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Voronoi diagram-based spheroid model for microwave scattering of complex snow aggregates

Ryan Honeyager*, Guosheng Liu, Holly Nowell

Department of Earth, Ocean and Atmospheric Science, Florida State University, Tallahassee, FL 32306, USA

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ABSTRACT

Methods to model snow aggregate scattering properties at microwave frequencies can be divided into structurally explicit and implicit techniques. Explicit techniques, such as the discrete dipole approximation (DDA), determine scattering and backscatter cross-sections assuming full knowledge of a given snow particle's structure. Such calculations are computationally expensive. Implicit techniques, such as using the T-matrix method (TMM) with optically soft spheroids, model equivalent particles with variable mass, bulk density and aspect ratio according to an effective-medium approximation. It is highly desirable that there should be a good agreement between modeled aggregate cross-sections using both methods.

A Voronoi bounding-neighbor algorithm is presented in this study to determine the bulk equivalent density of complex three-dimensional snow aggregates. While mass and aspect ratio are easily parameterized quantities, attempts to parameterize the bulk density of snowflakes have usually relied on a bounding ellipsoid, which can be determined from a flake's radius of gyration, root mean square mean or simply from its maximum diameter. We compared the Voronoi algorithm against existing bounding spheroid approaches and mass–effective density relations at ten frequencies from 10.65 to 183.31 GHz, using a set of 1005 aggregates with maximum dimensions from a few hundred microns to several centimeters.

When using the Voronoi-determined effective density, the asymmetry parameter, scattering, and backscatter cross-sections determined using the TMM reasonably match those for DDA-computed snow aggregates. From K_u to W-band, soft spheroids can reproduce cross-sections for aggregates up to 9 mm in maximum dimension. Volume-integrated cross-sections always agree to within 25% of DDA. As the DDA is computationally expensive, this offers a fast alternative that efficiently evaluates scattering properties at microwave frequencies.

1. Introduction

Accurate modeling of how ice crystals scatter radiation in clouds is a fundamental concern for meteorological remote sensing by microwave radars and radiometers. In order to correctly interpret the overall scattering signal, it becomes necessary to computationally model large samples of algorithmically generated ice particles.

* Correspondence to:Department of Earth, Ocean and Atmospheric Science Florida State University 1017 Academic Way, 404 Love Building Tallahassee, FL 32306-4520 Tel.: + 1850 644-6716; fax: + 1 850 644-9642.

E-mail address: rhoneyager@fsu.edu (R. Honeyager).

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These particles are structurally constrained using various models in the hope that the collective set properly represents reality in a substantial portion of clouds [1].

A substantial portion of in-cloud water exists in a solid state. Ice hydrometeors exhibit a wide variation in possible shapes, and each shape scatters light differently. The scattering signal for each ice particle can be determined using two general types of solution to the electromagnetic field equations. The first is to use a structurally-direct solution such as the discrete dipole approximation (DDA) [2,3], the finite-difference time-domain (FDTD) method [4,5] and the Rayleigh–Gans approximation [6,7]. In the DDA, the ice structure is discretized onto a fixed, regular and orthonormal lattice of polarizable dipole elements (dipoles) [8]. The DDA can resolve changes in overall scattering behavior caused by small variations in internal and surface structure. Based on convergence constraints, however, snowflakes must be modeled at resolutions of at least 10-100 microns at microwave frequencies, and fine structural features should be resolvable [9–11]. Processing time and memory requirements increase exponentially for finer resolutions, larger particles and higher frequencies [12]. Assuming fully random particle orientations, DDA calculations must be repeated over many possible orientations of a particle relative to the incident radiation to determine scattering properties [13,14]. Furthermore, a large number of representative particles must be considered that ideally have modeled structures which are similar to those found in nature [2,15]. This overall is quite computationally expensive.

