Efficient calculation of CBFs for the modeling of scattering by complex-shaped snow aggregates

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Abstract—The Sherman-Morrison-Woodbury formula-based algorithm is applied to enhance the computational performance of the characteristic basis function method (CBFM) when applied in a context of 3D full-wave model to the scattering by complex-geometry precipitation particles. The improvement brought by this algorithm, particularly to the compression rate achieved by the CBFM, enables us to simulate electrically larger particles while maintaining a satisfactory level of accuracy and a reasonable computational cost.

I. Introduction

Recent studies have pointed out the importance of a realistic and efficient modeling of electromagnetic scattering by complex-shaped hydrometeors for a better analysis of precipitation active and passive sensors observations. In this context, we have previously developed a 3D full-wave model for EM scattering by complex-geometry and electrically large snow particles, based on an integral representation of the electric fields inside the scatterer. The model is applied, in the frequency range of 3 GHz < f < 200 GHz, to a realistic set of particles modeling aggregate ice particle with different shapes and sizes (OpenSSP). The volume electric integral equation, solved using the conventional Method of Moments (MoM), places a heavy burden on the CPU time and memory usage. To address this problem, the Characteristic Basis Function Method (CBFM) [1], which handles large radiation and scattering problems using the domain decomposition approach, was applied in order to significantly enhance the computational performance of our 3D model. The CBFM has shown good computational performance and satisfactory level of accuracy when compared to the conventional MoM and to DDScat [2], the commonly used implementation of the discrete dipole approximation (DDA). It enables us to solve electrically large snow aggregates of upward 10 million of unknowns for the lower frequencies, on a 64 GB shared memory workstation while consuming only a reasonable amount of CPU time, which is as example up to 16 times lower than DDScat for a particle discretized into 130 000 cells. Nevertheless, the model still places a heavy demand on the memory storage as well as on the CPU time for larger EM scenes. In this work, we focus on enhancing the CBFM algorithm in order to cope with the computational challenges we encounter when dealing with the simulation of electrically larger snow aggregates. This entails

the use of the Sherman-Morrison-Woodbury Formula (SMWF) to speed up the generation of the characteristic basis functions.

In this paper, we review the impact of the block size on the computational performance of the CBFM to justify the application of the SMWF for the calculation of the CBFs. We briefly detail the fast CBFs generation via SMWF. Finally, numerical results are presented to compare the performances of the new code with the conventional CBFM and DDScat.

II. EFFICIENT CALCULATION OF CBFs BASED ON THE SMWF

The CBFM algorithm begins with the decomposition of the computational domain of Nb_c elementary cubic cells into M blocks, and then proceeds to generate the Macro-basis functions (MBFs) for these blocks by solving, for each block i, the following system of linear equations

$$Z_{ii}^{MoM} E_i^{MBFs} = E_i^{IPWs} \tag{1}$$

where Z_{ii}^{MoM} is the self-coupling matrix of block i and E_i^{IPWs} represents the N_{IPWs} plane waves excitation illuminating the block i. A singular value decomposition (SVD) and a threshold of 10^{-3} are then applied to the MBFs to remove the redundancy and down-select a reduced number of basis functions for the block i. Next, the initial $3Nb_c$ basis functions and the total obtained K CBFs are combined using the Galerkin method to generate the final reduced matrix Z^c .

A. Impact of the size block on the CR

The number of CBFs K retained is much lower than the number of original low-level basis functions. The resulting compression rate is the ratio between the number of the original basis functions and the number of post-CBFM unknowns $(CR = (3Nb_c)/K)$. It is well known that increasing the size of the blocks have a positive impact on the compression rate CR achieved by the CBFM [1]. However, using large blocks also leads to a dramatic increase of the CPU time, particularly the one needed to compute the CBFs, since we increase the size of the self-coupling matrix Z_{ii}^{MoM} . To avoid this increase in the CPU time associated with the large CBFM block, while maintaining the achieved high compression rate, we use the SWMF while solving Eq. 1 for each block i. This formula was used in [3] to ensure a fast direct solution of the reduced

matrix Z^c . Here, we apply it when dealing with large blocks, in the process of generating the CBFs, to maintain a high CR without having to bear the associated computational burden both in terms of CPU time and memory requirement.

