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Comparison and Improvement of the Computational Efficiencies of Two FFT-Based Iterative Solution Methods for the Scalar Multiple-Scattering Equation

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Abstract. We consider two existing FFT-based fast-convolution iterative solution techniques for the scalar T-matrix multiple-scattering equation [1]. The use of the FFT operation requires field values be expressed on a regular Cartesian grid and the two techniques differ in how to go about achieving this. The first technique [6,7] uses the non-diagonal translation operator [1,9] of the spherical multipole field, while the second method [11] uses the diagonal translation operator of Rokhlin [10]. Because of its use of the non-diagonal translator, the first technique has been thought to require a greater number of spatial convolutions than the second technique. We establish that the first method requires only half as many convolution operations as the second method for a comparable numerical accuracy and demonstrate, based on an actual CPU time comparison, that it can therefore perform iterations faster than the second method. We then consider the respective symmetry relations of the non-diagonal and diagonal translators and discuss a memory-reduction procedure for both FFT-based methods. In this procedure, we need to store only the minimum sets of near-field and far-field translation operators and generate missing elements on the fly using the symmetry relations. We show that the relative cost of generating the missing elements becomes smaller as the number of scatterers increases.

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1 Introduction

The scattering of acoustic waves from an ensemble of discrete scatterers is an important, age-old problem that finds applications in areas as diverse as sonar and medical

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imaging. In many applications, multiple scattering effects cannot be ignored in determining the overall scattering characteristics, but their numerical determination can be computationally challenging. They can be determined, for example, by solving the governing multiple-scattering equation [1] based on the T-matrix formalism [2]. If there are N_p scatterers in the ensemble and each scatterer requires P partial waves to represent its scattering behavior, one then needs to solve a system of linear equations of size N by N, where $N \equiv PN_p$. When N is modest, one may be able to solve the matrix equation using either a direct method such as the LU decomposition or an iterative technique such as the conjugate gradient (CG) method [3, 4]. A direct method would require $\mathcal{O}(N^3)$ floating point operations (FPOs) and $\mathcal{O}(N^2)$ memory units (MUs), while an iterative method would require $\mathcal{O}(N^2)$ FPOs per iteration and $\mathcal{O}(N^2)$ MUs. However, as N increases, with these unfavorable computational complexities, one quickly finds oneself unable to store the matrix even on a supercomputer, let alone solve the matrix equation.

Significant efforts have been directed at reducing the aforementioned undesirable computational complexities over the last decade and a half, and a number of efficient algorithms have been proposed. Among the useful algorithms that have emerged is the FFT T-matrix technique [6, 7] that was originally developed for electromagnetic scattering applications. This technique was later adopted by [11] for the acoustic case as part of its comparative study on efficient prediction techniques for scattering from a cluster of particles. The idea is to use the FFT-based fast-convolution technique to expedite matrix-vector multiplications, which are the most costly part of an iterative solution process.

In this paper we compare and improve the computational efficiencies of two existing FFT T-matrix methods for the scalar T-matrix multiple-scattering equation [1]. The use of the FFT operation requires field values be expressed on a regular Cartesian grid and the two versions differ in how to go about achieving this. The first method [6, 7, 11] uses the non-diagonal translation operator [1, 9] of the spherical multipole field, while the second method [11] uses the diagonal translation operator of Rokhlin [10]. Because of its use of the non-diagonal translator, the first version is thought to require a greater number of spatial convolutions than the second one [11]. We first establish that the first method requires half as many spatial convolutions as the second method for a given numerical accuracy and show, based on a CPU time comparison, that the first method indeed performs matrix-vector multiplications faster.

As alluded to earlier, when solving scattering from a volume distribution of scatterers, it is often the memory requirement that sets the upper limit on the problem size that can be solved on a given computer. Therefore, it is highly desirable to be able to reduce the memory requirement. Since storage of the translation matrix (TM) drives the overall memory requirements of the FFT T-matrix methods [13], we discuss the respective symmetry relations of the non-diagonal and diagonal TMs and develop a memory-reduction procedure for both FFT T-matrix methods. The procedure requires only the minimum sets of the translators be stored and generates missing elements from them on the fly using the symmetry relations. We show that the procedure reduces the memory requirements of both FFT T-matrix methods by non-trivial factors. These symmetry relations