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Comparison of scattering calculations for aggregated particles based on different models

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Abstract

Various theoretical methods and corresponding computer programs exist which can be used to compute electromagnetic scattering by a cluster of several arbitrarily shaped particles. The aim of this paper is to compare results of various theories to find the range of applicability of the different methods. At first some comments will be made on the programs employed: the order-of-scattering Mie program (OS-Mie), the discrete dipole approximation (DDSCAT) and the multiple multipole program (MMP). As examples, results for four spheres within varying distance will be compared. In addition computations of the scattering of one bigger transparent sphere with two smaller absorbing ‘satellite’ spheres and of the scattering of two small oblates will be presented. A table includes data to give a hint on the computational demands. © 1999 Elsevier Science Ltd. All rights reserved.

1. Introduction

There is increasing interest to simulate multiple scattering by a cluster of spheres because agglomerates of aerosol particles may be modeled in this way. In addition, it is possible to approximate irregular particles by a cluster of spheres, see e.g. [1].

Scattering of such agglomerates can be simulated most effectively by a program employing Mie-theory and the translation addition theorem for vector spherical harmonics. Various schemes utilizing this method have been developed and different ways to calculate the addition coefficients have been discussed by Fuller [2], Bruning and Lo [3], Borghese et al. [4], Hamid et al. [5], Mackowski [6], Quinten [7] and others. This approach can also be extended to the *T*-Matrix

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method [8] to compute scattering of neighboring spheroidal particles. Yet the T -Matrix method is restricted to clusters of which the enclosing spheres of the individual spheroids do not overlap. As we are especially interested in closely packed clusters we looked for other scattering methods.

Of course every volume discretization method can be used, e.g. the discrete dipole approximation (DDA), as was done by Xu [9] and Flatau [10] or the finite difference time domain method (FDTD), as shown by Videen [11], but the computational demand of these methods is very high.

Therefore surface-based methods, like variants of generalized multipole technique (GMT), are considered to be of advantage and have already demonstrated their capabilities as Dahl [12,13], Ludwig [14] and Eremin [15] investigated. But the GMT methods may suffer from a different problem which will be investigated in this paper. It may be difficult to handle small distances between the scattering particles.

The programs DDSCAT and MMP were selected for different reasons:

The discrete dipole approximation (DDA) code DDSCAT by Draine [16] is public domain software, well worked out and a *relatively fast* volume integral equation (VIE) technique.

The MMP program by Hafner and Bomholt [17] is very flexible concerning the choice of geometry of the scatterer and type of expansion functions, as well as capable of considering symmetries of a scattering problem and is therefore quite effective.

There are already some papers comparing one or the other of the spherical translation addition theorem-schemes to a different scattering computation approach, e.g. by Flatau [10] and Xu [9]. They found a satisfying agreement between the extended Mie-programs and DDA.

In this paper each method will at first be introduced shortly. The multiple scattering Mie program is based on the translation addition theorem coefficients calculated as proposed by Mackowski [6] and the order-of-scattering iterative scheme introduced by Fuller and Kattawar [2]. We will give a short description of DDA with a remark on the integral over the singularity, and excerpt the theory of MMP for the sake of completeness. Then numerical examples will follow, including a table showing computational demands and scattering intensity diagrams.

As there are many parameters which may influence the scattering behavior of agglomerates of arbitrary shaped particles of different materials, we chose to begin with the investigation of simple configurations of spheres. The idea was to attain an impression as to the reliability and capability of the programs employed.

As examples we will show simulational results of scattering by four-sphere chain-like aggregates with various distances between the spheres, as well as solutions for an aggregate of one larger transparent sphere with two smaller absorbing ‘satellite’ spheres. One example of two closely packed oblate spheroids will demonstrate the ability of MMP and DDSCAT to handle clusters of more complex particles.

2. The order-of-scattering Mie-program

Many methods have been developed to solve the scattering problem of neighboring spheres [2–7]. Most of them use a superposition ‘ansatz’ to construct the total solution for the external field by a summation over all individual solutions.

All fields are expanded into spherical vector wave functions (SVWF):

$$\mathbf{E}_i^s = \sum_{n=1}^{\infty} \sum_{m=-n}^n [a_{mn}^i \mathbf{N}_{mn}^{(3)}(\mathbf{r}_i) + b_{mn}^i \mathbf{M}_{mn}^{(3)}(\mathbf{r}_i)], \quad (1)$$

where \mathbf{E}_i^s is the scattered field of the i th sphere, a_{mn}^i , b_{mn}^i are the unknown expansion coefficients, $\mathbf{M}_{mn}^{(3)}(\mathbf{r}_i)$ and $\mathbf{N}_{mn}^{(3)}(\mathbf{r}_i)$ are the vector spherical harmonics, defined by

$$\mathbf{M}_{mn}^{(1,3)}(\mathbf{r}) = \nabla \times \mathbf{r} \begin{pmatrix} j_n(r) \\ h_n(r) \end{pmatrix} P_n^m(\cos \Theta) e^{im\phi}, \quad \mathbf{N}_{mn}^{(1,3)}(\mathbf{r}) = 1/k \nabla \times \mathbf{M}_{mn}^{(1,3)}(\mathbf{r}). \quad (2)$$

