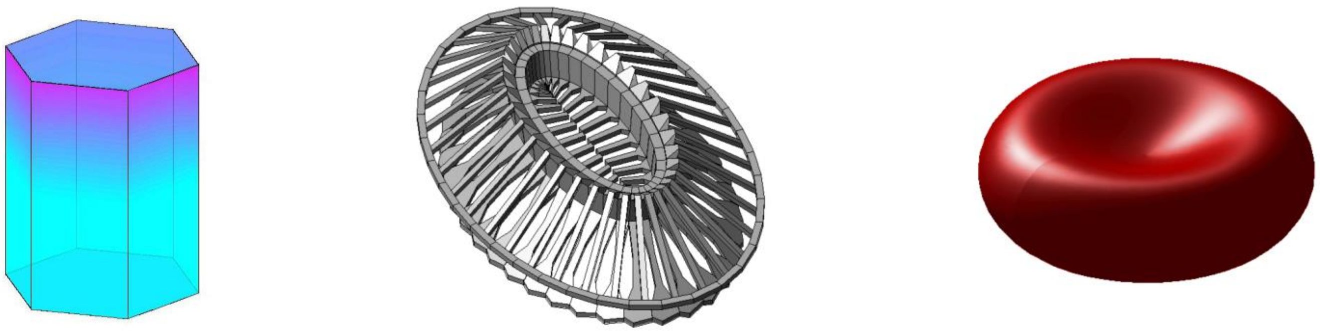
Simulation of Particle Optics: Applications in Geoscience and Biomedicine

Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta

Department of Atmospheric Sciences,
Texas A&M University



Simulation of Particle Optics: Applications in Geoscience and Biomedicine

Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

General Scattering Problems

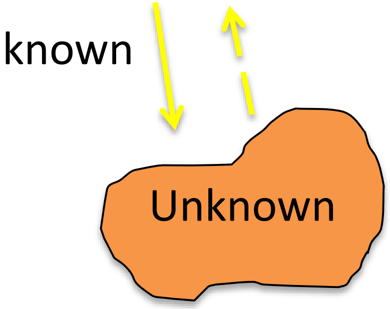
In “remote” or “non-invasive” sensing, a signal is sent at a target, The target scatters the signal, and the scattered signal is observed. The task is then to infer properties of the target from properties of the scattered signal. This is known as the inverse scattering problem.

Guidance in making the inference can be obtained by solving instances of the direct scattering problem: find the signal scattered by a target of known characteristics.

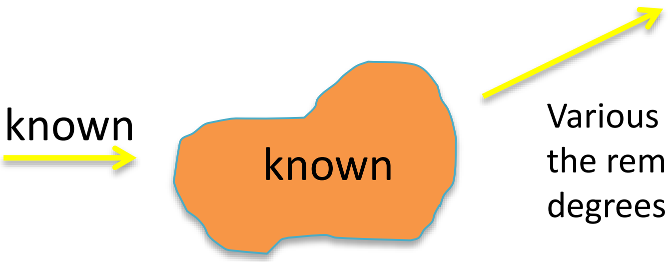
Our group uses a number of numerical methods to solve multiple instances of the direct optical scattering problem, and applies results to the inverse problem.

“Inverse” scattering problem

A source (here a satellite) sends down an optical signal of known wavelength(s) and observes back-scattering by atmospheric aerosols of unknown composition.



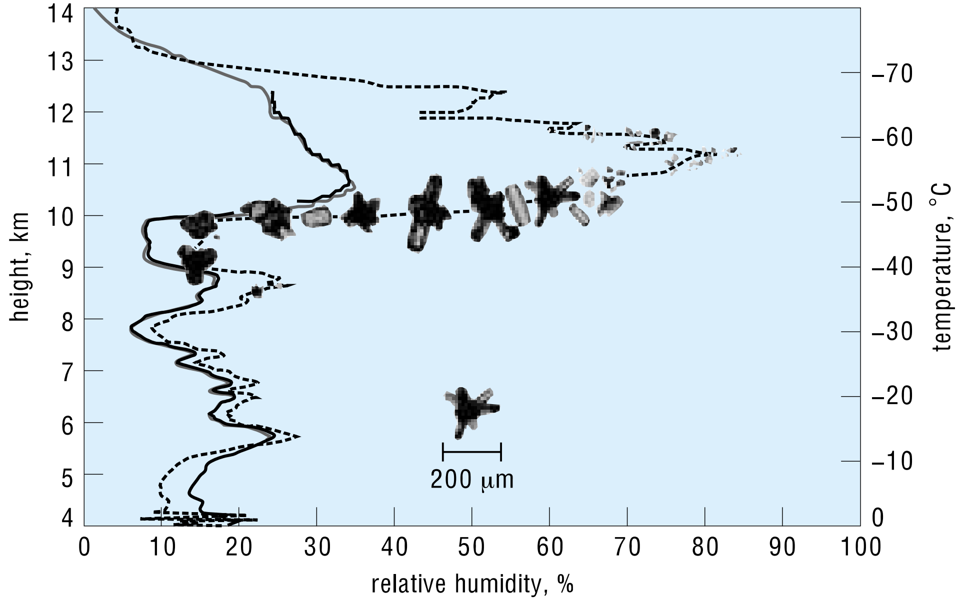
“Direct” scattering problem



Various methods are used to calculate the remote response, involving varying degrees of computational complexity

Effects of cirrus clouds

Cirrus clouds occur high in the atmosphere and consist of ice crystals rather than water droplets. Like water clouds, cirrus clouds have considerable effect on how the atmosphere responds to solar and infrared radiation.



