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Application of the iterative approach to modal methods for the solution of Maxwell's equations

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ABSTRACT

In this work we discuss the possibility to reduce the computational complexity of modal methods, i.e. methods based on eigenmodes expansion, from the third power to the second power of the number of eigenmodes by applying the iterative technique. The proposed approach is based on the calculation of the eigenmodes part by part by using shift-and-invert iterative procedure and by utilizing the iterative approach to solve linear equations to compute eigenmodes expansion coefficients. As practical implementation, the iterative modal methods based on polynomials and trigonometric functions as well as on finite-difference scheme are developed. Alternatives to the scattering matrix (S-matrix) technique which are based on pure iterative or mixed direct-iterative approaches allowing to markedly reduce the number of required numerical operations are discussed. Additionally, the possibility of diminishing the memory demand of the whole algorithm from second to first power of the number of modes by implementing the iterative approach is demonstrated. This allows to carry out calculations up to hundreds of thousands eigenmodes without using a supercomputer.

1. Introduction

Over the past decades an increasing interest has been devoted to the rigorous solution of Maxwell's equations in order to study the optical properties of optoelectronic devices including image sensors, nanostructured solar cells, photonic crystals and diffraction gratings [1,2]. Due to a rapid increase in complexity of the simulated devices and the continuously rising demand of accuracy that leads to the need of solving very large systems of linear equations, the application of iterative techniques [3,4] to the solution of Maxwell's equations in frequency domain may be very promising.

In recent years a number of algorithms to solve Maxwell's equations within iterative approach have been proposed [5–10]. Its implementation can significantly reduce the computational time. For example, iterative implementation of Generalized Source method, differential and Green's function approaches can reduce the number of arithmetic operations from cubic to linear dependence on the number of Fourier modes [5–7].

In case of modal methods iterative approaches are also exploited to speed up calculations, for instance to solve eigenvalue problems using Arnoldi method [8–10]. However, the computational complexity of these approaches is of order of the third power of the number of used eigenmodes, which is the same of the direct approach. The additional difficulty is due to the

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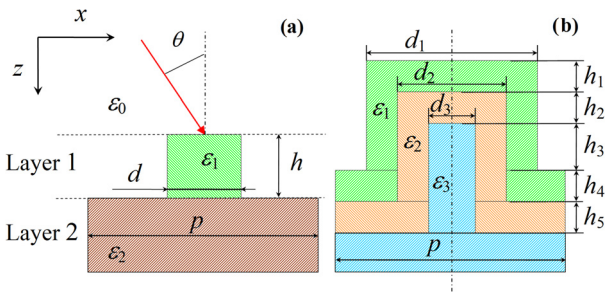

Fig. 1. Sketch of the gratings configuration. One period is depicted.

fact that modal methods include two significantly different stages: solution of the eigenvalue problem and calculation of the expansion coefficients with which eigenmodes represent the electromagnetic field. To decrease the order of computational complexity of the entire algorithm, both of these stages should be appropriately reformulated.

As it is well known according to modal methods, i.e. the algorithms based on eigenmode expansion, the simulation domain is divided into layers featuring parallel interfaces. The permittivity varies only in the plane of the layer and is assumed to be constant along the perpendicular direction allowing the separation of spatial variables (Fig. 1). Within each layer the eigenmodes of the electromagnetic field are calculated and the general solution is then expressed by means of an eigenmode expansion. The expansion coefficients can be found by applying proper boundary conditions. Due to their relative simplicity, two-dimensional (2-D) structures are often considered in order to discuss potentialities, drawbacks and features of the proposed algorithms. Indeed, in the case of 2-D structures, for which the dielectric constant within each parallel layer depends only on one spatial coordinate, in order to obtain the eigenmodes the one-dimensional Helmholtz equation has to be solved.

Most proposed implementations of the modal method use a set of predetermined basis functions to express the eigenmodes such as the complex Fourier series used in the Fourier modal method (FMM) known also as rigorous coupled-wave analysis method (RCWA) [11], orthogonal polynomials adopted in polynomial expansion modal methods [12–14] or B-splines [15,16]. The eigenmodes may be computed also by finite-difference approach [17] or by pseudospectral methods [18,19]. It is worth noting that all these methods are developed for periodic structures, however, using perfectly matched layers (PML) [20] they can be reformulated for implementing a general aperiodic case. From this point of view the FMM (RCWA) is especially thoroughly researched [21,22]. The extension of polynomial expansion modal method initially developed for periodic structures to aperiodic case is discussed in [23]. The direct solution of the eigenvalue problem in any of these methods demands an order of M^3 operations, where M is the number of eigenmodes included to computation. The only exception is the analytic or true modal method (AMM) [24,25] in which eigenmodes are expressed in an exact analytical form requiring order of operations equal to M to compute the eigenvalues by finding the roots of the transcendental equation. This represents a complicated task especially in case of complex permittivity and often one of the above-listed methods are used to find the approximation to the roots with subsequent purification by Newton's method [26]. In case of transverse electric polarization, a simple algorithm based on perturbation theory can be implemented [26] to avoid the solution of the full eigenvalue problem. However, for transverse magnetic polarization such simple technique is absent. Another drawback of AMM is that it can be rigorously implemented only in the 2-D case.

The computation of the expansion coefficients by S-matrix or similar technique also requires about M^3 operations [12, 27–29], consuming a noticeable time in overall calculation.

In this work we have proposed the application of the iterative approach to modal methods based on two relevant enhancements that can significantly increase the efficiency of the algorithms:

1) the M eigenmodes are found *by batches* by using Arnoldi method and shift-and-invert technique;
2) in order to solve the system of linear equations an *iterative* procedure is used instead of an S- or an R-matrix formalism.

If the possibility to restrict the number of operations in one shift-and-invert iteration to a value proportional to the first power of the number of used basis functions (or mesh points in pseudospectral and finite-difference methods) exists, then in combination to point 1) this ensures a reduction in a number of arithmetic operations to the order of M^2 to solve the eigenvalue problem. In some cases it can be obtained by using fast Fourier transform (FFT), in others by using some features of considered matrix such as sparseness or band structure. The point 2) allows to minimize the computational time of determining the expansion coefficients. Additionally, the memory requirements are relaxed from M^2 to the order of M in some formulations of the algorithm.

The iterative modal methods formulated within proposed approach may have its already known direct counterpart or have not. In the next section we present two examples of application of this approach, one of which use Chebyshev polynomials as basis function and has its direct counterpart [18], the over based on trigonometric functions has not.

The remainder of the paper is organized as follows: in Section 2 the theoretical part concerning the 2-D implementation case is outlined. In particular in section "A" we describe the iterative solution of eigenvalue problem and in section "B"