These expansions have to be transformed using the translation addition theorem for SVWF from one expansion origin at the center of a sphere to another at the center of a second sphere:

$$\mathbf{M}_{mn}^{(3)}(\mathbf{r}_j) = \sum_{l=1}^{\infty} \sum_{k=-l}^l [A_{kl}^{mn} \mathbf{M}_{kl}^{(1)}(\mathbf{r}_i) + B_{kl}^{mn} \mathbf{N}_{kl}^{(1)}(\mathbf{r}_i)], \quad (3)$$

$$\mathbf{N}_{mn}^{(3)}(\mathbf{r}_j) = \sum_{l=1}^{\infty} \sum_{k=-l}^l [A_{kl}^{mn} \mathbf{N}_{kl}^{(1)}(\mathbf{r}_i) + B_{kl}^{mn} \mathbf{M}_{kl}^{(1)}(\mathbf{r}_i)],$$

to satisfy the boundary conditions.

In this way a linear equation system in terms of the scattering coefficients is determined.

$$a_{mn}^i = -\hat{a}_n^i \left(p_{mn}^i + \sum_{j=1, j \neq i}^N \sum_{l=1}^{\infty} \sum_{k=-l}^l [A_{mn}^{kl}(\mathbf{r}_{ji}) a_{kl}^j + B_{mn}^{kl}(\mathbf{r}_{ji}) b_{kl}^j] \right), \quad (4)$$

$$b_{mn}^i = -\hat{b}_n^i \left(q_{mn}^i + \sum_{j=1, j \neq i}^N \sum_{l=1}^{\infty} \sum_{k=-l}^l [A_{mn}^{kl}(\mathbf{r}_{ji}) b_{kl}^j + B_{mn}^{kl}(\mathbf{r}_{ji}) a_{kl}^j] \right)$$

$$\Rightarrow \mathbf{a}^i + \sum_{j=1, j \neq i}^N X^{ji} \mathbf{a}^j = \mathbf{p}^i \quad \text{with } \mathbf{a}^i = \begin{pmatrix} a_{mn}^i \\ b_{mn}^i \end{pmatrix}, \quad \mathbf{p}^i = \begin{pmatrix} -\hat{a}_n^i p_{mn}^i \\ -\hat{b}_n^i q_{mn}^i \end{pmatrix} \quad (5)$$

where \hat{a}_n^i , \hat{b}_n^i are the Mie-coefficients of the isolated i th sphere.

The vector addition coefficients A_{kl}^{mn} and B_{kl}^{mn} can be obtained by an iterative scheme, as was shown e.g. by Mackowski [6]. First the scalar addition coefficients C_{kl}^{mn} are calculated by recurrence relations. The next step is to take advantage of the equations, which relate the scalar to the vector addition coefficients, derived by Stein [18]. Finally, from Eq. (5) the coefficients of the individual expansions and therefore the total solution can be calculated by using a linear equation solution technique.

There is a way to reduce the computational demand by employing the numerical scheme derived by Mackowski [6]: first the corresponding coordinate system is rotated to provide coincidence between the vector \mathbf{r}_{ji} and the z -axis. Then an axial translation is executed, where the coefficients fundamentally simplify due to a common azimuth angle ϕ , which is shared by both of the coordinate systems. Finally, the coefficients are rotated back to their original orientation.

The order-of-scattering technique [2], which is implemented in our program, is based on the physical concept of multiple reflections. The main idea is, that the external field of each sphere can

be decomposed into the incident field and the fields deriving from first, second etc. order of reflections of the other spheres. Thus, the coefficients can be expressed as

$$\mathbf{a}^i = \sum_{or=0}^{\infty} \mathbf{a}_{or}^i \quad \text{with } \mathbf{a}_0^i = \mathbf{p}^i \quad \text{and} \quad \mathbf{a}_{or}^i = - \sum_{j=1, j \neq i}^N Y^{ji} \mathbf{a}_{or-1}^j. \quad (6)$$

In this way a very efficient iteration scheme can be executed with the Mie-solution as starting value (\mathbf{a}_0^i).

3. Discrete dipole approximation

A standard practice to formulate the scattering problem is to derive a volume integral equation, which describes the entire field in terms of the incident and internal fields:

$$\mathbf{E}(\mathbf{r}) = \mathbf{E}_{\text{inc}}(\mathbf{r}) + k_0^2 \int_V \chi(\mathbf{r}') \mathbf{G}(\mathbf{r}, \mathbf{r}') \mathbf{E}(\mathbf{r}') d^3 \mathbf{r}', \quad (7)$$

where $\mathbf{E}(\mathbf{r})$ represents the total, $\mathbf{E}_{\text{inc}}(\mathbf{r})$ the incident electrical field, $\chi = (\varepsilon_r - 1)$ the susceptibility and k_0 the wavenumber of free space. An arbitrary point is denoted by \mathbf{r} , any point inside the volume V of the scatterer by \mathbf{r}' . $\mathbf{G}(\mathbf{r}, \mathbf{r}') = [\mathbf{1} + 1/k_0^2 \nabla \nabla] 1/(4\pi|\mathbf{r} - \mathbf{r}'|) e^{ik_0|\mathbf{r} - \mathbf{r}'|}$ is the Green's Dyadic for unbound, free space. For the DDA-formula one relates the polarization $\mathbf{P}(\mathbf{r})$ to the total electric field by $\mathbf{P}(\mathbf{r}) = \varepsilon_0 \chi \mathbf{E}(\mathbf{r})$.

