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Simulating Light Scattering from Micron-Sized Particles

A parallel Fast Discrete Dipole Approximation

A.G. Hoekstra, M.D. Grimminck, and P.M.A. Sloot

The Parallel Scientific Computing & Simulation Group, Faculty of Mathematics, Computer Science, Physics, and Astronomy, University of Amsterdam, Kruislaan 403, 1098 SJ Amsterdam, the Netherlands, tel. +31 20 5257463, fax. +31 20 5257490, email alfons@fwi.uva.nl, URL http://www.fwi.uva.nl/research/pwrs/

Abstract

Employing the combination of a kernel with low computational complexity, implemented on powerful HPC systems, we are now able to push the limits of simulation of light scattering from arbitrary particles towards particles with dimensions up to 10 micrometer. This allows for the first time the simulation of realistic and highly relevant light scattering experiments, such as scattering from human white blood cells, or scattering from large soot - or dust particles. We use the Discrete Dipole Approximation to simulate the light scattering process. In this paper we report on a parallel *Fast* Discrete Dipole Approximation, and we will show the performance of the resulting code, running under PVM on a 32-node Parsytec PowerXplorer. Furthermore, we present results of a simulation of scattering from a model of a small Human White Blood Cell. This model is the largest possible particle fitting in memory of our parallel computer, and contains 1.1 million dipoles.

1. Introduction

Elastic light scattering (ELS) from arbitrary particles has many important applications. Examples are ELS from human white blood cells, [e.g. 1,2,3] from interstellar and interplanetary dust particles, [e.g. 4,5,6] from soot particles in combustion flames, [e.g. 7,8] or from airborne particles [e.g. 9,10]. In many cases these particles are not highly symmetrical (e.g. ellipsoidal or spherical), preventing separation of variables in the Maxwell equations and subsequent analytical solution of the ELS problem. Moreover, many of these particles also fall outside the range of approximation theories of ELS, such as Rayleigh-Debey-Gans theory or anomalous diffraction [see e.g. 11 or 12]. Yet, the need to calculate ELS from these particles definitely exists. For instance, when one has to verify models of particles, solely on the basis of ELS information, as was the case for the interstellar dust particles, [4] or if one has to define an optimal scattering experiment to detect subtle changes in particle morphology, as is the case in our Flowcytometric experiments on human white blood cells [1].

The need to simulate ELS from arbitrary particles prompted much research to develop methods that support numerical solutions of the ELS problem. One such method is the Discrete Dipole Approximation (DDA) method [14], which has recently been reviewed by Flatau and Draine [15].

In this paper we survey the computational requirements of the DDA for the simulation of ELS from realistic, micron-sized particles and report on a parallel implementation of a *Fast* DDA method (FDDA). Our major interest is ELS from human white blood cells. In this paper we investigate if the combination of the FDDA method, executed on a powerful parallel system allows simulations of ELS from these realistic, micron-sized particles. We will present results of the largest possible simulations that we have performed on a 32 node Parsytec PowerXplorer, modelling a small Human White Blood Cell.

2. The Discrete Dipole Approximation

Consider an arbitrary particle illuminated by a monochromatic electromagnetic field $\mathbf{E}^0(\mathbf{r})$ with wavelength λ. Our task is to calculate the scattered electric field $\mathbf{E}^s(\mathbf{r})$ in the full solid angle around the particle.

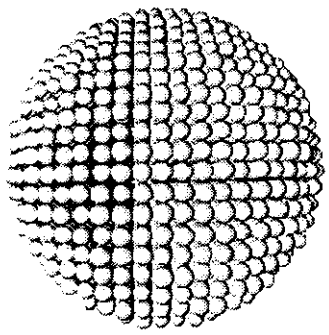

Figure 1: An example of a sphere discretised into 4226 isotropic dipoles, which are placed on a cubic grid.

The Discrete Dipole Approximation (DDA) method divides the particle into N equal sub volumes. The size of a sub volume, d, must be small enough to ensure that its response to an electromagnetic field is the response of an ideal induced dipole. Recommended values in the literature range from $\lambda/20 < d < \lambda/10$, with λ the wavelength of the incident light [13]. Figure 1 shows an example of a sphere discretised into dipoles.

