Cubature orientation-averaging scheme

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We propose the so-called cubature-on-the-sphere orientation-averaging scheme to be used in scattering computations. The cubature points are optimally arranged on the sphere to produce non-biased and fast convergence in scattering problems requiring numerical orientation averaging. Cubature clearly outperforms the conventional regular grid of sample points on the sphere.

INTRODUCTION

A common setup in scattering problems is to compute the orientation-averaged properties of the target. In many cases, we are interested to interpret and compare the scattering simulation results against observational data from a large ensemble of particles in random orientation. Therefore, we need to simulate particles with with different sizes and in different orientations. Usually, the orientation distribution can be considered to be evenly distributed over all Euler angles $(\alpha, \beta,$ and $\gamma)$.

There are computational methods that can perform the orientation averaging analytically, such as the T-matrix method for individual particles [1] or for cluster of spheres [2]. However, even with the T-matrix method the fixed orientation version of the code has some benefits, as Okada [3] has pointed out. The fixed-orientation superposition T-matrix code (F-ST) consumes less memory and can therefore be used for larger size parameters. Also, if accurate results can be achieved with a modest number or orientation angles, the F-ST can be even faster than the analytical orientation-averaging version (A-ST) for large problems. Another set of codes, where combining the fixed-orientation computations into averaged results is a must, are the volume-integral codes, e.g., the popular discrete-dipole approximation codes (DDA; e.g., [4, 5]).

The task in numerical orientation averaging is, in short, to compute the Mueller scattering matrix for a given set of Euler angles $(\alpha_i, \beta_i, \gamma_i)$ and then average the result over i. In many methods (e.g., in T matrix and DDA), the third angle γ can be sampled efficiently for given (α_i, β_i) by computing the result in several scattering planes. Therefore, the choice of orientation-averaging points reduces to the problem of selecting the (α_i, β_i) points on the sphere.

CUBATURE ON THE SPHERE

Currently, the standard method for selecting the (α_i, β_i) points on the sphere is to produce a regular grid by evenly distributing $\cos\alpha$ in $[0, \pi]$ and β in $[0, 2\pi]$. While there is nothing particularly wrong with this method, it is not the most efficient one. Because the Mueller

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matrix computation for every (α_i, β_i) can be very resource consuming, it would be beneficial to optimize the averaging (i.e., integration) as well as possible.

This optimization has been studied by Xu and Khlebtsov [6] and by Okada [3]. Xu and Khlebtsov state that using either Simpson rule or Gaussian quadrature will improve the accuracy in numerical orientation averaging. Okada proposes the quasi-Monte-Carlo (QMC) method for the same purpose. Both of these will improve the results compared to the standard regular grid on the sphere, but they leave space for improvements. The Simpson rule or Gaussian quadrature are only one-dimensional schemes which must be separately applied for α and β and then combined to a grid $\{\alpha_i\} \times \{\beta_i\}$. This will introduce again certain regularity to the point pattern on the sphere. The QMC points will not have a regular pattern on the sphere, but there is no guarantee that this is the optimal solution. Generally, for two-dimensional problem the optimal solution is a two-dimensional quadrature.

The term *cubature* is used for quadrature integration schemes in more than one dimension. For integration over spherical coordinates we need a cubature on the sphere. Fortunately, there exists some nice results on this subject, e.g., from Womersley and Sloan [7, 8]. They derive different sets of cubature-on-the-sphere points for slightly different minimization criteria, but the main point is that all the sets are very close to optimal and that, in all the sets, the cubature points are very evenly distributed on the sphere but without regular structure. In Fig. 1, we show the points in the regular grid and in the minimum-norm cubature (MN) having the same size.

The spherical cubature points and weights cannot be analytically solved for an arbitrary number of points; instead, they need to be computed using numerical optimization. Therefore it is most convenient that Womersley has a library of cubature-on-the-sphere points with tabulated sets to be downloaded*.

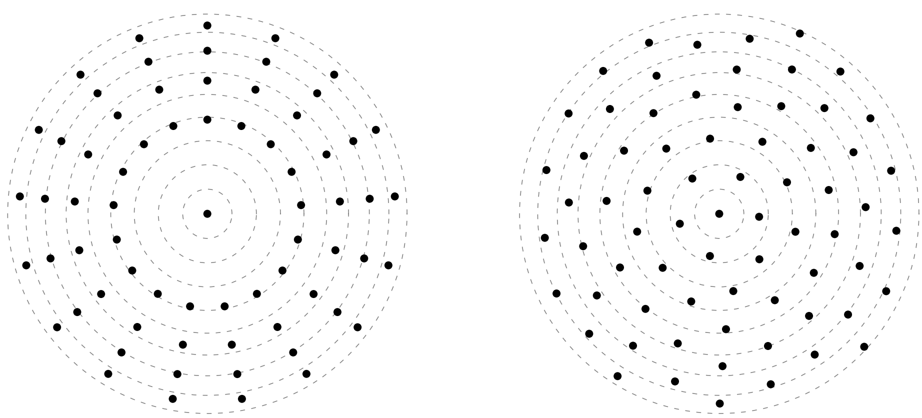

Figure 1. Upper hemispheres of regular grid points (in the left) and MN cubature points (in the right) in Lambertian projections. The regular grid has 69 points in the upper hemisphere and the MN cubature 70 points.

