The Discrete Dipole Approximation - Possibilities and Problems to Simulate Elastic Light Scattering

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The Discrete Dipole Approximation

Possibilities and Problems to Simulate Elastic Light Scattering

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Abstract

We give a short introduction to the Discrete Dipole Approximation (DDA), which is a method capable of simulating elastic light scattering from arbitrary particles. We survey the feasibility of large scale simulations using the DDA, both in terms of accuracy of the model and computational requirements. Finally, we show some examples of DDA simulations of scattering by small Human White Blood Cells.

1. INTRODUCTION

Methods to simulate Elastic Light Scattering from complex, arbitrary shaped particles with dimensions in the order of the wavelength of the incident light are slowly evolving into a state which facilitates routine calculations of scattering by such complex particles, much like the by now standard availability of Mie scattering codes. This optimistic statement is based partly on the ever increasing computational power which is present in today's (desktop) computers, but more importantly on some very relevant improvements in the models and/or algorithms underlying such simulations. This is certainly true for the Discrete Dipole Approximation (DDA), which, after its introduction by Purcell and Pennypacker in 1973 [1], has witnessed a steady development in both the model and the algorithms needed to solve the model equations. However, only after a major algorithmic improvement in 1991 by Goodman, Draine, and Flatau [2], involving the use of Fourier transformations, very large scale DDA calculations needed to model realistic particles became feasible.

We will shortly introduce the DDA model, describe the most widely used algorithms to solve the DDA equations, and give a number of examples of large scale simulations using the DDA method. Next, we will survey the ranges of particle size and refractive index which the DDA is currently able to cover. Finally, we will discuss some new directions in simulations using the DDA model.

2. THE DISCRETE DIPOLE APPROXIMATION

The Discrete Dipole Approximation (DDA) is a flexible and powerful model for Elastic Light Scattering from arbitrary shaped particles. The model is very intuitive and has a semi-microscopic flavour. However, as shown in a series of papers by Lakhtakia, the DDA method can be formally obtained from the macroscopic Maxwell equations, in the same way as the Method of Moments [3-5]. The DDA method was reviewed two years ago by Draine and Flatau [6]. For many details concerning the DDA we refer to this excellent review.

The DDA models a particle as a set of N point dipoles on a lattice. Each dipole i has a

polarisability $\tilde{\alpha}_i$ (in general a 3×3 tensor), is located at position $\mathbf{r}_i$, and has a polarisation $\mathbf{P}_i = \tilde{\alpha}_i \mathbf{E}_i$ with $\mathbf{E}_i$ the electric field on dipole i. The DDA consists of two phases, first the electric fields on all dipoles are calculated, and next, the (differential) scattering cross sections are obtained from these fields. The field on each dipole is obtained by summing the incident field on the dipole and the fields radiated by all other dipoles. This coupling between dipoles through their radiated fields gave the DDA its alternative name: Coupled Dipole method.

The electric field at $\mathbf{r}_i$ radiated by a dipole at $\mathbf{r}_j$ with polarisation $\mathbf{P}_j$ is given by [7]

$$\mathbf{E}(\mathbf{r}_i) = \left(k^2 (\mathbf{n}_{ij} \times \mathbf{P}_j) \times \mathbf{n}_{ij} \frac{e^{ikr_{ij}}}{r_{ij}} + (3\mathbf{n}_{ij}(\mathbf{n}_{ij} \cdot \mathbf{P}_j) - \mathbf{P}_j) \left(\frac{1}{r_{ij}^3} - \frac{ik}{r_{ij}^2} \right) e^{ikr_{ij}} \right), \tag{1}$$

k is the wave number, defined by $k = 2\pi/\lambda$; $\mathbf{n}_{ij}$ is the direction vector defined by $\mathbf{n}_{ij} = \mathbf{r}_{ij} / r_{ij}$, and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$; $r_{ij} = |\mathbf{r}_{ij}|$. Note that, in line with other authors, we use Gaussian units. For a discussion of units and dimensions, see the Appendix of Ref. [7]. In Cartesian coordinates Eq. 1 becomes

$$\mathbf{E}(\mathbf{r}_i) = \frac{e^{ikr_{ij}}}{r_{ij}} \left(-k^2 (\mathbf{n}_{ij}\mathbf{n}_{ij} - \mathbf{I}) + \left(\frac{1}{r_{ij}^2} - \frac{ik}{r_{ij}} \right) (3\mathbf{n}_{ij}\mathbf{n}_{ij} - \mathbf{I}) \right) \mathbf{P}_j \ , \tag{2}$$

