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Realistic Particle Designs for Ice Particle Scattering Calculations

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In retrievals of atmospheric hydrometeors using remote sensing, particularly hydrometeors composed of ice, accurate single scattering information is essential. For near-spherical liquid hydrometeors such as cloud droplets or smaller rain drops, Mie theory is generally sufficient for obtaining accurate single scattering parameters. However, nature is not this tidy for nearly all frozen hydrometeors and even larger rain drops. The Discrete Dipole Approximation (DDA) is capable of obtaining single scattering parameters for particles with general geometry. Currently, single-scattering studies using a freely available piece of software called DDSCAT developed by Draine and Flatau based on the DDA, have focused on non-spherical but still geometrically well-defined particles. To fully realize the potential of DDSCAT in advancing the retrieval of irregularly shaped ice or large, hydrodynamically-deformed drops, there needs to be a convenient means of generating "shape" information along with the concomitant dipole configuration information that serve as the required inputs to DDSCAT.

We present here a means to interactively generate hydrometeor designs and a method to automate the process of converting the designs to appropriate DDSCAT dipole configuration information. Results of a preliminary study are also presented on hexagonal prisms, hexagonal plates, and compound particles. With the addition of a flexible database, we will be able to systematically study shape effects on single scattering parameters and thus parameterize these effects so that the retrieval accuracy of irregular ice hydrometeors can be improved. The open-source subdivision surface modeler Wings3D is selected for interactively generating any type of hydrometeor shape. In the field of 3-dimensional computer graphics, a subdivision surface is a method of repre-

senting a smooth surface using a piecewise linear polygon mesh. In Wings3D, one can modify and combine geometric “primitives” to create subdivision surface models of complicated structures. The model can be saved in a variety of formats. We find the “.obj” format to be the most appropriate for our purpose. Wings3D binary is available for all major operating systems including Windows, Mac, and Linux. Its source code (written in ERLANG) and a user reference model are available for download from the associated web site: www.wings3d.com.

After a subdivision surface model of the hydrometeor design has been created, the interior and exterior of the hydrometeor in the model have to be distinguished so the interior can be populated with dipoles. If the hydrometeor is convex, finding its interior is simple. Concave designs are more problematic but doable. To allow maximum flexibility in hydrometeor design, we have found a general solution. The surface mesh is first triangularized in Wings3D before being saved as an “.obj” file. We then transform the “.obj” file into a format understood by another open-source computer program called TetGen (http://tetgen.berlios.de/), which converts the surface mesh into a tetrahedral mesh. Every tetrahedron is a convex object whose interior can be easily identified. The corresponding dipole configuration of the hydrometeor can thus be generated in a straightforward fashion.

The longest, second-longest, and shortest axes of the hydrometeor are automatically recognized. The hydrometeor is oriented by default with the plane (we call it the primary plane) spanned by the longest and second-longest axes perpendicular to the incident radiation. This is done because the incident radiation usually does not deviate far from local nadir, while the supposed hydrometeor, such as a snow flake, tends to fall with its primary plane perpendicular to zenith. With such a default orientation, it is straightforward to adjust the orientation actually used in a calculation with DDSCAT. In the future, we intend to incorporate a database and integrate the components into a complete system that produces hydrometeor designs, creates dipole configurations, performs DDSCAT calculations, and catalogs and archives parameter inputs and results outputs.

The single-scattering properties of irregularly shaped hydrometeors have applications across a wide region of the electromagnetic spectrum. In the optical and infrared spectrums, such information is needed for retrieving the microphysical properties of ice clouds, often cirrus clouds. The retrieval of solid- or mixed-phase precipitation requires single scatter information in the microwave spectrum. Other applications extend to situations in which aerosols play a role in the development of cloudiness and precipitation – or just aerosols themselves are the particles under investigation.

Since it is more efficient to exploit a community effort in gaining a comprehensive understanding of shape effects on irregularly-shaped particles across the applicable electromagnetic spectrum, we intend to develop a web interface to our end-to-end single scatter system system so that anyone with web access can benefit from it and contribute to it. Our plan is to develop the web site such that a user can determine whether single-scattering results associated with a given wavelength, a particular shape, and specific material properties ($i.e.$, complex refractive index) already exist in the database. If not, a user would presumably generate such information with the online software. Once the appropriate calculations are completed, the associated inputs and outputs would be automatically cataloged and archived into the database. Gradually, this would lead to the development of a comprehensive single scatter database associated with arbitrarily shaped particles for atmospheric remote sensing purposes.