

# Capabilities of the Discrete Dipole Approximation for Large Particle Systems

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**Abstract**— The discrete dipole approximation (DDA) is a general method to simulate light scattering by arbitrary particles. This talk reviews the DDA with focus on its application to very large particle systems, typically consisting of large numbers of particles with sizes comparable to or larger than the wavelength. Overall, the DDA is a viable option for such problems – it is conceptually simple, can naturally handle arbitrary inhomogeneous particles, and benefits from the availability of open-source codes. However, the major limitation is the computational complexity rapidly increasing with the size of the system. A few ideas to alleviate this issue are discussed, including the fast multipole method and the multi-grid DDA. While the DDA is equally applicable to both connected and disconnected particle systems, when applied to the latter it provides some insights into the notion of multiple scattering.

## I. INTRODUCTION

The discrete dipole approximation (DDA) is a general method to simulate scattering and absorption of electromagnetic waves by particles of arbitrary shape and internal structure [1], [2]. Initially, the DDA (sometimes referred to as the “coupled dipole approximation”) was derived on the basis of the physical picture of the point dipoles set [1], [3]. These dipoles interact with each other and the incident field, giving rise to a system of linear equations, which is solved to obtain dipole polarizations. The latter are further used to compute any measured scattering quantities. It is this appealingly simple description of the method coupled with the availability of optimized open-source codes [1], [4] that led to numerous applications of the DDA varying from interstellar dust to nanoparticles and biological cells.

Alternatively the DDA can also be derived by discretization of the volume integral equation for the electric field [5], [2]. This derivation rigorously proves the validity of the DDA and, thus, puts it in line with other numerically exact methods, i.e. its accuracy can be made as good as required given infinite computational resources. Moreover, it provides a solid base for the extension of the DDA to other physical phenomena and complex environments, which have recently become relevant to nanoscience [6], [7].

In this talk, I will review the DDA with focus on scattering by very large particle systems, typically consisting of large numbers of particles with sizes comparable to or larger than the wavelength  $\lambda$ . From a physical viewpoint, that is the simplest scattering problem, the same as it was 40 years ago [3]. The major challenge, however, is related to the required computer resources due to overall size of the particle system. That is why

the most interesting results have been obtained only recently. While the connectedness of the system has no effect on the DDA simulation *per se*, I will discuss several attempts to use the DDA to gain insights into the controversial notion of multiple scattering.

## II. COMPUTATIONAL CHALLENGE

The main computational bottleneck of the DDA is the solution of the system of  $3N_d$  complex linear equations, where  $N_d$  is the number of dipoles (volume discretization elements). Since  $N_d = 10^9$  is feasible [4], one has to resort to the iterative solution of the linear system. Moreover, a regular cubic discretization of the particle is commonly employed, allowing the use of the fast Fourier transform (FFT) to accelerate matrix-vector products [8]. The total computational complexity is then  $\mathcal{O}(N_{it}M\ln N)$ , where  $N_{it}$  is the number of required iterations and  $N$  is the number of dipoles, including the void ones, in the minimal rectangular box enclosing the scatterer.

The value of  $N$  is affected by three factors. The first one is the overall size parameter of the particle system  $x$  and the refractive index  $m$ . The rule of thumb is to use at least 10 dipoles per the wavelength in the medium [2], which implies  $N = \mathcal{O}((x|m|)^3)$ . The second factor is the porosity, i.e. the ratio  $N/N_d$ , which adds a constant factor to the previous estimate. While for compact shapes (e.g. ellipsoids) this ratio is of order 1, it can be much larger for particle systems. The third issue is the accuracy of the simulations. While it is hard to estimate *a priori*, more dipoles per  $\lambda$  are generally required to reach satisfactory accuracy when increasing  $x$  and/or  $m$  [2], [9]. Moreover, finer dipoles may be required to adequately model the shape of each monomer, if the latter is smaller than  $\lambda$ .

There exist at least two viable ideas to alleviate the effect of large porosity. The first one is to replace FFT acceleration by the fast-multipole method (FMM) [10], [11], which has potential scaling from  $\mathcal{O}(N_{it}N^{3/2})$  to  $\mathcal{O}(N_{it}N\ln^2 N)$  depending on the number of levels in multipole hierarchy. The problem is that such scaling can only be rigorously proven in combination with error analysis, which has not yet been done for the DDA, in contrast to the surface-integral-equation method [12]. Moreover, the FMM is much harder to parallelize efficiently, especially the multi-level variant.

The second option can be called a multi-grid DDA [13], [14]. A separate regular cubic grid is used for each of  $M$  compact particles, so the total number of grid points is comparable to  $N_d$ . Matrix-vector product is computed block-wise, where each block-block product is FFT-accelerated (with

a constant shift vector between two lattices). Assuming all particles to be comparable in size, the total complexity is  $\mathcal{O}(N_{it}N_d(\ln N_d + M))$ , which is faster than the standard DDA if  $N > N_d M$ . The only problem is that parallelization of this approach would require non-trivial load balancing, especially when monomers significantly vary in size.

The value of  $N_{it}$  increases with  $x$  and  $m$  and depends on the choice of iterative solver and DDA formulation. There is some progress in understanding (estimating) the behavior of  $N_{it}$  for particles smaller than  $\lambda$  [15], [16]. However, the known results for larger particles are fragmentary –  $N_{it}$  rapidly increases with  $x$  for real  $m$  [9], [17], but at a slower rate (linear with  $x$ ), when  $\text{Im}(m)$  is moderately large [18]. Moreover, large porosity should be of great help, since it reduces the overall interaction magnitude between the dipoles, hence, the condition number of the interaction matrix and  $N_{it}$ . As an extra benefit  $N_{it}$  only slightly depends on  $N_d$ ; thus, refining discretization for a fixed scattering problem implies predictable costs of computer resources.

