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Abstract  In a recent paper Fenni et al. (2021, https://doi.org/10.1029/2020jd034172) compared the code MIDAS, based on the direct solution of the volume-integral equation combined with advanced cubatures for orientation averaging, to the code DDSCAT, a state-of-the-art implementation of the discrete dipole approximation. This comment highlights methodological issues in this comparison and shows that the quantitative claims of Fenni et al. (2021, https://doi.org/10.1029/2020jd034172), related to superiority of MIDAS over DDSCAT, are based on very specific test cases with respect to particle symmetries or initial orientation, as well as to the selected scattering quantity of interest. Thus, these claims are not expected to hold for other similar particles. Moreover, the detailed discussion of these issues is relevant for all light-scattering simulation methods, except those allowing analytical orientation averaging. Thus, the comment constructs general guidelines for fair evaluation of orientation-averaging techniques in a wide range of light-scattering methods and computer codes.

Plain Language Summary  The paper discusses several issues that appear when one is comparing different orientation-averaging techniques (cubatures) in combination with the same or different light-scattering simulation methods. Fair evaluation of cubature performance in realistic general scenarios is important both for practitioners (to choose the most efficient combination of the existing codes and cubatures) and for code developers (to set their priorities on the new features with the largest expected benefits). Unfortunately, the performance of the cubatures is complexly interwoven with the internals of the simulation methods and depends on specific test particles and computed scattering quantities. This questions the generality of conclusions in some previous publications. Based on this discussion, the paper ends with general guidelines for fair evaluation of cubatures, allowing future studies to arrive at general conclusions, so that they can be directly used by other researchers.

1. Introduction

Fenni et al. (2018, 2021) have developed a modification of the discrete-dipole approximation (DDA) or, more generally, of the volume-integral equation (VIE) method, where the fast-Fourier transform (FFT) acceleration combined with iterative solution of the linear system (used in the production DDA codes) is replaced by the direct matrix inversion with matrix size reduced using the characteristic-basis-functions method (CBFM). This direct-solver-based (DSB) method has been shown to be superior to the standard (iterative-solver-based [ISB]) DDA for backscattering properties of large highly porous particles, when orientation averaging is required. In the latest paper (Fenni et al., 2021) the CBFM method, implemented in the code MIDAS, is combined with advanced cubatures (i.e., quadratures for 2D integrals) for orientation averaging and its performance is compared against the DDSCAT code.

The goal of this comment is to highlight certain issues in Fenni et al. (2021) which may affect the generality of its conclusions. The detailed discussion of these issues is distributed among the following five sections. While it is naturally focused on the DDA or VIE-based methods, the discussion mostly applies to any other light-scattering methods.
simulation methods as well. The only obvious exception is the T-matrix methods, which allow for analytic averaging over orientations once the T-matrix for a given scatterer is computed (Mishchenko et al., 1996). Note, however, that the fixed-orientation superposition T-matrix method, which is commonly employed for very large aggregates (Penttilä et al., 2021), do not compute the system T-matrix (despite the method name) and employ numerical orientation averaging. Finally, the conclusion summarizes the implications for validity of quantitative claims in Fenni et al. (2021) and provides general guidelines for fair evaluation of orientation averaging techniques in light-scattering simulations.