Ice crystal size and shape as a function of height, temperature, and relative humidity captured by a replicator balloon sounding system in Marshall, Colorado, on November 10, 1994. The broken and solid lines denote the relative humidity measured by cryogenic hygrometers and Vaisala RS80 instruments, respectively. (*Graphic by Andrew Heymsfield, National Center for Atmospheric Research. data from K. N. Liou, An Introduction to Atmospheric Radiation, 2d ed., Academic Press, 2002*)

http://pilotportalusa.atspace.com

The range of crystal shapes is considerable, being determined by various combinations of temperature and water vapor concentrations. Simple shapes are platelets or hexagons, but many elaborations on basic shapes, and aggregates of basic shapes occur.

Further complexity is introduced by surface roughening or inclusion of impurities. Numerical simulations indicate that different crystals interact differently with solar and infrared radiation.

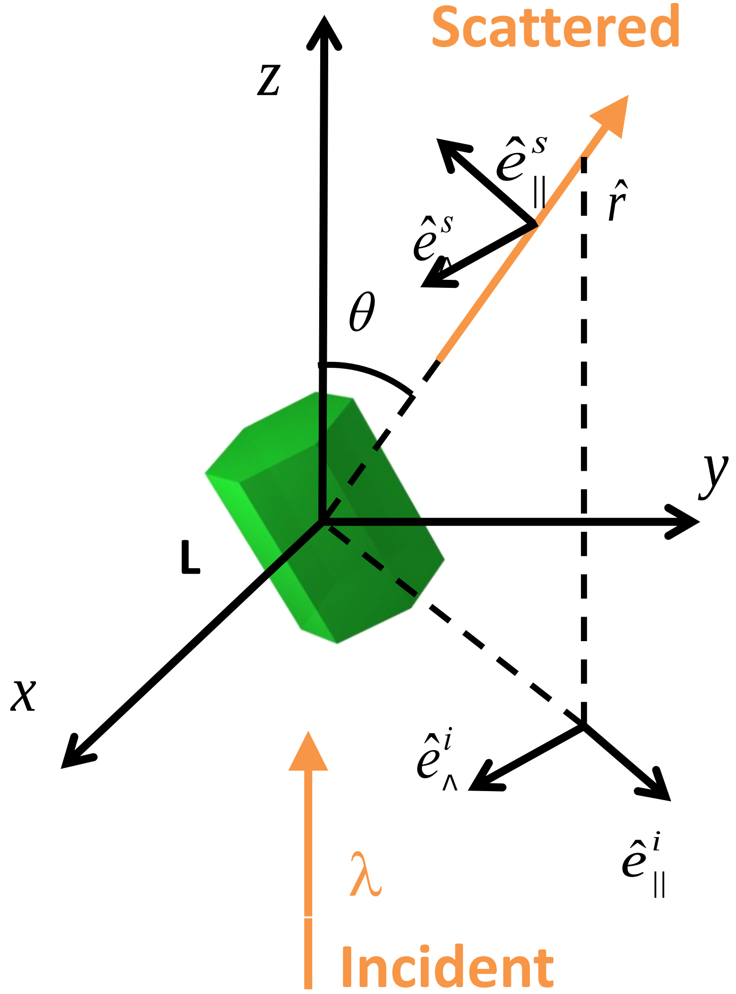
The optical direct scattering problem (single particle version)

When particles are small or large compared to the wavelength λ of incident light, approximate physical theories can be used to calculate the scattered response far from the target.

For particles with maximum linear dimension L, when (approximately)

$$1/3 < (L/\lambda) < 80,$$

the approximate theories break down. Maxwell's equations must be solved, numerically in most cases. A variety of methods exist: all become a computational challenge as soon as
L/ λ > 30: not only must the scattered signal be computed at all far-field angles q (see figure), but for all particle orientations in the case of non-spherical particles.



Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

Invariant Imbedding T-matrix Method

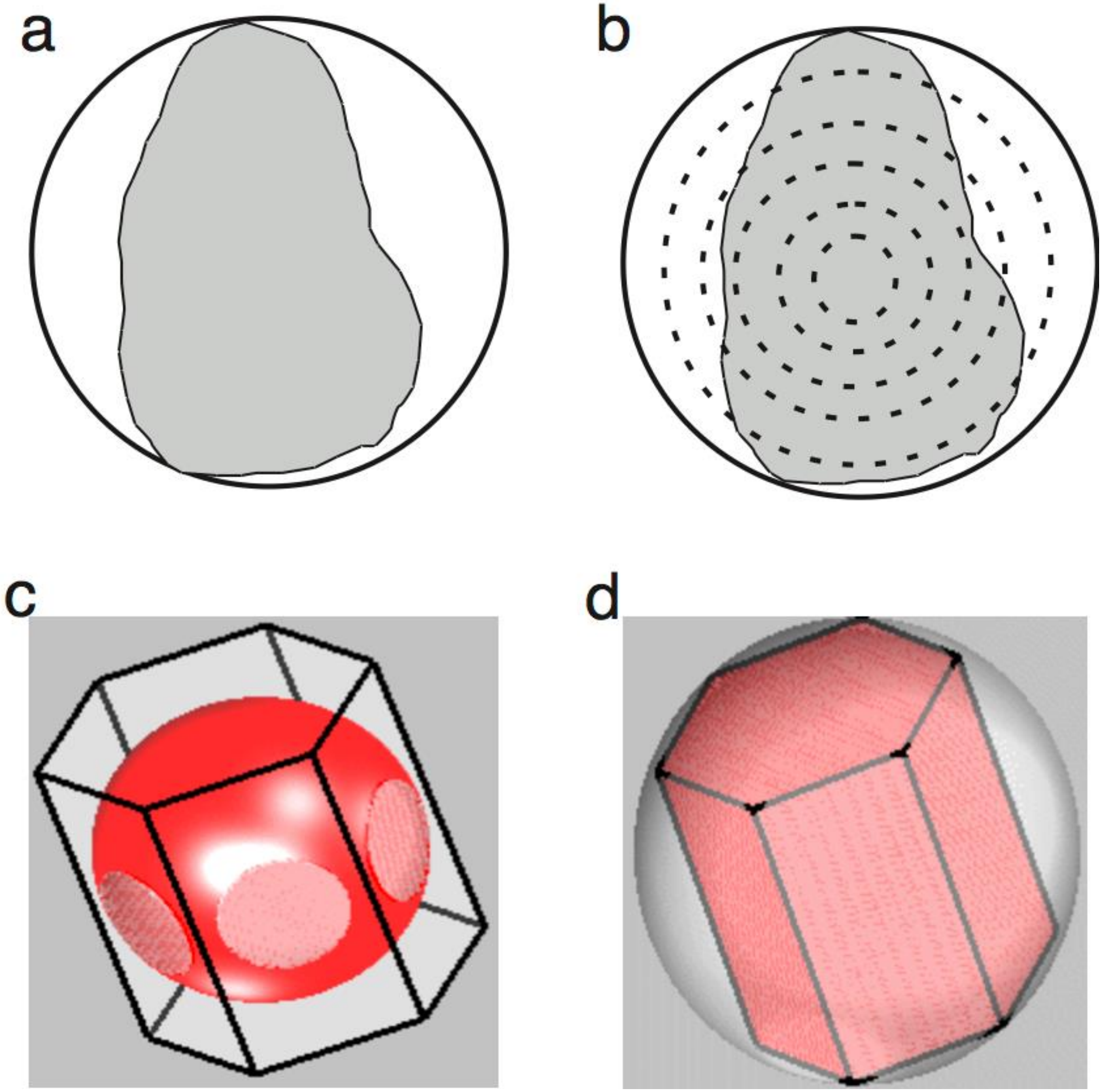
One of the methods for calculating the optical scattering properties of non-spherical particles we have developed is the “Invariant Imbedding T-matrix Method,” a method that considerably extends the range of computational feasibility of the standard T-matrix method. Steps in the method:

(a) a non-spherical particle is imbedded in a sphere. The portion of the sphere exterior to the non-spherical particle is vacuum (i.e. is given refractive index of 1).

(b) The calculation proceeds by iteratively considering successively larger concentric spheres. Homogeneous spheres can be treated with standard T-matrix.

(c) Internal spheres intersecting the surface of the embedded particle are treated using a field volume integral equation method.

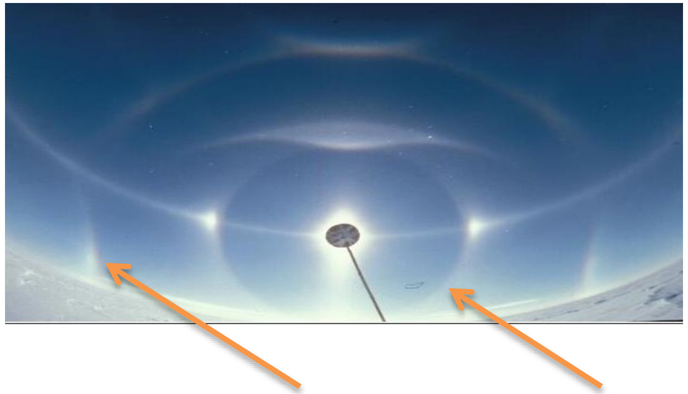
Fig (d): Hexagonal ice crystal example embedding, used in calculations reported below.



