Journal of Computational and Applied Mathematics 289 (2015) 296–305

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

Challenges in developing efficient Calderon preconditioners for resonating or high material contrast penetrable objects

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ARTICLE INFO

Article history:
Received 27 August 2014
Received in revised form 17 November 2014

Keywords:
Calderon preconditioning
Dielectric object
Electromagnetic scattering
Iterative solution
Surface integral equation
Transmission problem

ABSTRACT

Calderon preconditioning is a recently proposed technique for improving conditioning of ill-conditioned matrices arising from discretization of surface integral equations. In electromagnetics the method has been developed for both perfectly conducting and homogeneous penetrable objects. In the case of penetrable objects the large variety of possible material parameters poses additional challenges on the efficiency of the preconditioner. We demonstrate with numerical experiments that problems may appear in particular at high material parameter values, at the physical resonances of the object, and at negative or zero material parameters. As realistic examples of objects with zero or negative material parameters we consider plasmonic nanoparticles at optical wavelengths.

1. Introduction

Surface integral equation method provides elegant solutions for time-harmonic electromagnetic scattering by homogeneous penetrable objects. The method requires discretization of the surfaces and interfaces of homogeneous and isotropic domains only and thus essentially reduces the dimensionality of the problem by one and leads to much simplified data structures compared to methods based on volume discretization. Surface integral equations for penetrable objects can be written in infinitely many ways, see e.g. [1,2]. Most of the numerical integral equation solvers are based on so called Poggio–Miller–Chang–Harrington–Wu–Tsai (PMCHWT) [3] formulation. This formulation, however, is plagued with a couple of serious obstacles in particular as iterative or fast techniques are applied to solve the associated matrix equation. Discretization of the PMCHWT equations with conventional techniques, i.e., Galerkin's method with low order divergence conforming functions such as Rao–Wilton–Glisson (RWG) [4] functions, leads to a matrix in which condition number grows as the mesh density is increased or the frequency is decreased [5]. Thus, the PMCHWT formulation suffers from both the dense mesh and low frequency breakdowns, making the system matrix ill-conditioned and iterative solutions ineffective as the mesh density is high or the frequency is low.

Calderon preconditioning is a recently proposed technique for improving conditioning of the surface integral equations. In electromagnetics the method was originally developed for the electric field integral equation (EFIE) and perfectly conducting objects [6]. In [5] the method was extended for the PMCHWT formulation and homogeneous dielectric objects, and later in [7] for homogeneous chiral objects. The PMCHWT operator is shown to have a similar self-regularizing property as the electric field integral operator in the EFIE. However, due to the more complicated form of the PMCHWT operator (it contains also the magnetic field integral operator and operators with different material parameters), its self-regularizing property does not follow as straightforwardly from the Calderon integral identities as in the case of the EFIE. Despite that,

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http://dx.doi.org/10.1016/j.cam.2015.01.005

Calderon preconditioned PMCHWT formulation can be discretized using similar techniques as is used to discretize Calderon preconditioned EFIE [5]. Alternative forms and discretizations of the Calderon preconditioned PMCHWT formulation have been proposed and investigated e.g. in [8,9].

In the case of penetrable objects the large variety of possible material parameters poses additional challenges in developing efficient preconditioners that are not present in the case of metallic perfectly conducting objects. For example, as predicted in [5] with theoretical analysis, spectrum of the Calderon preconditioned PMCHWT formulation has two accumulation points, one depending on the material contrast of the object and the other one on the inverse of it. As these two points move further away from each other, e.g., as the material contrast of the object is increased, the efficiency of the preconditioner may decrease. In [9] a scaled form of the original Calderon preconditioner was proposed. The eigenvalue spectrum of the formulation called "method 3" in [9] is shown to have a single accumulation point and thus it is expected to lead to a more efficient preconditioner as the material contrast is high.

In this paper we investigate Calderon preconditioned PMCHWT formulations with numerical experiments. We consider both the original formulation [5] and the scaled one [9]. We show that the number of required iterations increase as the material contrast of the object is increased. This is found to be true for both considered forms of the Calderon preconditioner. We have also observed an increase on the iteration count at the physical resonances of the object, and at negative or zero material parameters. As realistic cases where permittivity is negative or zero, we consider plasmonic nanoparticles at optical wavelength. At these wavelengths (noble) metals, such as silver and gold, cannot be modeled as perfect conductors, rather they have to be modeled as penetrable dielectric objects with complex permittivity [10,11].

