Reduction of iterations for the linear equation solutions in DDA

- application for the orientation averaging of irregularly shaped particles -

Yasuhiko Okada,[1] Tadashi Mukai,[1] Ingrid Mann,[1]
Sano Itaru,[2] and Sonoyo Mukai[2]

[1] *Graduate School of Science, Kobe University*
1-1 Rokkodai, Nada Kobe 657-8501 Japan
[2] *Faculty of Science and Technology, Kinki University,*
3-4-1 Kowakae, Higashi-Osaka, 577-8502, Japan
tel: +81 (78) 803-6566, fax: +81 (78) 803-6483, e-mail: yasokada@gmail.com

Abstract

We introduce the method to shorten the number of iterations required in the linear equation solutions of DDA. In the linear equation solution in DDA, the solution is iteratively solved. We give the initial guess, which is close to the actual solution infered from parameters close to the selected one. We apply the method for the orientation averaging of scattering properties of non-symmetric particles. The method reduces the number of iterations into less than 10% for non-symmetric particles with moderate shape variations against the direction of incident light when the interval of the grid angles is set as 5 degree. On the other hand, non-symmetric particles with high shape variations against the direction of incident lights shows iteration ratio of less than 25%.

1 Introduction

Discrete Dipole Approximation (DDA) is a powerful tool to treat light scattering problems of irregularly shaped particles [1]. In the DDA calculations, the shape is described with a number of dipoles, then the multiple interactions of the incident light between the dipoles are solved. Compared with other methods, DDA has the advantage in treating shape with dipoles making the calculation possible for irregularly shaped particles without any symmetry. On the other hand, the disadvantage of DDA is that the linear equations are required to be solved for every variations in the parameter of the particle (e.g. size, shape, refractive index, etc.) and for the direction of incident lights.

In order to apply the calculation of DDA into the remote sensing, such as retrieval of atmospheric aerosol properties, cometary dust, and dust on the surface of Asteroids, reduction of the DDA calculations for parameter variations of the particles are indispensable. In this study, we apply the method to reduce the iterations in the DDA calculation for the variations in the particle orientation.

2 Reduction of the iterations

In the DDA calculation, the polarizability of all the dipoles are solved based on the iterative method (e.g. Conjugate Gradient Method) [1]. In the iterative method, the initial value of the dipole polarizability (hereafter as initial guess) is set arbitrarily (e.g. CMPLX(0.0, 0.0)) since the solution of the linear equations (i.e. dipole polarizability) is not known at the beginning of the iteration.

Muinonen and Zubko (2006) proposed the method to give the initial guess by extrapolating from the results of similar size or of similar refractive index to the selected parameter of the particle. This is because, small variations in the size or in the refractive index are considered to have only small influence in the polarizability of dipoles. Then the calculated initial guess is close to the solution of the selected parameter resulting in the reduction of iterations. In their study, extrapolation are used to calculate the initial guess of the polarizability for size variations or for variations in refractive indices.

In this study, we apply the same method for the orientation averaging of scattering properties. For the orientation variations, the interpolation of the initial guess is always possible by using values in both sides of the selected orientation. Since the interpolation is considered more accurate than extrapolation, the proposed method has more advantage in the proximity of the initial guess to the solution. We use spline interpolation [3] to calculate the initial guess of the selected orientation from the results of orientations close to the selected one.

We define the orientations, with which the interpolation is conducted, as “grid angles”. Before the calculation with the proposed method, the dipole polarizabilities for grid angles are calculated with the DDA method and are stored into the files. Then, the calculation with the proposed method is performed after interpolating initial guess from the stored polarizabilities of grid angles close to the selected orientation.

We define “iteration ratio” as the ratio between the number of iterations in proposed method and those in original calculation to investigate the efficiency of the method applied for orientation variation. We use public domain DDA code “DDSCAT6.1” developed by Dr. Draine and his colleague [1].

