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

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

The particle is discretized into N cubic cells \( \Omega_n \) of side \( c_m \) small enough to consider that the field inside is constant \([2]\).

\[
\vec{E}(f) = \sum_{n=1}^{N} \sum_{q=1}^{3} E_{R}^{E}(\vec{r}_q) \delta_{2}^n
\]

Application of a Method of Moments (MoM):

The particle is discretized into \( N \) cubic cells \( \Omega_n \) of side \( c_m \) to small enough to consider that the field inside is constant \([2]\).

\[
\epsilon_{R}^{E}(\vec{r}_q) \delta_{2}^n
\]

To select a set of test functions \( \psi_q^m \) the \( q \), \( x \), \( y \), \( z \) point matching method is used. So, \( N \times M \) and \( \psi_q^m \) is a delta target function concentrated at the center of the \( \Omega_n \).

\[
\Gamma_{\psi}^{E}(\vec{r}_q) = \sum_{n=1}^{N} \sum_{q=1}^{3} \psi_q^m \psi_q^m
\]

Application of the Characteristic Basis Function Method:

To overcome the computational burden associated with the VIEIM (O1(N^3)), we use the CBFM, a domain-decomposition method proven to be accurate and efficient when applied to large-scale EM problems.

Better adapted to multiple right-hand side problems

Highly amenable to \( \text{MPI} \) parallelization

Subject to a wide variety enhancement techniques

Tunable depending on 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 \( S \) Characteristic Basis Functions (CBFs) for each block \( n \) in order to generate a final reduced matrix of size \( K \times K \) where \( K = \sum_{n=1}^{N} S_n \). This results in a substantial size-reduction of the MoM matrix and enables us to use of a direct method for its inversion.

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 (\( \geq 5000 \)) of incident directions (\( \theta, \phi_s \))
- 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 compute 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:

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 compute resource, needed for an acceptably accurate orientation average.

\[
\epsilon_{R}^{E}(\vec{r}_q) \delta_{2}^n
\]

Variations of the relative error in averaged backscatter efficiency \( Q_{\text{bak}} \) using NESCoP, with respect to the convergence assumed achieved with aq and 2701 IDs, as function of \( x_d \) (\( \text{Tr(daq), \text{Tr(2701)}}, \) and \( x_d \) (\( \text{Tr(daq)} \) which \( Q_{\text{bak}} \) is calculated at 94 GHz with aq with 496 IDs and lb with 434 IDs.

2. Accurate & Efficient Orientation-Averaging:

The SSPs are computed for a sufficiently large number of incident directions (up to 7800 IDs only in \( \theta, \phi_s \)) 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

Staged with 48 cores & 256GB 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 \( \vec{E}_s \), and the resolution of \( \vec{E'} \) due to the use of SerialPACK.

3. Accuracy Assessment for scattering by mixed-phase hydrometeors

Using NESCoP with the sd and lb schemes enables a significant gain in computational cost, particularly for the calculation of the scattered field \( \vec{E}_s \). This gain increases with \( N \) (number of cells)

\[
\begin{array}{c}
\text{DDSCAT} \\
\text{NESCOP}
\end{array}
\]

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 JSIRT 2007

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\begin{array}{c}
\text{Solid-phase} \\
\text{Sphere}
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\text{mkd} = 0.27 \\
\text{mkd} = 3.0
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