2. Specific Single-Scattering Properties

The relative performance of various methods may largely depend on the calculated single-scattering property (SSP). The principal difference lies between integral or backscattering quantities (cross sections) and angle-resolved ones. The latter generally depend on all three Euler angles describing the orientation of the particle. I further use the “zyz-notation” for the angles $\alpha$, $\beta$, and $\gamma$ (Mishchenko & Yurkin, 2017; Okada, 2008; Um & McFarquhar, 2013; Yurkin & Hoekstra, 2011)—it corresponds, respectively, to $\gamma$, $\alpha$, and $\beta$ in Penttilä and Lumme (2011), and $\Phi$, $\Theta$, and $\beta$ in the DDSCAT code (which employs the xzx-notation) (Draine & Flatau, 2020). The first Euler angle, $\alpha$, can be equivalently represented by a rotation of the scattering plane around the propagation axis. On the one hand, such rotation is computationally cheap for iterative methods, since only a single solution of the DDA equations is required. The same applies to other light-scattering methods, which obtain orientation-averaged results from simulations for many fixed orientations. On the other hand, this rotation is irrelevant for integral and backscattering quantities—a single scattering plane with two incident polarizations is sufficient, see Equation 4 in Fenni et al. (2021). That is why only two angles are used for averaging in Fenni et al. (2021), specifically, $\theta$ and $\phi$ polar angles of the incident direction in the scatterer reference frame, which correspond to the Euler angles $\beta$ and $\gamma$.

For the DSB methods all rotation angles are equally cheap (a single matrix inversion is performed anyway), thus the relative comparison of the DSB versus ISB methods will depend on the scattering quantity. The quantities, involving orientation averaging only over $\beta$ and $\gamma$, are the most suitable for the DSB methods. This is especially so for the backscattering quantities, since they are known to require a lot of orientations for accurate results (Gasteiger & Wiegner, 2018; Kanngießer & Kahnert, 2021; Virkki et al., 2014), see also Figure 4 of Fenni et al. (2021). By contrast, angle-resolved scattering quantities, for example, the Mueller matrix for intermediate scattering angles, will require similar total number of orientations, but this number is now distributed over three angles, with the finest discretization used for the cheap $\alpha$. This can be qualitatively explained by Monte-Carlo arguments—the total integration error in several dimensions depends on the total number of function samples. Overall, previous studies (Gasteiger & Wiegner, 2018; Kanngießer & Kahnert, 2021) showed that the Mueller matrix and forward scattering quantities converge faster with total number of ($\beta, \gamma$) pairs than that for backscattering quantities. Thus, the same simulation accuracy can be achieved with fewer iterative solutions, making the ISB methods more favorable. Therefore, the conclusion of superiority of the DSB methods for backscattering quantities in Fenni et al. (2021), specifically MIDAS versus DDSCAT, do not necessarily hold for angle-resolved scattering quantities unless backscattering direction is relevant for a specific application (contrary to the general claims in the abstract).

3. Symmetric Scatterers

The comparison of different cubatures for a thin cylinder (Figures 3 and 7 of Fenni et al. (2021)) is artificially favorable for the advanced ones. The corresponding integrand is independent of the angle $\gamma$ due to the axial symmetry of the scatterer. Thus, the simple cubatures perform a lot of identically equivalent simulations wasting the computational resources. By contrast, the advanced cubatures incur less repetitions. In other words, using the same total number of pairs ($\beta, \gamma$), the advanced cubatures result in larger number of distinct values of $\beta$. Therefore, the drastic superiority of the advanced cubatures for a cylinder is largely due to the “irregular” placement of sample points, which makes them sub-optimal even for such symmetric case. This is a nice-to-have property, however, all cubatures would benefit from explicit consideration of the existing symmetry, reducing the integral to a 1D one, as recommended by the manuals of the DDA codes (Draine & Flatau, 2020; Yurkin & Hoekstra, 2020). Using high-order quadratures for the remaining 1D integral is still beneficial, but the difference
is not expected to be that large. Moreover, the total number of required orientations for symmetric scatterers is significantly smaller, making the ISB methods artificially more favorable to the DSB ones.

Therefore, although a cylinder is understandably a convenient test object, exemplified by a lot of data in Figure 8 of Fenni et al. (2021), the corresponding conclusions cannot be directly generalized to non-symmetric objects. This is similar to the issue encountered during comparison of several DDA codes (Penttilä et al., 2007). When non-symmetric aggregates were considered, all four tested codes showed very similar accuracy. By contrast, for axisymmetric scatterers (cylinder and oblate spheroid, see Figures 3 and 4 of Penttilä et al. (2007)) the accuracy of the ADDA code seems to be significantly worse than that for other codes. However, as explained in that paper this was caused by minor differences in the default orientation-averaging schemes of the code (using even or odd number of points per full angular range) and can be easily corrected. More details are given in (Comparison with Other DDA Codes [at ADDA Wiki], 2021).

