

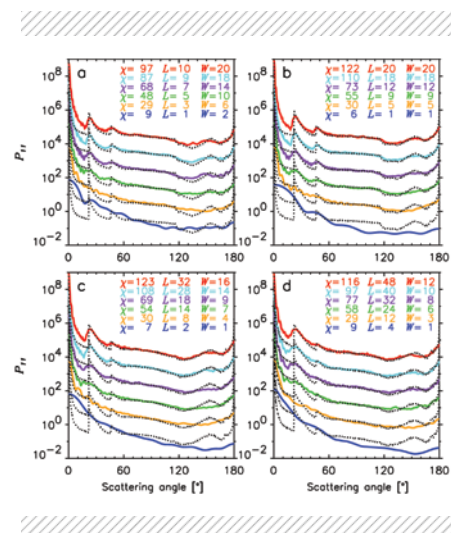
# APPLICABILITY OF GEOMETRIC OPTICS METHOD FOR CALCULATIONS OF SINGLE-SCATTERING PROPERTIES OF ATMOSPHERIC ICE CRYSTALS

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## EXECUTIVE SUMMARY:

Ice clouds exhibit a cooling impact on Earth's climate by reflecting solar radiation and a warming impact through absorption of infrared radiation and thermal emission towards Earth's surface. Ice clouds consist of non-spherical ice crystals with various shapes and sizes. To determine the influence of ice clouds on Earth's radiation budget and hence climate, knowledge of how they scatter and absorb radiation, henceforth called their single-scattering properties, is required. A geometric optics method (GOM), an asymptotic solution that is appropriate when a particle is much larger than the wavelength of incident light, has been widely used to calculate the single-scattering properties of ice crystals. However, the exact size range of applicability of GOM has not been well established and should be determined through comparison against numerically exact methods.



In this study, single-scattering properties of ice crystals were calculated using both GOM and a numerically exact method to determine the range of applicability of GOM.

## INTRODUCTION

Ice clouds exhibit a cooling impact on Earth's climate by reflecting incoming solar radiation and a warming impact through absorption of thermal emission from the Earth and lower atmosphere and emission of infrared radiation at colder temperatures. The relative importance of these two effects depends on the optical thickness of ice clouds and has large impacts on the terrestrial climate system and climate feedbacks. Despite the importance of ice clouds and their large spatial coverage and temporal frequency, their representation in numerical models and assumptions used in remote sensing retrieval algorithms have large uncertainties caused mainly by the non-spherical shape of ice crystals and their wide variety of shapes and sizes.

A geometric optics method (GOM) has been exclusively used to calculate the scattering properties of non-spherical ice crystals. However, a GOM is an asymptotic solution and its range of applicability has not been well established and should be determined through comparison against numerically exact (though computationally expensive) methods, such as the discrete dipole approximation (DDA). In this study, the range of applicability of GOM was determined, and the impacts of crystal size and shape on the applicability of GOM were also quantified. Since the required computing time and memory for numerically exact methods rapidly increase with particle size, knowledge of the range of applicability of a GOM method can save computing time.

## METHODS & RESULTS

In order to determine the applicability of GOM, the single-scattering properties of randomly oriented hexagonal ice crystals were calculated using the Amsterdam DDA (ADDA) [1] and conventional GOM [2] at a non-absorbing wavelength  $\lambda=0.55 \mu\text{m}$ . Observations of naturally occurring ice crystals were used to determine the range of morphological features of the crystals used in the calculations [3]. A width

(W) of up to  $20 \mu\text{m}$  and a length (L) of up to  $48 \mu\text{m}$  of hexagonal ice crystals with aspect ratios ( $\text{AR}=L/W$ ) of 0.5, 1.0, 2.0, and 4.0 were thus used in the simulations. These crystals correspond to a volume-equivalent-sphere size parameter ( $\chi$ ) of up to 123, where  $\chi$  is defined as the ratio of the perimeter of a sphere that has the same volume of a non-spherical particle to the wavelength of incident light. Since there is no size effect on the scattering calculations using GOM at  $\lambda=0.55 \mu\text{m}$ , only one simulation using the GOM was performed for each AR.