By using the same finite grid for integration and field discretization a system of equations in terms of the polarizations is obtained:

$$\mathbf{a}_{ii} \mathbf{P}(\mathbf{r}_i) = \mathbf{E}_{\text{inc}}(\mathbf{r}_i) - \sum_{j, j \neq i} \mathbf{a}_{ij} \mathbf{P}(\mathbf{r}_j). \quad (8)$$

Subsequently, the scattered far-field can be approximated as originating from a cloud of dipoles with the given polarisations.

The discrete dipole approximation was introduced by Purcell and Pennypacker [19] in 1973. Since then the theory has been greatly improved, including enhancement of the solving algorithms. A very important contribution is the use of a conjugate gradient algorithm combined with a fast Fourier transformation to solve the equation system [16]. Still special attention has to be paid to the singularity of the Green's function (in the \mathbf{a}_{ii} -terms in DDA), since inaccurate evaluation of the diagonal terms can lead to significant errors of the solution.

The classic procedure, excellently shown by Laktakhia [20] and Peltoniemi [21], yields for a polarizability α as follows:

$$\Rightarrow \alpha = 1/a_{ii} = \frac{\alpha_{\text{CM}}}{1 - \alpha_{\text{CM}}/\varepsilon_0 2/3 [(1 - ik_0 r_0) e^{ik_0 r_0} - 1]}, \quad (9)$$

with α_{CM} being the Clausius–Mosotti polarizability and r_0 being the dipole spacing. Still this derivation seems to be too bad an approximation to give satisfactory results. Several approaches try to surpass this point:

- The lattice correction technique by Draine and Goodman [22] gives really good results for relative refractive indices up to $\Delta n \approx 2.5$ for small particles.

- Assuming an electric field that changes over the sub-volume V_i , as shown by Peltoniemi [21], leads to one additional integral that contains the difference $\mathbf{E}(\mathbf{r}) - \mathbf{E}(\mathbf{r}')$. The polarizabilities gained by his results proved to be correct for relative refractive indices up to $n \approx 4 + 0.0i$.
- Sampling of the electric field can be handled just as in signal processing employing sampling theory as shown by Piller [23]. By convoluting the filter function with the Green's function a new *filtered Green's function* is obtained analytically, which no longer has singularities!

But there is still no satisfactory way of evaluating the quality of the results other than comparing it to other methods.

4. The multiple multipole program

The very first multiple multipole program (MMP) was written by Hafner [24] in 1980 and later on became an easy to handle 3D-program in Fortran77, running on a PC [17]. It is based on a method which was proposed to be called generalized multipole technique (GMT) by Ludwig [25] in 1989.

The field domain is separated into a number of subdomains D_i , each filled with linear, homogeneous and isotropic material. In each D_i a separate expansion of the field (e.g. into a series of multipole fields with different origins) is made:

$$\begin{pmatrix} \mathbf{E}^i \\ \mathbf{H}^i \end{pmatrix} = \begin{pmatrix} \mathbf{E}_{\text{inc}}^i \\ \mathbf{H}_{\text{inc}}^i \end{pmatrix} + \sum_{l=1}^{\infty} a_l^i \begin{pmatrix} \mathbf{E}_l^i \\ \mathbf{H}_l^i \end{pmatrix}, \quad (10)$$

where any choice of the unknown coefficients a_l^i results in a correct solution of Maxwell's equations, since each $(\mathbf{E}_l^i, \mathbf{H}_l^i)$ is such a solution. $(\mathbf{E}_{\text{inc}}^i, \mathbf{H}_{\text{inc}}^i)$ is the incident field generated by sources in domain D_i . Generally MMP demands one domain per material region. In our case, spherical multipole expansions with hankel functions were applied, see Eq. (2). This implies, that the origins of these functions (the poles) have to be situated outside the respective domain, where they are used as expansion functions.

This is why one may call MMP a semi-analytical method: the differential equations in each subdomain D_i are solved analytically, whereas the boundary conditions on the boundaries ∂D_{ij} between the subdomains D_i and D_j are fulfilled numerically by point matching. The employed extended point matching method is numerically equivalent to a Galerkin projection technique (test functions f_j are the same as expansion functions f_l) and to a least-squares error minimization. For example to approximate $f(\mathbf{r})$ by a liner combination of a complete system of $f_l(\mathbf{r})$, we consider the following minimization problem:

$$a_i: \min \left(\int_{\partial D} \left(f(\mathbf{r}) - \sum_{l=1}^L a_l f_l(\mathbf{r}) \right)^2 dA \right), \quad (11)$$

$$\Leftrightarrow \sum_{k=1}^K \omega_k \left(f(\mathbf{r}_k) - \sum_{l=1}^L a_l f_l(\mathbf{r}_k) \right) f_j(\mathbf{r}_k) = 0. \quad (12)$$

Since $K \geq L$, the resulting system of equations is overdetermined. The weight function ω_k may be interpreted as the surface elements dA due to the integration which is represented by the sum over

k . In our case the known incident fields on the boundary ∂D_{ij} are approximated by the expansions in the neighboring domains D_i and D_j at K matching points to obtain L expansion coefficients a_i^k and a_j^k .

