Light Scattering Simulations with a Massively Parallel Computer at the IC^{3}A

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Abstract

The Coupled Dipole method, as originally formulated by Purcell and Pennypacker, is a very powerfull method to simulate the Elastic Light Scattering from arbitrary particles. This method however has one major drawback: if the size of the particles grows, or if scattering from an ensemble of randomly oriented particles has to be simulated, the computational demands of the Coupled Dipole method soon become too high. In this paper we present a new computational technique to solve this problem. We have implemented the Coupled Dipole method on a Massively Parallel Computer in our Interdisciplinary Center for Computer based Complex systenm research in Amsterdam. The parallel efficiency is close to one, implying that attained computational speed scales perfectly with the number of processors.

1 Introduction

1.1 Definition of the physical problem and the computational challenge

Elastic Light Scattering (ELS) is of general interest to an enormous dynamic field with an impact on a large variety of disciplines, spanning the fields of solid-state physics, via meteorology, to chemistry, biophysics, and astronomy. For instance, light scattered from (nucleated) blood cells contains information on both the cell size and the morphology of the cell. This nondestructive sensing of a single cell has led to numerous analytical and preparative applications in cell biology. The number of theories describing light scattering from biological cells is, however, limited. Moreover, no adequate general

theory is yet known to describe analytically the ELS characteristics of arbitrarily shaped particles (although the need for such a theory is generally appreciated). This is mainly due to the complex nature of the phenomena and the numerical instability of the existing algorithms.

The Coupled Dipole (CD) method [3] is a powerful method to calculate Elastic Light Scattering (ELS) from arbitrary particles. However, to be useful in practical applications, a huge computational challenge must be met. Especially if orientational averages have to be calculated, or if the size parameter of the particle grows, the CD method soon needs computing power far beyond the possibilities of desktop computers or even beyond the possibilities of super computers. In this report we present a computational technique that can make the CD method suited for routine light scattering calculations of arbitrary particles.

The basic technique is parallel computing, which is an adaptation at the implementation level. The merits of parallel computing are demonstrated on the basis of CD calculations of systems containing up to 33.000 dipoles. Such large systems require very powerful computers. In our case the CD method is implemented on a 512 node parallel transputer system (a Parsytec GCel-3/512).

1.2 Interdisciplinary Center for Computer based Complex systen research Amsterdam IC^{3}A

The work presented in this paper was carried out at the IC^{3}A. The foundation of the IC^{3}A has been initiated by Prof. dr. L.O. Hertzberger and has been motivated by the success and growing importance of two multidisciplinary research thrusts, namely, computational science and complex systems. These two themes are synergistically linked by their reliance on high performance computers. In each case, we expect these fields to grow in importance with the continuing increase of performance of parallel supercomputers. It is the major objective of IC^{3}A to stimulate the computer supported research of complex systems. Studying the behaviour of such complex system models is essential for a better understanding of large classes of problems in a wide field of science and engineering. Such complex system models are helpful in better understanding problems in physics such as fluid flow, multi particle interaction, crystal nucleation, mechanical engineering, such as crash worthiness analysis, turbulent flow analysis for instance required in aeroplane design etc. Computer supported study of these complex systems via modelling and simulation is a methodology that offers the possibility of explanation, prediction and optimisation of these systems. IC^{3}A aims to be a focusing point for this research on the national as well as international level.

To promote the study of complex systems in science and technology applications through the usage of high performance computing the centre aims to have open facilities for the academic as well as industrial community. This implies that the software environment of the centre will be such that its facilities can be easily accessed over the national and international networks. Moreover experience of the centre in parallelising applications will be made available via a staff of scientific programmers that will be able to assist the domain experts in their tasks. In addition training courses and hands-on workshops will be organised among others on such aspects as the usage of the facilities, generic solver methods and

algorithms, the exploitation of parallelism for various large scale application etc.
The research programme of the centre focuses on the following aspects:

- Computational methods and techniques to realise and support the study of complex systems in order to realise large application in science and engineering,
- Methods and techniques to create new computer functionality's and systems.

