Improving Accuracy and Computational Efficiency for Orientation-averaged Single-Scattering Properties of Nonspherical Ice Particles

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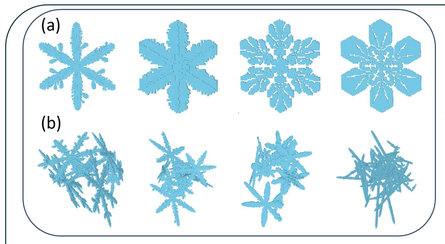
I – Introduction

We have developed a 3D full-wave model for Scattering by Complex-shaped Particles (NESCoP). The key idea behind this model is the use of a direct solver-based domain decomposition method, known as the Characteristic Basis Function Method (CBFM). Our model maintains the advantages of the DDA, namely full-wave solution to arbitrarily-shaped scatterer with inhomogeneous composition, while significantly surpassing the DDA implementations in computational efficiency, particularly when considering a large number of particle orientations. A wide spectrum of enhancements is worth considering to further optimize the numerical efficiency of our model and to improve its accuracy.

II – MoM/CBFM-based Full-Wave Scattering Model



Pristine crystals **(a)** simulated using the snowflake algorithm [1] and aggregate snow particles **(b)**

3D full-wave model based on the use of the **volume integral equation method (VIEM)** with **piecewise constant basis functions.**
The model is applied here to pristine ice crystals and aggregate snow particles simulated by Kuo et al [1] using a 3D growth model pioneered by Gravner and Griffeath.

Frequencies of interest : (35 - 380 GHz)

Integral representation of the total electric field (EFIE) :

$$\bar{E}(\bar{r}) = \bar{E}^i(\bar{r}) + \left(k_0^2 + \nabla\nabla.\right)\int_{\Omega} \chi(\bar{r}')\, G(\bar{r},\bar{r}')\, E(\bar{r}')\, d\bar{r}'$$

where $\bar{E}(\bar{r})$ is the field inside the scatterer, $\bar{E}^i(\bar{r})$ is the incident field, $\chi(\bar{r}')$ is the dielectric contrast at the location r', k_0 is the wavelength number in air and $G(\bar{r},\bar{r}')$ is the free space Green's function. We rewrite the integral equation above as :

$$\boxed{\Gamma\bar{E}(\bar{r}) = E^i(\bar{r})} \quad \text{where} \quad \Gamma = \underline{I} - \left(k_0^2 + \nabla\nabla.\right)\int_{\Omega} \chi(\bar{r}')\, G(\bar{r},\bar{r}')\, d\bar{r}'$$

Application of a Method of Moments (MoM) :

The particle is discretized into **N** cubic cells Ω_n ,of side c_n, small enough to consider that the field inside is constant [2]

$$c_n = \frac{\lambda_s}{10} \; ; \; \lambda_s = \frac{\lambda_0}{\sqrt{Re(\varepsilon_r)}}$$

$$\bar{E}(\bar{r}) = \sum_{n=1}^{N}\sum_{q=1}^{3} E_q^n \; \bar{F}_q^n(\bar{r})$$

where E_q^n is the constant unknown of $\bar{F}_q^n$, the nth basis function for the component (q=x, y or z) of the field inside the particle.

To select a set of test functions W_p^m (m=1,..,M and p= x, y, z), the point matching method is used. So, M=N and W_p^m is a Dirac delta function concentrated at the center of the cell Ω_n.

$$\boxed{\Gamma\bar{E}(\bar{r}) = E^i(\bar{r})} \Rightarrow \boxed{\sum_{n=1}^{N}\sum_{q=1}^{3} Z_{pq}^{mn} E_q^n = E_p^{i,m}} \Rightarrow ZE = E^i$$

Z is the 3N x 3N full matrix representing the interactions between the cells composing the particle. E^i is the incident field of size 3N and E is the unknown solution vector of size 3N that represents the total electric field inside the particle in the x, y and z directions.

