Iterative solvers for T-matrix and Discrete-Sources Methods

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The different iterative approaches (GMRES, MINRES, BiCGStab, BiCGStab(2)) to solve linear systems in scattering problems based on surface-integral-equation methods (Discrete-Sources Method, T-matrix) are compared. The case where the kernel matrix is relatively small but ill-conditioned is considered. Different preconditioning techniques (diagonal, block-diagonal preconditioning matrix) are also compared.

INTRODUCTION

The numerical simulation of light scattering by small particles is a modern and effective approach to investigate many physical processes. During the centennial history, a lot of numerical methods have been developed and extended. Most of them require or imply to solve the linear system problem.

Solving the linear system can be subjected to numerical difficulties because of the ill-conditionality of the kernel matrix and the finite-precision arithmetic in computers. The iterative methods help to reduce the influence of this factor and to decrease the required time to estimate the solution. The extremely large, sparse, ill-conditioned kernel matrix is the case where the iterative methods are mostly preferable. Therefore, they are used in volume-integral-equation methods like DDA (discrete-dipole approximation). Preconditioning techniques also allow to strongly improve the convergence of iterative processes.

Here, different iterative methods and preconditioning techniques for the Discrete-Sources Method (DSM) and the T-matrix Method labeled as surface-integral-equation methods are compared. Cases with relative small but highly ill-conditioned kernel matrices are considered.

MATHEMATICAL STATEMENT OF THE SCATTERING PROBLEM

Let us consider scattering in an isotropic homogeneous medium R^3 of an electromagnetic wave by a local homogeneous penetrable obstacle D_i with the smooth boundary ∂D. We assume the time dependence to be $\exp(j\omega t)$. Scattering is described by the electromagnetic fields $\{\mathbf{E}_{e,i}, \mathbf{H}_{e,i}\}$ satisfying the Maxwell equations

$$\begin{aligned} \nabla \times \mathbf{H}_{e,i} &= jk\varepsilon_{e,i}\mathbf{E}_{e,i}, \\ \nabla \times \mathbf{E}_{e,i} &= -jk\mu_{e,i}\mathbf{H}_{e,i}, \end{aligned} \qquad \text{in } D_{e,i}, \qquad D_e := R^3/\bar{D}_i, \tag{1}$$

the boundary conditions enforced on the particle surface

$$\begin{aligned} \mathbf{n}_p \times (\mathbf{E}_i(P) - \mathbf{E}_e(P)) &= \mathbf{n}_p \times \mathbf{E}^0(P), \\ \mathbf{n}_p \times (\mathbf{H}_i(P) - \mathbf{H}_e(P)) &= \mathbf{n}_p \times \mathbf{H}^0(P), \end{aligned} \qquad P \in \partial D, \tag{2}$$

and the Silver-Muller radiation condition at infinity,

$$\lim_{r\to\infty} \left(\sqrt{\varepsilon_e}\mathbf{E}_e \times \frac{\mathbf{r}}{r} - \sqrt{\mu_e}\mathbf{H}_e\right) = 0, \qquad r = |M| \to \infty, \tag{3}$$

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where $\{\mathbf{E}^0, \mathbf{H}^0\}$ is an exciting field, $\mathbf{n}_p$ is the unit outward normal to ∂D , index e belongs to the external domain D_e and i to the domain inside the particle D_i, $\varepsilon_{e,i}$ is the permittivity, and $\mu_{e,i}$ is the permeability of media. This boundary value scattering problem is well-known to have an unique solution.

T-matrix Method

The T-matrix approach is a modern and effective numerical tool for exactly solving the scattering problem for particles of arbitrary shape. It was proposed by Waterman [1] and extensively reviewed by Mishchenko et al. [2]. The further extension of the method is called the Null-Field Method with Discrete Sources (NFM-DS) [3].

In the terms of NFM-DS the internal electromagnetic field is expanded by a suitable basis of vector wave functions, e.g. in an isotropic medium regular vector spherical wave functions are used

$$\mathbf{E}_i(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[p_{mn}\mathbf{RgM}(k_s\mathbf{r}) + q_{mn}\mathbf{RgN}(k_s\mathbf{r})\right], \quad k_i = \sqrt{\varepsilon_i \mu_i}. \tag{4}$$

