Improvements of the Discrete Dipole Approximation method

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Abstract

We report improvements in complex conjugate gradient algorithms applied to the discrete dipole approximation (DDA). It is shown that computational time is reduced by using the Bi-CGSTAB version of the CG algorithm, with diagonal left preconditioning.

Key words: scattering, non-spherical particles, discrete dipole approximation.

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The discrete-dipole approximation (DDA) is a flexible technique for computing scattering and absorption by targets of arbitrary geometry. In [1] the discrete dipole approximation (DDA) for scattering calculations is reviewed. Rather than “direct” methods for solving linear system of equations arising in DDA problem iterative methods for finding the solution have proven effective and efficient.

In this paper we perform systematic study of various non-stationary iterative (conjugate gradient) methods in search for the most efficient one. We document implementation of these methods in our public domain code DDSCAT.5a code[1].

Numerical aspects of the discrete dipole approximation continue to be of great interest. Yung [2] applied a conjugate gradient method to the in DDA approach. Hoekstra [3] identifies Yung’s scheme as the conjugate gradient (CG) algorithm proposed by Hestenes [4]. Rahola [5] discusses solution of dense systems of linear equations in the discrete-dipole approximation and choice of of the best iterative method in this application. Draine [6] implemented a conjugate gradient method based on work of Petravic and Kuo-Petravic. [7] This implementation is quite robust and has been used for many years. [1] However, Lumme and Rahola [8] applied the quasi-minimal residual (QMR) conjugate gradient algorithm to the system of linear equations arising in the DDA applications. They claim that the QMR method is approximately 3 times faster in comparison to the one employed in the DDSCAT code. [1] It was this work which prompted us to perform the analysis reported here.
PIM[2] is a collection of Fortran 77 routines designed to solve systems of linear equations on parallel and sequential computers using a variety of iterative methods.

PIM contains implementations of various methods: conjugate-gradient (CG); Conjugate-Gradients for normal equations with minimization of the residual norm (CGNR); Conjugate-Gradients for normal equations with minimization of the error norm (CGNE); Bi-Conjugate-Gradients (BiCG); Conjugate-Gradients squared (CGS); the stabilised version of Bi-Conjugate-Gradients (BiCGSTAB); the restarted, stabilised version of Bi-Conjugate-Gradients (RBi-CGSTAB); the restarted, generalized minimal residual (RGMRES); the restarted, generalized conjugate residual (RGCR), the quasi-minimal residual with coupled two-term recurrences (QMR); the transpose-free quasi-minimal residual (TFQMR); and Chebyshev acceleration. The routines allow the use of preconditioners; the user may choose to use left-, right- or symmetric-preconditioning.

The convergence rate of iterative methods depends on the coefficient matrix. Hence one may attempt to transform the linear system into one that is equivalent (in the sense that it has the same solution) but is easier to solve. A preconditioner is a matrix $M$ that effects such a transformation. It is possible to introduce left- and right preconditioners. The simplest preconditioner consists of just the diagonal of the coefficient matrix. This is known as the (point) Jacobi preconditioner.

To compare these different algorithms we have used them to find solutions to the problem of scattering by a homogeneous sphere. The scattering problem is specified by the usual size parameter $x = 2\pi a/\lambda$, where $a$ is the radius.

Tables 1 and 2 presents the number of iterations and CPU time for size parameter $x = 0.1$ and $x = 1$ and for several values of refractive index. The conjugate gradient methods are defined as above. Label (L) indicates left Jacobi preconditioning. For example CGNE(L) is the conjugate gradient method for normal equations with minimization of the error norm and left Jacobi preconditioning. Similarly, (R) indicates right Jacobi preconditioning. CPU time (sequential Silicon Graphics workstation) is normalized to the “best” method. Star indicates that the method did not converge in the maximum allowed number of iterations or that the method failed to converge. Fractional error $10^{-5}$ was used as the stopping criterion. The DDSCAT.5a code[1] with the newly implemented GPFA fast Fourier transform method was used. For Bi-CGSTAB and CGNE we used left and right Neumann polynomial preconditioner truncated after the first term. Thus, Bi-CGSTAB(N)(L) indicates the stabilised version of Bi-Conjugate-Gradients method with left Neumann polynomial preconditioner.