where $\mathbf{I}$ is the 3×3 identity matrix and $\mathbf{n}_{ij}\mathbf{n}_{ij}$ denotes a dyadic product. The electric field on dipole i ($1 \le i \le N$), due to the external field $\mathbf{E}^0(\mathbf{r}) = \mathbf{E}^0 \exp(i\mathbf{kr}\text{-}i\omega t)$ and the field radiated by all other dipoles, is

$$\mathbf{E}(\mathbf{r}_i) = \mathbf{E}^0(\mathbf{r}_i) + \sum_{j \neq i}^{\mathbf{N}} \mathbf{F}_{ij} \mathbf{P}_j \ , \ 1 \le \mathrm{i} \le \mathrm{N}, \tag{3}$$

with the matrix $\mathbf{F}_{ij}$ defined by Eq. 2. All fields are assumed to be monochromatic, and from now on we simply skip the $\exp(-i\omega t)$ term. Furthermore, the particle is assumed to be non-magnetic. Singham [8] extended the original DDA method to intrinsic optical active particles. For the more general case of bianisotropic scatterers we refer to Ref. [4,5]. Note that the summation in Eq. 3 runs over all dipoles, except dipole i. This term, the eigen-term or self-term, is neglected in the original DDA method, but is present in the strong form DDA of Lakhtakia [5]. It accounts for the field that is radiated by the small volume, which the dipole models, to its own centre. Draine has also introduced such a term in the DDA [9], but he introduced it through the expressions for the polarisability (see the discussion at the end of this section).

Eq. 3 defines a set of $3N$ equations for the $3N$ unknowns ($\mathbf{P}_x(\mathbf{r}_i)$, $\mathbf{P}_y(\mathbf{r}_i)$, $\mathbf{P}_z(\mathbf{r}_i)$). These equations can be reformulated as a matrix equation $\mathbf{Ax} = \mathbf{b}$, with

$$\mathbf{x} = \begin{pmatrix} \mathbf{P}(\mathbf{r}_1) \\ \vdots \\ \mathbf{P}(\mathbf{r}_N) \end{pmatrix}, \ \mathbf{b} = \begin{pmatrix} \mathbf{E}^0(\mathbf{r}_1) \\ \vdots \\ \mathbf{E}^0(\mathbf{r}_N) \end{pmatrix}, \text{ and } \mathbf{A} = \begin{pmatrix} \alpha_{11}^{-1} & -\mathbf{F}_{12} & \cdots & & -\mathbf{F}_{1N} \\ -\mathbf{F}_{21} & \alpha_{22}^{-1} & & & \\ \vdots & & \ddots & & \vdots \\ & & & \alpha_{N-1,N-1}^{-1} & -\mathbf{F}_{N-1,N} \\ -\mathbf{F}_{N1} & & \cdots & -\mathbf{F}_{N,N-1} & \alpha_{N,N}^{-1} \end{pmatrix}. \tag{4}$$

The matrix $\mathbf{A}$ is the $3N \times 3N$ interaction matrix. It is obvious from the definition of $\mathbf{F}_{ij}$, that $\mathbf{F}_{ij} = \mathbf{F}_{ji}$. The polarisability tensor is symmetric, and so is its inverse. Therefore, the interaction matrix $\mathbf{A}$ is complex symmetric.

After having solved Eqs. 3 the scattering cross sections can be expressed in terms of the polarisation $\mathbf{P}_i$. Draine shows that extinction and absorption cross sections C_{ext} and C_{abs} can be expressed as [9]

$$C_{ext} = \frac{4\pi k}{\left|\mathbf{E}^0\right|^2} \sum_{i=1}^{N} \mathbf{Im}(\mathbf{E}^0(\mathbf{r}_i)^* \cdot \mathbf{P}_i) \tag{5}$$

$$C_{abs} = \frac{4\pi k}{\left|\mathbf{E}^0\right|^2} \sum_{i=1}^{N} \left\{ \mathbf{Im}\left[\mathbf{P}_i \cdot (\tilde{\alpha}_i^{-1})^* \mathbf{P}_i^*\right] - \frac{2}{3} k^3 |\mathbf{P}_i|^2 \right\} . \tag{6}$$

The scattering cross section is found through $C_{sca} = C_{ext} - C_{abs}$. Finally, the scattered field can be calculated from the internal field by summing all the electric fields radiated by the dipoles. Draine shows that in the far field the scattered electric field can be expressed as [9]

$$\mathbf{E}_s = \frac{k^2 e^{ikr}}{r} \sum_{i=1}^{N} e^{-ik\mathbf{n}\cdot\mathbf{r}_i} (\mathbf{nn} - \mathbf{I})\mathbf{P}_i \tag{7}$$

If we calculate the scattered field for perpendicular and parallel polarisation of the incident light we can obtain the total scattering matrix **S** of the particle, as described in chapter 3.3 of Ref. [10].

