BiCG-FFT T-Matrix Method for Solving for the Scattering Solution from Inhomogeneous Bodies

J. H. Lin and W. C. Chew
Electromagnetics Laboratory
Department of Electrical and Computer Engineering
University of Illinois
Urbana, IL 61801

Abstract

A BiCG-FFT T-Matrix algorithm is proposed to efficiently solve three dimensional scattering problems of inhomogeneous bodies. The memory storage is of $O(N)$ (N is the number of unknowns) and each iteration in BiCG requires $O(N \log N)$ operations. A good agreement between the numerical and exact solutions is observed. The convergence rate for lossless and lossy bodies of various size are shown. It is also demonstrated that the matrix condition number for fine grids is the same as that for coarse grids.

1. Introduction

The scattering of electromagnetic fields by inhomogeneous bodies is a research topic that finds applications in many fields. In this paper, we propose a method of solving the inhomogeneous body problem by approximating the inhomogeneous body with small dielectric cubes. The dielectric cubes are then approximated by equivolume spheres [1-4]. In this manner, the T matrix [5,6] of each individual sphere can be found in closed form. A set of linear algebraic equations can be easily derived to solve for the scattering amplitudes from each of the spheres. By using this T-matrix formulation, the Green's function singularity problem is avoided, while other formulations, such as the method of moments, such a singularity has to be handled with caution [7-9].

When the inhomogeneous body is discretized into a regular grid, the resultant equation has a block-Toeplitz structure. An iterative solver such as BiCG (bi-conjugate gradient) method [10,11] can be used to solve for the solution of the matrix equation iteratively. When an iterative solver is used, the main cost of seeking the solution is the cost of performing a matrix-vector multiplication. Exploiting the block-Toeplitz structure, we can perform the matrix-vector multiplication in $O(N \log N)$ operations by FFT [7-9,12], where N is the total number of spheres involved.

The method can be shown to require $O(N)$ memory storage. Hence, it can be used to solve fairly large problems. A volume scattering problem with 90,000 unknowns is solved on a Sparc 10 workstation. It is shown that iterative solvers converge faster for lossy bodies than lossless ones. This is because the matrix condition number for the former cases is smaller than that for the latter ones, as a lossless body could have high Q internal resonance modes.

As the simulation results show, by using the T-matrix formulation, the condition number of the resultant matrix is independent of the mesh size of

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a uniform grid. Therefore, the number of iterations does not grow when the body is gridded finer in order to achieve better resolution.

2. Formulation and Implementation

When a number of scatterers are placed on a uniform array, their scattering solution can be obtained efficiently by using FFT and an iterative method.

The total field due to an array of non-identical scatterers can be written as

$$\mathbf{E}(\mathbf{r}) = \boldsymbol{\psi}^t(k_0, \mathbf{r}_s) \cdot \mathbf{a}_s + \sum_{i=1}^{N} \boldsymbol{\psi}^t(k_0, \mathbf{r}_i) \cdot \mathbf{b}_i, \tag{1}$$

where $\mathbf{r}_i = \mathbf{r} - \mathbf{r}'_i$ and $\mathbf{r}'_i$ is the location of the scattering center of the i-th scatterer. $\boldsymbol{\psi}^t(k_0, \mathbf{r}_i)$ is a row vector containing the vector spherical harmonics from each scatterer. The first term in (1) comprises the incident field while the second term is the scattered field. The vectors $\mathbf{a}_s$ and $\mathbf{b}_i$ contain the amplitudes of the incident field harmonics and the scattered field harmonics from the i-th scatterer respectively.

