r = \left( \partial_v \mathbf{F} \cdot \mathbf{F}^{-1} \right) \mathbf{f}_r = \mathbf{D} \mathbf{f}_r,
\]

where \( \mathbf{D} \) is the matrix of DtN map operator. Knowing the DtN map operator matrices \( \mathbf{D}_1 \) and \( \mathbf{D}_2 \) for two spectral elements with a shared border \( \Gamma' \):

\[
\begin{align*}
\left( \begin{array}{c}
\partial_v \mathbf{f}_{r_1} \\
\partial_u \mathbf{f}_{r_1,2} \\
\end{array} \right) &= \left( \begin{array}{c}
\mathbf{D}_{1,2} \mathbf{f}_{r_1} \\
\mathbf{D}_{1,2,2} \mathbf{f}_{r_2} \\
\end{array} \right), \quad
\left( \begin{array}{c}
\partial_u \mathbf{f}_{r_2} \\
\partial_u \mathbf{f}_{r_2,2} \\
\end{array} \right) &= \left( \begin{array}{c}
\mathbf{D}_{2,2} \mathbf{f}_{r_2} \\
\mathbf{D}_{2,2,2} \mathbf{f}_{r_2} \\
\end{array} \right),
\end{align*}
\]

and taking into account boundary conditions on \( \Gamma' \), which for TM polarization are: \( \mathbf{f}_{r,2} = \mathbf{f}_{r,2,r} \), \( \partial_u \mathbf{f}_{r,2} = -\beta \cdot \partial_u \mathbf{f}_{r,2} \), where \( \beta = \varepsilon_2 / \varepsilon_1 \) is the ratio of the permittivities of the materials at points on both sides of the shared boundary \( \Gamma' \), the DtN map operator matrix of these two elements combining can be obtained:

\[
\begin{align*}
\left( \begin{array}{c}
\partial_u \mathbf{f}_{r_1} \\
\partial_u \mathbf{f}_{r_2} \\
\end{array} \right) &= \left( \begin{array}{c}
\mathbf{D}_{1,2} \mathbf{f}_{r_1} \\
\mathbf{D}_{2,2} \mathbf{f}_{r_2} \\
\end{array} \right), \quad
\left( \begin{array}{c}
\partial_v \mathbf{f}_{r_1} \\
\partial_v \mathbf{f}_{r_2} \\
\end{array} \right) &= \left( \begin{array}{c}
\mathbf{D}_{1,2} \mathbf{f}_{r_1} \\
\mathbf{D}_{2,2} \mathbf{f}_{r_2} \\
\end{array} \right),
\end{align*}
\]

where

\[
\begin{align*}
\mathbf{D}_{1,2} &= \mathbf{C} \cdot \left( \mathbf{D}_{1,2} \right)^{-1}, \quad \mathbf{D}_{2,2} = \beta \mathbf{C} \cdot \left( \mathbf{D}_{2,2} \right)^{-1}, \quad \mathbf{C} = -\left( \mathbf{D}_{1,2} + \beta \mathbf{D}_{2,2} \right)^{-1}.
\end{align*}
\]

Such approach significantly simplifies the program implementation of spectral element method, allowing to divide the task into many small subtasks and to avoid operating with large matrices. The
DtN map matrices of spectral elements can be calculated in parallel. It is also possible to connect the DtN maps of individual elements into one in parallel in $\log M$ stages, dividing the elements into groups, each consisting of two elements. In the Schur complement iterative method this problem is solved iteratively. Some iteration schemes are presented in [13]. The iterative algorithm is even more convenient for distributed parallel computing. In each computational node the DtN problem is solved for one or for a group of spectral elements and the nodes exchange only by the boundary condition information of the neighboring elements. In this point of view, the method is promising for calculations of large complex structures on distributed computing systems.

Once a similar calculation is made for the domain $\Omega_2$, the DtN map matrix of problem (1) for entire calculation region $\Omega = \Omega_1 \cup \Omega_2$ can be obtained. This matrix connects the values at the upper and lower boundaries of the domain $\Omega$ with the corresponding normal derivatives. Using this matrix we can find the S-matrix as was made in paper [14].

The spectral element method can be also used for iterative calculation of eigenmodes, for example, in resonators, or as an integral part of the modal methods. In paper [15], such iterative approach was used to calculate hundreds of thousands of eigenmodes within modal method based on 1-D spectral elements.

3. Conclusions

The implementation of the spectral element method based on the Dirichlet-to-Neumann map for solving Maxwell’s equations is discussed. The main advantage of the method is: it combines geometric flexibility of finite elements with the high accuracy of spectral methods. Besides, it can be effectively parallelized with minimal interprocessors data exchange that makes it promising for calculations of large complex structures on distributed computing systems.

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