Before we can proceed we need to settle two more matters of the DDA model, first the location of the dipoles and second expressions to find the polarisability of the dipoles as a function of macroscopic optical properties of the scattering volume, i.e. the refractive index.

In principle the point dipoles in the DDA represent the polarisability of a small volume of the scatterer. This means that one has complete freedom over the size, shape, and position of the dipoles, as long as dipole i with polarisability $\tilde{\alpha}_i$ is an accurate enough representation of the real polarisation of the finite volume element V_i. Despite this flexibility, most DDA models assume that the dipoles are located on a cubical grid. The grid spacing d has to be much smaller than the wavelength of the radiation, usually by a factor of 10 to 20. Furthermore, the graininess of the resulting model particle must be small enough to allow for accurate simulations of the scattering matrix (see for a discussion of these matters see e.g. Ref. [6, 9, 11]). The reasons to choose for a cubical grid are twofold. First it allows a more accurate analysis of the question how to find the polarisability of the dipoles. Next, as will become clear in section 3, such regular lattice allows to drastically reduce the execution time of the DDA simulation. It should however be noted that some authors have tried other configurations in modelling very thin layers or helical structures (see e.g. [12, 13].

In our discussion on the polarisability we will assume that the dipoles are isotropic, i.e. $\tilde{\alpha}_i = \alpha_i \mathbf{I}$. Originally, Purcell and Pennypacker obtained α_i via the Clausius-Mossotti relation

$$\alpha_i^{\mathrm{cm}} = \frac{3d^3}{4\pi} \frac{m_i^2 - 1}{m_i^2 + 2} , \tag{8}$$

with m_i the refractive index of the volume element V_i. The Clausius-Mossitti relation is exact in the dc limit, for an infinite cubical lattice of equal dipoles and it is assumed that for the finite DDA lattice it is a good approximation. An important limitation of the use of the Clausius-Mosotti relation lies in the fact that the optical theorem is violated. This is a well-known problem and is treated in many textbooks in the context of e.g. Rayleigh scattering. Non-absorbing particles with real m yield dipoles with real α according to Eq. 8. However, the single dipoles in the simulation do scatter light and their polarisabilities should have an imaginary part. As was noted by several authors [9, 14], this restriction does not introduce severe errors in the simulation of the differential cross sections. Nevertheless, it remains an important point of principle. As a consequence, the optical theorem cannot be used to calculate

total scattering cross sections of particles.

Several solution to this problem have been suggested. First, Draine [9] introduced an imaginary part into the polarisability by considering a radiative reaction field on the dipoles. Dungey and Bohren [15] introduce an exact formulation of the electric dipole polarisability of small spheres in the DDA formalism. This formulation basically is the first term in the Mie series, and includes the radiative reaction term of Draine as the third order term of an expansion in the size parameter of the spherical dipole. Finally, Draine and Goodman derived the Lattice Dispersion Relation by considering the question what polarisability α of an infinite cubical lattice of dipoles would result in the same dispersion relation of a continuum with refractive index m. [16] They show that

$$\alpha^{\mathrm{ldr}} \approx \alpha^{\mathrm{cm}}\left(1+\left(\alpha^{\mathrm{cm}}/d^3\right)\left[\left(b_1+m^2b_2+m^2b_3S\right)(kd)^2-(2/3)i(kd)^3\right]\right)^{-1}, \tag{9}$$

$$b_1=-1.891531, \qquad b_2=0.1648469,$$

$$b_3=-1.7700004, \qquad S=\sum_{j=1}^{3}\left(\hat{a}_j\hat{e}_j\right)^2,$$

where $\hat{a}$ and $\hat{e}$ are unit vectors defining the direction and polarisation of the incident light. The use of the Lattice Dispersion Relation results in more accurate DDA simulations, as compared to other methods to obtain the polarisability [16].

3. SOLVING THE DDA EQUATIONS

The DDA method consists of three parts. First an initialisation, in which the dipole positions, the incident field, and the other model parameters are specified. Second the calculation of the field at the dipoles and third the calculation of the scattering cross sections.

Calculation of the electric field on the dipoles, Eq. 3, is the computational most expensive part of the DDA method. From a numerical point of view, this calculation boils down to solving a very large system of linear equations $\mathbf{Ax} = \mathbf{b}$, with $\mathbf{A}$ a $n \times n$ complex symmetric matrix, $\mathbf{b}$ a known complex vector and $\mathbf{x}$ the unknown complex vector. Generally speaking linear systems are solved by means of direct or iterative methods [17]. In the past both approaches were applied to solve the DDA equations. For instance, Singham et al. used a direct method (LU factorisation) [8], Singham and Bohren described a reformulation of the DDA method, which from a numerical point of view is a Jacobi iteration to solve the matrix equation [18], and Draine applied a Conjugate Gradient iteration [9].