Focusing on the j-th scatterer, we can use the addition theorem or the translation matrix [4,13] to change the coordinates of all the spherical harmonics to that of the j-th scatterer to obtain

$$\begin{aligned}\mathbf{E}(\mathbf{r}) = \Re g \boldsymbol{\psi}^t(k_0, \mathbf{r}_j) \cdot \overline{\boldsymbol{\alpha}}_{js} \cdot \mathbf{a}_s + \Re g \boldsymbol{\psi}^t(k_0, \mathbf{r}_j) \cdot \sum_{\substack{i=1 \\ i \neq j}}^{N} \overline{\boldsymbol{\alpha}}_{ji} \cdot \mathbf{b}_i \\ + \boldsymbol{\psi}^t(k_0, \mathbf{r}_j) \cdot \mathbf{b}_j.\end{aligned} \tag{2}$$

Looking at the above, we see that the first two terms are incident waves impinging on the j-th scatterer while the third term is the scattered field off the j-th scatterer. Therefore, the amplitude of the third term must be related to the total amplitude of the first two terms via the isolated scatterer T matrix of the j-th scatterer, i.e., $\overline{\mathbf{T}}_{j(1)}$. Here, $\overline{\mathbf{T}}_{j(1)}$ is diagonal for the spherical scatterer. Consequently, we have

$$\mathbf{b}_j = \overline{\mathbf{T}}_{j(1)} \cdot \left[\overline{\boldsymbol{\alpha}}_{js} \cdot \mathbf{a}_s + \sum_{\substack{i=1 \\ i \neq j}}^{N} \overline{\boldsymbol{\alpha}}_{ji} \cdot \mathbf{b}_i \right], \quad j = 1, \cdots, N. \tag{3}$$

Essentially, we match the boundary condition at the surface of the j-th scatterer instead at the center of the scatterer. This explains why this formulation avoids the singularity problem.

Equation (3) could be rewritten as

$$\mathbf{b}_j - \overline{\mathbf{T}}_{j(1)} \cdot \sum_{\substack{i=1 \\ i \neq j}}^{N} \overline{\boldsymbol{\alpha}}_{ji} \cdot \mathbf{b}_i = \overline{\mathbf{T}}_{j(1)} \cdot \overline{\boldsymbol{\alpha}}_{js} \cdot \mathbf{a}_s \tag{4}$$

or

$$\mathbf{B} - \overline{\mathbf{T}} \cdot \overline{\mathbf{A}} \cdot \mathbf{B} = \overline{\mathbf{T}} \cdot \mathbf{S}, \tag{5}$$

where $\overline{\mathbf{T}}$ and $\overline{\mathbf{A}}$ are block matrices, and $\mathbf{B}$ and $\mathbf{S}$ are block vectors whose block elements are given by

$$[\overline{\mathbf{T}}]_{ij} = \delta_{ij} \overline{\mathbf{T}}_{j(1)}, \tag{6a}$$

$$[\overline{\mathbf{A}}]_{ij} = \begin{cases} \overline{\boldsymbol{\alpha}}_{ij}, & \text{if } j \neq i \\ 0, & \text{otherwise}, \end{cases} \tag{6b}$$

$$[\mathbf{B}]_j = \mathbf{b}_j, \tag{6c}$$

$$[\mathbf{S}]_j = \overline{\boldsymbol{\alpha}}_{js} \cdot \mathbf{a}_s. \tag{6d}$$

Equation (5) can be solved with iterative methods like the bi-conjugate gradient (BiCG) method. In such a method, the major computational cost would be in the matrix-vector multiplication $\overline{\mathbf{A}} \cdot \mathbf{B}$. For a dense matrix, the cost of such a matrix-vector multiplication requires $O(N^2 M^2)$ operations, where M is the dimension of the $\overline{\boldsymbol{\alpha}}_{ij}$ matrices.