Table 1 presents results for size parameter $x = 0.1$ and real refractive index $n = 1.33, 2, 3, 5$ as well as one case with small complex part of refractive index $n = (5, 0.0001)$ and size parameter $x = 0.1$. In Table 1 the CPU times are normalized to the CG(L) method, which was found to be the best method. For example it is 4.0 times faster in comparison with the CGNE for $n = (1.33, 0)$. For larger values of real refractive index the CGNE is almost an order of magnitude slower in comparison to CG. This is because more iterations are needed for the same convergence and because cost of one CG iteration is less than cost of one CGNE iteration. The QMR algorithm is never competitive and actually fails to converge for large real refractive indices. For small refractive index the Bi-CGSTAB algorithm is comparable to the CG and requires less iterations. However, the cost per iteration is larger in comparison to CG which offsets the advantage of lesser number of iterations. The Petravic and Kuo-Petravic [3] algorithm used by us...
for many years [3] is similar to CGNR and CGNE. However, we observed on occasion slightly different convergence rates due to stabilization of Petravic and Kuo-Petravic algorithm every 10th time step. [3] This is true for all other cases. The storage requirements of CG, CGNE, CGNR is $6 \times N$, for BiCG it is $8 \times N$, for CGS, Bi-CGSTAB, TFQMR it is $10 \times N$, QMR requires $11 \times N$. Thus, for pure real refractive index, the CG is not only the fastest method but also it requires the least amount of temporary storage. It can be seen that left preconditioning by the inverse of diagonal of the DDA matrix [3] reduces the number of iterations needed. The added time needed for division by diagonal elements is generally negligible in comparison to the time saved by smaller amount of iterations. It can be seen that for Bi-CGSTAB, Bi-CGSTAB(L), and Bi-CGSTAB(R) the left Jacobi preconditioning is the only method converging for larger refractive index. Restarted methods (RBi-CBSTAB and RGCR) appear to be not competitive but further study may be needed (we used the orthogonal base of 10 vectors for all restarted methods). The CG method is also competitive in cases with small absorption (see last column of Table 1). We have also calculated (not presented) results for size parameter of $x = 0.1$ and increasing complex part of refractive index $n = (1.33, 0), (1.33, 0.01), (1.33, 0.1), (1.33, 1), (1.33, 2), (1.33, 3)$. The BiCGSTAB(L), which proved to be the most robust method. However the CGS(L) is competitive and faster for $n = (1.33, 3)$. Both CGS(L) and BiCGSTAB(L) require the same amount of iteration for convergence and their cost is similar. These methods are between 2.9 and 1.6 times faster in comparison to CGNR — the method used in DDSCAT code. The QMR and TFQMR which Lumme and Rahola [8] claim to be faster in comparison to CGNR and the DDSCAT implementations do not converge on occasion and when they work they are only slightly better in this case. As before, left Jacobi preconditioning is almost always beneficial. The CG(L) algorithm is faster than BiCGSTAB(L) for refractive index $n = (1.33, 0), (1.33, 0.01), (1.33, 0.1)$. Table 2 is for size parameter $x = 1$. All the results are normalized to Bi-CGSTAB(L). This method is clearly superior to the CGNR method and it is 2-4.3 faster. It can be seen that CGNR converges slowly, and has not satisfied the stopping criterion in 140 iterations for $n = (3, 0.0001)$. For this larger value of size parameter the QMR algorithm doesn’t converge well but its smooth version TFQMR does. However, TFQMR is slower in comparison to Bi-CGSTAB(L) and comparable to CGNR. The CG(L) method for refractive index $n = (1.33, 0)$ and $n = 1.33, 0.01$ is faster than the reference scheme Bi-CGSTAB(L). It can be seen that the Neumann polynomial preconditioning Bi-CGSTAB(N)(L) or Bi-CGSTAB(N)(R) does reduce the number of iterations needed for certain cases of refractive index. However the cost associated with the additional calculations always offsets this improved convergence rate. As before, the left Jacobi preconditioner is superior to right or no-preconditioner cases. CG(L) works well for small refractive index but is comparable to Bi-CGSTAB(L). The QMR algorithm fails to converge but the transpose-free quasi-minimal residual (TFQMR) algorithm converges well and is comparable to CGNR. The CG method is theoretically valid for Hermitian positive definite matrices. The matrix arising in the DDA is not Hermitian but symmetric. Therefore, strictly speaking, the CG method is not valid for use in the DDA. The users are advised to test the CG method when extrapolating results presented here to different size parameters, particle sizes, and refractive index values.

We recommend use of the stabilized version of the Bi-conjugate gradient algorithm with left Jacobi preconditioning [Bi-CGSTAB(L)]. This algorithms requires 67% greater storage than the
CGNR algorithm, but is typically 2-3 times faster.