Direct methods require $O(n^3)$ floating-point operations to find a solution, whereas iterative method require $O(n^2)$ floating-point operations, provided that the number of iterations is much smaller than n. In many cases the size of the DDA interaction matrix alone forces us to use iterative methods.

The Jacobi iteration is not very well suited for a large number of dipoles; already for a relative small number of dipoles ($N \sim 500$), the Jacobi iteration becomes non-convergent [19]. A very efficient iterative method is the Conjugate Gradient method [17]. Draine [9] showed that the Conjugate Gradient method is very well suited for solving the DDA equations. The number of iterations needed to find the solution is much smaller than the dimension of the matrix. For instance, for a typical small particle with 2320 dipoles (n = 6960) the Conjugate Gradient method only needs 17 iterations to converge. Rahola and Lumme have recently compared the performance of a number of different Conjugate Gradient methods for solving DDA equations

[20,21]. They show that the Quasi-Minimal Residual (QMR) algorithm can be 2 to 4 times faster to find the solution of the DDA equations.

Although the use of direct methods to solve the equations has clear advantages (for orientational averaging, see next section), currently most groups apply iterative CG methods, allowing to handle systems with up to 5×10^3 dipoles, or when executed on very powerful (parallel) computers, up to 10^5 dipoles [see e.g. 22]. However, the execution time needed for such large systems is still to high. The $O(n^2)$ complexity of the CG methods needs to be reduced to allow for real production - type of simulations of light scattering using DDA (see also next section).

The major breakthrough came in 1991, when Goodman, Draine, and Flatau, inspired by comparable techniques which are well-known in the Method of Moments, showed how to reduce the $O(n^2)$ complexity to $O(n\log n)$ by using 3D Fast Fourier Transformations in the CG methods [2]. The key point is that due to the property $\mathbf{F}_{ij} = \mathbf{F}_{i-j}$, the matrix vector products, accounting for the $O(n^2)$ complexity in the CG methods, are in fact discrete convolutions. If the dipoles are located on periodic lattices, FFT methods can be used to evaluate these convolutions in $O(n\log n)$ complexity. Using FFT techniques allows to run DDA simulations with 10^4 dipoles in only a few minutes on workstations, and to move to systems with 10^6 to 10^7 dipoles by executing the DDA on powerful supercomputers (see e.g. [23], and section 6).

A public domain DDA scattering code, by Draine and Flatau, employing CG iterations and FFT kernels is available via anonymous ftp from astro.princeton.edu in the directory draine/scat/ddscat. See also the links on the "scattering codes" home page of Dr. Wriedt; http://imperator.cip-iw1.uni-bremen.de/fg01/codes2.html.

4. CURRENT RANGES OF APPLICABILITY

In principle the DDA is able to simulate light scattering by any arbitrary particle, only limited by computational power and memory of a computer. In this section we will survey the current ranges of applicability of the DDA. First, we ask the question how many dipoles we expect to be needed in typical particle models. As our own interest lies mainly in scattering by complex biological cells [see e.g. 22-25], we concentrate this discussion on compact particles. However, comparable estimates can be made for porous aggregates as considered in e.g. [21, 26]. Next, we will show the computational requirements for large DDA models and discuss the influence of the refractive index of the particles on the applicability of DDA and the added problems when orientational averaging is required in the simulations.

Fig. 1 gives an estimate of the number of dipoles needed to model a compact particle, as a function of the size parameter α[1], with grid spacing d equal to $\lambda/20$, $\lambda/10$, and $\lambda/5$. Even for modest size parameters the number of dipoles is $O(10^4)$ or larger. In our specific application, simulation of elastic light scattering from human white blood cells, α is in the range of 20 to 80. This means that we should be able to handle models with up to 10^8 dipoles, assuming that we will need 20 dipoles per wavelength for e.g. accurate depolarisation simulations. Fortunately, in many cases it is possible to employ larger dipoles, resulting in smaller models (see e.g. the results on the simulation of total cross sections in Ref. [6]).

In general, if the size parameter is in the range of 80 or larger it becomes possible to employ other, computationally less expensive approximate methods to simulate light scattering, such as

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1 The size parameter is defined as $\alpha = 2\pi r/\lambda$, with r the radius of the particle

physical optics approximations. This means that if it is possible to compute DDA models with up to 10^8 dipoles we are able, with DDA, to cover the gap between low- and high-frequency approximations of Elastic Light Scattering.