3 Efficiencies and Accuracies

As non-symmetric particles, we use “Gaussian Sphere (hereafter as GSP)” and “Overlapping mixture of multiple tetrahedra (hereafter as OMMT)” as shown in Fig.1. The former is produced to have moderate surface roughness with the selected parameters of Gaussian Sphere while the latter shape has high surface roughness causing high orientation dependence of the shape against the direction of incident light. The GSP described originally with a number of triangular facets [4] are converted into the shape described with dipoles following Muinonen et al. (in Press) [5]. OMMT is created by using the tetrahedra composed of dipoles, which is produced with “calltarget” program in DDSCAT6.1 [1], then, by sequentially adding randomly rotated tetrahedra into the particle.

In the DDSCAT6.1, the angle of the particles against the direction of incident light is configured with *beta*, *theta* and *phi* [1]. In this study, we arbitrarily set theta=20.0 and phi=15.0, then rotate the particles in the direction of beta from 0 to 360 degree.

In this study, we set grid angles as 5 degree. Therefore the precalculation of dipoles for 73 grid angles are required. After calculating for 73 grid angles, we performed the calculation with the proposed method with interpolation. The interpolation for orientations is conducted by using 8 grid angles close to the selected angle. The “8” is arbitrarily chosen in this study. We investigate for the particle size parameter for the equivolume sphere as 7.0. The refractive index is selected as m=1.60 + 0.01i.

Fig.2 shows the iteration ratio for GSP and for OMMT. The iteration ratios are less than 10% for GSP and less than 25% for OMMT. This iteration ratio depends on the interval of grid angles, which is set as 5 degree in this study. We also investigate the iteration ratio for GSP and OMMT with the grid angle interval of 10 degree. The result (not shown here) is that the iteration ratio is increased for the central angle between grid angles, while for the orientations close to the grid angles, the iteration ratio become small similar to those shown in Fig. 2.

In order to investigate the accuracies of calculated scattering properties, we have compared scattering properties calculated 1) with original DDASCAT and 2) those with the proposed method for the angles *beta* from 0 to 360 degree with the step of 0.5 degree. Fig.3 shows the example of the comparison of absorption (*Qabs*) and scattering properties (*Qsca*) of the OMMT for the variation of the *beta* angles. Fig.4 shows the comparison for the scattering function S11 and polarization -S12 / S11 where *beta*=113.5 for OMMT. The errors (i.e. *| Qoriginal- Qproposed | / Qoriginal*100* [%]) caused by the proposed method are less than 0.013%, 0.08%, 0.09%, 5.58% for Qabs, Qsca, S11, -S12 / S11, respectively. The errors of S11 and -S12 / S11 for different *beta* angles are also in the same order.