The recent version of Discrete Dipole Approximation code DDSCAT5a developed by Draine and Flatau contains improvements documented in this paper. The code is available via anonymous ftp from the ftp.astro.princeton.edu site or from the Light Scattering and Radiative Transfer Codes Library — SCATTERLIB (http://atol.ucsd.edu/~pflatau).

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Table 1: CPU time (normalized) and number of iterations for $x=0.1$.

| Method         | $n=(1.33,0)$ | (2.0)  | (3.0)  | (5.0)  | (5.0,0001) |
|----------------|--------------|--------|--------|--------|------------|
| CGNE           | 4.0(9)       | 4.9(24)| 8.7(76)| *(540) | *(540)     |
| CGNE(L)        | 3.3(7)       | 4.0(19)| 7.8(67)| *(540) | *(540)     |
| CGNE(R)        | 4.1(9)       | 4.9(24)| 8.8(76)| *(540) | *(540)     |
| CGNE(N)(L)     | 3.1(4)       | 4.1(13)| 19.3(113)| *(540)| *(540)   |
| CGNE(N)(R)     | 4.4(6)       | 7.7(25)| *(140) | *(540) | *(540)     |
| CGNE(N)(L)     | 3.1(4)       | 4.1(13)| 19.3(113)| *(540)| *(540)   |
| CGNE(N)(R)     | 4.4(6)       | 7.7(25)| *(140) | *(540) | *(540)     |
| CGNR           | 4.0(9)       | 4.7(23)| 8.0(69)| *(540) | *(540)     |
| CGNR(L)        | 3.3(7)       | 4.0(19)| 5.9(50)| 4.6(329)| 3.5(330) |
| CGNR(R)        | 4.1(9)       | 4.7(23)| 8.0(69)| *(540) | *(540)     |
| QMR            | 3.7(6)       | 3.3(11)| 3.3(19)| *(111) | *(78)      |
| QMR(L)         | 2.6(4)       | 2.8(9) | 2.7(15)| *(75)  | *(92)      |
| QMR(R)         | 3.8(6)       | 3.4(11)| 3.4(19)| *(268) | *(540)     |
| CG             | 1.4(6)       | 1.2(11)| 1.2(20)| 1.2(163)| 1.1(213) |
| CG(L)          | 1.0(4)       | 1.0(9) | 1.0(16)| 1.0(138)| 1.0(182) |
| CG(R)          | 1.4(6)       | 1.2(11)| 1.2(20)| 1.1(157)| 1.2(213) |
| BiCG           | 2.3(6)       | 2.1(11)| *(140) | *(540) | *(540)     |
| BiCG(L)        | 1.6(4)       | 1.8(9) | *(140) | *(540) | *(540)     |
| BiCG(R)        | 2.4(6)       | 2.2(11)| *(140) | *(540) | *(540)     |
| Bi-CGSTAB      | 1.8(4)       | 1.5(7) | 1.5(13)| *(540) | *(540)     |
| Bi-CGSTAB(L)   | 1.4(3)       | 1.3(6) | 1.3(11)| *(540) | *(540)     |
| Bi-CGSTAB(R)   | 1.8(4)       | 1.5(7) | 1.6(13)| *(540) | *(540)     |
| Bi-CGSTAB(N)(L)| 1.9(2)       | 6.8(17)| 14.9(65)| *(540) | *(540)     |
| Bi-CGSTAB(N)(R)| 2.1(2)       | 13.1(33)| 27.9(122)| *(540) | *(540)     |
| TFQMR          | 3.8(5)       | 3.4(9) | 4.3(19)| *(540) | *(540)     |
| TFQMR(L)       | 3.1(4)       | 3.1(8) | 4.1(18)| *(540) | *(540)     |
| TFQMR(R)       | 3.9(5)       | 3.5(9) | 4.4(19)| *(540) | *(540)     |
| CGS            | 1.7(4)       | 1.5(7) | 1.4(12)| *(540) | *(540)     |
| CGS(L)         | 1.4(3)       | 1.3(6) | 1.2(10)| *(540) | *(540)     |
| CGS(R)         | 1.8(4)       | 1.5(7) | 1.4(12)| *(540) | *(540)     |
| RGCR           | 4.3(2)       | 2.8(2) | 2.5(3) | *(14)  | *(14)      |
| RGCR(L)        | 2.0(1)       | 2.4(2) | 2.1(2) | *(14)  | *(14)      |
| RGCR(R)        | 4.4(2)       | 2.8(2) | 2.7(3) | *(14)  | *(14)      |
| RBi-CGSTAB     | *(12)        | *(12)  | *(12)  | *(12)  | *(12)      |
| RBi-CGSTAB(L)  | *(12)        | *(12)  | *(12)  | *(12)  | *(12)      |
| RBi-CGSTAB(R)  | *(12)        | *(12)  | *(12)  | *(12)  | *(12)      |
Table 2: CPU time (normalized) and number of iterations for x=1