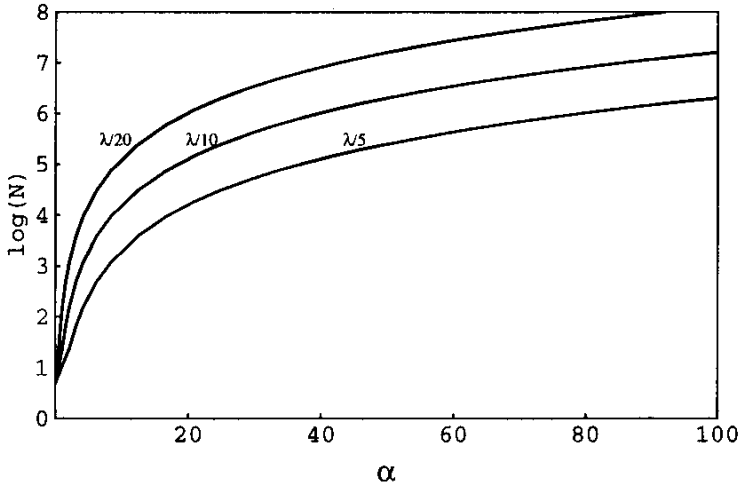

Figure 1. Estimation of the number of dipoles needed to model a compact particle.

In Fig. 2 we indicate the number of floating point operations needed for 1 iteration of the DDA (the line *direct DDA*, i.e. DDA with a Conjugate Gradient solver, *without* employing the FFT's), as a function of the number of dipoles N. In order to simulate ELS from human white blood cells, which have diameters up to 16 μm, the number of dipoles needs to be in the range 10^5 to 10^8. In reference [22] we describe a parallel version of the direct DDA, and based on this work we are able to indicate the range of operations which can be performed in less than 10 minutes[2], when executed on a typical workstation (a Sun Sparcstation 20 at 50 MHz) or a powerful parallel computer (a 32 node Parsytec PowerXplorer). It is obvious that the direct DDA iteration is too demanding if we wish to simulate scattering from realistic, micron sized particles (see also the discussion in [22]).

The operation count for one iteration of the *fast* DDA (i.e. DDA using the fast Fourier transforms) is also indicated in Fig. 2. This suggests that Goodman's fast DDA, when executed on powerful supercomputers allows to cover a significant range of numbers of dipoles N needed to model realistic, micron-sized particles. We therefore developed a parallel fast DDA, using the previously developed parallel version of the direct DDA, and demonstrated DDA simulations with up to 1.1 10^6 dipoles (see section 5 and Ref. [23]). The size of the models was only limited by the available memory. Even for this large model the execution time for 1 iteration is only 150 s.

Another important issue is the memory consumption of the simulations. The fast DDA program of Flatau and Draine requires ~$0.58(N_xN_yN_z/1000)$ Mbytes, where $N_xN_yN_z$ is the volume containing all the N dipoles [6]. The calculations are performed in double precision. This means that for a particle fitting in a 32^3 portion of a lattice (such as a sphere modelled with 17,904 dipoles) ~19Mbyte of RAM is needed. We have recently optimised the memory consumption of the fast DDA by only storing the dipoles, and not the complete computational box holding the particle. Furthermore, we perform our calculations in single precision, which give the same accuracy as in double precision [27]. This results in a memory consumption of 234 bytes/dipole, resulting in a requirement of ~ 4 Mbyte for the sphere model mentioned

[2] A typical DDA run requires 30 to 50 iterations. An upperbound of 10 minutes per iteration therefore is realistic if one wants to work in a production mode.

above.