When the scattering centers are placed on a uniform grid, then $\overline{\boldsymbol{\alpha}}_{ij} = \overline{\boldsymbol{\alpha}}(\mathbf{r}'_i - \mathbf{r}'_j)$. The translation matrix is only a function of $\mathbf{r}'_i - \mathbf{r}'_j$. When the formulation is implemented, the summation in Equation (4) is actually replaced with a three dimensional summation. In such a case, $\overline{\mathbf{A}}$ can be expressed as a block-Toeplitz matrix. By grouping the elements of same harmonics into one block, the block-Toeplitz matrix is converted to a Toeplitz-block matrix (i.e. each block is Toeplitz). Then the fast Fourier transform (FFT) method can be used to expedite the matrix-vector multiplication $\overline{\mathbf{A}} \cdot \mathbf{B}$ with operation count of $O(NM \log N)$.

If the spheres are small compared to λ_0, it possesses only electric dipole moments which correspond to the first three harmonics in $\overline{\mathbf{T}}_{j(1)}$. Therefore, $M = 3$ and furthermore there are only 6 independent elements in the 3 by 3 matrix $\overline{\boldsymbol{\alpha}}_{ij}$ due to the rotational symmetry.

In order to perform the matrix-vector multiplication more efficiently, the Fourier transform of $\overline{\mathbf{A}}$, $\tilde{\overline{\mathbf{A}}}$ is calculated only once outside the iteration loop and stored. Note that $\overline{\mathbf{A}}$ has been extended to a circulant matrix in the x-, y- and z-directions and zeros have to be padded to the original vector to prevent aliasing. Hence, whenever a matrix-vector multiplication is required in each iteration, three forward 3D-FFT corresponding to three harmonics are first performed, then they are multiplied by $\tilde{\overline{\mathbf{A}}}$ in the frequency domain and finally three inverse 3D-FFT are carried out. Then the product can be obtained by discarding those entries with zero-padding in the first place.

The memory requirement of the method is still $O(N)$ since each block matrix in $\overline{\mathbf{A}}$ can be represented by one of its rows or columns.

3. Results and Conclusions

A good agreement is observed both in Figure 1 for a dielectric layered sphere and in Figure 2 for a dielectric cube [9]. It converges in 53 iterations for the case in Figure 1 and takes about $1\frac{1}{2}$ hours CPU time on Sparc 10 workstation working in double precision.

Shown in Figure 3 are the number of iterations vs. the number of unknowns for lossless and lossy objects. As we have observed in 2D cases [14], the number of iterations increases with the size of the object and in the lossy medium, less number of iterations is required to converge than in the lossless medium. This shows that in the lossy medium, the complex permittivity shifts the otherwise small eigenvalues in the lossless medium away from the origin. Physically, the resonant frequencies of the lossy dielectric body are complex, while in practice, the operating frequency is always real, which precludes the eigenvalues from being too close to zero.

The number of iterations is approximately proportional to N for lossless objects and seemingly to $N^{0.75}$ for lossy ones when N is large. Without preconditioners, the eigenvalue distribution seems dispersive without confinement as N grows and the erratic convergence of BiCG algorithm worsens the already poor condition number. In order for BiCG-FFT or its like to be more favorable, a suitable preconditioner is needed.

Finally, we demonstrate that when the object is gridded finer, the T-matrix formulation is still stable. The first example is a homogeneous dielectric sphere with $\epsilon_r = 4.0$ and the radius $= 10^{-5}\lambda_0$. The simulation results show that the number of iterations remains as 6 for the cases of $8 \times 8 \times 8$, $16 \times 16 \times 16$ and $32 \times 32 \times 32$ grids. Figure 4 shows one of the results and it agrees very well with the exact solution. We have also run a second example (not shown here) which is a homogeneous dielectric cube with $\epsilon_r = 9.0$ and the side length $=0.34\lambda_0$. Similar to the first example, the number of iterations is 16 for all the three different grids as mentioned above.

