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A stochastic model for density-dependent microwave Snow- and Graupel scattering coefficients of the NOAA JCSDA community radiative transfer model

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ABSTRACT

A structural model is developed for the single-scattering properties of snow and graupel particles with a strongly heterogeneous morphology and an arbitrary variable mass density. This effort is aimed to provide a mechanism to consider particle mass density variation in the microwave scattering coefficients implemented in the Community Radiative Transfer Model (CRTM). The stochastic model applies a bicontinuous random medium algorithm to a simple base shape and uses the Finite-Difference-Time-Domain (FDTD) method to compute the single-scattering properties of the resulting complex morphology.

1. Introduction

The Community Radiative Transfer Model (CRTM) is a flagship radiative transfer model of the U.S. National Oceanic and Atmospheric Adiministration (NOAA) and has been actively improved at the Joint Center for Satellite Data Assimilation (JCSDA). As described in the CRTM user guide by Delst, [15] the CRTM is a fast scalar radiative transfer solver, whose primary purpose is its usage as a forward operator for satellite observational data assimilation in conjunction with the Global assimilation with Gridpoint Statistical Interpolation (GSI) code by Hu et al., [26], in order to provide initial conditions and drift corrections for numerical weather prediction (NWP). Specific procedures for satellite data assimilation as conducted at the JCSDA are given for instance by Weng et al., [58], while basic introductions to the topic of observational data assimilation can be found in Rodgers, [48] and Kalnay, [31]. In this context, Rodgers, [48] puts a stronger focus on the remote sensing aspect, while Kalnay, [31] approaches the subject from the perspective of NWP. A more recent example, specifically including solid hydrometeors, has been published by Wood et al., [59]. The CRTM itself has been extensively validated in the past, by Chen et al., [12], Yi et al., [64] or Ding et al., [18] in comparison with high accuracy solvers such as DISORT by Stamnes et al., [51].

In addition to algorithms to deal with atmospheric absorption, the official CRTM release also includes two solvers to handle electromagnetic scattering by particles. In particular, these two solvers are the so-called "Advanced Doubling-Adding Method" (ADA) by Liu et al., (2006) and the Successive-Order-of-Interaction Radiative Transfer Model by Heidinger et al., [24], with the ADA being the default solver. As detailed in the CRTM user guide by Delst, [15], scattering particles are broadly categorized into aerosol and cloud particles, with optical property data sets for each category stored in a separate unformatted binary file. This study focuses on the cloud scattering properties retained as Look-Up tables (LUTs) in the CRTM CloudCoeff binary file. Due to its application for satellite data assimilation, the description of cloud particles in the CRTM aligns itself with cloud microphysical parameterizations used in NWP models, as described for instance by McCumber et al., [39]. The CRTM does not include a continuous, so-called spectral ice scheme, but uses a four-class, type 1 classification of cloud ice in the terminology of McCumber et al., [39] instead. Aside from liquid water droplets, the CRTM distinguishes solid hydrometeors into cloud ice, and precipitating ice in the form of either snow, graupel, or hail. The distinguishing feature of the solid hydrometeor categories is their associated mass density, which is given in Table 1.

The original computations of the default single-scattering properties of the hydrometeors listed in Table 1 include certain incon-

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Table 1
Solid hydrometeor categories and associated densities in the CRTM Release 2.1.3.

Category	Density (g/cm^3)
Cloud ice	0.900
Graupel and hail	0.400
Snow	0.100

sistencies, which are discussed in further detail in Section 3.1 and Section 4. A recent update of the CRTM ice optical properties has been provided by Yi et al., [64], where the default ice optical properties are replaced by the so-called MODIS Collection 6 ice cloud optical properties (Platnick et al., [46]) in the infrared and microwave regime and on the basis of the temperature dependent ice refractive index tabulated by Iwabuchi and Yang, [28].

Consequently, this manuscript will focus on providing density-variable scattering properties for the remaining solid hydrometeor optical properties in the microwave regime, namely snow and graupel. The second section of this manuscript discusses the model proposed for the morphology of the graupel and snow scattering particles. Its third section describes the computation of the particle single-scattering properties and the fourth section deals with the corresponding bulk scattering properties and their adaption to the CRTM format. The fifth section investigates the changes brought about in the radiative transfer calculations involving scattering cloud layers, and the sixth section comprises the conclusion of the manuscript.

