Journal of Computational Physics 261 (2014) 130–144

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

On the complexity of aperiodic Fourier modal methods for finite periodic structures

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ARTICLE INFO

Article history:
Received 28 September 2013
Received in revised form 22 December 2013
Accepted 24 December 2013
Available online 2 January 2014

Keywords:
Fourier-modal method
FMM
Rigorous coupled-wave analysis
RCWA
Perfectly matched layers
PML
Computational costs
Logarithmic complexity
Aperiodic Fourier-modal method
AFMM-CFF
Alternative discretization

ABSTRACT

The Fourier modal method (FMM) is based on Fourier expansions of the electromagnetic field and is inherently built for infinitely periodic structures. When the infinite periodicity assumption is not realistic, the finiteness of the structure has to be incorporated into the model. In this paper we discuss the recent extensions of the FMM for finite periodic structures and analyze their complexity both with respect to the main discretization parameter $\hat{N}$ as well as with respect to the number of periods R. We show that among the three FMM-based approaches able to represent finiteness, the aperiodic Fourier modal method with alternative discretization has the lowest computational cost given by either $\mathcal{O}(\hat{N}^3 \log_2 R)$ or $\mathcal{O}(\hat{N}^2 R)$ depending on the values of $\hat{N}$ and R. This result demonstrates that the method is highly suited for rigorous modeling of scattering from large periodic structures. For instance, for $\hat{N} = 100$ and $R < 1000$ the complexity of the aperiodic Fourier modal method with alternative discretization is comparable to the complexity of the standard FMM.

1. Introduction

Periodicity encountered in a structure is often responsible for its special electromagnetic properties. Examples are the creation of higher orders during wave propagation in diffraction gratings or effective imitation of a negative refractive index [1] or even invisibility [2,3] by metamaterials. In the process of modeling periodic structures and solving the underlying Maxwell's equations, an important assumption is routinely made: it is considered that the periodic structure, which is finite in reality, is approximated reasonably well by an idealized infinitely periodic structure. In this case the field is quasi-periodically repeating from one period to another and it suffices to compute the solution in a single period of the structure as shown in Fig. 1(a). Obviously, this leads to low computational costs. The disadvantage however lies in the "infinite periodicity" assumption. As the periodic structure gets smaller (e.g. due to being driven by Moore's law in the semiconductor industry) the approximation becomes less accurate and a different approach is required.

If infinite periodicity can be assumed then standard numerical techniques for Maxwell's equations may be applied to solve for a single period of the structure. These techniques include the finite-element method (FEM) [4–6], the finite-difference time–domain method (FDTD) [7–9] and the integral equation methods (IEM), which include the boundary element method (BEM) [10–12] and the volume integral method (VIM) [13–17].

The enumerated methods are derived from general-purpose numerical discretization schemes. In the field of computational diffractive optics one specialized method has gained a large popularity due to its simplicity and natural interpretation of the field expansions. It is known under several names and abbreviations: rigorous coupled-wave analysis (RCWA), modal

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0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.12.051