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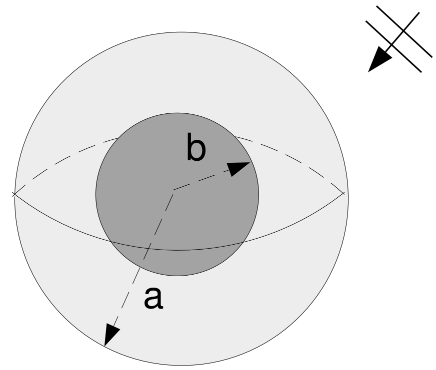


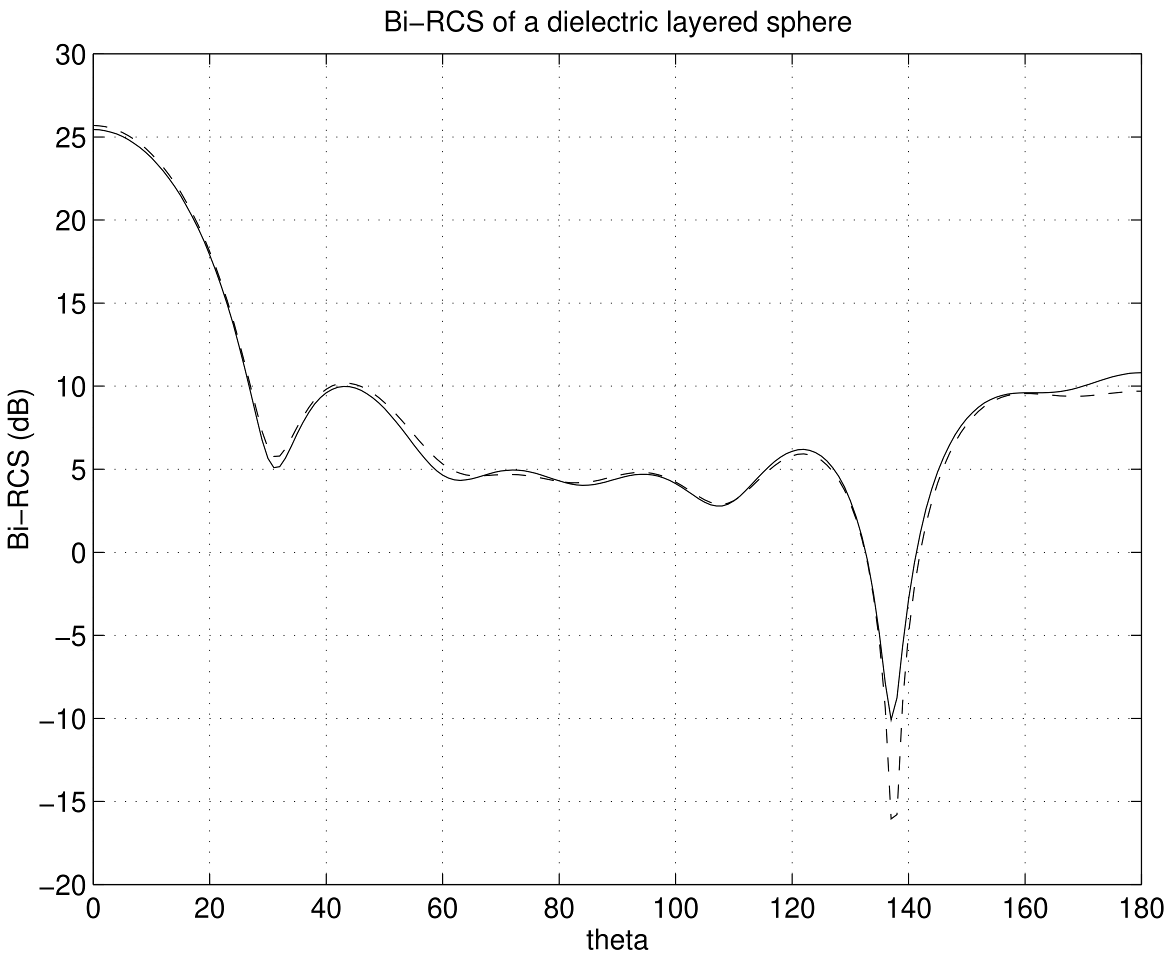
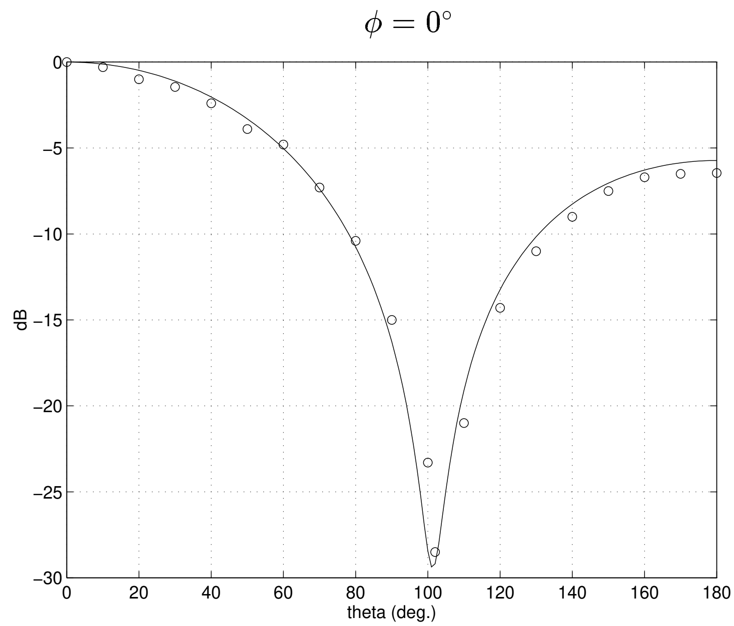
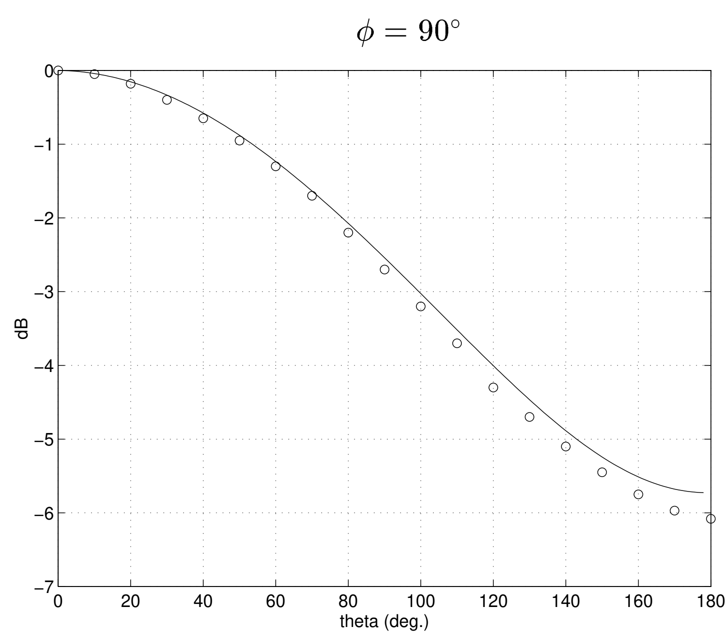