2. Particle morphology model

2.1. Bicontinuous random medium (BRM) theory

As shown in Table 1, the crucial aspect distinguishing cloud ice, snow and graupel in the CRTM is the assumed bulk mass density. Consequently, the first and primary requirement for the morphological model is its ability to create a scattering particle that can cover the entire range of bulk mass density as given in Table 1. Moreover, observations of snow, graupel, and especially rimed snow documented in e.g. Pruppacher and Klett, [47] or Kikuchi et al., [32] show that these particles may often display a highly irregular, random structure that is often covered in rime for precipitating ice, which the model also needs to be able to reproduce. A natural response is to first look for a deterministic model that is able to reproduce the natural diffusive growth process of ice crystals in the atmosphere, such as the cellular automata of Gravner and Griffeath, [23] or the subsequent parametric interface FEM model by Barrett et al., [1]. However, reproducing the full spectrum of possible solid precipitation shown by Kikuchi et al., [32] using these methods is computationally not feasible in the scope of this project. Furthermore, random physical processes such as mesoscale surface roughness, riming, and turbulent convection cannot be considered using these methods alone. The importance of taking these processes into account in order to match the optical properties of real ice crystals has been demonstrated for instance for the case of surface roughness by Stegmann et al., [52]. In these cases, the chosen deterministic ice growth model would have to be supplemented by the approach of Zhang et al., [67] for surface roughness, Criscione et al., [14] for riming, and Wang, [54] for turbulent convection, further increasing the computational complexity and strain of this method. Instead, a much simpler solution is the application of a bicontinuous random spatial partitioning scheme known from the theory of heterogeneous materials (see Sahimi, [49] for an overview). The term bicontinuous in this context means that the two separated phases, which are ice and air for the case of snow and graupel, may display connected structures extending over the entire domain upon which the Bicontinuous Random Medium (BRM) algorithm is applied. This scheme had first been developed and applied to scalar scattering by a bulk medium by Berk, [4] and Berk, [5] as the so-called leveled-wave model. Later, the model has been applied to scattering of electromagnetic waves by particles by Ding et al., [17] and Tang et al., [53]. Subsequently, the model has also been utilized by Xiong and Shi, [60] in the context of polarized radiative transfer through layers of settled ground snow.

The basis of the BRM model as originally defined by Berk, [4], is a finite superposition of stochastic standing cosine waves $S(\vec{r})$. Its mathematical definition is given in Eq. (1), while an illustration can be found on the left hand side of Fig. 1.

$$S(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{n=1}^{N} \cos\left(\vec{k}_n \cdot \vec{r} + \phi_n\right) \tag{1}$$

Using differential geometric terminology, $S(\vec{r})$ in Eq. (1) is a level set over a Euclidean manifold with coordinates $\vec{r}$, and as such it is a simplified stochastic special case of more general methods to track the dynamic evolution of interfaces as developed by Osher and Sethian, [43]. In Eq. (1), the integer N is the total number of superimposed cosine waves. The scalar $\phi_n \in [0, 2\pi)$ is the random phase shift associated with the nth cosine wave $S_n(\vec{r})$ and follows a uniform distribution. In the current study, an xorshift 1024* pseudo-random number generator (PRNG) from the Xorshift class of PRNGs by Marsaglia, [37] is used to obtain uniformly distributed random numbers. The 3D vector $\vec{k}_n = k_n \cdot \hat{k}_n$ is the wave vector of $S_n(\vec{r})$. Its direction $\hat{k}_n$ is uniformly distributed on the unit sphere and its scaling wavenumber k_n determines the geometric properties and structural length scales of the BRM. Its selection is *a priori* arbitrary and as this work is primarily dealing with solid hydrometeors consisting of ice crystals, the gamma distribution suggested by Chen and Chang, [11] is selected. It should be noted that this choice is strongly dependent on the material under scrutiny. Berk, [5] for instance used a shifted delta distribution to study water–oil microemulsions, i.e. only one specific wavenumber. In a notable analogy to the present study, the resulting morphologies obtained via the delta distribution bear a remarkable similarity to the structures computed by solving the deterministic Cahn-Hilliard PDE by Cahn and Hilliard, [10], albeit at a fraction of the computational cost. As a consequence, the wavenumber may randomly take on any value in the interval $[0, \infty)$, under the sole condition that the frequency of occurrence of wavenumbers follows a gamma probability distribution function $p(k)$ as defined in Eq. (2).

$$p(k) = \frac{1}{\Gamma(b+1)} \frac{(b+1)^{b+1}}{\langle k \rangle} \left(\frac{k}{\langle k \rangle}\right)^{b} \exp\left(-(b+1)\frac{k}{\langle k \rangle}\right) \tag{2}$$

In Eq. (2), $\Gamma(\bullet)$ is the Gamma function, $\langle k \rangle$ is the mean wavenumber, and b is a shape parameter related to the standard deviation of $p(k)$.

An algorithm for drawing pseudo-random numbers from a gamma probability distribution can be found for instance in Marsaglia and Tsang, [36]. After a realization of the random level set $S(\vec{r})$ has been drawn, the interface separating the two phases ice and air needs to be defined by choosing one specific level. This can be achieved by introducing a threshold level θ given by Eq. (3).

$$\theta = erf^{-1}(1 - 2f_V) \tag{3}$$

Eq. (3) relates the threshold θ of $S(\vec{r})$ to the volume fraction f_V of ice in the total volume on which the BRM model is applied via the inverse of the error function $erf^{-1}(\bullet)$. The introduction of the threshold on a 2D example wave field is illustrated in Fig. 1, with the resulting ice structure shown on the right side. The original field $S(\vec{r})$ is mapped to a new field $\tilde{S}(\vec{r})$, which is defined by Eq. (4).