To conclude, the tests of the orientation averaging can be considered general only if performed on non-symmetric particles. The optimization of orientation averaging for symmetric particles is also a relevant problem. But, although some cubatures may perform sub-optimally out of the box, better efficiency can always be obtained by explicitly reducing the integration domain based on the symmetry. In any case, the relative behavior of various cubatures (and simulation methods) will be specific to these cases and cannot be directly generalized to particles with other symmetries.

4. Particularly Unfavorable Initial Orientation

From all the considered irregular aggregates, Fenni et al. (2021) have focused on “a0012,” which was the most problematic for DDSCAT (see Figures 10 and further from that paper). However, this case is artificial, not even due to specific shape of the aggregate, but mostly due to its specific orientation. This aggregate has a strong dependence of backscattering intensity on rotation angles with a peak at the default orientation (due to a specular reflection from one plane constituent). Thus, the angular region, where most of the integral value is gathered, happens to be greatly undersampled by the default orientation averaging scheme of DDSCAT, see Figure 11 of Fenni et al. (2021). A simple fix for this issue is a random initial (one-time) rotation of the aggregate before further averaging is performed. Actually, such random initial orientation is implicitly included in any random generation of the scatterer, which is commonly used in large-scale simulations of irregular particles. By contrast, Fenni et al. (2021) have used a “representative” set of manually chosen aggregates, from which one turned out to be very non-representative.

The conclusion is similar to that for symmetric scatterers above. The advanced cubatures do have a nice property of being (almost) invariant to the initial rotation of the scatterer, while simple ones need special attention not to stumble on a particularly unfavorable case. Still, even if such case is encountered it can be easily circumvented. In any case, the relative performance of cubatures, especially of the one built into the production DDA codes, should not be judged on such special cases. In particular, the quantitative conclusions of Fenni et al. (2021), including relative computational times of MIDAS versus DDSCAT, should be based on other nine aggregates (considered in Figure 9 of that paper, which does not include DDSCAT results) rather than on the aggregate a0012.

5. Choice of a Proper Reference

Although the DDA is often regarded as a method with moderate accuracy at best, this opinion is an implication of relatively large computational requirements, motivating users to search for a compromise between accuracy and simulation time. In fact, the DDA is a numerically exact method, that is, it can reach any predefined accuracy given sufficient computational resources (Yurkin & Hoekstra, 2007). On the one hand, the convergence with refining discretization is slow due to the used low-order approximation of the fields inside each voxel (discretization element); the error is linear or quadratic in the voxel size (Yurkin et al., 2006a). On the other hand, this voxel size is the main parameter determining the final simulations accuracy for scatterers with fixed orientation. This allows simple error control in the DDA varying a single parameter (Draine & Flatau, 2020; Yurkin & Hoekstra, 2020) and even increasing the order of the numerical scheme using the Richardson extrapolation (Yurkin & Kahnert, 2013; Yurkin et al., 2006b).
When orientation averaging is employed, another parameter comes into play—the number of orientations. The error control is still straightforward, but varying only one parameter (e.g., the number of orientations) leads not to the exact solution, but rather to a well-orientation-averaged result for a given voxel size. The latter determines the remaining error. Importantly, the FFT acceleration used in the ISB DDA incurs no approximations, that is, it does not affect the simulation results (above the level of machine precision).

By contrast, MIDAS employs the CBFM that accelerates computations through a certain truncation, which necessarily implies approximation. The parameters of this truncation affects the final accuracy and further complicates the error control. Moreover, the errors introduced by some values of these parameters depends on the specific problem, voxel size, and number of orientations. Therefore, further analysis is somewhat speculative due to the limited amount of data in Fenni et al. (2021).