At every surface one has to use about 10 grid points per wavelength to get useful results and about 20–30 gpts/ λ will be needed in the neighborhood of nearly touching surfaces to obtain good solutions ($\approx 5\%$ accuracy).

The origin as well as the order of the poles are chosen, so that all surface points, which do not have to lie on a closed surface(!), are “illuminated” by at least one expansion function. The choice of the poles is done quite experimentally, a good criterium is to look for a set of poles, of which the regions of influence do not “overlap” too much. That means that even for a spherical particle multiple origins are employed to represent the internal fields. For aggregated spheres naturally even the outer field is expanded in a series over functions having poles at the centers of those spheres. For more complex-shaped particles the choice of poles should lead to a total “illumination” of the surface. In addition the “illumination” should be as uniform as possible.

The far-field is easily computed by inserting expansion coefficients into approximate equations (far-field behavior of the hankel functions) for those far fields.

5. Numerical investigations

The programs were compared by the exactness of their solution. For some exemplary cases the discretization points or the number of expansion functions, respectively, were enlarged until convergent solutions were gained, of which at least two were not to differ by more than 5% maximum relative difference in the scattering diagrams. Because the OS-Mie-program turned out to be very reliable and fast converging to such solutions, we compared other results to those obtained by this code.

The DDA-Code used was the public domain software DDSCAT,¹ version 5, by Draine and Flatau [16]. The MMP program was a version of Hafner [17] improved by Dahl [13].

The refractive indices were chosen to be $n = 1.5 + i0$ for four-sphere configurations, $n = 1.5 + i0.1$ for larger particles, $n = 1.5 + i1.0$ for small ‘satellites’ and $n = 1.33 + i0$ for oblates. As a result, diagrams of the scattered intensities and of the corresponding relative differences and a table listing the required storage, the CPU-time used and again an rms-difference as scale for the deviation are given.

5.1. Clusters of spheres

Figs. 1–6 are the results of our first example. The behavior of the programs is investigated for the case of four close spheres within one row perpendicular to the direction of wave propagation. Figs. 1 and 2 show the scattering patterns obtained by DDSCAT and OS-Mie as well as their deviation for the case of touching spheres, whereas Figs. 3 and 4 represent the other ‘extreme’: they

¹ <ftp://astro.princeton.edu/draine>.

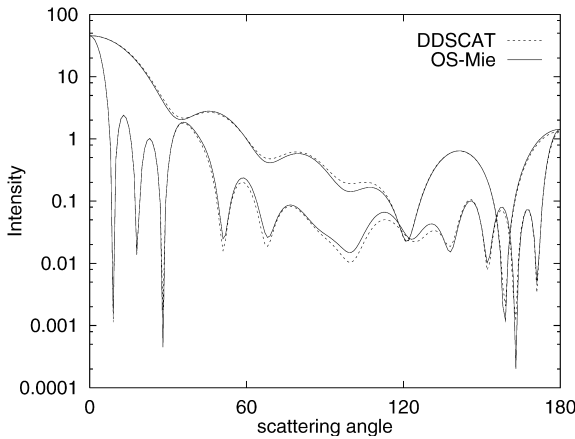


Fig. 1. Scattering diagram of four touching spheres with $x = 5$ and $n = 1.5 + i0.0$. The DDA-data was computed with $96 \times 24 \times 24$ dipoles, the OS-Mie program used 25 expansion coefficients for each sphere.

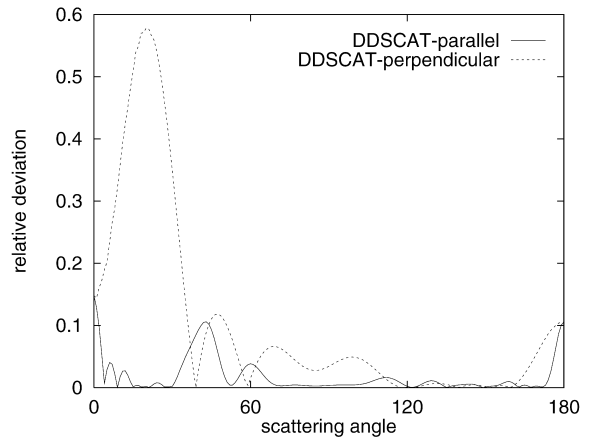


Fig. 2. Relative deviation of Fig. 1.

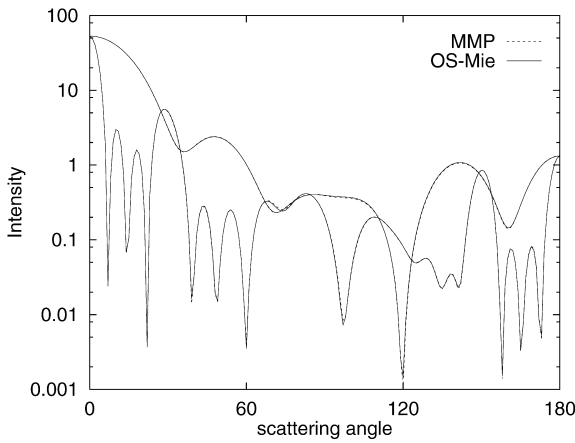


Fig. 3. Scattering diagram of four spheres with $x = 5$ and $n = 1.5 + i0.0$ being separated by $0.5R$. The MMP-data was computed with 572 matching points, the OS-Mie program used 25 expansion coefficients for each sphere.