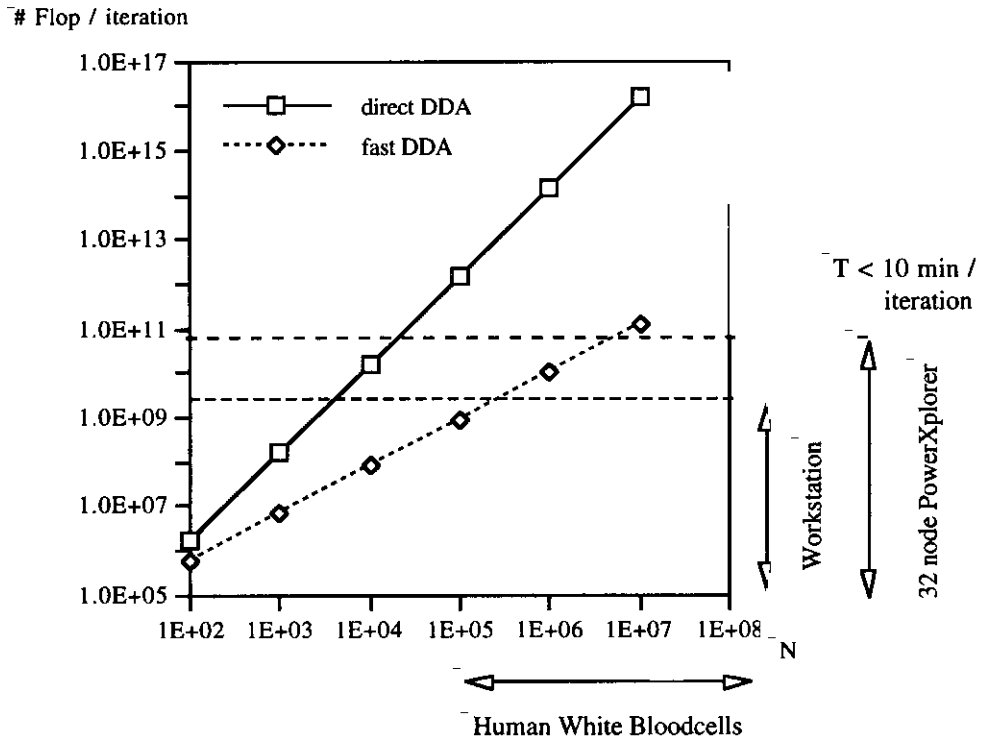

Figure 2: The required number of floating point operation per iteration in the DDA, as a function of the number of dipoles N used to discretise the particle. Lines for the direct DDA, and the Fast DDA (i.e. accelerated using FFT) are shown. The range of N, needed to model Human White Blood cells is indicated, and, by demanding that the maximum time for an iteration is smaller than 10 minutes, the range of workstations and a 32 node PowerXplorer are also indicated.

One may conclude that DDA models with up to 10^4 dipoles can now easily be handled on powerful PC's or workstations. Larger models of $O(10^5)$ dipoles can still be handled on workstations, provided that enough RAM (say 64 or 96 Mbyte) is available. Even larger models not only require more memory than usually available on the desk-top, the execution times of such large models will also become to high for current workstations. Therefore, such simulations should be performed on powerful supercomputers. We are currently preparing for DDA simulations of models with 10^7 dipoles on a parallel IBM SP2 computer.

Up till now we have only investigated to what extend DDA simulations are feasible, from a computational point of view. A more important question is the quality of the DDA model itself, i.e. the accuracy of the DDA model. Usually the accuracy is measured by performing DDA simulations of particles allowing analytic solutions of the light scattering problem, and comparing the DDA results with exact theory. In most cases the particles are spheres or concentric spheres, however recently a two-sphere system was simulated with DDA and compared to exact theory [28].

The conclusion of many of these comparisons (see e.g. [6,9,16,21-23,25] is that for slightly absorbing particles, with refractive indices up to 1.5 + i 0.1, the accuracy of the total cross sections can be (much) better than 1 % provided that $|m|kd < 0.5$. The is also true for the rms error in the differential cross sections. However, for specific scattering angles, the errors in DDA can easily increase above 5 %. Usually this happens for scattering angles where the differential cross section itself is quite small, and therefore small absolute errors result in relative large relative errors. The results presented in [6], and also our own experiments [22,25], show that it is always possible to decrease the errors in the differential cross sections

by decreasing the size of the dipoles (to e.g. $d/\lambda = 1/20$). In some cases other elements of the scattering matrix have been calculated [6,11,12]. All elements have an accuracy comparable to that of the S_{11} element, except the S_{34} element which usually has larger errors.

If the refractive index of the particle is large, and if it becomes more absorbing, the number of iterations needed in the CG methods sharply increases [see e.g. 21]. Furthermore, the errors in the differential cross sections increase. However, again we observe that it is always possible to decrease the errors by decreasing the dipole size.

In general we can conclude that in the ranges of particle sizes and refractive indices ($|m|<\sim 2$) surveyed up till now the DDA allows for accurate simulations of light scattering.

Many light scattering simulations require an orientational averaging of the (differential) cross sections over a particle's position. If one solves the system of equations with a direct method (LU decomposition, which has the disadvantage that the number of dipoles cannot be to large), the randomising of the orientation of the particle can be accomplished by explicitly solving the matrix equation just once for one orientation and applying rotation matrices to calculate the solution for other orientations [29]. If iterative methods are used it is necessary to actually calculate the cross sections for a large number of orientations. As was shown by Singham [19], orientational averaging requires simulations in 1000 to 2000 random positions of the particle. This problem places a severe burden on the DDA method, as compared to other methods, such as the T-matrix approach, which allows for a much more efficient way of orientational averaging [30-32].