With computational methods and techniques (like Computational Fluid Dynamics, Multi Particle models, Monte Carlo techniques or non linear dynamics techniques) it becomes possible to model and simulate complex real world systems and problems such as a chemical reactor, light scattering on complex particles, a wing of an aeroplane, or the long term changes in the atmosphere and get a better understanding of their behaviour. The realisation of large realistic applications, based on the better understanding of complex systems, is one of the main targets of the research programme of the centre.
To be able realise complex system studies the current models, and computational techniques for simulation are not sufficient. Moreover realistic problems will often require orders of magnitude more computing power than is available with sequential computer systems and can only be realised through the usage of parallel systems and computational techniques. Therefor important research issues in this part of the program is the study and development of generic parallel solver methods that are applicable to a wide range of application domains and a wide area of parallel and distributed platforms. The programme will also study complex systems for which no a priori model is available and for which models have to be developed along phenomenological lines.
To support the previous research line a second line concentrates on the study of computer systems as a complex system with the aim to extent its functionality. Emphasis will be on the methodologies to create high performance parallel and distributed systems that provide flexible user interaction. The realisation of new interactive control methods (for instance via visualisation) to enable user controlled simulation experiments are the main objective. In the study of parallelism through the interaction between application and machine emphasis will be on scalability effects, to be able to exploit massive parallel systems.
Additional important research issues are software integration over multiple levels of the technology chain (e.g. application, system software, computer hardware), machine and application modelling and parametrisation, multi modal information storage and retrieval, sensor based computer interaction (including virtual reality)
The center has a 64-node Meiko, a 512 node T805 based Parsytec GCel -3/512 and will have a 64 node T9000 based Parsytec GC-2/64 in the near future to be extended by the end of the year towards 128 nodes. The installation of an IBM SP_1 is under negotiation. Access to the recourses of the centre will be provided on basis of a short proposal stating, among others, the goals of the research and its importance, the amount of facilities and services required etc. The scientific board of the centre
judges the potentialities of the proposal advised if necessary by outside referees.

2 Computational structure

The CD method divides a particle into N small subvolumes, whose size must be small enough to ensure that it can be viewed as an ideal dipole. Usually one chooses $\lambda/20 < d < \lambda/10$, with d the size of a subvolume, and λ the wavelength of the incident light. From now on we refer to the subvolumes as dipoles. First the electric field on dipole i, $\mathbf{E}(\mathbf{r}_i)$ $(1 \le i \le N)$, due to the external field $\mathbf{E}^0(\mathbf{r})$ and the field radiated by all other dipoles is calculated. This can be formulated as a matrix equation $\mathbf{Ax} = \mathbf{b}$, with

$$\mathbf{x} = \begin{pmatrix} \mathbf{E}(\mathbf{r}_1) \\ \vdots \\ \mathbf{E}(\mathbf{r}_N) \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} \mathbf{E}^0(\mathbf{r}_1) \\ \vdots \\ \mathbf{E}^0(\mathbf{r}_N) \end{pmatrix} \text{ and}$$

$$\mathbf{A} = \frac{\gamma}{4\pi\varepsilon_0} \begin{pmatrix} \mathbf{I} & -\mathbf{F}_{12} & \cdots & & -\mathbf{F}_{1\mathrm{N}} \\ -\mathbf{F}_{21} & \mathbf{I} & & & \\ \vdots & & \ddots & & \vdots \\ & & & \mathbf{I} & -\mathbf{F}_{\mathrm{N}-1,\mathrm{N}} \\ -\mathbf{F}_{\mathrm{N}1} & & \cdots & -\mathbf{F}_{\mathrm{N},\mathrm{N}-1} & \mathbf{I} \end{pmatrix}.$$

The matrix $\mathbf{A}$ is the n×n interaction matrix (n = 3N), $\mathbf{F}_{ij}$ is a functional describing the field, radiated by dipole j on dipole i, and γ is the polarizability of the dipoles. 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 $\mathbf{r}_{obs}$. The dipoles are placed on a cubic grid with grid spacing d. The diameter of the spherical dipoles is equal to the grid spacing d.

Figure 1 gives an estimate of the number of dipoles needed to describe a compact particle, as a function of the size parameter α, with 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.

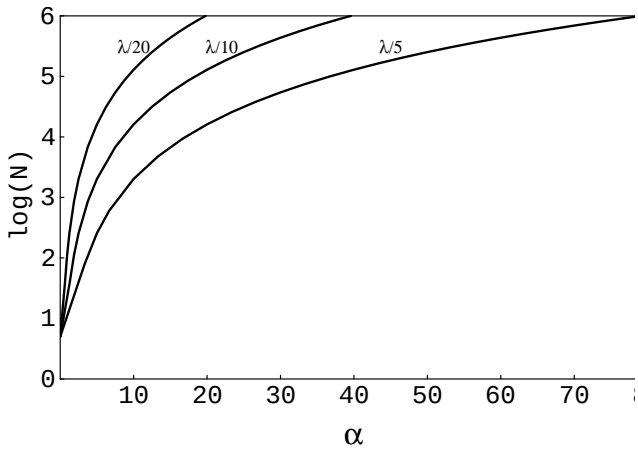


Figure 1: Estimation of the number of dipoles needed to model a compact particle.