The electromagnetic fields outside the circumscribed sphere are expanded into a series of spherical vector wave functions

$$\mathbf{E}_e(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[a_{mn}\mathbf{M}(k_s\mathbf{r}) + b_{mn}\mathbf{N}(k_s\mathbf{r})\right], \quad k_s = \sqrt{\varepsilon_s \mu_s}, \tag{5}$$

$$\mathbf{E}_s(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left[f_{mn}\mathbf{RgM}_i(k_s\mathbf{r}) + g_{mn}\mathbf{RgN}_i(k_s\mathbf{r})\right], \tag{6}$$

where k_s is the wave number of the isotropic surrounding medium, and a_{mn}, b_{mn} and f_{mn}, g_{mn} are the expansion coefficients of the incident and scattered fields, respectively. Considering the null-field equations (2) and the expansions (4-6), the transition matrix $\mathbf{T}$ can be obtained from the following linear system:

$$\mathbf{T} \cdot \mathbf{Q}^{31} = -\mathbf{Q}^{11}, \quad \begin{pmatrix} f_{mn} \\ g_{mn} \end{pmatrix} = \mathbf{T} \begin{pmatrix} a_{mn} \\ b_{mn} \end{pmatrix}, \tag{7}$$

where the matrices $\mathbf{Q}^{31}$, $\mathbf{Q}^{11}$ include surface integrals over the particle surface. In real simulations, the matrix size depends on the expansion order $1 \leq n \leq N_{rank}$ in (4-6) and is typically less than 10000.

Discrete Sources Method

In the frame of DSM, an approximate solution of the scattering problem is constructed as a finite linear combination of the field of dipoles and multipoles $\{z_n\}_{n=1}^{N}$ deposited in a supplementary domain ω_0. Detailed review can be found in the book by Wriedt et al. [4]. In the case of a P-polarized incident plane wave and an axially symmetric particle, the approximate solution can be presented in the form

$$\begin{pmatrix} \mathbf{E}_{e,i}^N \\ \mathbf{H}_{e,i}^N \end{pmatrix} = \sum_{m=0}^{M} \sum_{n=1}^{N_{e,i}^m} \left\{p_{mn}^{e,i} D_1 \mathbf{A}_{mn}^{1,e,i} + q_{mn}^{e,i} D_2 \mathbf{A}_{mn}^{2,e,i}\right\} + \sum_{n=1}^{N_{e,i}^0} r_n^{e,i} D_1 \mathbf{A}_n^{3,e,i} \tag{8}$$

with vector differential operators D_1, D_2, the vector potentials in a cylindrical coordinate system $\mathbf{A}_{mn}^{1,e,i}$, $\mathbf{A}_{mn}^{2,e,i}$, $\mathbf{A}_n^{3,e,i}$, and the amplitudes of the corresponding multipoles $p_{mn}^{e,i}$, $q_{mn}^{e,i}$, $r_n^{e,i}$.

The unknown amplitudes of the discrete sources are to be determined from the boundary conditions (2). To solve this problem, the Generalized Point-Matching Technique is used. The matching of the approximate solution and the external excitation over the particle surface is replaced by the matching over particle generatrix $\{\eta_n\}_{n=1}^{L}$ for each Fourier harmonic m separately. As a consequence, the unknown vector of amplitudes $\mathbf{p}_m = \{p_{mn}^{e,i}, q_{mn}^{e,i}\}_{n=1}^{N_{e,i}^m}$ can be found as a pseudosolution of an over-determined system of linear equations:

$$\mathbf{B}_m \mathbf{p}_m = \mathbf{q}_m, \qquad m = 0, ..., M, \tag{9}$$

where $\mathbf{B}_m$ is a rectangular matrix of dimension $4L \times 2(N_i^m + N_e^m)$. Similarly, the amplitudes $\mathbf{p}_{-1} = \{r_n^{e,i}\}_{n=1}^{N_{e,i}}$ corresponding to the vertical electric or magnetic dipoles can be found.

Solving this problem we transform (directly or formally) the equation (9) to its 'equivalent' normal form ($n = m$) (10) through multiplication by the conjugate transpose matrix,

$$A_m \mathbf{p}_m = \hat{b}_m, \quad A_m = \mathbf{B}_m^T \mathbf{B}_m, \quad \hat{b}_m = \mathbf{B}_m^T \mathbf{q}_m. \tag{10}$$

Here A_m is a Hermitian, non-singular, positive definite matrix with the dimension $2(N_i^m + N_e^m) \times 2(N_i^m + N_e^m)$. Usually, the matrix size lies in the range between 500 and 5000.