Figure 1. The Bi-RCS of a spherically layered scatterer. The solid line is from the Mie series solution; the dash line is the numerical solution. Here, $b = 0.5\lambda_0, \epsilon_{r1} = 1.2, a = 1.0\lambda_0$ and $\epsilon_{r2} = 2.4$. A $30 \times 30 \times 30$ grid is used.



(a) The far field $\|\mathbf{E}_\theta\|$ as a function of θ



(b) The far field $\|\mathbf{E}_\phi\|$ as a function of θ

Figure 2. The far fields as a function of θ computed for a lossless dielectric cube with $\epsilon_r = 9$ and $k_0 a = 0.628319$. The solid lines represent the results by the BiCG-FFT T-matrix method and the symbols $\circ$ represent the results by Zwamborn and van den Berg. A $7 \times 7 \times 7$ grid is used.

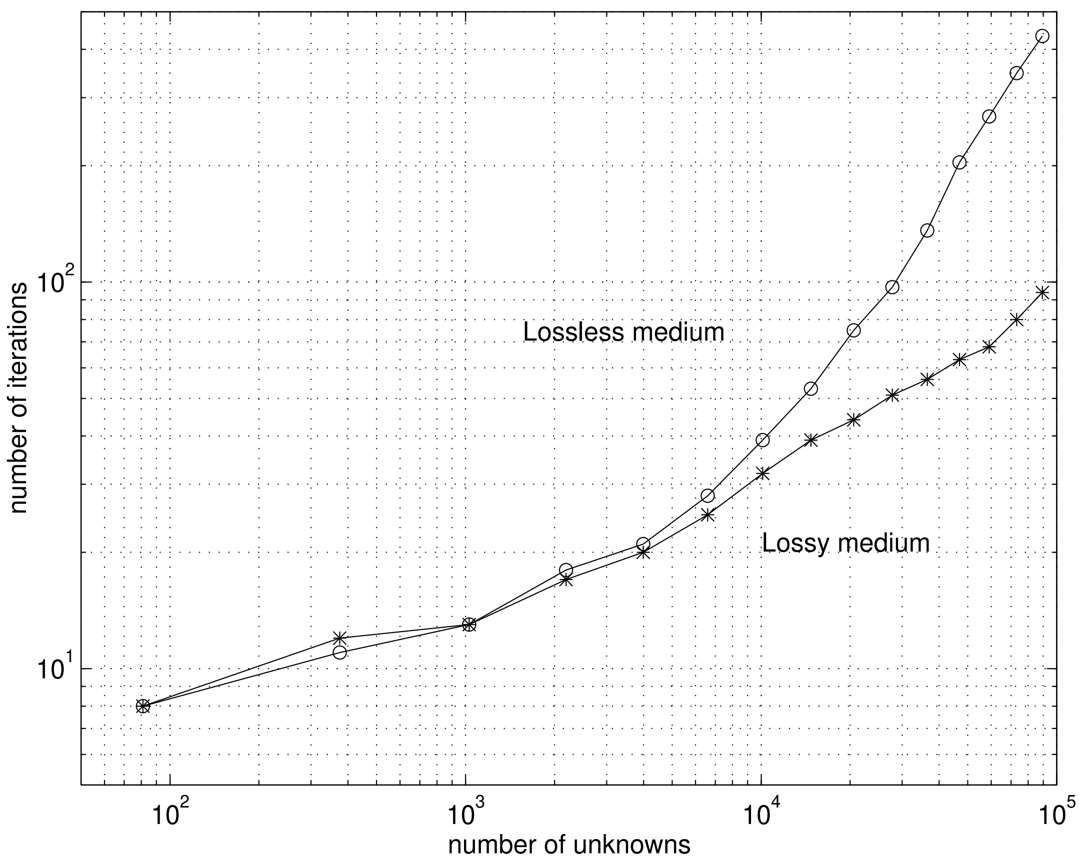
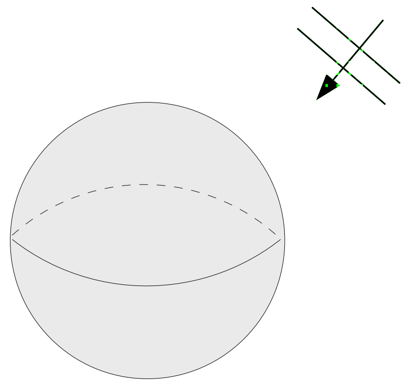


Figure 3. The number of iterations vs. number of unknowns for lossless cubes of $\epsilon_r = 9.0$ and for lossy cubes of $\epsilon_r = 9.0 + i3.0$.