Calculation of the electric field on the dipoles, that is, to solve the system of linear equations $\mathbf{Ax} = \mathbf{b}$ is the computationally most demanding part of the CD method. Generally speaking linear systems are solved by means of direct or iterative methods [4]. In the past both approaches were applied to solve the

coupled dipole equations. For instance, Singham et al. used a direct method (LU factorization) [5], Singham and Bohren described a reformulation of the CD method, which from a numerical point of view is a Jacobi iteration to solve the matrix equation [6], and Draine applied a Conjugate Gradient iteration [7].

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. We want to simulate Elastic Light Scattering of particles with $\alpha > 20$, i.e. $N = O(10^5)$. This vast number of dipoles forces us to use iterative methods. Suppose that the implementation can run at a sustained speed 1.0 Gflop/s, and $n = 3.0\ 10^5$. In that case a direct method roughly needs O(10) months to find a solution. An iterative method needs O(100) seconds per iteration. If the number of iterations can be kept small enough, execution times can be acceptable.

The Jacobi iteration is not very well suited for a large number of dipoles; already for a relative small number of dipoles (N= ~500), the Jacobi iteration becomes non-convergent [8]. A very efficient iterative method is the Conjugate Gradient method [4]. Draine [7] showed that the Conjugate Gradient method is very well suited for solving the coupled dipole 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. We apply a Conjugate Gradient method, the so-called CGNR method [9], to find the electric field on the dipoles.

3 Parallel Computing

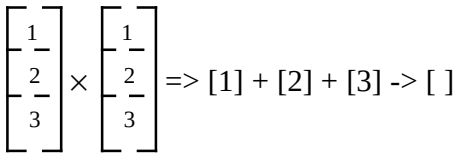
3.1 Parallel calculation of the dipole fields

The dipole fields are calculated in parallel by assigning N/p dipoles to each processor (with p the number of processors of the parallel computer), and each processor calculates the fields on these dipoles, using our parallel implementation of the CGNR method [10]. The CGNR method was implemented on a ring of transputers, with a rowblock decomposition of the matrix. Rowblock decomposition means dividing **A** in blocks of rows, with every block containing n/p consecutive rows.

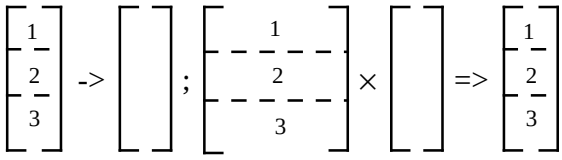
The CGNR method contains two matrix vector products, three vector updates and three inner products per iteration. Figure 2 schematically shows how these operations are performed in parallel.

$$\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} + [\text{factor}] \times \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

2.a: parallel vector update



2.b: the parallel inner product.



2.c: the parallel matrix vector for a rowblock decomposed matrix.

Figure 2: A schematic drawing of the parallel implementation (here with 3 processors) of the numerical operations. The decomposition of the vector and matrix is symbolized by the dashed lines; a single arrow (->) means a communication, and the implication mark (=>) means a (parallel) calculation.

The total computation time is $O(n^2/p)\tau_{calc}$, the communication time is $O(n)\tau_{comm}$. [10]. The parameters τ_{calc} and τ_{comm} are the times to perform one floating-point operation on a processor and to send one byte from a processor to a neighbouring processor. Thus, the efficiency of the parallel CGNR is

$$\varepsilon = \frac{T_1}{p\,T_p} \approx \left(1 + O\left(\frac{p}{n}\right)\frac{\tau_{comm}}{\tau_{calc}}\right)^{-1}, \qquad [1]$$

with T_1 the execution time on 1 processor and T_p the execution time on p processors. Here we neglegted many details of the communications and computations, for this see reference [10]. Still, equation 1 contains the most important conclusion. If n/p is large, the efficiency of the parallel CGNR method can be very close to one. This means that the execution time of the parallel CGNR is almost inversely proportional to the number of processors available in the parallel computer. Performance measurements of the actual implementation support this conclusion [10, 11].

3.2 Parallel calculation of the scattered fields

The scattered electric field is calculated in parallel by calculating the radiated electric fields from the dipoles in parallel, and summing them afterwards. This strategy matches the data decomposition used in the parallel CGNR implementation. After convergence of the CGNR every processor has the electric field on its local dipoles in memory. All processors calculate the scatterd fields due to their local dipoles in all observation points (e.g. the scattered field as a function of the scattering angle θ). Subsequently the results of all processors are accumulated and summed in the root processor, which writes the results

to disk for further analysis.