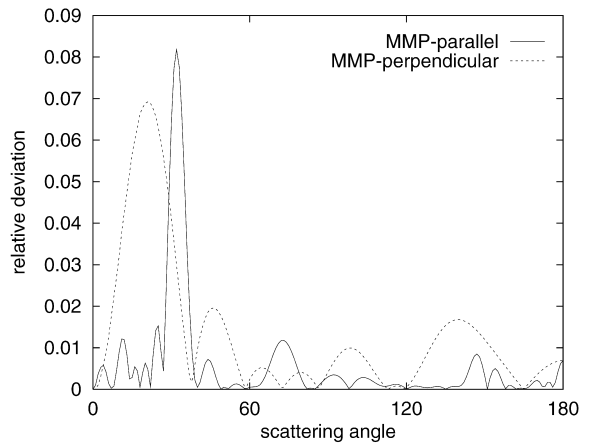


Fig. 4. Relative deviation of Fig. 3.

give the results of MMP and OS-Mie for spheres separated by half a radius, being the largest distance of our variation. The programs are best suited for these constellations which was why these figures were chosen.

Figs. 5 and 6 show the most suitable parameter ranges:

- DDSCAT gives reliable results of ‘medium’ accuracy even in the case of touching scatterers, although the accuracy may be ameliorated by utilizing huge amounts of computer power. In our

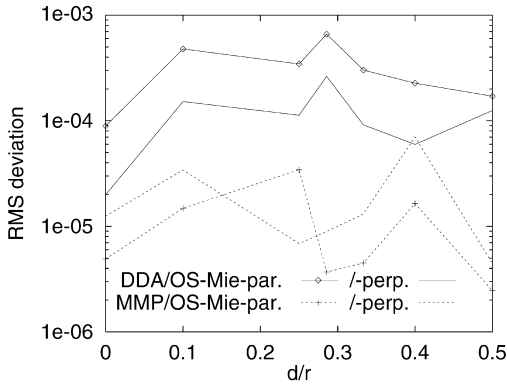


Fig. 5. RMS deviation of DDSCAT/OS-Mie and MMP/OS-Mie for a four-sphere configuration over the distance-per-radius ratio.

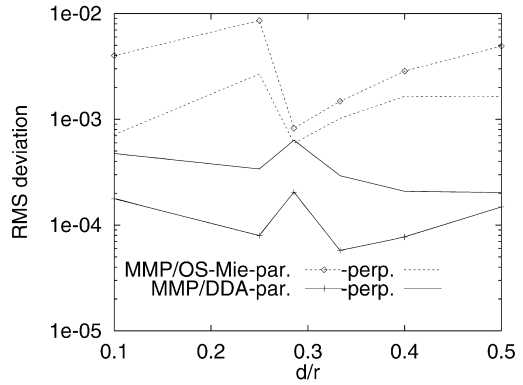


Fig. 6. RMS deviation of MMP/DDSCAT for a four-sphere configuration over the distance-per-radius ratio. As a validation trial: RMS deviation of the MMP and the OS-Mie-result of the next smaller distance.

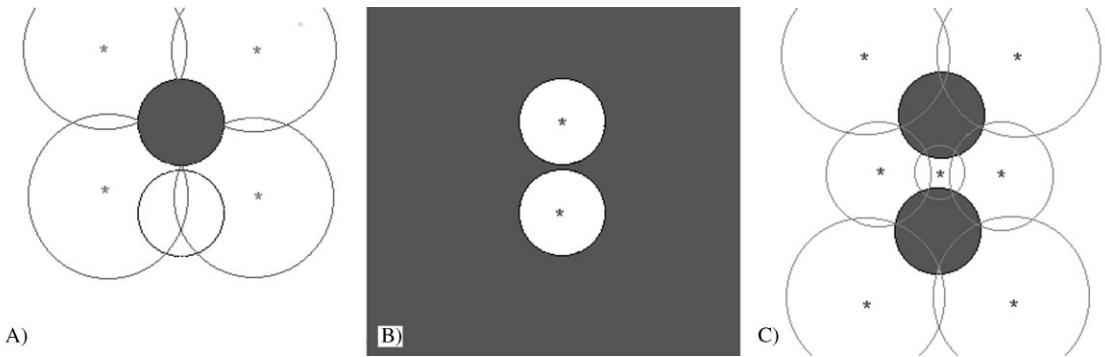


Fig. 7. (A)–(C): Scheme of poles and their related domain for two sphere configurations. The dark area is the respective domain, the poles are represented by small stars and their circle of influence. (A) illustrates one internal field expansion for the case of nearly touching scatterers. For each sphere a separate domain and a related set of poles is chosen, (B) gives the poles for the external field expansion, (C) demonstrates the total all-over internal field ‘ansatz’, when the scatterers are far enough from each other to insert poles in between and consequently only one domain/expansion is needed for the internal fields of both scatterers.

example a *doubled* refinement of the grid steps was necessary to achieve any remarkable improvement.