Simulation of Particle Optics: Applications in Geoscience and Biomedicine

Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

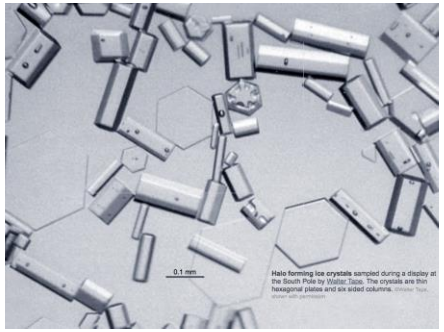
Sun halos seen in the atmosphere



46°

22°

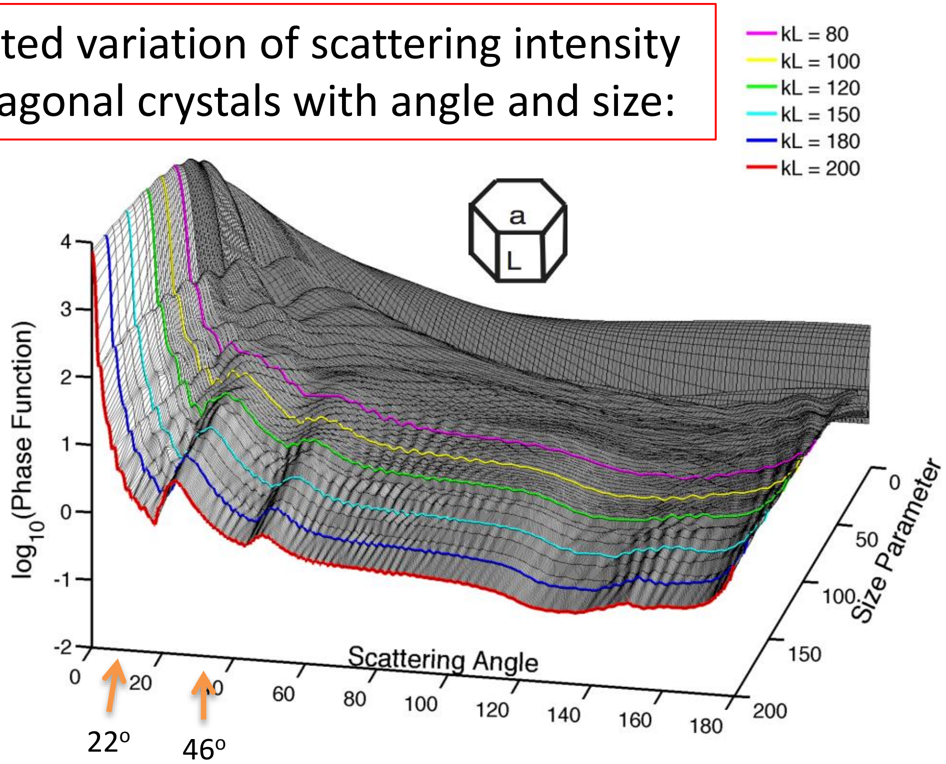
Ice crystals falling to ground at time of photo



The photo above left, taken in Antarctica, shows several optical phenomena, including the 22o and 46o halos. In the photo, the direct view of the sun is blocked by a circular disk. At the time of the photo, crystals that were falling to the ground are shown at top right.
(Photos from Tape 1994)

Our calculations indicate that hexagonal crystals must be above a critical size that depends on wavelength in order for halos to form. The numerical results shown at right show how the scattering intensity varies as a function of angle for a range of sizes (but constant aspect ratio L/a) of hexagonal crystals. The sharp ridges in scattering intensity that develop as the size increases correspond to the halos. (Other features in the photo above are due to other shapes.)

Computed variation of scattering intensity for hexagonal crystals with angle and size:

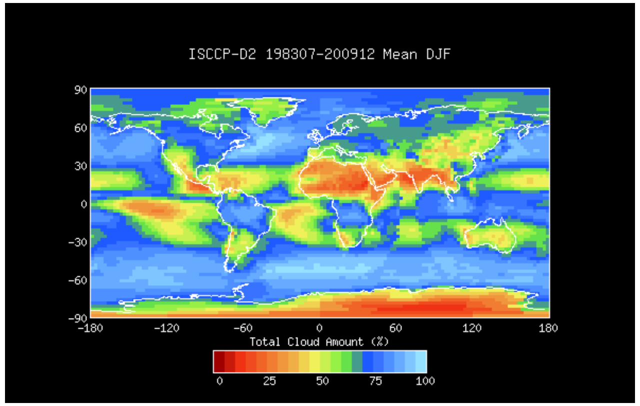


Simulation of Particle Optics: Applications in Geoscience and Biomedicine

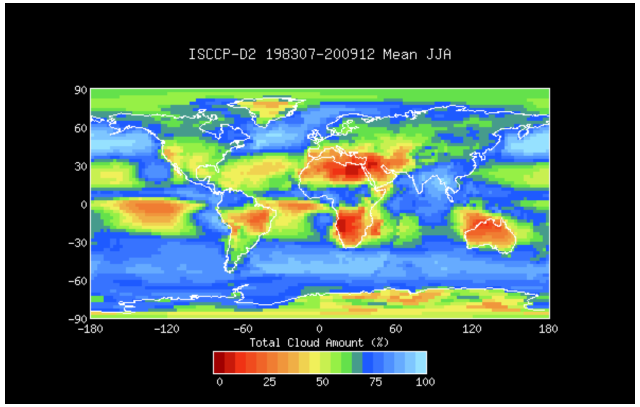
Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

Cirrus clouds – global distribution and radiative heating

Winter (DJF)