For example, the MIDAS accuracy of backscattering quantities for particles in a fixed orientation is on the order of several percent; 7% is mentioned in Fenni et al. (2021) for one case. This inaccuracy propagates into orientation averaged properties (with some reduction due to averaging), that is, convergence of the orientation-averaged results with increasing number of orientations, for example, down to 0.1% does not imply the same accuracy of the obtained value. Consider, for instance, Figure 10 (top-right panel) of Fenni et al. (2021). Here the DDSCAT result seems to be well-converged, which is expected for low frequencies, since then the specular reflection is not present. The MIDAS also converges (using any cubature), but to a value, which is 1.3% off the DDSCAT limit. Given the same discretization used for both methods, one can conclude that this difference is due to the CBFM error. This implies that the discussion of this figure in the text is misleading, for instance “the relative differences … stabilizes at 1.3% for DDSCAT” suggests that DDSCAT cannot reach better accuracy, which is not true. Moreover, this panel shows that the default orientation scheme of the DDSCAT converges faster than the simplest cubature (“aq”) used in MIDAS. This reiterates the conclusion of Section 4 that the former is not inherently inferior but rather very unsuitable for the case with strong specular reflection.

For 35.6 GHz (bottom-left panel at the same figure), DDSCAT also seems to converge (albeit not so conclusively) to a value about 1%–2% off the MIDAS value. Note also that the error of the CBFM is expected to increase with frequency (or, equivalently, scatterer size parameter) unless special care is exercised in tuning its parameters. Therefore, any comparison of MIDAS versus DDSCAT should be considered keeping this uncertainty of a couple of percent in mind. This, however, does not affect the conclusion of bottom-right panel of the same figure (for 94 GHz), where the orientation averaging scheme of the DDSCAT definitely fails. Still, the quantitative claims of Fenni et al. (2021) that MIDAS can reach 1% accuracy of backscattering quantities using some number of orientations is misleading, since the real error can be a few times larger.

To conclude this section, a general piece of advice for comparing simulations methods is to treat the produced results as experimental ones, by including uncertainties. Naturally, the uncertainties of numerical experiments need to be justified (properly estimated) and include all sources of errors. While, unfortunately, it is not common for the published results of the DDA-like codes, the methods to estimate such uncertainties do exist (Yurkin et al., 2006b). Then one can unambiguously choose the proper reference for any computed quantity as the one with the smallest uncertainty (Gilev et al., 2010; Kanngießer & Kahnert, 2021; Liu et al., 2018; Yurkin & Kahnert, 2013). And the latter uncertainty would quantify the confidence level associated with any computed differences.

6. CBFM Truncation as Regularization

Let us further consider the CBFM errors in more details. The corresponding truncation is similar to the one used when the optical properties of a scatterer are represented by a finite T-matrix (Mishchenko et al., 1996). In this case the truncation of high-order multipoles directly corresponds to a smoother light-scattering pattern and smoother dependence of any SSP on the particle orientation. This is beneficial for advanced cubatures since they are designed to be exact for spherical harmonics of up to a certain order. Thus, MIDAS with advanced cubatures seems to be almost equivalent to computation of the (truncated) T-matrix from the VIE with further analytic orientation averaging (Herranen et al., 2017; Løke et al., 2009; Mackowski, 2002). Importantly, there is a synergetic effect between the CBFM used for simulations of fixed-orientation SSPs and the orientation-averaging cubature.
On the one hand, such synergy is definitely useful, as ultimately fewer number of orientations are required. Moreover, this is analogous to spectral filtering or regularization—well-established techniques to improve the convergence of a wide range of numerical techniques. On the other hand, the regularization has a drawback—the final result is somewhat different. The more one smoothes the integrated function—the faster orientation averaging converges but the larger is the error due to the smoothing itself. Moreover, the final accuracy is determined not so much by the number of orientations (as mentioned above, potentially even analytical averaging can be used), but rather by the CBFM truncation.

