Theoretical and computational aspects of the SVM, EBCM, and PMM methods in light scattering by small particles

V.B. Il'in[*,1,2,3], V.G. Farafonov[2], and A.A. Vinokurov[2,3]

[1] *St. Petersburg University, Universitetskij pr. 28, St. Petersburg, 198504 Russia.*

[2] *State University of Aerospace Instrument., Bol. Morskaya 67, St. Petersburg, 190000 Russia.*

[3] *Pulkovo Observatory, Pulkovskoe chaussee 65/1, St. Petersburg, 196140 Russia.*

We consider the generalized separation of variables, extended boundary condition, and generalized point-matching methods that apply single expansions of the electromagnetic fields in terms of wave functions to solve the light-scattering problem. We consider especially theoretical studies related to analysis of infinite linear systems, questions of field-expansion convergence, and the Rayleigh hypothesis. The passage from the infinite systems to truncated ones used in calculations will be discussed, and numerical solutions provided by the methods will be compared.

INTRODUCTION

The behavior of the electromagnetic (EM) fields $\vec{E}, \vec{H}$ in any medium is governed by the macroscopic Maxwell equations. In the light scattering (LS) theory one usually considers time-harmonic fields $\vec{E}(\vec{r}, t) = \vec{E}(\vec{r})\, e^{-i\omega t}$, where ω is the radiation frequency [1]. So, for most of the media the Maxwell equations transform into

$$\Delta \vec{E}(\vec{r}) + k^2(\vec{r})\, \vec{E}(\vec{r}) = 0, \quad \vec{\nabla} \cdot \vec{E}(\vec{r}) = 0, \tag{1}$$

where $k(\vec{r})$ is the wavenumber in the medium, and similar equations for the magnetic field $\vec{H}(\vec{r})$ related to the electric one as $\vec{H}(\vec{r}) = (i\mu(\vec{r})k_0)^{-1}\, \vec{\nabla} \times \vec{E}(\vec{r})$, where $\mu(\vec{r})$ is the magnetic permeability, k_0 the wavenumber in vacuum.

The boundary conditions to Eqs. (1) are provided by continuity of the tangential components of the fields at any interface, which gives for a scatterer with the surface $\partial\Gamma$

$$\left.\begin{aligned} (\vec{E}^{\rm inc}(\vec{r}) + \vec{E}^{\rm sca}(\vec{r}) - \vec{E}^{\rm int}(\vec{r})) \times \vec{n}(\vec{r}) = 0, \\ (\vec{H}^{\rm inc}(\vec{r}) + \vec{H}^{\rm sca}(\vec{r}) - \vec{H}^{\rm int}(\vec{r})) \times \vec{n}(\vec{r}) = 0, \end{aligned}\right\}_{\vec{r}\in\partial\Gamma} \tag{2}$$

where $\vec{E}^{\rm inc}, \vec{H}^{\rm inc}, \vec{E}^{\rm sca}, \vec{H}^{\rm sca}$, and $\vec{E}^{\rm int}, \vec{H}^{\rm int}$ are the fields of incident, scattered, and internal radiation, respectively, $\vec{n}(\vec{r})$ is the outward normal to $\partial\Gamma$. There is also the well-known radiation condition at infinity for the scattered field.

Various methods are used to solve the LS problem for non-spherical scatterers (see, e.g., the reviews [1, 3]). One often applies the separation of variables (SVM), extended boundary condition (EBCM), and point-matching (PMM) methods based on the same single expansions of the EM fields in terms of vector wave functions $\vec{F}_\nu(\vec{r})$

$$\vec{E}(\vec{r}) = \sum_\nu \alpha_\nu\, \vec{F}_\nu(\vec{r}), \quad \vec{H}(\vec{r}) = \sum_\nu \beta_\nu\, \vec{F}_\nu(\vec{r}), \tag{3}$$

* Corresponding author: Vladimir Il'in (ilin55@yandex.ru)

where α_ν, β_ν are some coefficients.

METHODS UNDER CONSIDERATION

Generalized SVM approach

Here one usually substitutes the expansions (3) in the boundary conditions (2), multiplies these conditions by the angular part of different index wave functions and integrates the results over the scatterer surface $\partial\Gamma$ (see, e.g., [1, 4]). As a result one gets a set of linear algebraic equations relative to unknown coefficients of the external ($\alpha_\nu^{\rm sca}$) and internal ($\alpha_\nu^{\rm int}$) field expansions

$$\left\{ \begin{array}{l} A\,\vec{x}^{\,\rm sca} + B\,\vec{x}^{\,\rm int} = E\,\vec{x}^{\,\rm inc}, \\ C\,\vec{x}^{\,\rm sca} + D\,\vec{x}^{\,\rm int} = F\,\vec{x}^{\,\rm inc}, \end{array} \right. \tag{4}$$

where $A, B, ..., F$ are matrices whose elements are integrals of the wave functions and their derivatives, $\vec{x}^{\,\rm sca,int} = \{\alpha_\nu^{\rm sca,int}\}_{\nu=1}^{\infty}$, and $\vec{x}^{\,\rm inc}$ is a vector of the known coefficients of the incident field expansion. Solution to the system (4) gives the unknown coefficients which allows one to calculate any optical properties of a scatterer [4]. We consider the *generalized* SVM when the approach is applied to particles of arbitrary shape (see for more details [4]).