ITERATIVE SOLVERS

Krylov subspace

Many powerful and effective methods are Krylov subspace projection methods. These methods were initiated in the early 1950s with the introduction of the conjugate gradients methods [5]. For a given non-singular matrix A, an approximate solution is constructed in the so-called Krylov subspace

$$x_k \in x_0 + K^k(A; r_0), \quad K^k(A; r_0) = span\{r_0, Ar_0, \dots, A^{k-1} r_0\},$$

where $r_0 = b - Ax_0$ is an initial residual, x_0 is a given initial solution, and k is the iteration step. Because of the non-singularity of A, the vectors $r_0, Ar_0, \dots, A^{k-1}r_0$ are linearly independent and the Krylov subspace is a k-dimensional space. This means that the dimensionality of the subspace will increase by 1 up to n per iteration. The Krylov subspace methods should give the exact solution after at least n iterations, but they give a suitable approximate solution much earlier. By the criteria on 'optimality', these methods fall in three different classes:

The Ritz-Galerkin approach — Construct the $x_k \in x_0 + K^k(A, r_0)$ for which the residual $r_k = b - Ax_k$ is orthogonal to the current subspace $r_k \perp K^k(A, r_0)$. The commonly used methods for symmetric (Hermitian) matrices are CG, SYMMLQ, for non-symmetric matrices are FOM, CGNE, CGNR.

The minimum residual approach — Construct the $x_k \in x_0 + K^k(A, r_0)$ for which the Euclidian norm $\|b - Ax_k\|_2$ is minimal over the current subspace. The commonly used algorithms of the current group are GMRES, RGMRES, FGMRES, GMRESR and version of GMRES for symmetric (Hermitian) matrices MINRES.

The Petrov-Galerkin approach — Construct the $x_k \in x_0 + K^k(A, r_0)$ for which the residual r_k is orthogonal to some other suitable k-dimensional subspace. If we select $L^k =$

$K^k(A^T, s^0)$ for some vector s^0, then we obtain the BiCG and QMR methods and their further modifications CGS, BiCGStab, BiCGStab(l) and TFQMR, respectively.

Based on preliminary simulations, for further comparisons, the following methods RGMRES(m), BiCGStab, BiCGStab(l) (PIM library [6]) and MINRES were chosen.

Preconditioning techniques

One of the advantages of the iterative methods is the availability of preconditioning techniques. The convergence of an iterative process and the accumulation of round-off errors strongly depend on the condition number $\kappa(A) = \max \|\lambda_i\| // \min \|\lambda_i\|$, where λ_i is the i-th eigenvalue of the matrix A. By multiplication (left- and/or right-sided) by some other matrix K, we can change the condition number and therefore improve the iterative process.

Because the calculation of well-known preconditioners (*ILU*, *ILUT*, *IC*, polynomial preconditioner) for ill-conditioned dense matrices could be numerically difficult and unstable, diagonal matrix preconditioners $D = diag\{d_{11}, d_{22}, \ldots, d_{nn}\}$ with different filling rules as well as two-diagonal preconditioners are chosen. To keep the Hermitian symmetry of the matrix A, we used the left and right preconditioning $\hat{A} = D^{1/2} A D^{1/2}$, $P = D^{1/2}$.

In Fig. 1, the iterative behavior of the scattering computation using the DSM method is plotted. The scatterer is a prolate spheroidal particle with size parameter $kR = 50$, aspect ratio $e = 10$, and refractive index $m_r = 1.6$. As a measure of the quality of the solution, the discrepancy of the surface fields ($\|\mathbf{n}_p \times (\mathbf{E}_i - \mathbf{E}_e - \mathbf{E}^0)\| / \|\mathbf{E}^0\|$) is used.

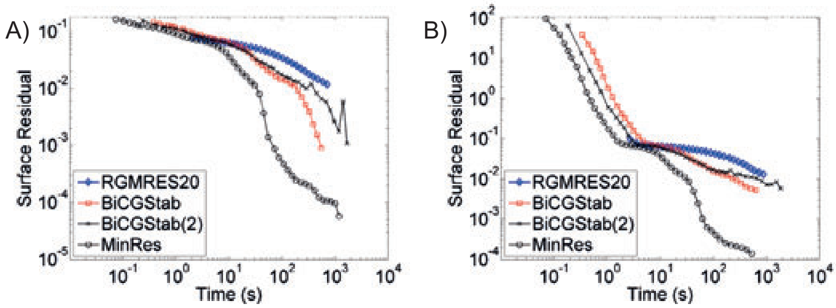

Figure 1. The iterative behaviour of scattering computation using iterative solvers (a) without preconditioning techniques and (b) with a block-diagonal preconditioning matrix.

Acknowledgments: We acknowledge support by Deutsche Forschungsgemeinschaft (DFG).

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