Application of the Characteristic Basis Function Method :

To overcome the computational burden associated with the VIEM (O[(3N)^2]), we use the CBFM, a domain-decomposition method proven to be accurate and efficient when applied to large-scale EM problems.

- ❖ **B**etter adapted to multiple right-hand side problem
- ❖ **H**ighly amenable to **MPI** parallelization
- ❖ Subject to a wide variety of enhancement techniques
- ❖ **T**unable depending on to the needs (memory or CPU)

After dividing the 3D complex geometry of the particle of **N** cells into **M blocks**, the **CBFM** process [3] consists in generating $\mathbf{S_i}$ Characteristic Basis Functions (CBFs) for each block **i** in order to generate a final reduced matrix of size **K x K** where $K = \sum_{i=1}^{M} S_i$. This results in a substantial size-reduction of the MoM matrix and enables us to use of a direct method for its inversion.

Direct solver

Solving the resulting reduced system of equations, instead of the original one, enables us to achieve a significant reduction both in terms of CPU time and memory.

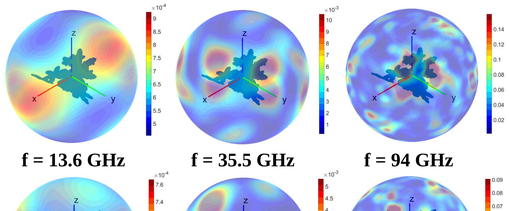
III – Enhancing Accuracy and Computational Capabilities

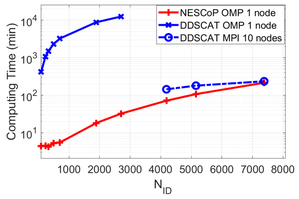
The main current objectives in terms of optimization of the accuracy and computational efficiency of our scattering model NESCoP are:

- ✓ Reducing the computational expense, both time and memory requirements, when computing the scattering properties of electrically large hydrometeors for a large number (≥ 5000) of incident directions (θ_i, Φ_i)
- ✓ Accurately and efficiently determining orientation-averaged Single Scattering Properties (SSPs), after evaluating the efficacy of several quadrature schemes in minimizing the number of orientations, and hence computation resources, needed for an acceptably accurate orientation average.
- ✓ Ensuring the accuracy of the MoM/CBFM solution when considering scattering from mixed-phase hydrometeors, featuring a problematic high dielectric contrast between ice and water.

The ultimate goal is to enable users to obtain satisfactorily accurate SSPs of large complex-shaped solid and mixed-phase hydrometeors for a large number of incident directions (or equivalently target orientations) at a reasonable computational cost.

1. Optimization of computational efficiency :



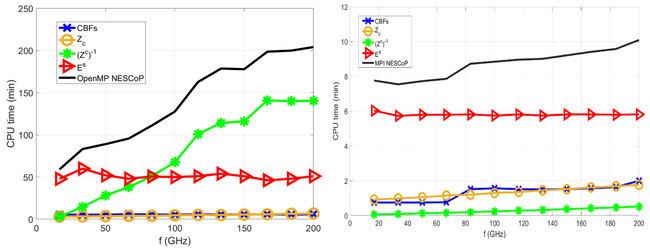


Variation of computing time for OMP-parallelized NESCoP and OMP & MPI DDSCAT when increasing the number of incident directions N_{ID}

The SSPs are computed for a sufficiently large number of incident directions (up to 7800 IDs only in θ_i, Φ_i) by virtue of the high computational efficiency of NESCoP.