- MMP on the other side seems better suited if the individual spheres are separated more than a fourth to a fifth of a radius. If they are packed more closely, it is necessary to assume an individual expansion, i.e. a different domain, for each neighboring sphere. Fig. 7 schematically illustrates the varied ‘ansatz’ for closely lying scatterers. In our example this causes a loss of symmetry of the configuration and therefore a longer computation time. As soon as the spheres are half a radius apart, convergence is fast and the accuracy of the solution is high and it fits the OS-Mie results excellently.

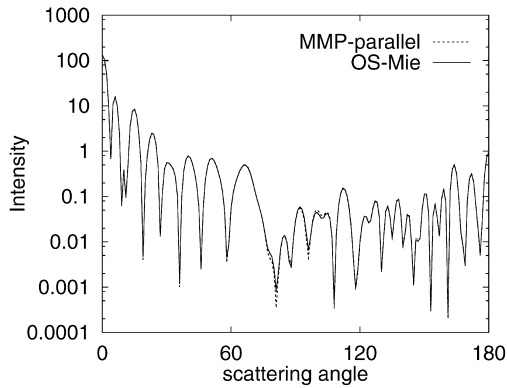


Fig. 8. Scattering diagram of two spheres with $x = 20$ and $n = 1.334 + i0.0$ being separated by $0.4R$. The MMP-data was computed with 1341 matching points, the OS-Mie program used 40 expansion coefficients.

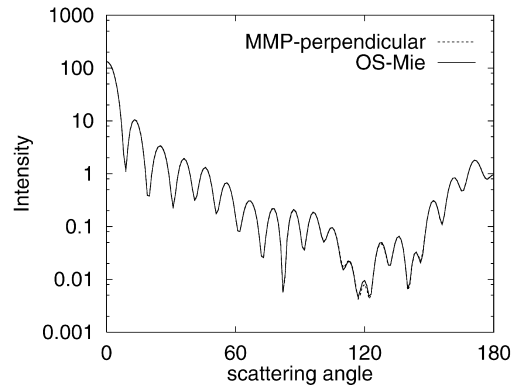


Fig. 9. Same as Fig. 8 for the perpendicular case.

Fig. 6 gives the DDA–MMP deviation, which is clearly less than the MMP-to-‘shifted’-OS-Mie deviation, shown as a comparison. This ‘shifted’ curve was obtained by calculating the deviation of an MMP-result to the OS-Mie result of the configuration with the next smaller distance between the scatterers. That means, the differences between the methods are smaller than those between the results for different configurations.

As the deviation of DDA and MMP fits to the maximum-curve of the respective deviation of the methods to OS-Mie, there is one more hint, that the assumption of a ‘correct’ result from OS-Mie is true.

Figs. 8 and 9 show the simulation results for two spheres of radius r with $2\pi r/\lambda = 20$, separated by $0.4r$, computed by MMP and OS-Mie for two polarization cases. Figs. 10 and 11 are the scattering diagrams of two spheres in contact calculated by DDSCAT and OS-Mie. These four diagrams support the assumptions made for the ranges of applicability of the programs. There is good agreement between OS-Mie and MMP for a non-touching scattering problem, even for larger particles, whereas the agreement between OS-Mie and DDSCAT for touching scatterers is only almost satisfactory, spoiled by the usual problems of DDA for larger scatterers, since the discretization cannot be chosen as fine as is necessary for a more exact calculation.

In our final example we applied the OS-Mie program and MMP for one large transparent sphere ($x_1 = 20$, $n = 1.5 + 0.0i$) and two smaller absorbing spheres ($x_2 = 4$, $n = 1.5 + 1.0i$), which were $0.5r_1$ apart. Figs. 12 and 13 again show that the curves match as well as expected.

Table 1 lists the computer storage and CPU-time needed by the different codes. Results were obtained with the following parameters:

The MMP-surface consisted of 472 matching points for the four-sphere examples and of about 1200 points for the other cases, the discretization was $30 \text{ gpts}/\lambda$.

DDSCAT used $20 \times 20 \times 20$ dipoles to simulate each sphere for the first examples and $80 \times 80 \times 80$ dipoles for each sphere for larger particles, leading to a discretization of about 10 dipoles/ λ .

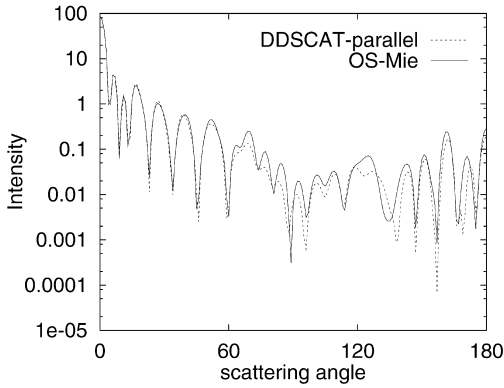


Fig. 10. Scattering diagram of two spheres in contact with $x = 20$ and $n = 1.334 + i0.0$.