Generally, any comparison is the most conclusive if a single parameter is varied at a time, for example, if the DDSCAT with both default and advanced cubatures is compared against that for MIDAS. But the above synergy makes such separation of effects not possible. In particular, the improvement in MIDAS itself when switching from a simple to an advanced cubature is probably more pronounced than it would be for the DDSCAT. Thus, one has to resort to the strategy of comparing the accuracy of final results when several parameters are changed at once. This is exactly what is done in Fenni et al. (2021) but with the focus on varying the same parameter, specifically the number of orientations. By contrast, unambiguously comparing the final accuracy requires varying different parameters (the most relevant ones) for each method. While the number of orientations seems a suitable option for DDSCAT (or any DSB-DDA) when sufficiently fine discretization is employed, the CBFM parameters need to be considered for MIDAS (as discussed in Section 5).

7. Conclusion

Overall, this comment does not question the qualitative conclusions of Fenni et al. (2021): First, advanced cubatures are indeed more versatile and efficient than the simple ones for orientation averaging of SSP, whatever is the underlying simulation method (among the VIE family). Second, the DSB methods with CBFM acceleration may outperform the ISB DDA for backscattering properties of large highly porous and/or very non-compact particles (which volume is much smaller than that of the circumscribing rectangular box), when orientation averaging is required. Note, however, that this specific superiority niche is not accurately described in the abstract of Fenni et al. (2021), where too general phrase “complex-shaped” is used. Moreover, one can also add another conclusion to this list, namely inherent smoothing in CBFM can accelerate orientation averaging for a fixed required accuracy (at the cost of more complicated error control). However, the comment shows that many of the quantitative conclusions of Fenni et al. (2021), like “can be greater than three orders of magnitude more efficient” are based on very specific test cases, and need significant changes (and further research) to be generalized to other ones.

Finally, based on this discussion, let us formulate the following guidelines for a fair evaluation of orientation-averaging cubatures in any light-scattering method (unless analytic averaging is possible):

- Perform separate tests for SSPs requiring averaging over two or three Euler angles. While one of them can be sufficient for a specific application, do not blindly apply conclusions from one class of SSPs to the other.
- Base all conclusions on tests for general non-symmetric particles. If orientation averaging for symmetric particles is required, this symmetry should be explicitly accounted for (reducing the range of Euler angles) before any cubature is applied.
- Avoid special initial orientations of the scatterers, for example, ones with strong specular backscattering. If such scatterers appear in practice, apply one-time random rotation before averaging.
- Separate the accuracy (or convergence speed) of the cubature from the accuracy of the underlying method. Specifically, compare the same method with different cubatures and the same cubature with different methods.
- The above separation may be hard for the light-scattering methods that perform some truncation, filtering, or regularization. Then the parameters of the method may affect the convergence of the cubatures, especially high-order ones (the stronger filtering—the faster cubature convergence). In this case compare the final obtained accuracy of a combination method + cubature.
- When comparing any computed values, always consider associated uncertainties. The latter should be estimated accounting for all relevant sources or errors (internal method parameters) that may be largely different for different methods.
- These uncertainties are critical for selecting a proper reference and making quantitative statements about the optimal values of parameters. In particular, requiring each method to reach a certain accuracy under variation of a single parameter (e.g., the number of orientations) is only meaningful if the uncertainty of the limiting value (due to other method parameters) is less than this prescribed level.
These guidelines should help researchers to make general conclusions from their data. This, in turn, can further be used to reliably select the optimal combination of a method and cubature for a specific application and to steer further development of light-scattering methods and corresponding computer codes.

Data Availability Statement

Data were not used, nor created for this research. Software (other than for typesetting) was not used for this research.

References