OpenMP : 16 CPUs with 64 GB RAM
Total : 28 h 26 min

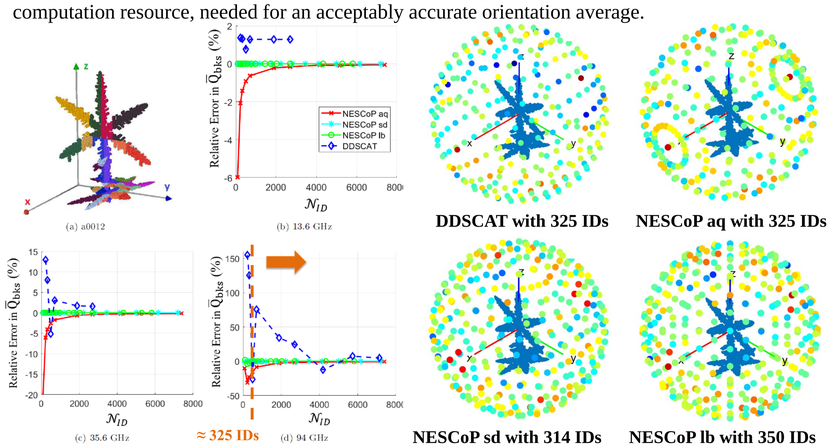
MPI : 96 MPI tasks; 2 nodes on TACC Stampede2 with 48 cores & 192GB of RAM each
Total : 1 h 56 min



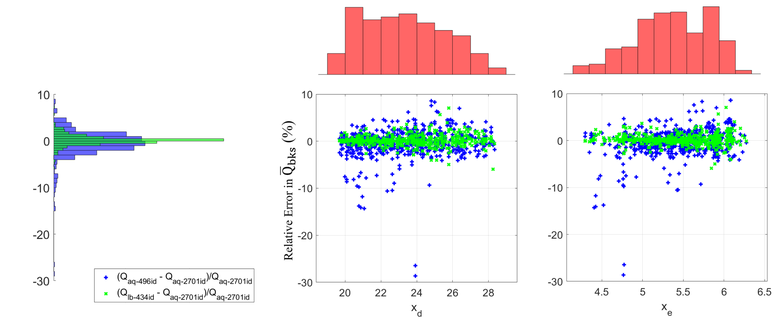
The MPI parallelization reduces drastically the computation time particularly for the embarrassingly parallel loops in **the calculation of the scattered field E^s, and the resolution of $Z^c\alpha = E^c$ due to the use of ScaLAPACK.**

2. Accurate & Efficient Orientation-Averaging :

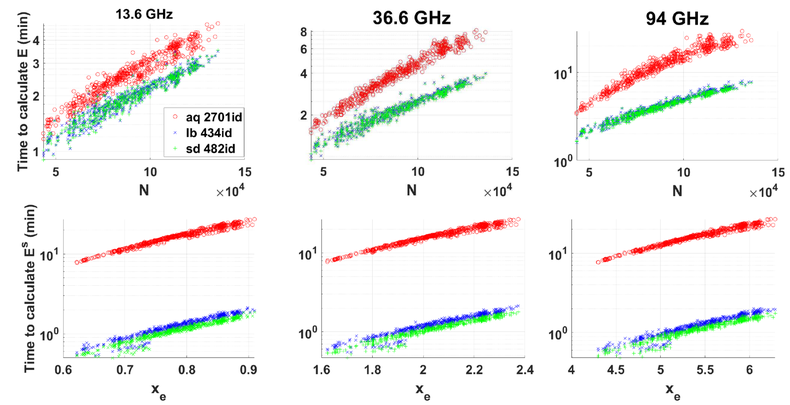
We evaluate the efficacy of several quadrature schemes namely adaptive quadrature (aq), spherical design (sd), and Lebedev quadrature (lb), in minimizing the number of orientations, and hence computation resource, needed for an acceptably accurate orientation average.