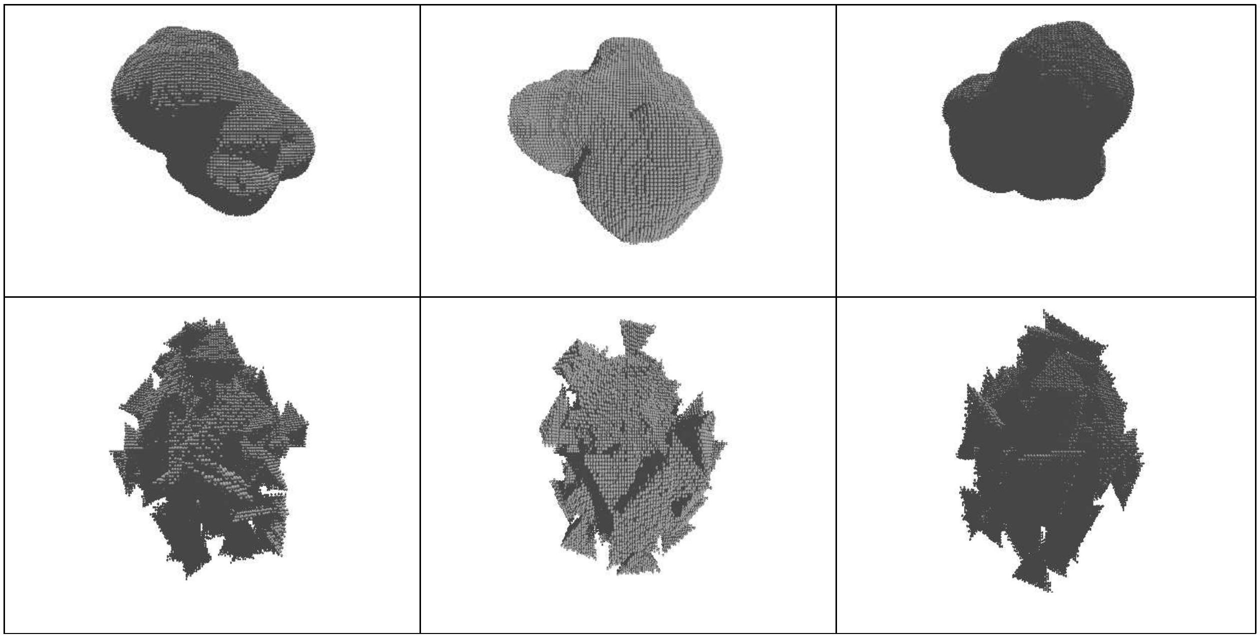

Figure 1: Shapes of the particles composed of a number of dipoles shown in XY (left), YZ (middle), and XZ plane (right). Gaussian sphere (upper panel) and overlapping mixture of multiple tetrahedra (lower panel) are considered.

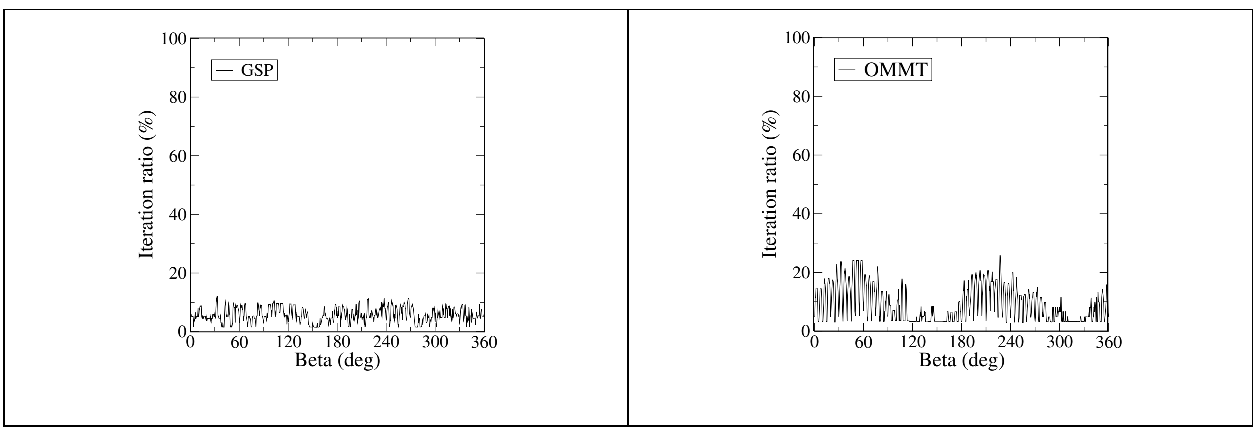

Figure 2: The iteration ratio for GSP and OMMT where the interval of grid angles is 5 degree.

4 Summary

The reduction method of the iterations in the linear equations are applied for the orientation variations of irregularly shaped particles. Non-symmetric particles with moderate orientation dependence of the shape (i.e. Gaussian Sphere) have gained large advantage with the iteration ratio of less than 10%. While, non-symmetric particles with large orientation dependence of the shape (i.e. OMMT) has also gained advantage with iteration ratio of less than 25%. We have known that the iteration ratio becomes larger for larger intervals of grid angles at central angles between grid angles. We are now trying to devise efficient division of orientation angles to reduce total number of iterations in DDA calculations in order to conduct DDA calculation efficiently for the 3D orientation averaging.