*Interpolation and Cubature on the Sphere in WWW at http://web.maths.unsw.edu.au/∼rsw/Sphere/

TEST WITH CUBATURE

We have been using cubature averaging with the F-ST code and with the DDA code ADDA already for various scattering computations and have been satisfied with its performance. In this section, we present a small example using both the regular grids and MN cubatures with various sizes. We use the same 4-sphere and 50-sphere aggregates that were used in a recent article about the accuracy and performance of different DDA codes [9]. For both geometries, we consider equal-volume-sphere size parameters of 3.80 and 5.11 and refractive indices of $1.5 + i0.001$. The geometries are shown in Fig. 2.

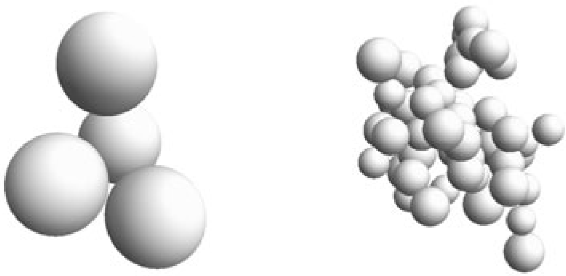

Figure 2. The two geometries used in testing the cubature. On the left, a 4-sphere cluster and, on the right, a 50-sphere cluster.

We run the computations using the F-ST code with regular grids having 23, 38, 80, 138, and 255 (α_i, β_i) points on the sphere (k points for α and $2(k-2)+1$ for β), and with the MN cubature having 25, 36, 81, 144, and 256 points. Both methods use 61 scattering planes (angle γ). The mean absolute relative error (MARE) for the intensity ($\Delta\theta = 1°$, θ is the scattering angle),

$$\mathrm{MARE}(I) = \frac{1}{181} \sum_{j=0}^{180} \frac{|I_A(j\Delta\theta) - I(j\Delta\theta)|}{I_A(j\Delta\theta)}, \tag{1}$$

and the mean absolute error (MAE) for the linear-polarization ratio,

$$\mathrm{MAE}(P) = \frac{1}{181} \sum_{j=0}^{180} |P_A(j\Delta\theta) - P(j\Delta\theta)|, \tag{2}$$

are calculated for all the cases. With I_A and P_A we denote the accurate values of intensity and linear polarization ratio (in percents) using the analytical averaging, and with I and P the corresponding values using numerical orientation averaging. The results are quite similar for both geometries and for both sizes, so we present the averaged behavior of MARE and MAE over all the cases in Fig. 3.

It is evident that the MN cubature outperforms the regular grid points when the size of the cubature exceeds 40–50 points. The improvement with the same number of orientation points is about 3.5-fold (error using grid divided by error using cubature) for intensity and about 4.5-fold for polarization ratio.

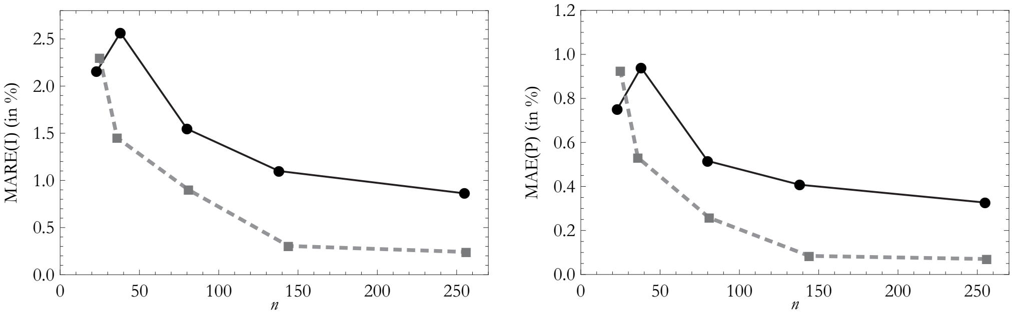

Figure 3. The average error for intensity and linear polarization ratio using regular grid and MN cubature points in orientation averaging. The number of (α_i, β_i) points is n, and the black solid line is for the regular grid and the grey dashed line for the cubature.

CONCLUSIONS

We conclude that the cubature orientation averaging scheme has better accuracy than the common method of regular grid. We recommend that the cubature points should be included as an option for orientation averaging for the popular DDA codes such as DDSCAT and ADDA.

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