Shape and variations of averaged Qbks with NESCoP and DDSCAT at Ku, Ka and W bands , depending on the numerical integration scheme used with NESCoP and on the number of incident directions NID

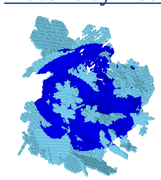


Variations of the relative error in averaged backscatter efficiency $\bar{Q}_{bks}$ using NESCoP, with respect to the convergence assumed achieved with aq and 2701 IDs, as function of x_d ($\pi d_{max}/\lambda$) and x_e ($\pi d_{equ}/\lambda$) when $\bar{Q}_{bks}$ is calculated at 94 GHz with aq with 496 IDs and lb with 434 IDs.



These lb and sd schemes exhibit significantly higher ability to capture the essence of Q_{bks}, independently from the complex geometry or orientation of the aggregate, and perform well with much fewer quadrature nodes.
Using NESCoP with the sd and lb schemes enables a significant gain in computational cost, particularly for the calculation of the scattered field E^s. This gain increases with N (number of cells)

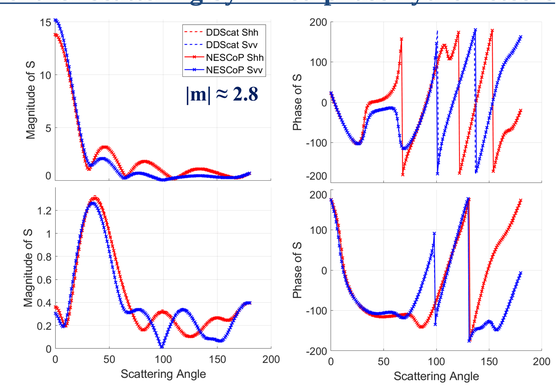
3. Accuracy Assessment for scattering by mixed-phase hydrometeors



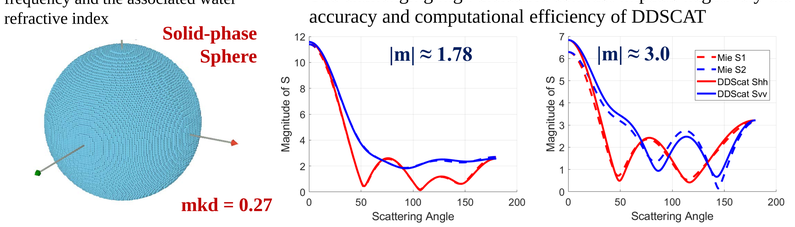
d_{equ} = 2.72 mm d_{max}=8.20 mm
Nb_c =86164 cells

f (GHz)	13.6	35.5	94
$\lvert m_{water}\rvert$	6.3	4	2.8
NESCoP	5	6	9
DDSCAT	≥ 1e3		19

Computing time (min) for NESCoP and DDSCAT depending on the frequency and the associated water refractive index



The challenging high dielectric contrast impacts negatively the accuracy and computational efficiency of DDSCAT



It is worth recalling that "the main difference between DDA-based codes and derivations based on the integral equations such as NESCoP is that the latter give more mathematical insight into the approximation, thus pointing at ways to improve the scattering solution" Yurkin JQSRT 2007

References : [1] Kuo, K. S., Olson, W. S., Johnson, B. T., Grecu, M., Tian, L., Clune, T. L., ... & Meneghini, R. (2016). The Microwave Radiative Properties of Falling Snow Derived from Nonspherical Ice Particle Models. Part I: An Extensive Database of Simulated Pristine Crystals and Aggregate Particles, and Their Scattering Properties. Journal of Applied Meteorology and Climatology, 55(3), 691-708. [2] Nguyen, H., Roussel, H., & Tabbara, W. (2006). A coherent model of forest scattering and SAR imaging in the VHF and UHF-band. IEEE transactions on geoscience and remote sensing, 44(4), 838-848.E. [3] Lucente, G. Tiberi, A. Monorchio, and R. Mittra, "An iteration-free MoM Approach Based on Excitation Independent Characteristic Basis Functions for Solving Large Multiscale Electromagnetic Scattering Problems", IEEE Trans. Antennas Propag., Vol. 56, no. 4, pp.999-1007, Apr. 2008.