

An Adaptive Finite Element Method with a Modified Perfectly Matched Layer Formulation for Diffraction Gratings

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Abstract. For numerical simulation of one-dimensional diffraction gratings both in TE and TM polarization, an enhanced adaptive finite element method is proposed in this paper. A modified perfectly matched layer (PML) formulation is proposed for the truncation of the unbounded domain, which results in a homogeneous Dirichlet boundary condition and the corresponding error estimate is greatly simplified. The a posteriori error estimates for the adaptive finite element method are provided. Moreover, a lower bound is obtained to demonstrate that the error estimates obtained are sharp.

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1 Introduction

Due to its wide applications in micro-optics, diffraction gratings have recently received considerable attentions in both engineering and computational sciences [1, 2, 14]. There are various methods for the numerical simulation of diffraction gratings; among which the finite element method is one of the most popular approaches due to its capability in handling complicated geometries and boundary conditions. There are two challenges in applying the finite element method to diffraction grating simulation. One is to truncate the unbounded domain into a bounded one with some adequate approximation accuracy,

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and the other is to resolve the solution singularity caused by the discontinuity of the dielectric coefficient. To address these two issues, the perfectly matched layer (PML) [7] technique combined with a posteriori error estimate based adaptive finite element method have been applied [4, 16].

Since the pioneering work of Babuška and Rheinboldt [6], the adaptive finite element methods based on a posteriori error estimates have become a central theme in scientific and engineering computations. For appropriately designed adaptive finite element procedures, the meshes and the associated numerical complexity are quasi-optimal, see, e.g., [4, 9, 11–13, 15, 16]. This makes the adaptive finite element method attractive for grating problems, which is often combined with the PML technique. In [16], Chen and Wu introduced an adaptive linear finite element algorithm with PML for domain truncation. A posteriori error estimate is derived to determine the PML thickness parameters automatically. Moreover, an exponential decay factor is introduced so that the a posteriori error estimate decays exponentially with respect to the distance to the computational domain, which makes the computational cost insensitive to the thickness of the absorbing layer. Later in [4], a second-order adaptive finite element method with error control was developed by Bao et al. for one-dimensional grating problems. The method has been applied to solve problems such as the 2D acoustic problem [17] and the 3D electromagnetic scattering problem [8].

Based on the work of Chen and Wu [16], several important improvements on the PML-based adaptive finite element method will be made in this paper:

(a) The PML formulation in [16] is modified by subtracting an auxiliary function from the electric field variable which satisfies the Helmholtz equation. The modification results in a homogeneous Dirichlet condition for all the boundaries, while in [16], the boundary condition on the upper boundary is not homogeneous. As a consequence, the exponential decay factor used for the error estimation in [16] is deleted here and accordingly the error analysis and practical implementation of the PML algorithm are greatly simplified.

(b) Furthermore, the error estimate for the PML is improved on the situation where the imaginary part of dielectric coefficient is small and positive, and the error bound is much better than that in [16]. The derived error estimate also implies that the solution of the PML problem converges exponentially to the solution of the grating problem when either the thickness of the PML layers or the PML medium parameters approaches infinity.

(c) A posteriori error estimates between the solution of the grating problem and the finite element approximation of the PML problem are derived. Since the modification of PML formulation results in a homogeneous Dirichlet boundary condition, both the estimations and proving are much simpler than that in [16]. And a lower bound of the a posteriori error estimates is obtained, which is missed in [16]. The lower bound is not used in the practical adaptive finite element procedure, however it illustrates that the derived error estimates are sharp.

The remainder of this paper is organized as follows. In Section 2 the 1D diffraction gratings model is presented. In Section 3 the modified PML formulation is introduced