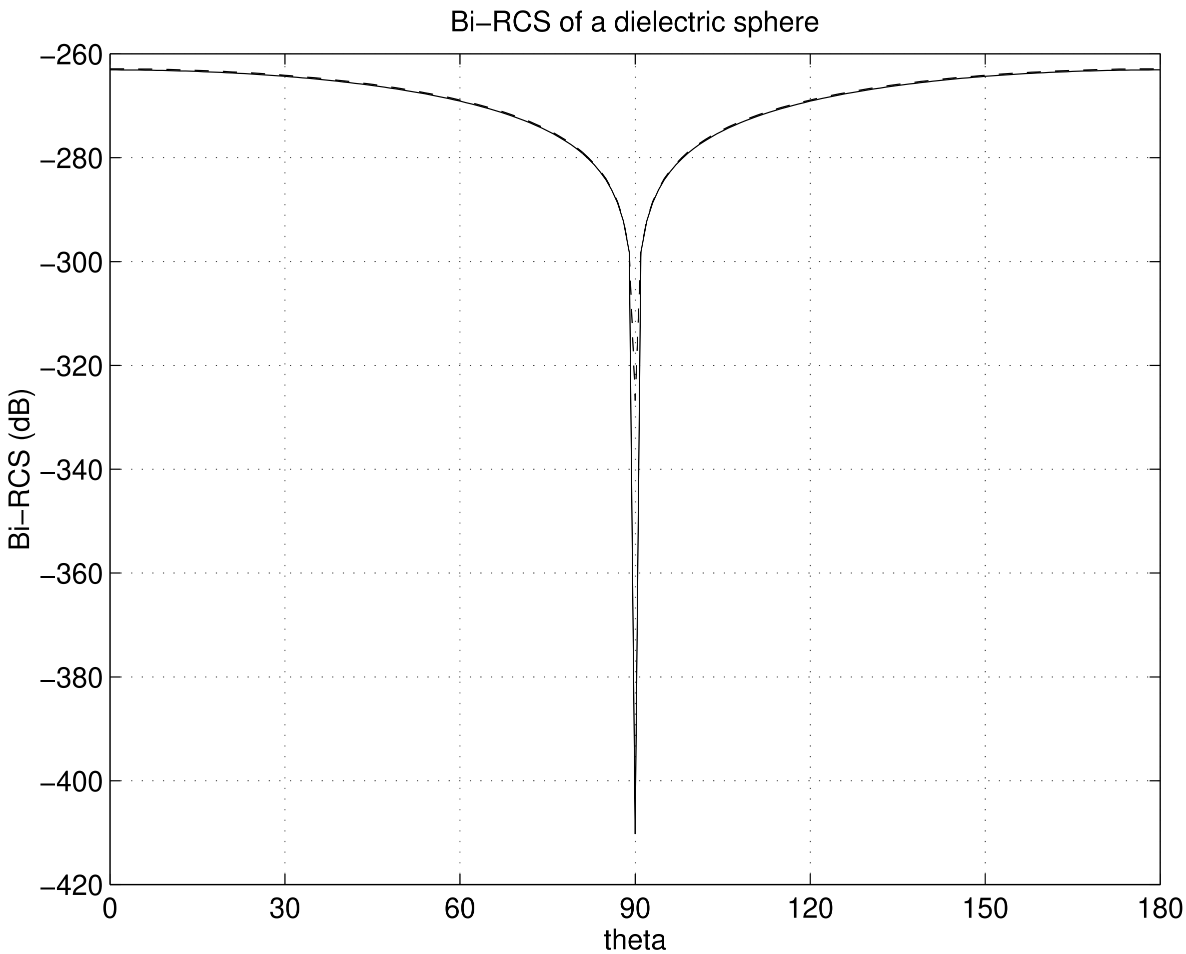


Figure 4. The Bi-RCS of a dielectric sphere. The solid line is from the Mie series solution; the dash line is the numerical solution. Here, the radius = $10^{-5}\lambda_0$ and $\epsilon_r = 4.0$. A $16 \times 16 \times 16$ gird is used.