The electric field on each dipole, due to an external field and the fields radiated by all other dipoles, must be calculated. Once the electric field on the dipoles is known, the scattered field is calculated by summing the contributions of all dipoles in the far field region. The electric field on dipole i ($1 \le i \le N$), due to the external field $\mathbf{E}^0(\mathbf{r})$ and the field radiated by all other dipoles, is

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

The 3×3 matrix $\mathbf{F}_{ij}$ describes the radiation from dipole j on dipole i (see e.g. [3,16] for an exact definition). Eq. 1 defines a set of $3N$ equations for the $3N$ unknowns ($\mathbf{E}_x(\mathbf{r}_i)$, $\mathbf{E}_y(\mathbf{r}_i)$, $\mathbf{E}_z(\mathbf{r}_i)$).

After solving the matrix equation, the scattered electric field $\mathbf{E}^s$ is calculated by summing the fields, radiated by the dipoles, at the observation point $\mathbf{r}_{obs}$:

$$\mathbf{E}^s(\mathbf{r}_{obs}) = \sum_{i=1}^{N} \mathbf{F}_{obs,i}\mathbf{E}(\mathbf{r}_i) \; . \tag{2}$$

Calculation of the electric field on the dipoles, Eq. 1, is the most expensive computational 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. This system of equations is solved using a Conjugate Gradient method. We apply the so-called CGNR method [17]. In previous work we have parallelised the CGNR method for distributed memory computers, in the Single Program Multiple Data paradigm [3,18], and used it to develop a parallel DDA simulation [16].

In Fig. 2 we indicate the number of floating point operations needed for 1 iteration of the DDA (the line *direct DDA*), 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 [16] 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, when executed on a typical workstation (a Sun Sparcstation 20 at 50 MHz) or a 32 node Parsytec PowerXplorer (see Fig. 2). It is obvious that the direct DDA iteration is to demanding

if we wish to simulate ELS from realistic, micron sized particles (see also the discussion in [16]).

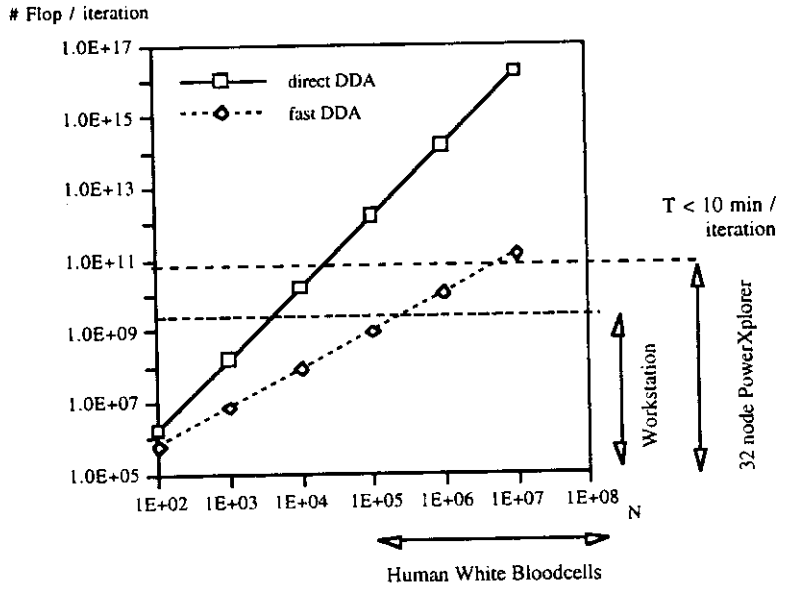

Figure 2: The required number of floating point operation per iteration in the DDA, as a function of the number of dipoles N used to discretise the particle. Lines for the direct DDA, and the Fast DDA (i.e. accelerated using FFT) are shown. The range of N, needed to model Human White Blood cells is indicated, 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.

Goodman et al., pointed out that due to the property $\mathbf{F}_{ij} = \mathbf{F}_{i-j}$, the matrix vector products which appear in the DDA iterations can be reformulated as discrete convolutions of electric fields on the dipoles [19]. These convolutions can be calculated in an O(Nlog$N$) complexity (using fast Fourier transformations), which is an enormous reduction in operations as compared to the direct (O(N^2)) calculation. The operation count for one iteration of this *Fast* DDA (FDDA, i.e. DDA using the fast Fourier transforms) is also indicated in Fig. 2. This suggests that Goodman's FDDA, when executed on a 32 node PowerXplorer (i.e. a low complexity kernel executed on a powerful HPC system) allows to cover a significant range of numbers of dipoles N needed to model realistic, micron-sized particles. We therefore developed a parallel FDDA, using the previously developed parallel version of the direct DDA [16].