As ice aggregates are quite porous, it is also possible to use the Rayleigh–Gans approximation [6,7] to determine backscatter. The Rayleigh–Gans formulation has been applied to both spheroidal [7,13,16] and aggregate [17,18] shapes. As with the DDA, aggregate structure can be discretized onto a lattice. Calculations are much faster than with the DDA because interdipole interactions are neglected. However, the accuracy of the results depends on the aggregate shape model [18,19].

The other class of methods use techniques that indirectly use structural information. For example, Mie theory provides an exact scattering solution for spherical particles [20]. Similar approaches include the T-matrix method, which uses an extended boundary technique to handle nonspherical morphologies [9,21–23].

In the T-matrix method, a more realistic ice particle is commonly represented by an equivalent homogeneous spheroid. This approximation is tailored to preserve important quantities such as particle mass, aspect ratio and bulk effective density [24,25]. Implementations assuming randomly-oriented [23] and arbitrarily aligned [26] scatterers are both readily available. This is much faster than using a DDA solution and, depending on the approximation algorithm used, may preserve only the structural information that has a significant impact on scattering behavior.

Aggregate formulations have been proposed using collections of columns [18,27,28], bullet rosettes [1,18,29], planar dendritic snowflakes [18,30,31], hexagonal plates [18,32,33], stellar type crystals [34] and spheres [35]. Several studies provide explicit comparisons of DDA aggregate results with other methods. Kim [27] compared a Mie-based representation of simple columnar aggregates with the DDA and established that Mie theory did not adequately predict single-scattering properties such as cross-sections and asymmetry parameter for size parameters greater than 2.5. Westbrook et al. [36] presented early small bullet rosette aggregates. Hogan and Westbrook [16,17] expanded these aggregate formulations in the domain of small particles using a modified version of Rayleigh–Gans theory. Nowell et al. [1] compared bullet rosette aggregates using the DDA with combinations of solid and soft spheres and oblate ellipsoids.

Fractal shape models have also been developed [31,33,35,37]. Maruyama and Fujiyoshi [35] aggregated low-density spheres with variable densities. Ishimoto [37] considered particles with no particular shape and various fractal dimensions. Schmitt and Heymsfield [33] used an iterative algorithm were repeating hexagonal crystals were randomly added to a growing seed crystal. Tyynelä et al. [31] used a fractal model based on results from Ishimoto [37] and compared against an aggregation models based on Westbrook et al. [29] comprised of either stellar or fernlike dendrites.

The DDA, Rayleigh–Gans and T-matrix methods, however, usually produce very different results when applied to aggregate snowflakes [1,30,31]. Aggregates are larger ice particles resulting from collision, deposition and repeated freezing/melting processes [38]. They have very complicated shapes. When modeling aggregates using the DDA, their lattice structures should ideally match observed projected size-density, aspect ratio and fractal dimension relations [1]. These parameters are easy to incorporate into a DDA model. For validation, comparisons have been commonly made against a hard-sphere model [27,39], in which Mie theory calculates scattering properties of equivalent solid ice spheres. These spheres preserve ice particle mass while ignoring other information such as effective density and aspect ratio. As aggregate morphologies incorporate a significant amount of air into the ice lattice, this approach produces equivalent spheres that are much smaller in diameter (microns vs. mm). The resulting hard-sphere backscatter is frequently an order of magnitude larger than DDA results for high frequencies and large particles [1,27,40].

Soft spheroid models have also been used [13,24,30,31,41–46]. In such models, it is possible to preserve particle mass, size and aspect ratio. However, the shape of the particle being considered is different. Instead of having separate regions of ice and air, these models construct ellipsoids made of a combined ice/air medium. This medium has a refractive index intermediate to ice and air, and the refractive index is determined by a mixing relation [47–49]. This mixing relation is itself dependent on the effective (ice + air) density of the source snowflakes. The concept of effective density is poorly-defined for snowflakes [42]. While soft spheroid models preserve mass, a reference volume must be selected.

A common trend in soft-spheroid results is to use the concept of a geometric bounding surface [24,30,50], such as a circumscribing circle/sphere/ellipsoid [16,34,51], a root mean square (RMS) sphere [30], or a radius of gyration (RG) sphere