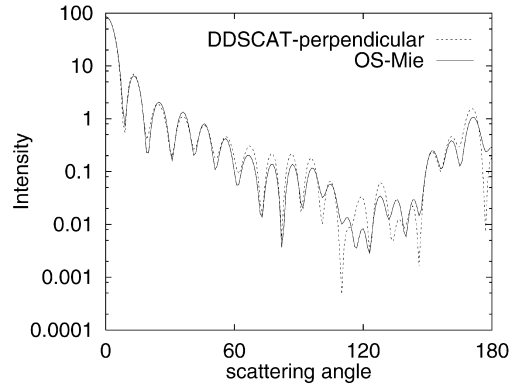


Fig. 11. Same as Fig. 10 for the perpendicular case.

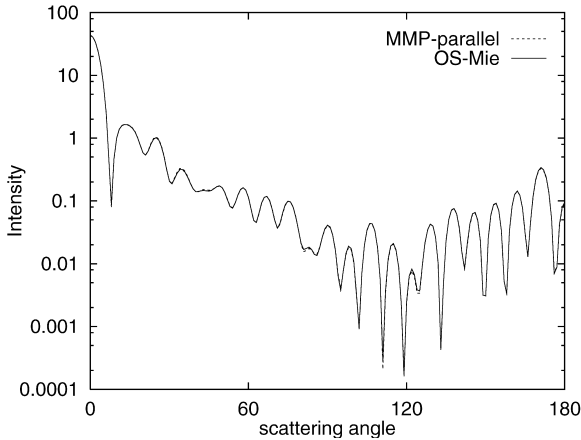


Fig. 12. Scattering diagram of one transparent sphere with $x = 20$ and $n = 1.5 + i0.0$ and two satellite spheres with $x = 4$ and $n = 1.5 + i1.0$.

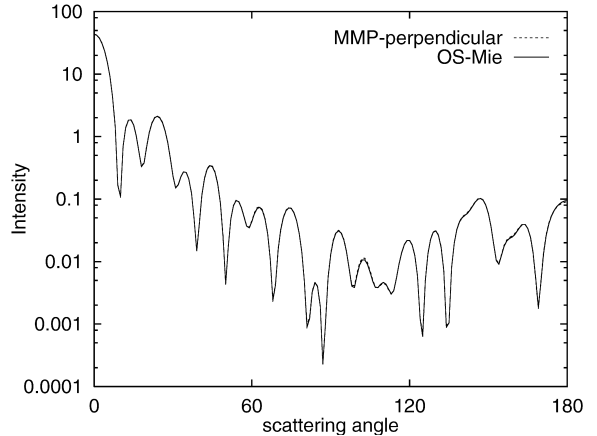


Fig. 13. Same as Fig. 12 for the perpendicular case.

The OS-Mie-program employed 25 or 40 expansion coefficients for every sphere.

As expected the discrete dipole approximation has an enormous demand of memory, still it is quite fast if the particles considered are relatively small, i.e., some wavelengths. MMP is quite modest concerning storage demand, but needs CPU-times comparable to DDSCAT. Results quality was very good for our examples.

More complex configurations would show the full extent of the OS-Mie program's advantages. The cases chosen here were quite suited for DDA and MMP, as the enclosing rectangular block was minimal ('small' volume for DDA) and the configurations were symmetric (symmetric matrices for MMP). The CPU-time was taken on an IBM RISC/6000-595-workstation.

Table 1
Computational demand

Program	Storage (/kB)	CPU-time (/sec)	Deviation (rms)	
4 spheres $x = 5$				
DDSCAT	33,000	90	2E-5	9E-5
MMP	7000	190	4E-6	2E-6
OS-Mie	10,000	20	—	—
2 spheres $x = 20$				
DDSCAT	240,000	13,000	1E-5	1.4E-5
MMP	24,000	4400	4E-6	2E-6
OS-Mie	10,000	30	—	—
1 sphere $x_1 = 20$				
2 spheres $x_2 = 4$				
MMP	17,000	3400	5E-5	5E-5
OS-Mie	9,000	12	—	—
2 oblates $x = 5$				
DDSCAT	112,000	900	—	—
MMP	35,000	6300	—	—

5.2. Clusters of oblate spheroids

As an outlook as to the possibilities of MMP and DDSCAT two examples for close oblates of volume-equivalent Mie parameter $x = 5.0$, refractive index $n = 1.33 + i0.0$ and axis ratio $a/b = 4$ were calculated. Figs. 14 and 15 present the computed result of the scattering of two plates within a distance of $dist = b/2$. Figs. 16 and 17 show the scattering of two touching plates. The curves show a merely satisfactory fitting. Since the DDSCAT result did still change depending on discretization, this program probably caused the deviation of results.

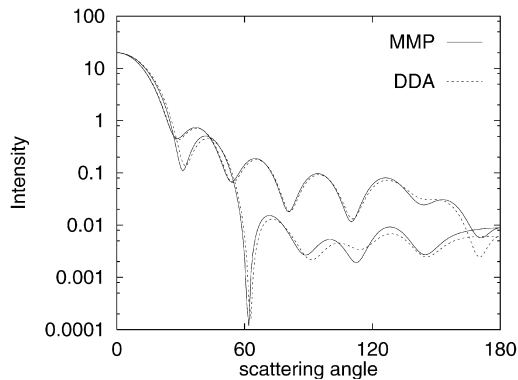


Fig. 14. Scattering diagram of two oblate spheroids with $x = 5$, $n = 1.33 + i0.0$, $a/b = 4$ and a distance $dist = b/2$.

