# Efficient numerical orientation average for calculations of single-scattering properties of small atmospheric ice crystals

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## 1. INTRODUCTION

- Except for a few large crystals, most ice crystals do not have preferred orientations and the corresponding single-scattering properties typically calculated using averages over random orientations.
- Numerical methods, such as geometrical optics, *T*-matrix, discrete dipole approximation, and finite difference time domain, use averages over several orientations to calculate single-scattering properties.
- Past studies showed advanced orientation schemes (e.g., Quasi Monte Carlo) were more efficient than equal spaced orientation average schemes (i.e., Lattice grid division) for calculating single-scattering properties of spheres and sphere aggregates.
- Atmospheric ice crystals have non-spherical shapes and the single-scattering properties depend heavily on orientation.
- The optimal orientation averaging scheme and minimum number of orientations required to calculate the average single-scattering properties of realistically shaped atmospheric ice crystals within predefined accuracy level (i.e., 1.0%) are determined in this study.

## 2. METHODOLOGY

- Amsterdam discrete dipole approximation 1.0 (Yurkin and Hoekstra 2011) used to calculate the scattering phase matrix $P_{11}$, asymmetry parameter $g$, single-scattering albedo $\omega_o$, extinction efficiency $Q_{ext}$, scattering efficiency $Q_{sca}$, and absorption efficiency $Q_{abs}$.
- Single-scattering properties of 4 different idealized models with $D$=10 μm (Fig. 1) are calculated at 3 wavelengths ($\lambda$=0.55, 3.78, and 11.0 μm).
- 2 orientation average schemes used:
  - Lattice grid (equal spaced) and Quasi Monte Carlo (QMC)
  - Maximum of 135,168 orientation averages are made for each crystal habit
- Since there is no exact solution for calculations of single-scattering properties of nonspherical particles, single-scattering properties averaged over 135,168 orientations using QMC are assumed as reference values in this study.

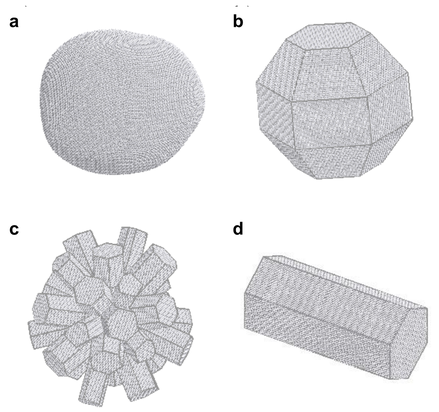


Fig.1. Idealized shapes of ice crystals used in this study: (a) Gaussian random sphere (GS, Nousiainen and McFarquhar 2004), (b) droxtal (DX, Yang et al. 2003), (c) Budding Bucky Ball (3B, Um and McFarquhar 2011), and (d) column (COL). GS, DX, and 3B have an area ratio of 0.85. COL has an aspect ratio ($D/L$) of 0.5.

## 3. RESULTS

- Figures 2 - 5 show convergence of single-scattering properties ($g$, $\omega_o$, $Q_{ext}$, $Q_{sca}$, $Q_{abs}$, $P_{11}(90°)$, and $P_{11}(180°)$) of ice crystals as a function of number of orientations using two different orientation average schemes (QMC vs. Lattice grid).
- The minimum number of orientations to achieve 1.0% accuracy using QMC and Lattice grid are indicated with different colors. A ratio (black) between the minimum number of orientation using QMC and that using Lattice grid is also embedded.