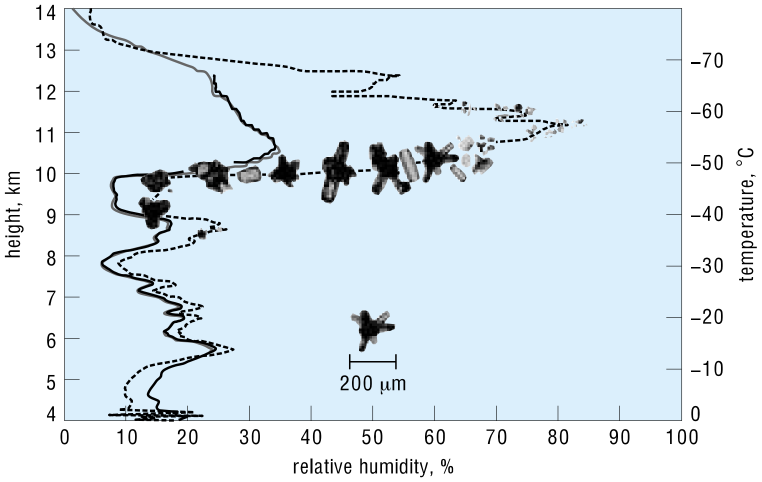


Summer (DJF)



Satellite observations are used to make estimates of global cirrus cloud cover. As shown above, coverage varies from season to season(source: http://isccp.giss.nasa.gov). High cloud amounts extend over much of extra-tropical oceanic regions, as well as regions of deep convection over land.

Cirrus clouds, composed of ice crystals, are found relatively high in the atmosphere, typically at temperatures below -40 C. The actual form the ice crystals take is the result of a complex interaction of ambient water vapor levels and temperatures. Crystals undergo both growth and aggregation,
and details of shape and even surface texture affect the amount of absorption and scattering of both shortwave (solar) and longwave (terrestrial) radiation. Estimating the net effect on heating/cooling of the atmosphere is difficult both in terms of physical understanding and numerical simulation.

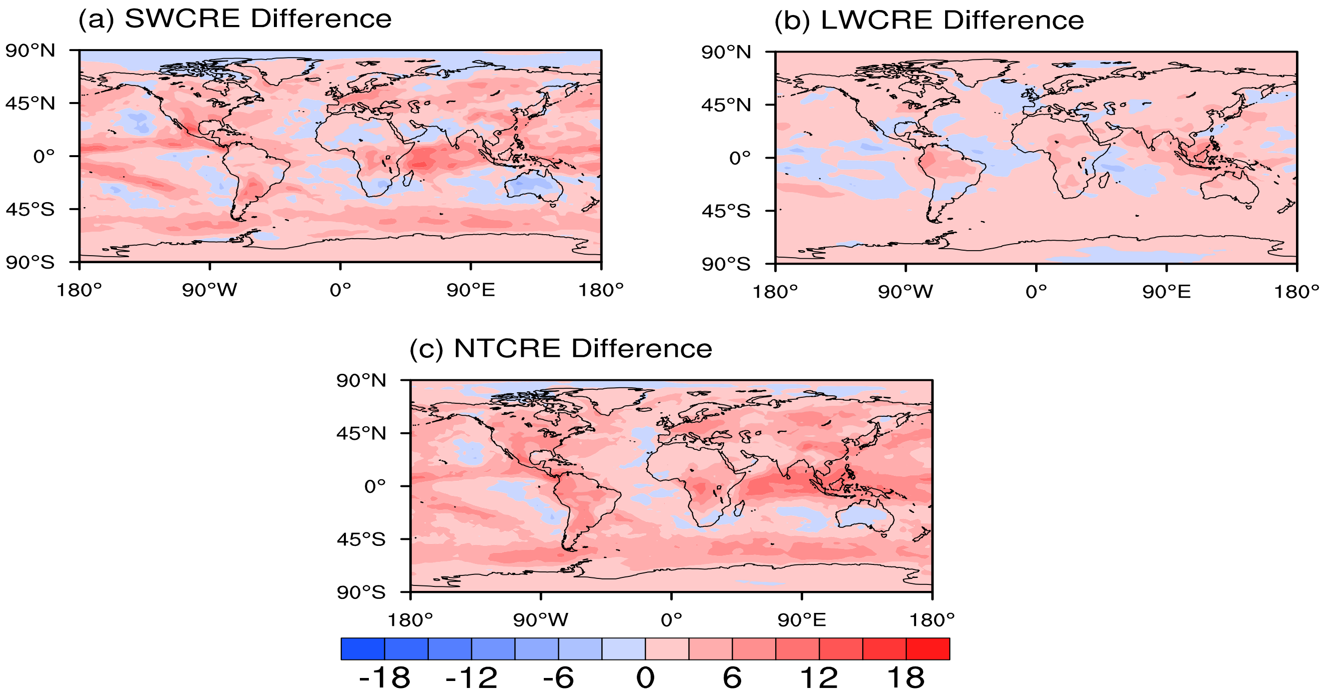


Ice crystal size and shape as a function of height, temperature, and relative humidity captured by a replicator balloon sounding system in Marshall, Colorado, on November 10, 1994. The broken and solid lines denote the relative humidity measured by cryogenic hygrometers and Vaisala RS80 instruments, respectively. (*Graphic by Andrew Heymsfield, National Center for Atmospheric Research. data from K. N. Liou, An Introduction to Atmospheric Radiation, 2d ed., Academic Press, 2002*)

http://people.atmos.ucla.edu/liou/Group_Papers/Liou_Yearbook_2005.pdf

Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

Ice Crystal Optics in a Global Circulation Model



Differences in simulated cloud radiative effect between the cases with the Lorenz–Mie theory and the nonspherical-ice optical properties. Units: W m^{-2}.