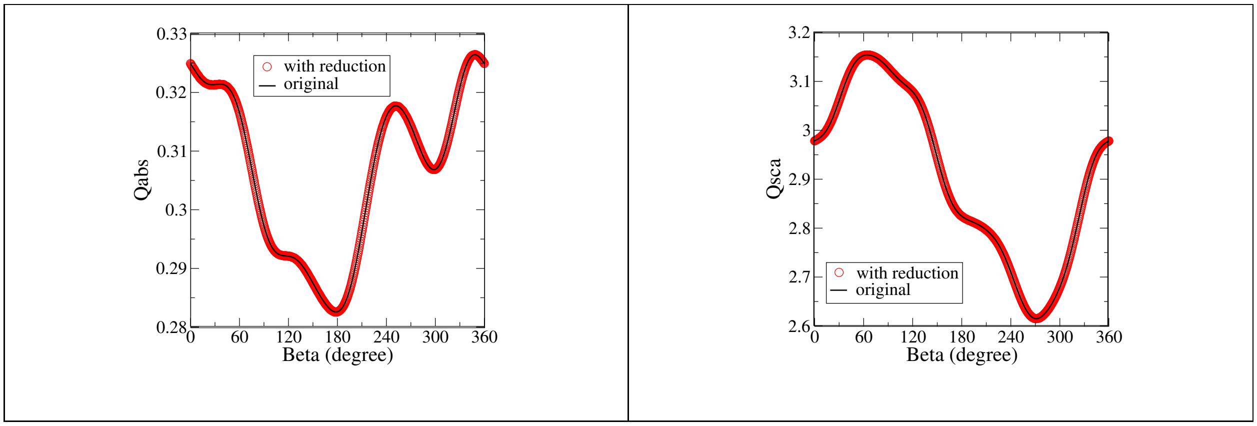

Figure 3: The comparison of Qabs and Qsca of OMMT for the original and the proposed method

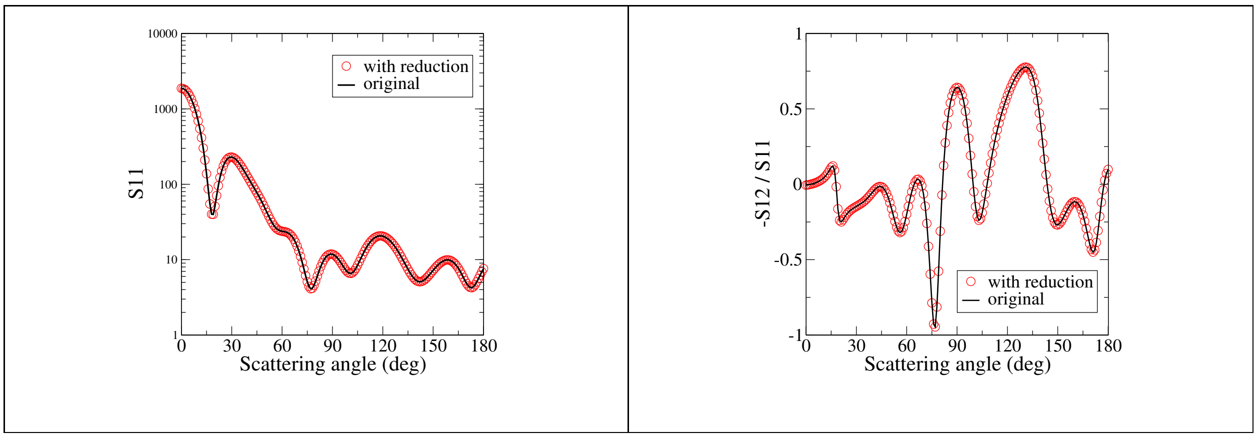

Figure 4: The comparison of S11, and -S12 / S11 of OMMT where *beta*=113.5.

Acknowledgments

Some of the data analysis were performed on the general common use computer system at the Astronomical Data Analysis Center (ADAC) of the National Astronomical Observatory of Japan. DDSCAT6.1 is provided from http://www.astro.princeton.edu/~draine/. This research is supported by “The 21st Century COE Program of Origin and Evolution of Planetary Systems” of the Ministry of Education, Culture, Sports and Technology (MEXT).

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