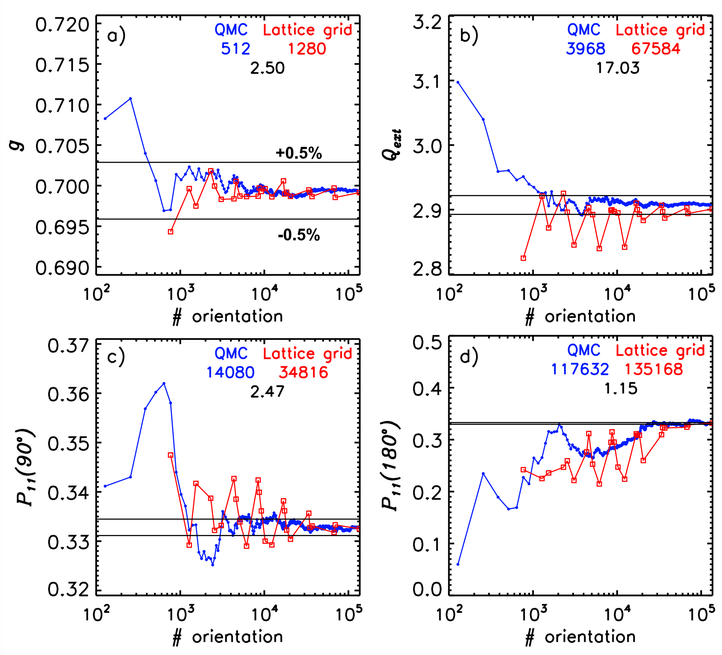


Fig.2. Calculated (a) $g$, (b) $Q_{ext}$, (c) $P_{11}(90°)$, and (d) $P_{11}(180°)$ of 3B as function of number of orientations at $\lambda$=0.55 μm. If a single-scattering property lies between ±0.5% lines and further orientation averages still fall between the lines, then it is assumed to have converged. In Fig.2a, for example, the required number of orientations for calculating $g$ within 1.0% accuracy using QMC and Lattice grid is 512 and 1280, respectively. The lattice grid requires 2.5 times more orientations, and hence 2.5 times more computing time.

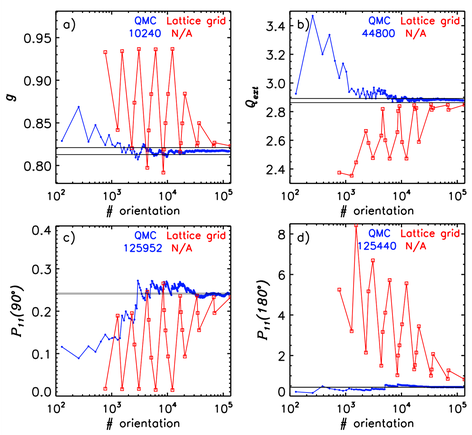


Fig.3. Same as Fig. 2, but for COL. The N/A indicates that single-scattering property does not converge within 1.0% accuracy.

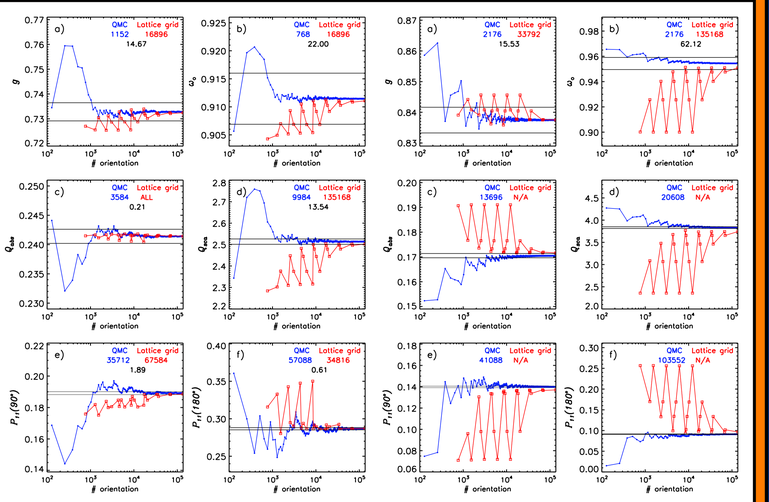


Fig.4. Calculated (a) $g$, (b) $\omega_o$, (c) $Q_{abs}$, (d) $Q_{sca}$, (e) $P_{11}(90°)$, and (f) $P_{11}(180°)$ of GS as function of number of orientations at $\lambda$=3.78 μm