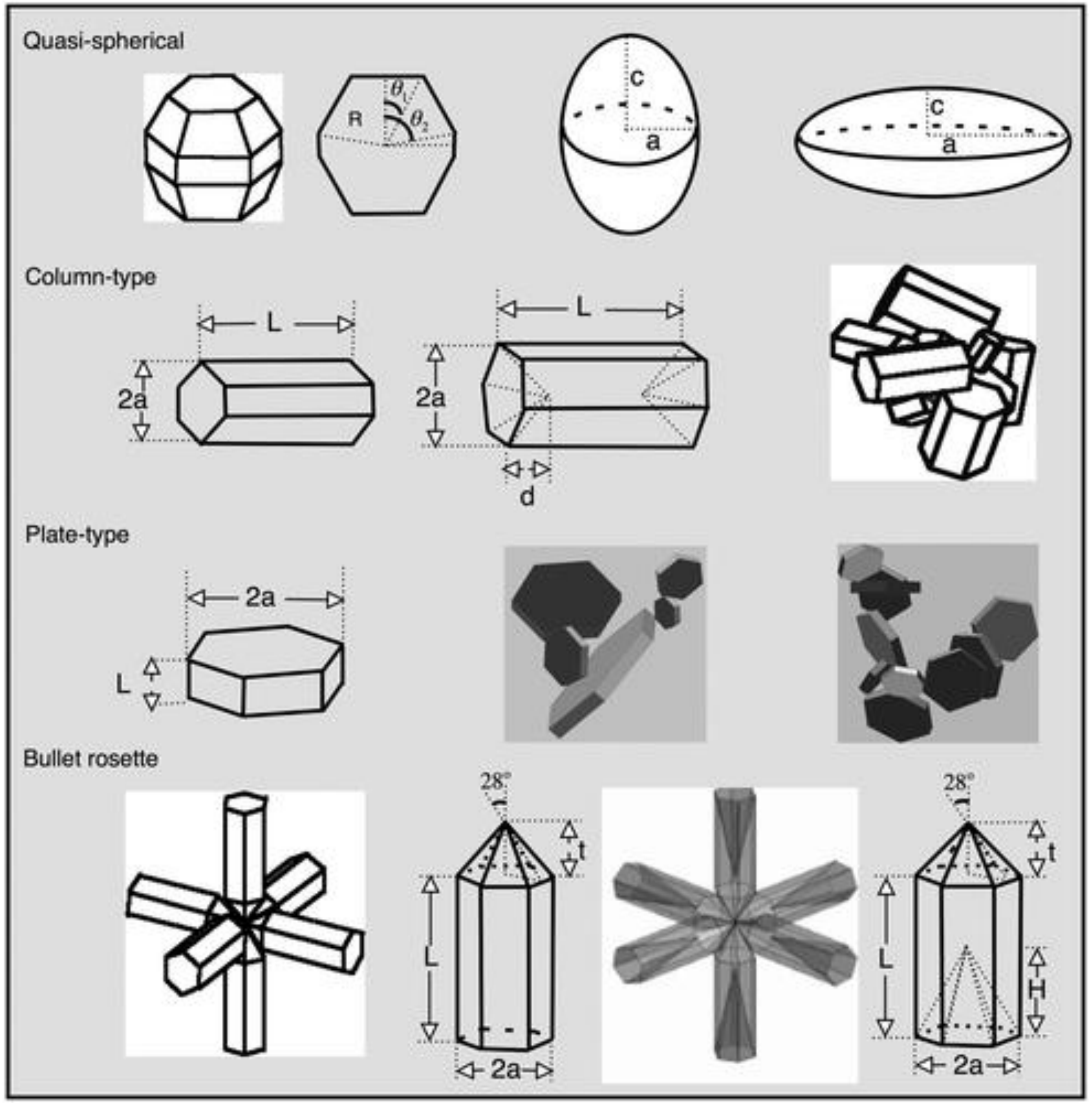
Because of the considerable cpu challenge in calculating scattering properties of non-spherical particles, parametrizations of cirrus cloud radiative effects were first based on assumption of spherical crystals. We have found that the differences between calculations of the net radiative heating based on assumption of spherical vs more realistic non-spherical crystals are substantial. In the figure above, the upper left figure is for short wave (solar) radiation, upper right is for longwave (terrestrial) radiation, and at bottom is the total difference.

Ice Crystal Optics DATABASE Simulated from EOS/ADA

Using the Invariant Imbedding and other methods, our group has built up a data-base of optical scattering properties of a variety of crystal shapes known to occur in cirrus clouds.

This provides a ``look-up" table for use in the interpretation of satellite observations. Building this table took several hundreds of thousands of cpu hours on the A&M clusters Eos and Ada. The database is now being put into operational use.

One example of operational use of the the table, built from many solutions of direct scattering problems, to solve an inverse scattering problem is next.

