

ERROR ESTIMATION FOR NUMERICAL METHODS USING THE ULTRA WEAK VARIATIONAL FORMULATION IN MODEL OF NEAR FIELD SCATTERING PROBLEM*

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Abstract

In this paper, we investigate the use of ultra weak variational formulation to solve a wave scattering problem in near field optics. In order to capture the sub-scale features of waves, we utilize evanescent wave functions together with plane wave functions to approximate the local properties of the field. We analyze the global convergence and give an error estimation of the method. Numerical examples are also presented to demonstrate the effectiveness of the strategy.

Mathematics subject classification: 65N12, 65N55.

Key words: Helmholtz equation, Ultra weak variational formulation, Plane wave function, Evanescent wave function, Absorbing boundary condition.

1. Introduction

Near field optics could provide an effective approach to break the diffraction limit in conventional far-field optics [1, 2], so it has developed dramatically and been applied in diverse aspects in recent years, such as nondestructive imaging of biological samples, nanotechnology, near-field optical microscopy [3]. In order to theoretically understand the physical mechanism of this fascinating feature, it is desirable to accurately solve the underlying scattering problem.

In this paper, we focus on a typical scattering problem in the near field optics that models the total internal reflection microscopy (TIRM). More specifically, we consider a sample deposited on a homogeneous substrate and illustrated from below (transmission geometry). When the incident angle is greater than a critical value, the total internal reflection happens. Then the evanescent wave appears at the other side of the interface which is used as illumination to encode the sub-wavelength structure of the scattering object. This phenomenon is formulated mathematically by Helmholtz equation, which models time-harmonic electromagnetic wave scattering for the case of TM (transverse magnetic) polarization. However, at medium and high frequency, resolution requirements and so-called pollution effect entail an excessive computational efforts and prevent standard finite element method from effective use. Thus, numerically simulating the wave propagation is a challenging task. But the wave-based methods offer a possible way to deal with this problem. The main idea is to use special solutions of the underlying partial differential equation in each element to build the discrete space, thus a priori information about the

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solution is directly incorporated in the approximation space. Possible techniques include least squares methods (LSM) [4–6], the partition of unity method (PUM) [7, 8], the discontinuous Galerkin method (DG) [9, 10], and the ultra weak variational formulation (UWVF) [11, 13, 14]. It is the last of these techniques that will be considered for this work.

The ultra weak variational formulation is originated from the domain decomposition technique and was proposed by Cessenat and Després. In [11], Cessenat and Després studied an obstacle scattering problem in homogeneous background medium by virtue of this method using plane wave functions. They proved an error estimate for the method showing that the solution of the UWVF converges to an appropriate impedance trace of the true solution on the boundary of the domain. Inspired by their ideas, we apply UWVF to solve our problem. By introducing a coupling parameter, an ultra weak variational formulation suitable to TIRM scattering model problem is derived. And in order to capture the sub-scale features of the wave field, evanescent wave functions which are also the solution of Helmholtz equation are introduced to enrich the plane wave functions. We analyze the error estimation and give a hp-version convergence result even away from the boundary. The argument is fundamentally different from that of [11].

The remainder of this paper is organized as follows. In Section 2, we give a ultra weak variational formulation appropriate to our model problem. Then we introduce the discrete problem including construction of the approximation space. In Section 3, we analyze the error estimate of our approach. First, via an auxiliary sesquilinear, we show that our ultra weak variational formulation has sufficient coercivity to provide an error estimate. Next, a basic estimate is given by means of the duality techniques. Finally, we derive convergence result from the best approximation error and a knowledge of the approximation properties of bases. In Section 4, numerical experiments are presented to demonstrate the validity of the method. In Section 5, we conclude.

2. Continuous and Discrete Problem

2.1. Formulation of the Model Problem

In this subsection, we introduce the model problem to be studied and give some related notations used later.

The point in the plane is denoted by $\mathbf{x} = (x, y) \in \mathbb{R}^2$. The whole space \mathbb{R}^2 is divided by the substrate $\Gamma_0 = \{\mathbf{x} | y = 0\}$ into $\mathbb{R}_+^2 = \{y > 0\}$ and $\mathbb{R}_-^2 = \{y < 0\}$. The corresponding refractive indexes are n_+ and n_- ($n_+ < n_-$) respectively. A sample S with refractive n_s is deposited on the substrate Γ_0 and illustrated from below by time harmonic plane wave $u^i = \exp(i\alpha x + i\eta y)$ at an angle θ greater than a critical value, where $\alpha = k_0 n_- \sin \theta$ and $\eta = k_0 n_- \cos \theta$, and k_0 is the free-space wave number (see Fig. 2.1 for geometry of the model). Throughout we assume nonmagnetic materials and TM polarization.

When there is no sample, the field in \mathbb{R}^2 denoted by u^{ref} is called reference field. According to the Maxwell electromagnetic theory, u^{ref} is the solution of the following equation

$$\Delta u^{ref} + k_0^2 m^2(\mathbf{x}) u^{ref} = 0, \quad \mathbf{x} \in \mathbb{R}^2, \quad (2.1)$$

where refractive is defined by

$$m(\mathbf{x}) = \begin{cases} n_+, & \mathbf{x} \in \mathbb{R}_+^2, \\ n_-, & \mathbf{x} \in \mathbb{R}_-^2. \end{cases}$$