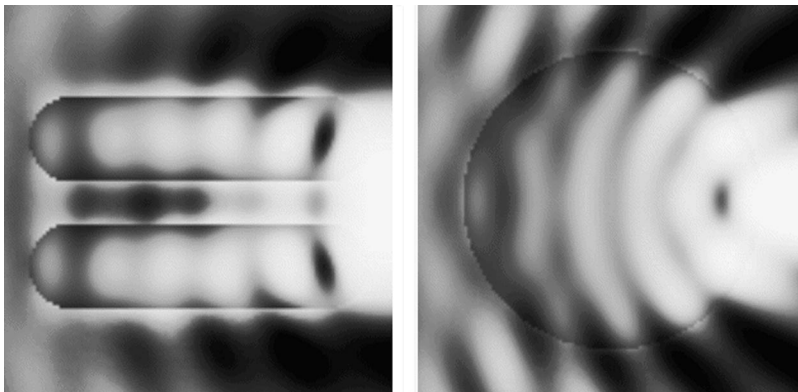


Fig. 15. Light intensity in the parallel/perpendicular plane of two oblate spheroids with $x = 5$, $n = 1.33 + i0.0$, $a/b = 4$ and a distance $dist = b/2$ in between.

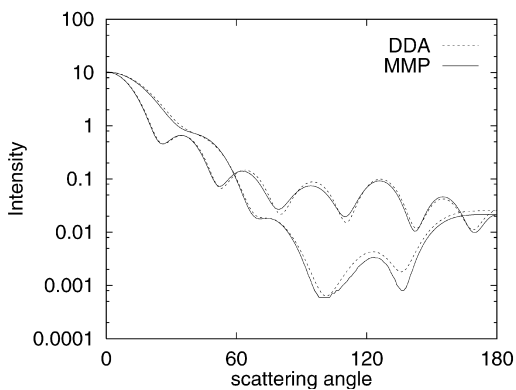


Fig. 16. Scattering diagram of two touching oblate spheroids with $x = 5$, $n = 1.33 + i0.0$ and $a/b = 4$.

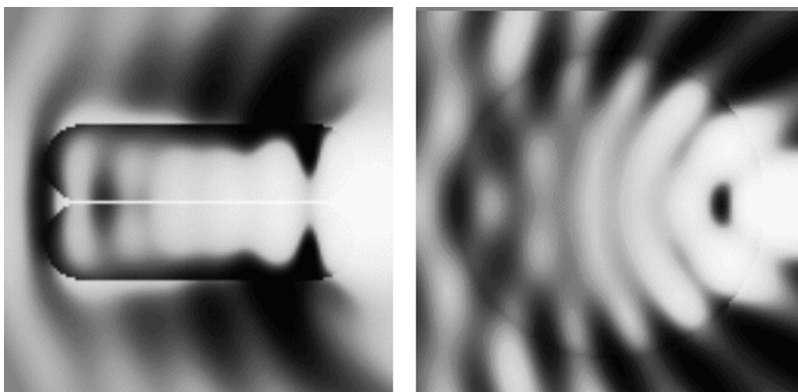


Fig. 17. Light intensity in the parallel/perpendicular plane of two touching oblate spheroids with $x = 5$, $n = 1.33 + i0.0$ and $a/b = 4$.

Once more MMP used separate domains for the inner fields of the scatterers leading to relative high computational demand due to loss of symmetry. Still the advantage in comparison to DDSCAT's storage demands is obvious.

6. Conclusion

This paper is not a full investigation on multiple scattering by different programs. But it may give a hint on the capabilities of these computer codes for simulating the scattering of 'densely packed' clusters.

The DDA method is very memory consuming, amplified by the high refractive index chosen, as any increase of discretization has to be taken into account by the order of three. This is most probably one reason for the differences to the MMP and OS-Mie results for our examples. Instead of our DDSCAT-'tailor-made' geometrical arrangement of the scatterers the number of cells for DDA may not have been large enough to reach high accuracy. But even with these restrictions quite reliable approximations can be obtained especially for touching scatterers.

MMP showed some difficulties for close particles making a separate expansion domain for neighboring particles necessary. As long as a minimum distance of app. $0.3-0.4R$ was maintained between the individual scatterers, one expansion domain per material was sufficient, i.e. for the inner fields of all scatterers the same superposition of expansion functions could be employed, whereas in the former case a separate domain with its own set of poles had to be chosen for each scatterer.

The final results were in good agreement with the OS-Mie-data. The program gave very reliable results, whose quality can be estimated by the matching error at the boundaries.

Our main intention was to test the reliability and exactness of MMP and DDA for closely packed agglomerates as well as to obtain a reference for the order-of-scattering Mie program, which may now be extended as a next step to other geometries of the individual scatterers.

The scattering diagrams correspond to the assumption, that all three programs give satisfactory results for the type of agglomerated particles considered. Especially, MMP turned out to be capable to calculate touching scatterers even for the case of oblate spheroids.

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