Both the calculation time and the communication time of the parallel calculation of the scattered fields are neglegible compared to the calculation - and communication time of the parallel CGNR. Therefore, the efficiency of the parallel CD method will be as good as the efficiency of the parallel CGNR. However, the parallel calculation of the scattered fields also has a very good parallel efficiency on its own right, as a straightforward analysis reveals (data not shown).

3.3 Results

The parallel CD method was implemented on a Parsytec GCel-3/512, a 512 node distributed memory computer, which was recently installed in Amsterdam. The nodes are Inmos T805 transputers. The implementation was carried out in the language C, under Parsytec's parallel programming environment Parix.

Figure 3 show the measured parallel efficiency of the CGNR for some small systems. As the number of dipoles increases the efficiency stays very close to 1 for a larger number of processors. It can be shown that for $N = O(10^4)$ or more, the efficiency is almost 1 for the maximum number of processors ($p = 512$). Most computing time is spent in the CGNR method, therefore these conclusions also hold for the complete parallel implementation of the Coupled Dipole method. This is also supported by actual measurements (data not shown).

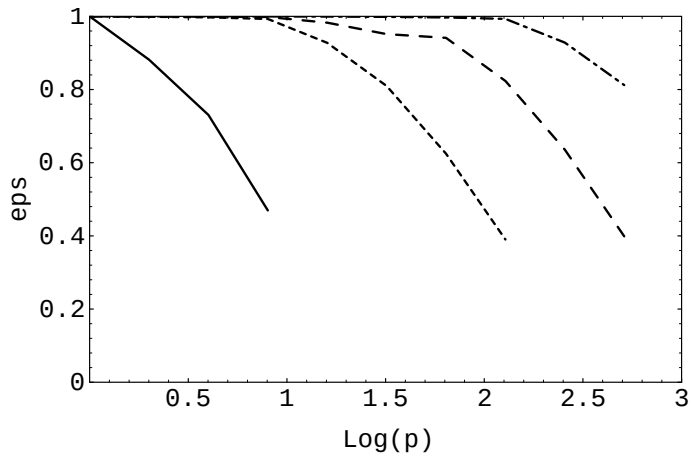


Figure 3: The measured parallel efficiency of the CGNR methodfunction of the number of processors; the straight line is for 8 dipoles, the short dashed line for 136 dipoles, the long dashed line for 552 dipoles and the point dashed line for 2176 dipoles

Figure 4 shows the result of a CD simulation of scattering by sphere, together with the analytical Mie result. The number of dipoles was 33552, the diameter of the dipoles was $\lambda/10$, resulting in a size parameter $\alpha = 12.6$; the refractive index was 1.05. This calculation required 11 hours on 512 processors. The parallel speedup was estimated to be larger than 500, the sustained computational speed was 250 Mflop/s. As soon as new updates of the C compilers are available, this number is expected to

be increased with a factor 2 (the current implementation was done with Parix 1.1).

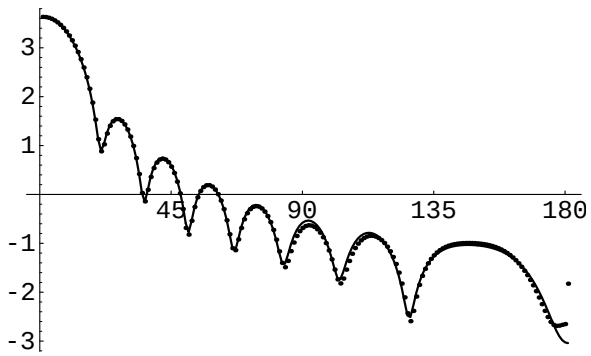


Figure 4: Coupled Dipole simulation (dots) of scattering by a sphere, and Mie calculations (line). The S_{11} element of the scattering matrix S, as a function of the scattering angle is shown. The size parameter of the sphere is α = 12.6, the refractive index is m = 1.05. The number of dipoles in the CD simulation was 33552, the size of the dipoles was $\lambda/10$.

The results of the CD simulations are in good agreement with the exact Mie results, except in the backscattering. This is probably due to the relative large size of the dipoles. The execution times are long, even on massively parallel computers. Note that we simulated a particle in only one orientation. If randomization is required, the execution times are no longer realistic. Furthermore, if the number of dipoles gets even larger, to $O(10^5)$ or $O(10^6)$, the execution time of the CD method for a particle in just one orientation already becomes too high.

4 Conclusions

The CD method allows, in principle, simulation of ELS of arbitrary particles. In practice however the calculation times to solve the CD equations soon become unrealistic. We have introduced a new technique to meet the computational challenge imposed by the CD method.

For the first time very large CD simulations can be performed on high end systems. In the future these advanced innovations will allow routine ELS calculations from arbitrary shaped particles, and serve more detailed optical particle characterizations.

5 Acknowledgement

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