The FDDA embeds the particle in a rectangular box, as demanded by the reformulation into discrete convolutions [19]. First, the box is decomposed in the z-direction, and the slices are allocated to processors. A fast Fourier transformation is first performed in the x-direction (completely in parallel). Next, the data box is transposed, giving rise to an expensive global communication operation, and then single y-z planes are (in parallel) 2D convoluted using fast Fourier transformations and inverse fast Fourier transformations. The data volume is transposed back again to the original z-decomposition and finally the total 3D convolution is completed by inverse fast Fourier transforms in the x-direction. This order of operations saves a large amount of memory. Details are described elsewhere [20].

The parallel FDDA was implemented in PVM. We have performed a number of performance measurements on a 32 node Parsytec PowerXplorer, which has an 80 MHz PowerPC-601 processor with 32 Mbytes RAM as compute node, and per node 1 T8 transputer as communication chip. In Fig. 3 we show the execution time of 1 iteration of the FDDA as a function of p, the number of processors and N, the number of dipoles. Even for the largest model fitting in memory of the full system ($N = 1.1\ 10^6$, executed on 32 processors), the execution time for 1 iteration is only 150 s. If we compare this execution time of FDDA to an execution time of 30 minutes per iteration for a much smaller number of dipoles ($N = 3.3\ 10^4$) for the direct DDA running on 32 nodes of the PowerXplorer (see [16]), the enormous gain is obvious.

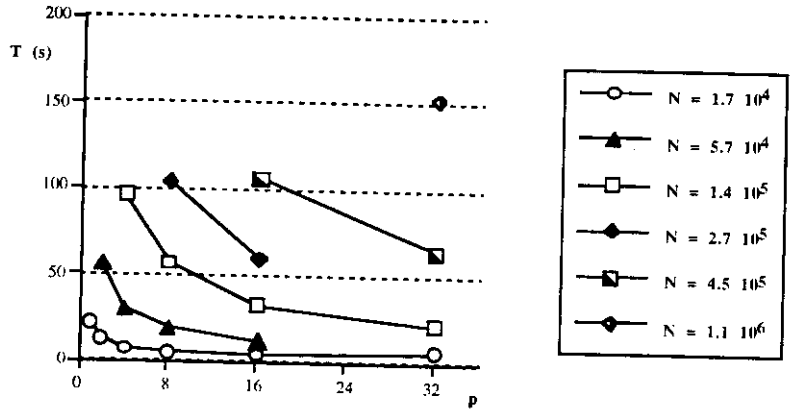

Figure 3: The execution time (in seconds) of one iteration of the parallel FDDA, as a function of the number of processors, for a range of the number of dipoles N. The program was executed on a 32 node Parsytec PowerXplorer.

Since only the smallest problem size ($N = 1.7\ 10^4$) fits in memory of 1 processor, we are not able to measure parallel efficiencies of the code. However, the data for $N = 1.7\ 10^4$, $5.7\ 10^4$, and $1.4\ 10^5$ suggest that after an initial good scaling of the execution time, the speedup levels off. This behaviour is due to the relative expensive transpose operation. We measured the total communication time per iteration. It turns out that this communication overhead is almost constant, independent of the number of processors (i.e. $O(N)$, data not shown). However, the time spent in calculations decreases with increasing p (i.e. $O(N \log N / p)$, which qualitatively explains the data in Fig. 3. In order to assess to what extent the parallel execution is communication bound, we plot, in Fig. 4, the percentage of communication overhead per iteration of the FDDA. We can conclude that as p increases, the parallel FDDA rapidly becomes communication bound. However, if the problem size is increased the communication overhead decreases again.

It is well known that the balance between communication speed and computation speed of the Parsytec PowerXplorer is not very good (see e.g. our own measurements [21]). We expect, with drastically increased link speeds of next generation systems, that the communication overhead will become less pronounced than in this current set of measurements.

However, for us the resulting execution times and the maximum size of the models which we can simulate now are much more important that the efficiency of the parallel code. The parallelisation not only allowed us to use the computational power which is present in the Parsytec PowerXplorer, it *also* allowed us to use the full one Gbyte

memory of the parallel system, which is much larger than what we have available in our local workstations. Therefore, the parallelisation not only results in small execution times per iteration, but more important, it allows to alleviate the memory bottleneck which we encountered on workstations, thus facilitating simulations of larger models. The parallel FDDA could also be executed on a cluster of workstations, thus allowing to use the combined memory which is present in the cluster.