Fig.5. Same as Fig. 4, but for COL

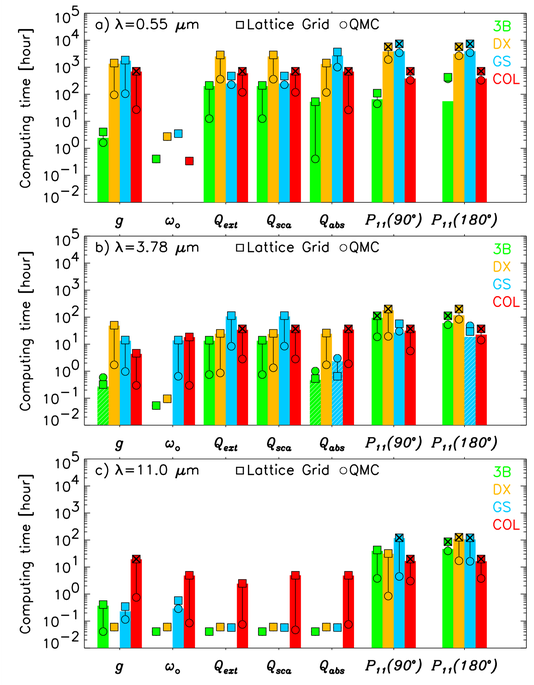


Fig.6. Computing time required to achieve 1.0% accuracy in single-scattering properties using the Lattice grid (square) and using the QMC (circle) as determined using 300 2.6 GHz CPUs. Differences in computing time (lattice - QMC) also shown with bar plots. Solid filled color bars indicate positive differences (computing time using lattice grid > QMC), whereas negative differences are shown as striped pattern color bars. Different ice crystal models indicated with different colors. When the single-scattering property using the lattice grid does not converge (i.e., N/A in Figs. 3 and 5), 2 times the maximum number of orientations (2X135,168) are assigned and indicated with an X inside the square.

- For all $\lambda$. the single-scattering properties of ice crystals calculated with QMC converge more efficiently than those calculated with the Lattice grid (Figs. 2 - 5) and hence less computing time (Fig.6) is required.
- Calculations of $P_{11}(90°)$ and $P_{11}(180°)$ require more orientations than calculations of other variables ($g$, $\omega_o$, $Q_{ext}$, $Q_{sca}$, $Q_{abs}$, ) (Figs. 2 - 5).
- The required number of orientations and required computing time decrease with an increase of $\lambda$.

## 4. CONCLUSIONS

- The QMC required fewer orientations than the Lattice grid for calculating the single-scattering properties of nonspherical atmospheric ice crystals within 1.0% accuracy.
- The QMC required less computing time than the Lattice grid and it saved 55.4 (60.1, 46.3), 3065 (117, 110), 3933 (65.8, 104), and 381 (22.8, 16.0) hours of computing time for calculating the single-scattering properties ($g$, $\omega_o$, $Q_{ext}$, $Q_{sca}$, $Q_{abs}$, $P_{11}(90°)$, and $P_{11}(180°)$) within 1.0% accuracy for Budding Bucky Ball, droxtal, Gaussian random sphere, and column, respectively, at $\lambda$=0.55 (3.78, 11.0) μm using 300 2.6 GHz CPUs.
- Calculations of scattering phase function (i.e., $P_{11}(90°)$, and $P_{11}(180°)$) required more orientations and computing time than other variables (i.e., $g$, $\omega_o$, $Q_{ext}$, $Q_{sca}$, $Q_{abs}$).
- For most ice crystals considered in this study, the minimum number of orientations and the corresponding computing time required to achieve 1.0% accuracy in the single-scattering calculations decreased with an increase of wavelength due to fewer interactions between light and ice crystals and an increase in absorption.

## REFERENCES & ACKNOWLEDGEMENTS

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This research was supported by DOE under grant number DE-FG02-09ER64770, DE-SC0001279, and DE-SC0008500. Data were obtained from the ARM program archive.