Standard EBCM approach

In this case a surface integral formulation of the LS problem arisen from the Stratton-Chu formula is utilized (see, e.g., [5])

$$\vec{\nabla} \times \int_S \vec{n}(\vec{r}\,') \times \vec{E}^{\,\rm int}(\vec{r}\,')\, g(\vec{r},\vec{r}\,')\, {\rm d}s' - \frac{1}{ik_0\varepsilon} \vec{\nabla} \times \vec{\nabla} \times \tag{5}$$

$$\int_S \vec{n}(\vec{r}\,') \times \vec{H}^{\,\rm int}(\vec{r}\,')\, g(\vec{r},\vec{r}\,')\, {\rm d}s' = \left\{ \begin{array}{ll} -\vec{E}^{\,\rm inc}(\vec{r}), & \vec{r} \in \Gamma_-, \\ \vec{E}^{\,\rm sca}(\vec{r}), & \vec{r} \in \Gamma_+, \end{array} \right.$$

where $g(\vec{r},\vec{r}\,')$ is the free space Green function, Γ_- and Γ_+ mean the interior and exterior of a scatterer, respectively, ε is the dielectric permittivity. The field expansions (3) and the known Green function expansion in terms of some wave functions are substituted in the extended boundary conditions (5). Linear independence of the basis functions allows one to equal the expansion coefficients for each function $\vec{F}_\nu$ (see for more details [4]). So, the equations (5) give two matrix equations relative to the unknown expansion coefficients

$$\left\{ \begin{array}{rcl} Q_{\rm S}\,\vec{x}^{\,\rm int} & = & \vec{x}^{\,\rm inc}, \\ \vec{x}^{\,\rm sca} + Q_{\rm R}\,\vec{x}^{\,\rm int} & = & 0, \end{array} \right. \tag{6}$$

where the matrices $Q_{\rm R}, Q_{\rm S}$ have the elements being integrals of the wave functions and their derivatives. The EBCM suggested by Barber [6] and used by us [4] and Waterman's null-field method discussed in [1] are practically the same.

Integral generalized PMM approach

In the PMM one considers a residual δ describing fulfillment of the boundary conditions (2) in a set of points $\{\vec{r}_s\}_{s=1}^{M}$ on the scatterer surface $\partial\Gamma$

$$\delta = \sum_{s=1}^{M} \left\{ \left| \left(\vec{E}^{\rm inc} + \vec{E}^{\rm sca} - \vec{E}^{\rm int} \right) \times \vec{n} \right|^2 + \left| \left(\vec{H}^{\rm inc} + \vec{H}^{\rm sca} - \vec{H}^{\rm int} \right) \times \vec{n} \right|^2 \right\}_{\vec{r}=\vec{r}_s \in \partial\Gamma} . \tag{7}$$

The first N (in the generalized PMM $N < M$) terms of the field expansions (3) are substituted in Eq. (7) and the residual is minimized in the least-square sense. The derivatives of the residual with respect to the unknown coefficients $\alpha_\nu^{\rm sca}, \alpha_\nu^{\rm int}$ for $\nu = 1, 2, ..., N$ are made equal to 0, which gives $2N$ linear algebraic equations relative to these coefficients. As a result, one gets a system like (4) but with other matrix elements [1, 4]. Replacing summation in Eq. (7) with integration provides more accurate results for smaller M being now the number of knots [7]. So, hereafter we discuss such an *integral generalized* PMM. In our theoretical analysis below this approach is considered for the case of $N = \infty$.

DISCUSSION OF THE METHODS

In computations one always deals with truncated expansions of the EM fields. They can be considered as approximations to the infinite expansions giving the exact values. We discuss theoretical aspects related to the infinite expansions (3), the infinite linear systems (4),(6) and a passage from them to truncated systems as well as some numerical results. Generally, we try to follow and extend the fundamental review [1, 2].

Convergence of infinite field expansions

This point is considered by analyzing singularities of the analytic continuations of the EM fields [8]. We discuss the role played by the expansion convergence in the methods under consideration and concern the Rayleigh hypothesis problem by debating a recent review [9].

Investigations of infinite linear systems

This aspect has not yet been discussed in the literature on the EBCM and generalized SVM. We investigate the infinite systems (4) and (6) arisen in these methods and find the condition of their solvability that involves distances to singularities of analytic continuations of the EM fields. We also explain the connection between the pattern equation method (see [10] and references therein) and the EBCM, which allows us to make important conclusions for the far-field zone. Though equivalence of the EBCM and generalized SVM was generally shown in [11], we demonstrate equivalence of the infinite systems arisen in all the methods under consideration in a more strict way.

Infinite system truncation and numerical comparison of methods

Our passage to truncated systems is based on a proof that infinite systems are regular in terms of [12]. Then they must have the only solution that can be found by the expansion truncation method. Using a homogeneous set of our generalized SVM, EBCM, integral generalized PMM codes, we confront results of calculations with the theoretical predictions. We also compare these numerical solutions for scatterers of different shape and structure. Special attention is paid to the behavior of the truncated system condition numbers.

REVIEW OF APPLICATIONS OF THE METHODS

Finally, keeping in mind the above discussion, we give a review of works on development and application of the SVM, EBCM and PMM approaches. We mainly concentrate on the SVM and PMM as works on the EBCM are well reviewed (see [13] and references therein) and discuss the use of different (spherical, cylindrical, spheroidal, and ellipsoidal) bases in treatment of homogeneous and layered scatterers and their systems.

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