5. EXAMPLES OF LARGE SCALE DDA SIMULATIONS

As an example of the use of DDA we show our first steps towards simulations of light scattering by Human White Blood Cells (HWBC). More examples of the use of DDA can be found in Refs. [13,21,26,33-40]

An important type of a small HWBC is the Lymphocyte, which normally is nearly spherical, and has a large spherical nucleus [41]. However, subtle morphological differences between Lymphocyte sub classes have been reported, and pathological stages of Lymphocytes usually show clear morphological signatures (such as a displacement or roughening of the nucleus; for a discussion of these issues, see Ref. 25, chapter 1.3.3). It is our purpose to detect such biologically important morphological differences through Elastic Light Scattering. The goal of our simulations is to search for suitable light scattering experiments which are most sensitive to specific morphological differences between (subsets) of HWBC or between healthy and malign HWBC. In this section we will demonstrate that with our current parallel fast DDA we will be able to pursue such large scale simulations.

The diameter D of HWBC is $4 \leq D \leq 16$ μm [see e.g. 41, 42 table I, or 43, chapter 1]. The relative refractive index m of HWBC is in the range $1.01 \leq m \leq 1.08$ [44].

In Fig. 3 we show results of a simulation of scattering from a homogeneous sphere with a diameter of 7.2 μm, resulting in a size parameter α of 36, and a relative refractive index of 1.05. Next, Fig. 4 shows a simulation of scattering from a small Lymphocyte, which is modelled as a concentric sphere with an outer diameter of 6.0 μm and an inner diameter of 4.2 μm. The refractive index of the nucleus, i.e. the inner sphere, is 1.05 and that of the cytoplasm is 1.02. In both cases the particles are modelled in the fast DDA with 1.1 10^6 dipoles. The number of iterations was 49 and 37 for the homogeneous and concentric spheres respectively.

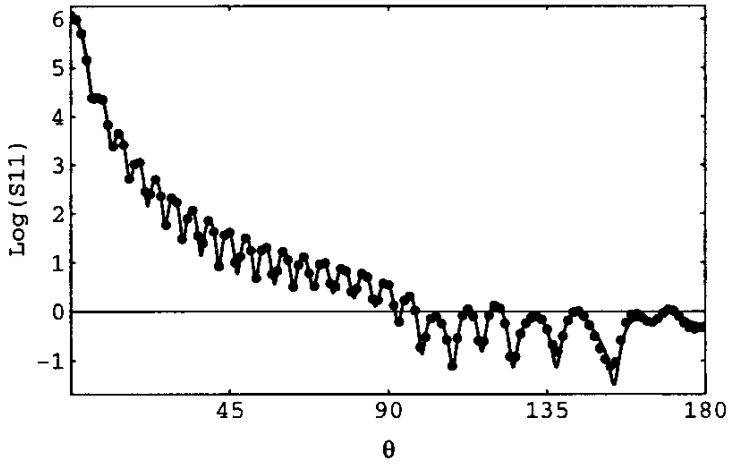

Figure 3: A fast DDA simulation, on the 32 node Parsytec PowerXplorer, of the scattered intensity from a homogeneous sphere with a diameter of 7.2 μm and a relative refractive index of 1.05; the number of dipoles in the simulation was 1.1 10^6, and the wavelength of the incident light was 632.8 nm. The dots are the results of the DDA simulation, the solid line is a Mie calculation.

The results are compared with analytical Mie theory. The correspondence between the analytical theory and the DDA simulations is good. In the future we plan to start simulations of scattering from Lymphocytes with a non-spherical or rough nucleus, with a displaced nucleus, or with non spherical cell shapes. Such simulations can no longer be performed with analytical theories, and for them we will employ our parallel fast DDA method.