2. Theoretical background

Consider time-harmonic electromagnetic scattering by a homogeneous penetrable object in a homogeneous background medium. Let Ω^i denote the interior of the object, Ω^e the exterior and Γ the interface of Ω^e and Ω^i. Let ε^i, μ^i and ε^e, μ^e be the constant electromagnetic parameters of the domains. The sources of the incident primary fields, $\boldsymbol{E}^{\mathrm{inc,p}}$ and $\boldsymbol{H}^{\mathrm{inc,p}}$, are in domain Ω^p. Here, and in the sequel, $p = e$ or i, indicating exterior (e) or interior (i) domains.

The task – the transmission problem for Maxwell's equations – is to find the secondary fields, $\boldsymbol{E}^{\mathrm{sec,p}}$ and $\boldsymbol{H}^{\mathrm{sec,p}}$, so that they satisfy homogeneous Maxwell's equations in Ω^p and on Γ the total fields, $\boldsymbol{E}^{\mathrm{inc,p}} + \boldsymbol{E}^{\mathrm{sec,p}}$ and $\boldsymbol{H}^{\mathrm{inc,p}} + \boldsymbol{H}^{\mathrm{sec,p}}$, satisfy transmission conditions

$$\begin{aligned} &\gamma_t(\boldsymbol{E}^{\mathrm{inc,e}} + \boldsymbol{E}^{\mathrm{sec,e}}) = \gamma_t(\boldsymbol{E}^{\mathrm{inc,i}} + \boldsymbol{E}^{\mathrm{sec,i}}), \\ &\gamma_t(\boldsymbol{H}^{\mathrm{inc,e}} + \boldsymbol{H}^{\mathrm{sec,e}}) = \gamma_t(\boldsymbol{H}^{\mathrm{inc,i}} + \boldsymbol{H}^{\mathrm{sec,i}}), \end{aligned} \tag{1}$$

where γ_t is the tangential trace operator on the surface Γ.

2.1. Formulation

We continue by giving the PMCHWT integral equations for the electromagnetic transmission problem formulated above. First, introduce Green's functions of the homogeneous domains

$$G^p(\boldsymbol{r}, \boldsymbol{r}') = \frac{e^{ik^p|\boldsymbol{r}-\boldsymbol{r}'|}}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}, \quad \text{with } k^p = \omega\sqrt{\varepsilon^p\mu^p}. \tag{2}$$

Next define two surface integral operators

$$\mathcal{K}^p[\boldsymbol{F}](\boldsymbol{r}) = \nabla \times \mathcal{S}^p[\boldsymbol{F}](\boldsymbol{r}), \tag{3}$$

$$\mathcal{T}^p[\boldsymbol{F}](\boldsymbol{r}) = \frac{-1}{ik^p}\nabla\mathcal{S}^p[\operatorname{Div}\boldsymbol{F}] + ik^p\mathcal{S}^p[\boldsymbol{F}](\boldsymbol{r}), \tag{4}$$

where

$$\mathcal{S}^p[\boldsymbol{F}](\boldsymbol{r}) = \int_\Gamma G^p(\boldsymbol{r}, \boldsymbol{r}')\,\boldsymbol{F}(\boldsymbol{r}')\,dS(\boldsymbol{r}'), \tag{5}$$

is the single layer potential operator and Div denotes surface divergence of a sufficiently regular tangential vector field. More precisely, this tangential vector field should be in $H_{\mathrm{Div}}^{-1/2}(\Gamma)$ [12]. On the interface Γ operators $\mathcal{K}^p$ and $\mathcal{T}^p$ are defined in the sense of Cauchy principal value integrals.

Let $\boldsymbol{n}^p$ denote the unit normal vector of Γ pointing into domain Ω^p and define the electric and magnetic equivalent surface current densities of the domains as $\boldsymbol{J}^p = \boldsymbol{n}^p \times \boldsymbol{H}^p$ and $\boldsymbol{M}^p = -\boldsymbol{n}^p \times \boldsymbol{E}^p$, where $\boldsymbol{E}^p$ and $\boldsymbol{H}^p$ are the total fields in Ω^p. The surface integral representations for the total fields in domains Ω^p can now be expressed compactly as [13]

$$\begin{aligned} &\Omega^p(\boldsymbol{r})\boldsymbol{E}^p(\boldsymbol{r}) = \eta^p\mathcal{T}^p[\boldsymbol{J}^p](\boldsymbol{r}) - \mathcal{K}^p[\boldsymbol{M}^p](\boldsymbol{r}) + \boldsymbol{E}^{\mathrm{inc,p}}(\boldsymbol{r}), \\ &\Omega^p(\boldsymbol{r})\boldsymbol{H}^p(\boldsymbol{r}) = \frac{1}{\eta^p}\mathcal{T}^p[\boldsymbol{M}^p](\boldsymbol{r}) + \mathcal{K}^p[\boldsymbol{J}^p](\boldsymbol{r}) + \boldsymbol{H}^{\mathrm{inc,p}}(\boldsymbol{r}). \end{aligned} \tag{6}$$