Fig. 1 shows that the calculated scattering phase functions (P11) of hexagonal crystals using ADDA approached those calculated using GOM more closely as the size of the crystal increases for all four ARs. Better agreement between the P11 calculated using ADDA and those using conventional GOM is also shown for large hexagonal crystals with compact shapes (e.g.,  $\text{AR}=1.0$ ) compared to those with oblate (e.g.,  $\text{AR}=0.5$ ) and prolate (e.g.,  $\text{AR}=4.0$ ) shapes. The most notable differences in P11 are in the forward scattering region with the differences caused by errors in Babinet's principle that was used in the GOM for calculation of diffraction.

Fig. 2 shows that the differences between ADDA and GOM simulations for parameters that describe the directional scattering of radiation (the asymmetry parameter g) and the extinction efficiency ( $Q_{\text{ext}}$ ) became smaller as the crystal size increased. The errors in the conventional GOM compared to ADDA were  $\sim 1.5\%$  ( $7.0\%$ ) for g ( $Q_{\text{ext}}$ ) of hexagonal crystals with  $\chi=90$  for all ARs, whereas they were  $\sim 1.2\%$  ( $3.3\%$ ) for hexagonal crystals with  $\chi=100$ . The GOM simulations (i.e. P11, g, and  $Q_{\text{ext}}$ ) for hexagonal crystals with compact shapes (i.e.  $\text{AR}=1.0$ ) were closer to the ADDA simulations for smaller sizes compared to the simulations for oblate and prolate hexagonal crystals. This indicates that the lower size limit of applicability of GOM depends on the crystal shape (i.e. habit) and on its morphological features (e.g., aspect ratio).

Since methods that directly solve Maxwell's equations (e.g., DDA) are computationally expensive for large particles, while GOM is a fast and flexible method to calculate scattering properties of non-spherical particles, inevitably GOM will continue to be used for scattering calculations. This work provides guidance on where errors in GOM are small enough that its

use is appropriate. The wide variety of shapes, sizes, and habits of ice crystals mean the development of more databases on scattering properties will continue to be needed.

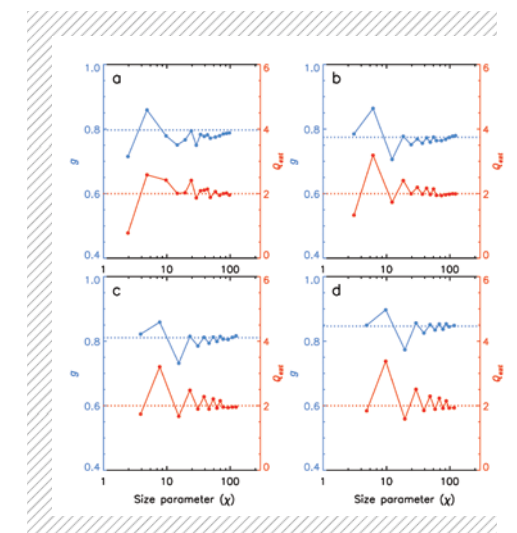
## WHY BLUE WATERS?

A conventional GOM is appropriate when a particle is much larger than the wavelength of incident light. Thus, numerically exact methods (e.g., DDA and T-matrix) are required for the calculations of scattering properties of particles with small size parameters, and errors of GOM in this region should be quantified through comparison with numerically exact methods. The required computing time and memory for numerically exact methods rapidly increase with particle size and large computing resources, like Blue Waters, were thus required to complete this study.

## PUBLICATIONS

Um, J., and G. M. McFarquhar, Formation of atmospheric halos and applicability of geometric optics for calculating single-scattering properties of hexagonal ice crystals: Impacts of aspect ratio and ice crystal size. *J. Quant. Spectrosc. Radiat. Transfer*, 165 (2015), pp. 134–152, doi:10.1016/j.jqsrt.2015.07.001.

Um, J., and G. M. McFarquhar, Formation of atmospheric halos by hexagonal ice crystals. 14th Conference on Atmospheric Radiation, Boston, Mass., July 7–11, 2014.



**FIGURE 2:** The asymmetry parameter (g, blue) and extinction efficiency ( $Q_{\text{ext}}$ , red) of hexagonal crystals with AR of (a) 0.5, (b) 1.0, (c) 2.0, and (d) 4.0 using ADDA (solid lines with circles) and GOM (dot lines).