Optimization of the discrete-dipole approximation for large optically soft particles

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Background

The discrete dipole approximation method (DDA) solves the direct light scattering problem, i.e. calculates the light scattering pattern (LSP) given the parameters of the particle (scatterer) and the incident wave [1]. The drawback of the DDA is the significant computational time. Moreover, a large number of launches with different scatterer parameters are often required. The latter is relevant in solving inverse problems (characterization of single particle by LSP), when a previously calculated database of LSPs (up to a million elements) is used. In biological applications of the DDA, we usually deal with large optically soft particles i.e. $|m-1| \ll 1$ and $x \gg 1$, where m – relative refractive index, $x = kR$ – size parameter, k is the wave vector, R is the (effective) radius of the particle. In this regard, the task of optimizing the DDA for such particles is relevant. The most time-consuming and resource-intensive part of DDA is the solution of a system of linear equations. This time depends on the initial electric field inside the particle (first guess in the iterative solver). Thus, it is important to have as accurate guess as possible, at least among those obtainable with little extra calculations.

Results

To solve this problem, we propose a modified Wentzel-Kramers-Brillouin approximation (WKBr). The original WKB takes into account the phase shift of the incident wave in a particle [2,3]. The WKBr accounts also for the refraction at the boundary. In this work, we showed that the WKB eliminates the error of order $x(m-1)$ in the internal field, and WKBr – all errors of order x (with any dependence on m). Our theoretical and numerical analysis uncovers the scaling of various optical phenomena (refraction, reflection, ray focusing) with m and x, which supports the design of the WKBr (leaving only the significant and easy to implement corrections). Refining the internal electric field, we also considered the problem of the additional phase $\pi/2$ at the passage of a focal line [4]. Simulation results for spheres shows that the WKBr both improves the accuracy of the internal fields and accelerates the DDA simulation. In some cases, such as a sphere with $x = 250$ and $m = 1.1$, the DDA iterative solver converges to the relative residual of 10^{-3} only when the WKB or WKBr are used as a first guess. Moreover, the WKBr is significantly superior to the WKB in this case.

References

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