| Method          | n=(1.33,0) | (1.33,0.01) | (1.33,1) | (2.0)  | (3.0,0001) |
|-----------------|------------|-------------|---------|--------|------------|
| CGNE            | 3.2(10)    | 3.2(10)     | 2.0(16) | 4.5(33)| *(140)     |
| CGNE(L)         | 2.7(8)     | 2.6(8)      | 1.7(13) | 3.8(27)| *(140)     |
| CGNE(R)         | 3.2(10)    | 3.2(10)     | 2.0(16) | 4.6(33)| *(140)     |
| CGNE(N)(L)      | 2.6(5)     | 2.6(5)      | *(140)  | *(140)| *(140)     |
| CGNE(N)(R)      | 3.6(7)     | 3.6(7)      | *(140)  | *(140)| *(140)     |
| CGNR            | 3.5(11)    | 3.5(11)     | 2.0(16) | 4.3(32)| *(140)     |
| CGNR(L)         | 2.7(8)     | 2.6(8)      | 1.7(13) | 3.7(27)| *(140)     |
| CGNR(R)         | 3.5(11)    | 3.5(11)     | 2.0(16) | 4.4(32)| *(140)     |
| QMR             | *6(47)     | *5(58)      | *2(25)  | *7(76)| *(50)      |
| QMR(L)          | 5.3(12)    | *5(59)      | *2(21)  | *7(71)| *(39)      |
| QMR(R)          | *(52)      | *(63)       | *(22)   | *(70)| *(37)      |
| CG              | 1.3(8)     | 1.3(8)      | *(140)  | *(140)| *(140)     |
| CG(L)           | 0.9(5)     | 0.9(5)      | *(140)  | *(140)| *(140)     |
| CG(R)           | 1.3(8)     | 1.3(8)      | *(140)  | *(140)| *(140)     |
| BiCG            | *(140)     | *(140)      | *(140)  | *(140)| *(140)     |
| BiCG(L)         | *(140)     | *(140)      | *(140)  | *(140)| *(140)     |
| BiCG(R)         | *(140)     | *(140)      | *(140)  | *(140)| *(140)     |
| Bi-CGSTAB       | 1.3(4)     | 1.3(4)      | 1.2(10) | 1.2(9)| 1.1(24)    |
| Bi-CGSTAB(L)    | 1.0(3)     | 1.0(3)      | 1.0(8)  | 1.0(7)| 1.0(21)    |
| Bi-CGSTAB(R)    | 1.3(4)     | 1.3(4)      | 1.2(10) | 1.3(9)| 1.1(24)    |
| Bi-CGSTAB(N)(L)| 1.4(2)     | 1.4(2)      | 1.5(6)  | 4.6(17)| *(140)     |
| Bi-CGSTAB(N)(R)| 1.5(2)     | 1.5(2)      | 1.6(6)  | *(140) | *(140)     |
| TFQMR           | 3.3(6)     | 3.3(6)      | 3.3(14) | 3.4(13)| 3.8(42)    |
| TFQMR(L)        | 2.8(5)     | 2.8(5)      | 3.0(13) | 3.0(11)| 3.7(40)    |
| TFQMR(R)        | 3.4(6)     | 3.4(6)      | 3.3(14) | 3.4(13)| 3.9(42)    |
| CGS             | 1.3(4)     | 1.3(4)      | 1.3(11) | 1.4(10)| 1.6(34)    |
| CGS(L)          | 1.0(3)     | 1.0(3)      | 1.2(10) | 1.3(9)| 1.1(23)    |
| CGS(R)          | 1.3(4)     | 1.3(4)      | 1.3(11) | 1.4(10)| 1.6(33)    |
| RGC             | 3.7(2)     | 4.5(2)      | *(14)   | 3.3(3)| *(14)      |
| RGC(L)          | 3.2(2)     | 3.1(2)      | 6.5(6)  | 2.9(3)| *(14)      |
| RGC(R)          | 3.7(2)     | 3.7(2)      | 7.4(7)  | 3.3(3)| *(14)      |