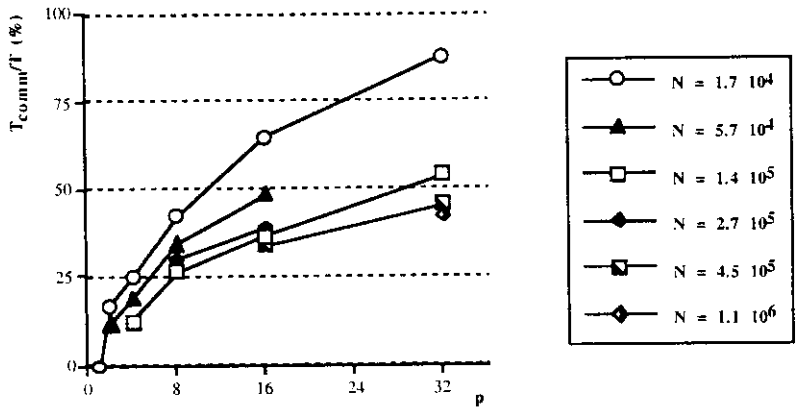

Figure 4: The percentage of communication overhead in one iteration of the parallel FDDA, as a function of the number of processors, for a range of the number of dipoles N. The program was executed on a 32 node Parsytec PowerXplorer

3. A DDA simulation, with more than 1 million dipoles, of a small Human White Blood Cell

An important type of a small Human White Blood Cell (HWBC) is the Lymphocyte, which normally is nearly spherical, and has a large spherical nucleus [22]. 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 reference 3, chapter 1.3.3). It is our purpose to detect such biologicaly important morphological differences through Elastic Light Scattering. The goal of our simulations is to search for suitable ELS 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 the current parallel FDDA 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. 21, 23 table I, or 24, chapter 1]. The relative refractive index m of HWBC is in the range $1.01 \leq m \leq 1.08$ [25].

In Fig. 5 we show results of a simulation of scattering from a homogeneous sphere with a diameter of 7.2 μm and a relative refractive index of 1.05. Next, Fig. 6 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 FDDA with $1.1\ 10^6$ dipoles, which, to the authors' knowledge, are the largest FDDA simulations ever reported.

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 FDDA method.

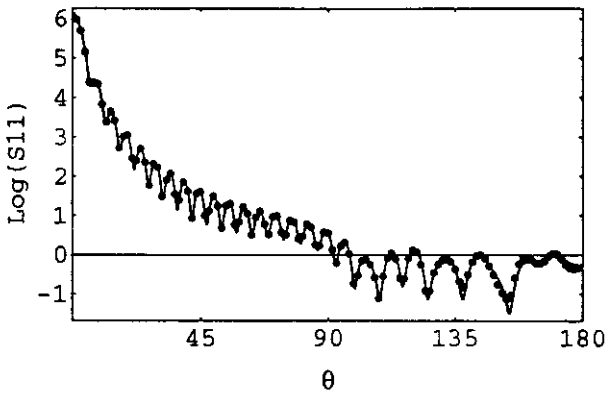

Figure 5: A FDDA simulation, on the 32 node Parsytec PowerXplorer, of the scattered intensity from a homogeneous sphere with a diameter of 7.2 μm and a relative refractive index of 1.05; the number of dipoles in the simulation was 1.1 10^6, and the wavelength of the incident light was 632.8 nm. The dots are the results of the DDA simulation, the solid line is a Mie calculation.

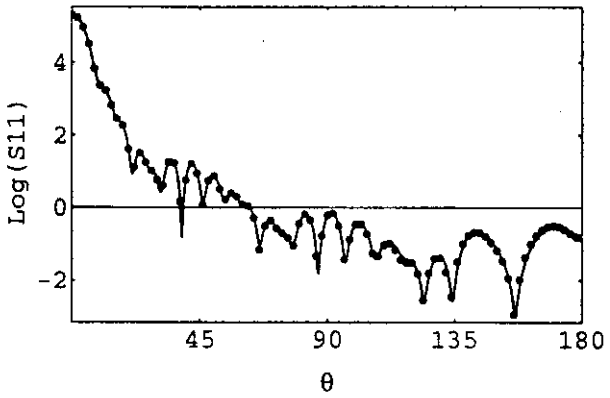

Figure 6: A FDDA simulation, on the 32 node Parsytec PowerXplorer, of the scattered intensity from a small Lymphocyte, modelled as a concentric sphere with an outer diameter of 6.0 μm, an inner diameter of 4.2 μm, an inner relative refractive index of 1.05 and an outer relative refractive index of 1.02; 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

4. Conclusions

In this paper we have presented a final step towards simulation of Elastic Light Scattering from realistic, micron sized particles.