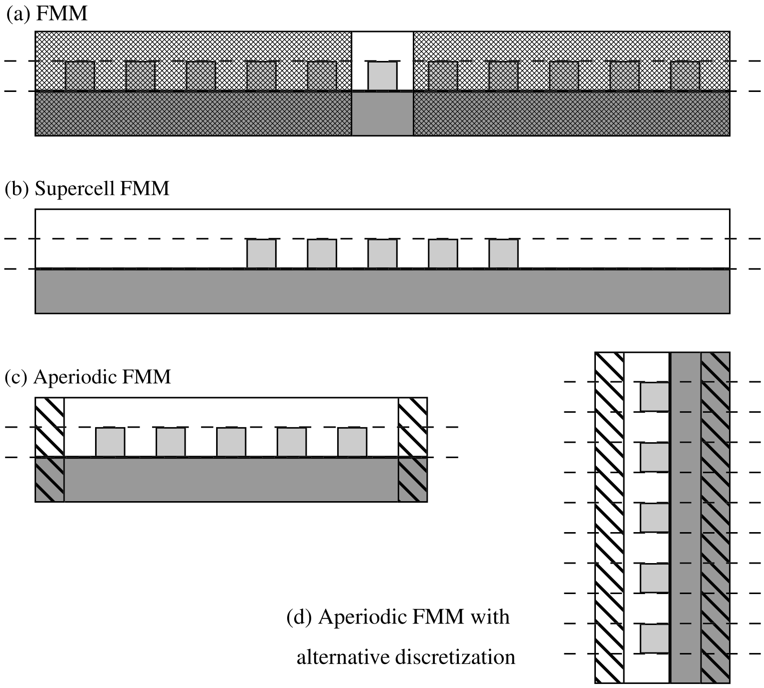

Fig. 1. Overview of FMM-based methods for modeling finite periodic structures. (a) Classical FMM employing the "infinite periodicity" assumption. Only the field in the highlighted cell needs to be computed. (b) Supercell FMM. (c) AFMM-CFF with classical discretization. (d) AFMM-CFF with alternative discretization.

method with Fourier expansion (MMFE), and the Fourier-modal method (FMM). The latter name is used throughout this paper. The FMM [18] was proposed in 1978 by Knop [19]. The method is analytical in one spatial direction and (for a broad range of applications) outperforms general-purpose approaches relying on a full numerical discretization of all directions. In the past decades the FMM has matured due to fundamental studies and improvements to its stability [20,21] and convergence [22–24]. Other important contributions to the evolution of the method are the techniques of *adaptive spatial resolution* [25] and *normal vector fields* [26–28]. Ref. [29] gives a mathematical perspective of the challenges that have been overcome in the FMM and of the open problems still to be addressed. For possible improvements of the method see Chapter 7 in [30].

Recently, several extensions of the FMM have been proposed which do not rely on the infinite periodicity assumption and rigorously model all the periods of the structure of interest. We illustrate the FMM-based approaches which incorporate finiteness in Figs. 1(b), (c), and (d). The most straightforward extension of the FMM to finite structures is the so-called *supercell* approach, depicted in Fig. 1(b). The computational domain is extended to include all periods of the structure. Moreover, extra space is left on both sides of the structure in order to decrease the coupling/reflections via the periodic boundary conditions which are built-in in the method due to the use of Fourier-mode expansions. The more empty space is left on the sides, the better the model represents finiteness. We note that, unlike the methods described below, the supercell FMM is not rigorous in the sense that the radiation condition is imposed indirectly by expanding the computational domain. The computational cost significantly increases both as the number of periods in the structure becomes larger and as the empty spaces are chosen wider. In practice, this means that supercell FMM can only be used for small structures (with a size of several tens of wavelengths).

A more efficient approach is to replace the wide (and expensive) empty spaces by narrow artificial absorbers as done in the *aperiodic Fourier modal method in contrast-field formulation* (AFMM-CFF) and depicted in Fig. 1(c). The AFMM-CFF [31–33] is a recent extension of the FMM to aperiodic structures. It builds upon the aperiodic Fourier modal method developed and refined by Lalanne and co-workers [34–38] with the key difference that the AFMM-CFF solves Maxwell's equations formulated in terms of a contrast (scattered) field instead of a total field. This reformulation allows prescription of arbitrary incoming fields onto the structure of interest [31]. Aperiodicity is achieved by using *perfectly matched layers* (PMLs) [39] on the vertical boundaries in order to annihilate the periodic boundary condition.

Finally, it turns out that the computational cost for AFMM-CFF can be further reduced by applying an *alternative discretization* [40], which can also be viewed as a classical FMM discretization applied to a rotated geometry as shown in Fig. 1(d). This alternative discretization is chosen based on complexity arguments and will be explained in Section 5.

Since in practical applications the number of periods can be quite large, an important criterion for comparing these methods is the scaling of computational costs with the number of periods and with the number of basis functions per period. We will discuss the complexity in terms of time and memory for all methods presented.

This paper is structured as follows. We describe the four FMM-based approaches in Sections 2–5. Computational results which illustrate the characteristics of the methods are presented in Section 6. In Section 7 the complexity of the AFMM-CFF