Averaging over the orientation of the particle system presents additional challenge, since the calculations need to be performed anew for each combination of two of the three Euler angles, in contrast to fast analytical averaging in T-matrix methods [19]. Moreover, the required number of orientation increases with  $x$ . While optimization of the integration scheme (cubature) is possible [20], [21], the major progress is expected from optimization of repeated DDA runs, either by educated guess of initial vector based on results for similar orientations [22] or by block-iterative methods [23]. Similar ideas can be employed to repeated calculations with other varying parameters, such as  $x$  and  $m$  [24] or  $\lambda$  [25].

### III. SIMULATION EXAMPLES

Despite the abovementioned computational challenges the DDA has already been used for simulation of different large particle systems [26]–[37], mostly enabled by the parallelized computer code ADDA [4]. The DDA has also been used for moderately sized systems with large number of particles, resulting in comparable computational requirements [38]–[42]. Both these cases can be considered a discrete random medium, as reviewed in [43]. Alternatively, one may use periodic boundary conditions to model infinite inhomogeneous media [44], [45]. However, this can adequately account only for those of the relevant effects that are determined by short-range interaction.

I will review most interesting simulation results from the above papers in my talk, but in this extended abstract only a single example is presented, adapted from [43]. While far from being the most challenging one ( $N_d \leq 1.1 \times 10^6$ ), this example shows that the DDA can produce accurate results even for complex inhomogeneous systems. The system is composed of a host sphere, filled with 10 randomly positioned spherical inclusions, illuminated by a plane wave. Their size parameters are 10 and 2.5 and refractive indices are 1.33 and  $1.55 + 0.003i$ , respectively. The results were averaged over orientation of the system. The DDA simulations were performed with the code ADDA 1.2 [4], using five levels of discretization between 64 and 128 dipoles per diameter of the host sphere. Then the results were extrapolated to infinite discretization [46]. The corresponding phase function is plotted

in Fig. 1 in comparison with the results of the superposition T-matrix method (STMM) [47]. The quantitative agreement between the two methods is quite good with relative differences less than 1% for almost all scattering angles.

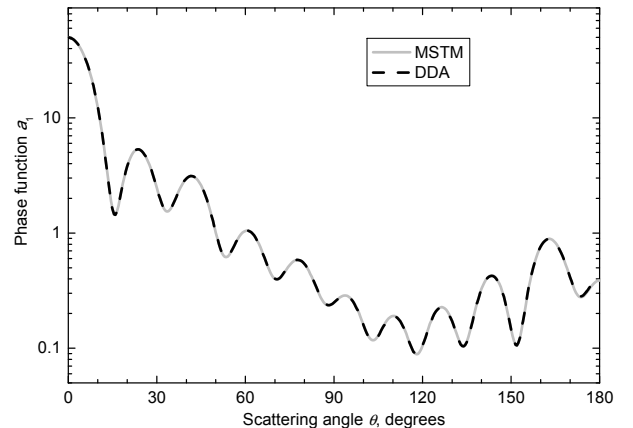


Fig. 1. Orientation-averaged phase function for a sphere filled with 10 smaller spheres (see text), computed with the DDA and STMM. Adapted from [43].

### IV. MULTIPLE SCATTERING

In the framework of frequency-domain electromagnetics, multiple scattering is not a real physical phenomenon, since the whole system interacts simultaneously with monochromatic (and, hence, infinitely long) incident wave. Still this notion can be a useful mathematical concept, related to the Neumann expansion of inverse operator (matrix). Generally, it is expressed as the order-of-scattering expansion of the Foldy equations for the electric field [43].

With respect to the DDA, the corresponding framework is called the scattering-order formulation (SOF) [48]–[50]. It is extremely simple to implement and gives a direct indication of magnitude of interaction between different particles in a system, i.e. how fast the expansion converges. However, the latter also depends on the self-interaction of constituent particles, which may become dominant if the particles themselves are large. The main drawback of the SOF is the limited domain of convergence (in terms of  $x$  and  $m$ ) [49] in contrast to the always solvable original Foldy or DDA equations. Moreover, from a numerical viewpoint, the SOF is a stationary Krylov-subspace iterative solver, which is always (even when rapidly converges) inferior to nonstationary ones discussed in Section II.

Still, the SOF can be useful in a following feasible two-level method for a sparse system of large particles. At the second level the DDA equations should be solved for each of the particles independently, while at the first level the interactions should be exchanged through the SOF to modify the incident fields for the second one. Such approach may additionally benefit from multi-grid or FMM ideas.

Alternatively, the effect of multiple scattering can be assessed directly varying the separation between the particles [27]–[29], [34], [40], [42], [44]. More subtle approaches include modification of DDA internals, e.g. removing parts of the Green’s tensor [51]. However, the interpretation of such results is ambiguous, since the modification may influence other DDA parts as well.

## CONCLUSION

Overall, the DDA is a viable option to simulate light scattering by large particle systems or particulate/porous media. The method is conceptually simple, can naturally handle arbitrary irregular and/or inhomogeneous particles, and benefits from the availability of open-source optimized user-friendly codes. Thus, it is especially promising for studies involving variations of system morphology, including particle shapes.

The major drawback is the reverse side of the DDA generality – the large computational requirements due to the employed volume discretization. Certain ideas to alleviate these problems do exist, especially for systems of significantly separated particles. However, the specialized methods are expected to always be superior to the DDA for systems with simple morphology, e.g., STMM for aggregates of spherical particles. Also, the combination (hybridization) of the DDA with simpler asymptotic methods, such as geometrical optics seems a promising direction of research, but no specific ideas are currently available. Alternatively, one can simply wait for more powerful supercomputers to become available and make a specific problem solvable with the DDA.

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