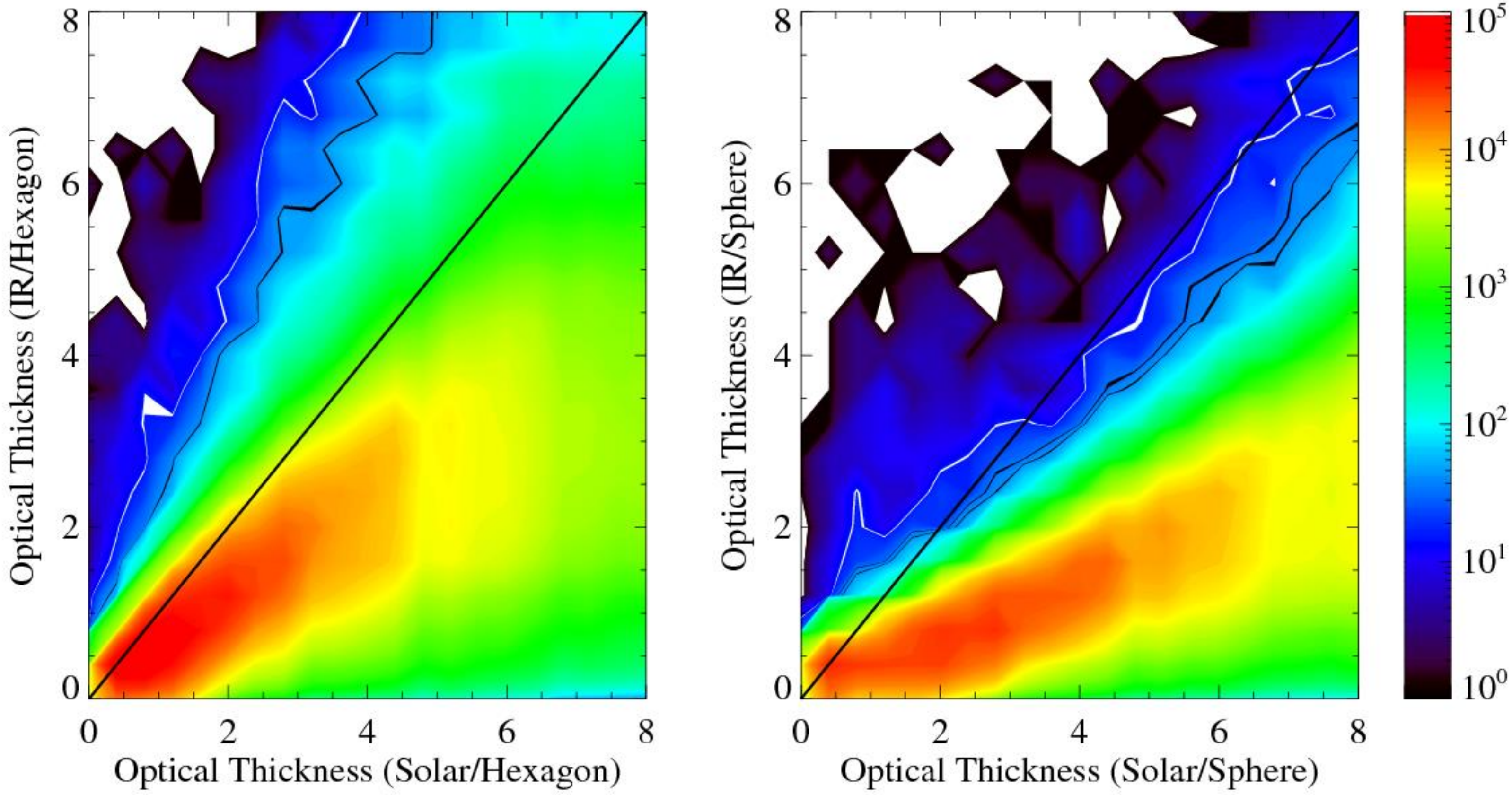


Ping Yang, Lei Bi, and co-authors, Journal of the Atmospheric Sciences, 70, 330-347, 2013.

Simulation of Particle Optics: Applications in Geoscience and Biomedicine

Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

Ice Crystal Optics and Remote Sensing



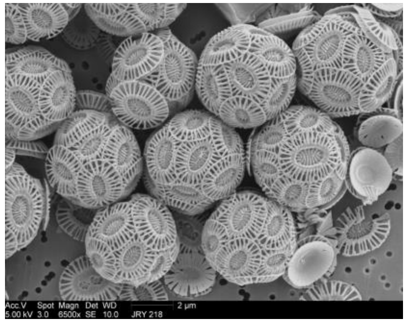
The scattering properties of a particle are dependent on wavelength as well as particle geometry. Satellite observations can be used to infer optical depth: observations at two different wavelengths should give the same answer, if the correct assumption is made about cloud crystal forms. Above: comparisons (histograms of pairs of thickness inferences) of ice cloud optical thicknesses retrieved from the solar-band-based and IR-band-based algorithms. Use of the single hexagonal column model (left panel) leads to far more points on the 45° line than using a more common sphere model (right panel).

