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The fast multipole method in electromagnetics applied to the simulation of metamaterials

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Abstract

In this paper the reader is introduced to an algorithm that revolutionized the complexity of problems that could be handled in electromagnetics in the past decennium. The algorithm, called fast multipole method, has allowed the solution of problems with many millions of degrees of freedom with reasonable computer resources. The method is explained on different levels of abstraction. It is illustrated by means of a wire scattering problem that is applied for the exact simulation of a piece of metamaterial with a negative index of refraction. It is the first time that an exact numerical verification of the lens effect in a negative index metamaterial is performed.

MSC: 65R20

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1. Introduction

One of the effects of Moore's law is the fact that simulations of ever larger and more complex problems are possible. However, the invention of new algorithms often allows for a much more dramatic increase in the complexity of problems that can be handled. One such example is the fast multipole method (FMM) and its multilevel extension called the multilevel fast multipole algorithm (MLFMA).

The FMM method finds its origin in interstellar interaction problems where the interactions between N objects are calculated. A direct calculation of these interactions requires $O(N^2)$ operations and $O(N^2)$ memory capacity to store them. An FMM as developed in [7] reduces the complexity of this problem to $O(N)$ operations and $O(N)$ memory capacity. [7] deals with a Laplacian problem. The method has been extended to wave equation problems in [12] and later a multilevel version has been developed, the MLFMA, in [10]. The MLFMA for so-called method of moments (MoM) problems has a computational complexity of $O(N)$ or $O(N \log N)$ and also a memory requirement of $O(N)$ or $O(N \log N)$ depending on the geometry.

In this paper we will provide the reader with an introduction to FMM and MLFMA. First, by application to a many particle problem, the concept of FMM will be explained. Then we explain the difference between low and high frequency multipole methods. To mathematically illustrate the method we consider the problem of the scattering of electromagnetic waves by thin wire structures. This problem is described by an integral equation that is solved by

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the Galerkin MoM on which we apply the MLFMA. Finally, we use this technique, to illustrate the scattering by a so-called negative index material that is artificially constructed by a complex wire configuration embedded in a host medium.

This paper does not aim to give a full review of FMM and MLFMA, nor proposes to provide the reader with all technical details to solve the wire scattering problem. We rather want to provide the reader with a touch of FMM and MLFMA at different levels of abstraction allowing him or her to grasp the ideas behind these methods as being used in electromagnetics. Perhaps, this will allow the reader to study these techniques more profoundly and lead him or her to use these algorithms in other fields of interest. For a rather thorough introduction in FMM and MLFMA we refer the reader to [2].

2. Many particle problem

To gain some insight in FMM it is useful to consider a set of N mutually interacting particles. One could think of a set of point charges as in an ionized plasma or a set of masses as the stars in a galaxy. Let $\mathbf{F}_{ij}$ denote the force exerted by particle j on particle i. Hence, the total force acting on particle i is

$$\mathbf{F}_i = \sum_{j=1}^{N} \mathbf{F}_{ij}. \tag{1}$$

If one wants to simulate the evolution of the interacting particles, using e.g. a finite difference approximation applied on the equations of motion, one needs to evaluate the forces $\mathbf{F}_i$, $i = 1, \ldots, N$, at each time step. This means a computational complexity of $O(N^2)$. For large problems this soon becomes unacceptable.

Consider a cloud of particles that is far away from two other particles A and B as shown in Fig. 1. To calculate the force exerted by the particles in the cloud on A and B it is obvious that one could replace the particles in the cloud by one large equivalent particle at its "centre of mass", i.e. a monopole representation, and just calculate the interaction between this equivalent particle and A and B as shown in Fig. 2. To increase the accuracy of the interaction one could also add a dipole, quadrupole, etc … to the "centre of mass" of the cloud.

To calculate the interactions between all particles, in a large set of N particles, one divides this set into a number of clouds, each containing a certain amount of particles as shown in Fig. 3. The interaction between particles that are in clouds that are separated far from each other are calculated using the multipole expansion as explained above. Interactions between particles in clouds that are close to each other or between particles within one cloud are calculated individually. It is clear that this procedure will drastically reduce the computational complexity.

This procedure could be improved further by clustering clouds in larger clouds and so on in order to obtain a hierarchical tree-like structure of clouds. In this way one can show that the computational complexity for a dense three-dimensional set of particles reduces to $O(N)$.

Fig. 1. A cloud of particles interacting with two other particles A and B.

Fig. 2. An equivalent particle (monopole) interacting with two other particles A and B.