B. SMWF for the calculation of the CBFs

The SMWF-based algorithm (SMWFA) is used to efficiently solve Eq.1. It proceeds by implementing a multilevel binary division of Z_{ii}^{MoM} , where the self-coupling submatrices are subject to the next level and the off-diagonal ones are approximated by using the adaptive cross approximation (ACA) algorithm. Indeed, the basic idea of implementing the SMWFA is to recursively substitute the equation ZI = E, rewritten as

$$\begin{pmatrix} Z_{11} & Z_{12} \\ Z_{21} & Z_{22} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} E_1 \\ E_2 \end{pmatrix} \tag{2}$$

by the following two smaller systems of linear equations

$$I_1 = \hat{E}_1 - \hat{U}_{12} x_2 \tag{3}$$

$$I_2 = \hat{E}_2 - \hat{U}_{21} x_2 \tag{4}$$

where $\widehat{E}_1=Z_{11}^{-1}E_1$, $\widehat{U}_{12}=Z_{11}^{-1}U_{12}$, $\widehat{E}_2=Z_{22}^{-1}E_2$ and $\widehat{U}_{21}=Z_{22}^{-1}U_{21}$. The sizes of U_{12} and U_{21} are $(3Nb/2)\times r_1$ and $(3Nb/2)\times r_2$, while the sizes of V_{12} and V_{21} are $r_1\times (3Nb/2)$ and $r_2\times (3Nb/2)$. Nb is the number of cells per block, and r_1 and r_2 are the effective ranks of Z_{12} and Z_{21} , which result from the compression of the off-diagonal submatrices Z_{12} and Z_{21} using the ACA algorithm. We refer the reader to [3] for further details about the implementation of the SMWF-based algorithm. The recursive application of the SMWFA enables us to implement the CBFM with numerically large blocks, which ensures a high CR, without having to calculate all the $3Nb\times 3Nb$ terms of Z_{ii}^{MoM} or to solve the associated expensive system of linear equation. Finally, in order to further reduce the CPU time needed for the generation of the CBFs, the self-coupling matrices $Z_{ii}^{MoM,L}$ of the finest level (level L) are sparsified by simply discarding any element lower than $10^{-3}\times Z_{ii}^{MoM,L}(1,1)$.

III. NUMERICAL RESULTS

To check the accuracy and the computational performance of CBFM-SMWF approach, we apply it to the electrically medium complex-geometry snow particle presented in Fig. 1.



Fig. 1: Snow Aggregate divided into M=27 and 4 blocks

The particle is discretized into $Nb_c=24385$ cells (73155 unknowns) and divided into M=27 CBFM blocks for

the application of the conventional CBFM, then into only M=4 blocks to compare with the new approach. The error criterion for the ACA algorithm ϵ_{ACA} is initially set to 10^{-2} , then 10^{-3} to check its impact on the accuracy of the CBFM-SMWF. Fig. 2 shows the extinction and backscattering efficiency factors Q_{ext} and Q_{bks} as functions of the frequency f, computed for 2701 incident directions with the CBFM codes and 2352 target orientations with DDScat. Fig. 2 shows a good agreement between the results obtained with DDScat and the CBFM and those derived by the CBFM-SMWF code for $\epsilon_{ACA} \leq 10^{-3}$. With 4 large blocks, the CBFM-SMWF achieved high CR going from 164 for the higher frequency to 754 for the lower one, and needed 230 min to calculate the averaged scattered quantities. Thus, it clearly outperforms the conventional CBFM wich needed 210 min, with smaller blocks, to achieve 39 < CR < 155. Note that applied to 4 large blocks, the conventional CBFM takes 1570 min to compute the scattering quantities, while DDScat requires 3458 min to yield comparable results.

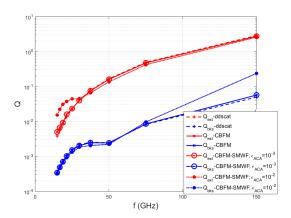


Fig. 2: Variation of orientationally averaged scattering coefficients calculated with DDScat and the two CBFM codes.

IV. CONCLUSIONS

The SMWF is used to speed-up the calculation of CBFs for scattering by complex-shaped snow particles. Results show that we can achieve a satisfactory level of accuracy, while significantly increasing the compression rate realized via the use of CBFM. We expect the CBFM-SMWF to provide even better computational performance when applied to electrically larger or to a volume of complex-geometry particles.

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