Simulation of Particle Optics: Applications in Geoscience and Biomedicine

Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

Remote sensing of calcification state of coccolithiphores and coccoliths

Coccolithophores, forms of calcifying plankton consisting of a central coccoid core covered with small calcite plates called coccoliths, play a fundamental role in the marine carbon cycle. They are sites of both CO_2 uptake and, in calcifying phases, CO_2 release. Quantifying the calcification state is important in understanding the control of marine alkalinity. Major bloom events can be detected as milky white or turquoise patches from satellites due to strong backscattering of sunlight by calcite platelets, which easily become detached.

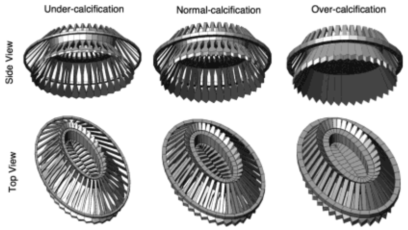


Observed occolithophores
http://www.co2.ulg.ac.be/peace/intro.htm

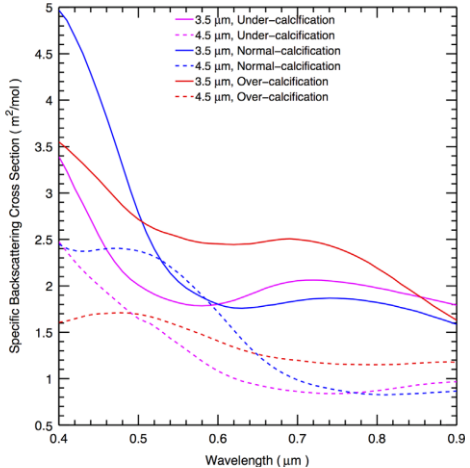
Our model coccolithophore

The amount of light a particle backscatters depends on several factors, including size, shape, and composition. A simple sphere gives a poor representation of the optical properties of coccolithophores. Our model (shown above, right) includes realistic structure as well as a way of representing degree of calcification (right).

Satellite image: a phytoplankton bloom, mainly coccolithophores, off the coast of Cornwall, UK.
http://oceancolor.gsfc.nasa.gov



Our model coccoliths



Shown above right are computations of backscattering cross sections of coccoliths with varying sizes and calcification states. These computations and others not shown indicate clear potential for use of remote sensing data in estimation of coccolith calcification states.

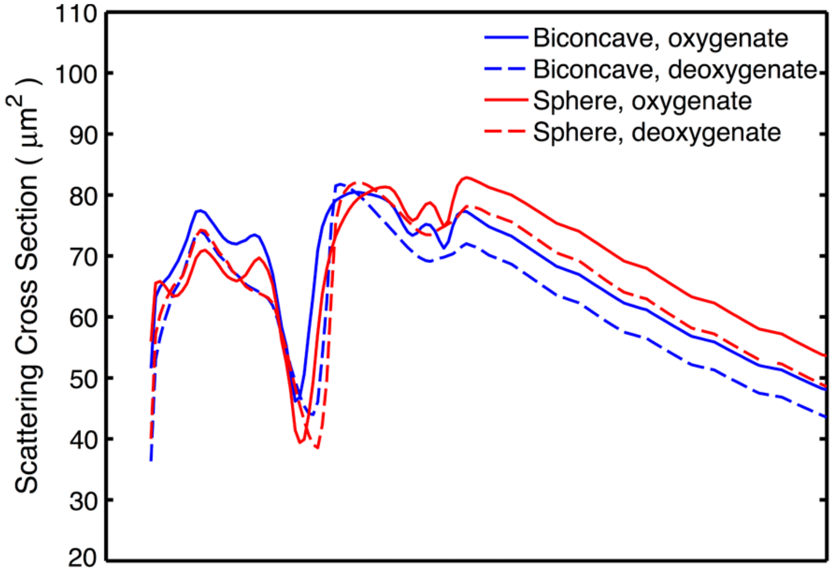
Simulation of Particle Optics: Applications in Geoscience and Biomedicine

Lei Bi, Bingqi Yi, Ping Yang, Lee Panetta
Department of Atmospheric Sciences, Texas A&M University

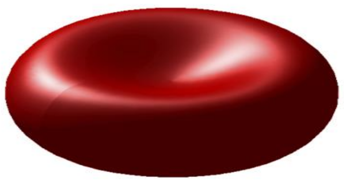
Red Blood Cells and Disease Detection

The normal shape of a human red blood cell (RBC), called biconcave, resembles a filled-in doughnut (see below). Deviations from this shape may impair O2 and CO2 transport efficiency, and may indicate such blood disorders as malaria and sickle-cell anemia.

Using our Imbedded T-Matrix method we have been able to demonstrate differences in scattering properties of biconcave and deformed RBC's, where the deformation chosen for examination is one seen
In observations. The Invariant Imbedding T-Matrix method offers considerable computational economies when compared with other numerical methods.



Biconcave RBC



Deformed RBC

The numerically calculated scattering cross-sections show clear differences between biconcave and deformed red blood cells, in both oxigenated and de-oxigenated states. The results show clearly the promise of disease detection by measuring optical scattering properties of blood samples.

Bi, L. and P. Yang, J. Biomedical Optics, 18(5),1-13,2013