The combination of a low complexity kernel, i.e. the *Fast* DDA method, implemented on a powerful HPC system allows us to run DDA simulation with more than one million dipoles. Although, even for the largest models, the parallel simulation spends a significant percentage on communication overhead, the execution time of the parallel FDDA is very small. Furthermore, the parallelisation allowed us to run much larger

models, because we are now able to exploit *all* memory available in the (distributed memory) parallel system. This conclusion, together with the small execution times is much more relevant than a good efficiency of the parallel code. Therefore, the relative high communication overhead is not of a great concern. The parallel FDDA is also suited to be executed on clusters of workstations, allowing to exploit the combined memory present in the workstations of the cluster.

The large scale simulations which we can now execute allow, for the first time, to model small Human White Blood Cells. We have presented an example of a simulation of scattering from a Lymphocyte, which was modelled as a concentric sphere with a diameter of 6 μm. In the future we plan to perform simulations on more realistic morphologies (i.e. a non spherical or rough nucleus, etc.). Furthermore, we plan to simulate the total scattering matrix, allowing to investigate more subtle light scattering experiments such as depolarization of the scattered light. Finally, with the availability of more powerful HPC systems we expect to be able to cover also the domain of larger Human White Blood Cells (such as Granulocytes or Monocytes), be able to include biological variability into the particle models, and be able to average over the orientation of the particles.

References

1. P.M.A. Sloot, A.G. Hoekstra, H. van der Liet, and C.G. Figdor, Applied Optics **28**, 1752 (1989).
2. B.G. Grooth, L.W.M.M. Terstappen, G.J. Puppels, and J. Greve, Cytometry **8**, 539 (1987).
3. A.G. Hoekstra, *Computer Simulations of Elastic Light Scattering, Implementation and Applications*, Ph.D. dissertation, University of Amsterdam, 1994.
4. J.I. Hage and J.M. Greenberg, Astrophysical Journal **361**, 251 (1990).
5. J.I. Hage, M. Greenberg, and R.T. Wang, Applied Optics **30**, 1141 (1991).
6. K. Lumme and J. Rahola, Astrophys. J. **425**, 653 (1994).
7. T.T. Charampopoulos, D.W. Hahn, and H. Chang, Applied Optics **31**, 6519 (1992).
8. C.M. Sorensen, J. Cai, and N. Lu, Applied Optics **31**, 6547 (1992).
9. W.L. Eberhard, Applied Optics **31**, 6485 (1992).
10. I. Colbeck, E.J. Hardman, and R.M. Harrison, J. Aerosol Sci. **20**, 765 (1989).
11. C.F. Bohren and D.R. Huffman, *Absorption and Scattering of Light by Small Particles* (John Wiley & Sons, 1983).
12. P.M.A. Sloot and C.G. Figdor, Applied Optics **25**, 3559 (1986).
13. A.G. Hoekstra and P.M.A. Sloot, Optics Letters **18**, 1211 (1993).
14. E.M. Purcell and C.R. Pennypacker, The Astrophysical Journal **186**, 705 (1973).
15. B.T. Draine and P.J. Flatau, J. Opt. Soc. Am. A **11**, 1491 (1994).
16. A.G. Hoekstra, P.M.A. Sloot, Int. J. Mod. Phys. C **6**, 663 (1995).
17. S.F. Ashby, T.A. Manteuffel, and P.E. Saylor, Siam J. Numer. Anal. **27**, 1542 (1990).
18. A.G. Hoekstra, P.M.A. Sloot, W. Hoffmann, and L.O. Hertzberger, Tech. Rept. CS-92-06, Faculty of Mathematics and Computer Science, University of Amsterdam, 1992.
19. J.J. Goodman, B.T. Draine, and P.J. Flatau, Optics Letters **16**, 1198 (1991).
20. M.D. Grimminck, Masters Thesis, University of Amsterdam, faculty of mathetics, computer science, physics, and astronomy (1996).
21. A.G. Hoekstra, P.M.A. Sloot, F. van der Linden, M. van Muiswinkel, J.J.J. Vesseur, and L.O. Hertzberger, Concurrency, Practice and Experience **8**, 19 (1996).
22. H. Begemann and J. Rastetter, *Atlas of clinical hematology* (Springer Verlag 1979).
23. P. Latimer, D.M. Moore, and F. Dudley Bryant, J. Theor. Biol. **21**, 348 (1968).
24. P.M.A. Sloot, *Elastic Light Scattering in the Development of Computer Assisted Cell Separation*, Ph.D. dissertation, University of Amsterdam, 1988.
25. K.W. Keohane and W.K. Metcalf, Quart. J. Exp. Physiol. Cog. Med. Sci. **44**, 343 (1959).