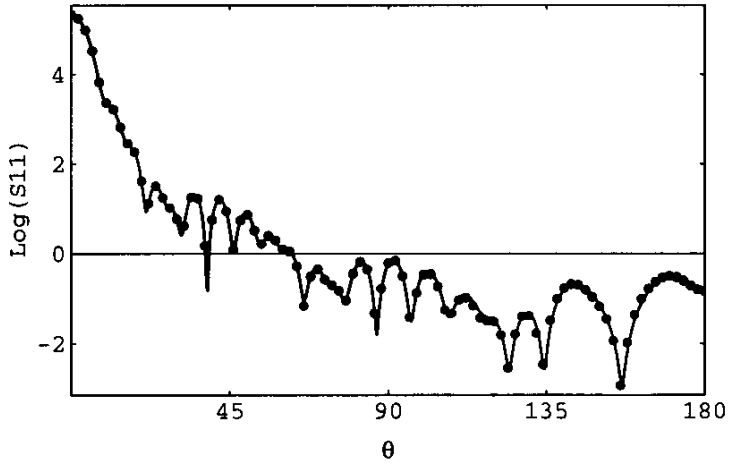

Figure 4: A fast DDA simulation, on the 32 node Parsytec PowerXplorer, of the scattered intensity from a small Lymphocyte, modelled as a concentric sphere with an outer diameter of 6.0 μm, an inner diameter of 4.2 μm, an inner relative refractive index of 1.05 and an outer relative refractive index of 1.02; the number of dipoles in the simulation was 1.1 10^6, and the wavelength of the incident light was 632.8 nm. The dots are the results of the DDA simulation, the solid line is a concentric sphere Mie calculation

6. OPEN QUESTIONS AND NEW DIRECTIONS

As we already noticed in section 4 the number of iterations needed to solve the DDA equations rises sharply if the refractive index of the particle is increased, i.e. an enormous slowing down of the convergence rate of the Conjugate Gradient method is observed [21, 25]. Furthermore, if the grid spacing d is kept constant, the accuracy of DDA seems to decrease,

which can be solved by making the grid spacing smaller [6]. The bottom line is that DDA calculations of large models with large refractive index are much more difficult from a computational point of view. It is still an open question if the current numerical procedures are robust enough to solve the equations with large m. We feel that for the situations of large m a good preconditioner for the Conjugate Gradient method needs to be developed. We have tried a simple first order polynomial preconditioner, but this was not successful [25].

Furthermore, just as we are able to settle a range of particle sizes which we should be able to model (see section 4), we should define a range of refractive indices which we should be able to cover with DDA. Draine and Flatau e.g. have shown that for $|m| >> 1$ the DDA is no longer a good model, because the DDA seems to result in to large polarisation in the surface layers, resulting in an overestimation of absorption cross sections for large m. [6,9] They suggest that in this case other techniques (such as the method of Rouleau and Martin [45]) are much more suited than DDA. A systematic study of DDA versus other methods for large m would be needed to find the range of refractive indices which we should be able to cover with DDA, and to answer the question if this is at all possible, both from a physical - (accuracy of DDA model) and from a computational (execution time of the simulation) point of view.

In principle the DDA method allows to simulate scattering by an arbitrary incident field, provided that the incident field is a solution of the Maxwell equations. We have studied the feasibility of the DDA method to simulate scattering by focused laser beams. We simulated scattering of strongly focused laser beams from a sphere with the DDA method, and compared the results with analytical calculations using the generalised Lorenz-Mie theory (GLMT). The first results show that DDA is perfectly capable of simulating scattering by focused beams, but that the accuracy of the simulation is somewhat less as compared to plane wave illumination [25, 27].

Other new directions are attempts to reduce the computational complexity of algorithms to solve the DDA equations using hierarchical methods. First, the work of Chew et al. could be very relevant for the DDA [46]. Chew et al. try, among others, to reduce the complexity of the direct $O(n^3)$ methods to solve the equations resulting from Integral Equation methods for scattering. These new algorithms could be combined with the straightforward orientational averaging which is possible when using direct methods to solve the DDA equations.

Hierarchical tree methods could be applied to reduce the complexity of the matrix vector products in the conjugate gradient method [20,22]. In most DDA applications the FFT does a great job. However, if the particles become very fluffy, the FFT has to do many unneeded calculations thus reducing the efficiency of the FFT's. Furthermore, if one wants to relax the demand to put the dipoles on a regular grid the FFT's can no longer be used. It is in these two situations that hierarchical methods could be applied to reduce the execution time of the matrix vector products. First results show that hierarchical tree methods are indeed suited to reduce the complexity of vector wave problems [20,47].

7. CONCLUDING REMARKS

The Discrete Dipole Approximation is a well established method to simulate light scattering from arbitrary shaped particles. Models containing an $O(10^4)$ dipoles with $|m| < 2$ can be easily simulated on powerful PC's or workstations. Larger models and higher refractive indices pose computational problems, forcing to run the models on more powerful computers. In all cases studied so far however the resulting (differential) cross sections are quite accurate. We have e.g. shown accurate DDA simulations of a model containing 1.1×10^6 dipoles.

More research is required to establish the quality of both the DDA model itself and the numerical algorithms for large refractive indices. Furthermore, efficient techniques for orientational averaging have to be developed.

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