Demonstration of an overlap range of size parameters for reliable exact and approximate methods of computing single-particle scattering optical properties

R. Lee Panetta[a,b*], Ping Yang[a], Jiachen Ding[a], Michael Mishchenko[c], and Siyao Zhai[a]

[a]*Department of Atmospheric Sciences, Texas A&M University, College Station, Texas, USA*
[b]*Department of Mathematics, Texas A&M University, College Station, Texas, USA*
[c]*NASA Goddard Institute for Space Studies, 2880 Broadway, New York, NY 10025, USA*

[*]*Presenting author (panetta@tamu.edu)*

Using any of several numerical methods based directly on Maxwell's equations to calculate single particle scattering becomes increasingly demanding of computational resources as the size parameter of the particle increases, and as the particle's index of refraction departs significantly from unity. With these so-called "exact" methods, at any given time there is an upper bound on the size parameter that is feasible for general and practical use, i.e., for "random orientation" calculations of particles that have arbitrary shapes and have indices of refraction that are not close to 1. The bound depends essentially on the state of hardware and software development at that time: beyond the size parameter bound exact methods may be used only under specializing assumptions like symmetry, or single-orientation, or index of refraction differing only slightly from unity. On the other hand, for large enough size parameters, numerical methods that are based on variously improved versions of geometrical and physical optics methods are adequate for computing single scattering properties of practical interest. These methods are not based directly on Maxwell's equations but on physical approximations to the scattering process, and there is an effective lower bound on the size parameter for reliable calculations set by the physical approximations made.

Until recently there has been a gap in sizes between the upper bound of what can be feasibly handled handled by an exact method and the lower bound on what an approximate method can reliably treat. In this talk we describe success in closing the gap that has recently been achieved by using the exact Invariant Imbedding T-Matrix (II-TM) method in conjunction with an approximate Physical Geometric Optics Method (PGOM). The gap is closed in the sense that there is an overlap range of size parameters, roughly 100–300 in which the two methods agree well in their calculation of single-scattering optical properties. The II-TM method requires no special assumptions on particle symmetry, but it is possible to accelerate the computation of properties when some symmetries are present by improvements in the II-TM algorithm.

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