Supercomputing aware electromagnetics

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***Abstract*—The Fast Fourier Transform (FFT) extension of the conventional Fast Multipole Method (FMM) has demonstrated that it reduces the matrix vector product (MVP) complexity while preserving the propensity for parallel scaling of the single level FMM. An efficient hybrid MPI/OpenMP parallel implementation of the FMM-FFT and, subsequently, an improved nested scheme of the algorithm, and a combination with MLMFMA have been employed successfully for the solution of challenging problems with hundreds of millions of unknowns.**

***Index Terms*—Fast Multipole Method, Fast Fourier Transform, Multilevel Fast Multipole Algorithm, Supercomputing**

I. Introduction

The last decade sustained a great effort in the development of fast and efficient algorithms to reduce the computational cost of the method of moments (MoM). One of the most important advances was the development of the fast multipole method (FMM) [1] and its multilevel version, the MLFMA [2]. The FMM reduces the computational complexity from $\mathcal{O}(N^2)$ -using an iterative resolution of the MoM-, to $\mathcal{O}(N^{3/2})$, and the multilevel versions have achieved $\mathcal{O}(N \log N)$. So, while substantially more difficult to implement, the MLFMA has become the choice when solving large-scale electromagnetic scattering problems. Simultaneously to these algorithmic advances, the sustained growth in computer technology has lead to the availability of computer clusters and multi-core processors with very large memory and computational capabilities. In this context, the parallelization of the MLFMA has been an objective of great interest [3], [4], due to its low computational complexity. However, the parallelization of this algorithm requires sophisticated load distribution strategies, often involving different partitions of work across the multilevel oct-tree, which limits the parallel scalability in modern high performance computers (HPC).

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A. High scalability algorithms

To deal with the aforementioned trade-off between low-numerical complexity and high-scalability behavior, we have concerned with a variation of the FMM, namely the FMM-Fast Fourier Transform (FMM-FFT). We have demonstrated that this variation allows to take advantage of the large amount of computational resources that are available in current HPC systems. The FMM-FFT was first proposed in [5] as an acceleration technique applied to almost planar surfaces. Later on, a parallelized implementation was applied to general three-dimensional geometries [6]. The method consists of employing the FFT to speedup the translation stage in the framework of the FMM strongly reducing its computational complexity. Although in general it is not algorithmically as efficient as the MLFMA, it has the advantage of preserving the natural parallel scaling propensity of the single-level FMM in the spectral (k-space) domain. The concurrence of the reduced complexity with the propensity for high scalability makes the FMM-FFT algorithm a very attractive alternative in massively parallel supercomputers. An efficient parallel implementation of the method has been used by the authors to solve, among others, a problem with more than 150 millions of unknowns [7].

To deal with very large problems involving hundreds of millions of unknowns where the amount of memory becomes a critical issue, we have proposed a variation of the algorithm [8], [9]. It applies a nested FMM-FFT scheme to calculate the near-field contributions and the aggregation and disaggregation matrices, achieving a slightly worse parallel performance but in exchange for lower memory consumption. From one or more refinement steps of the hierarchical oct-tree decomposition, the nested algorithm carries out the far-field computation at the coarsest oct-tree level as in the original FMM-FFT, while obtaining the near-field interactions at the finest level by using one or more local shared memory FMM-FFT algorithms inside each computing node. Finnally a combination of the FMM-FFT techniques with MLFMA deal with a problem of 620 million unknowns, the bigger problem solved in electromagnetics as far as we know.

As it is described in Figure 1, more and more demanding problems have been tackled by means of these approaches and the available computational resources. These world record challenges has resulted in various international awards in computationally intensive applications in 2009 (International PRACE Award and Itanium Innovation Award).

II. FMM-FFT, nested FMM-FFT and MLFMA-FFT parallel implementations

A hybrid parallel programming by combining the Message Passing Interface (MPI) with the OpenMP standard has been

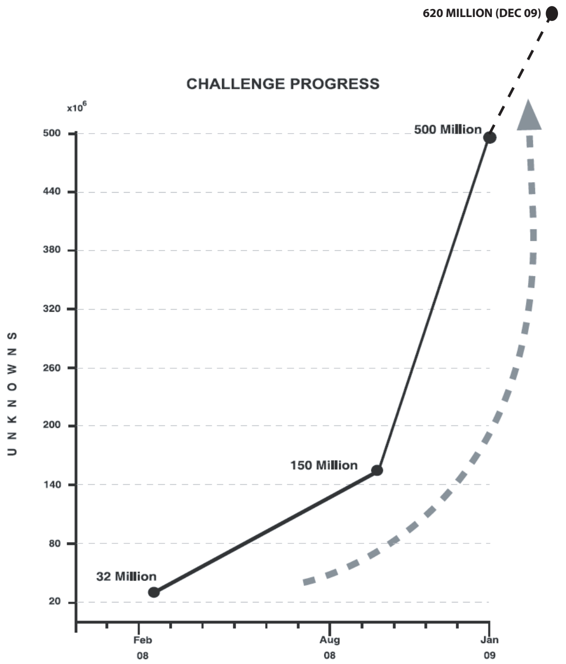

Fig. 1. Challenges course.

selected for the MLFMA-FFT, the FMM-FFT method and the nested algorithm implementations. This hybrid parallel programming allows to fit the architecture characteristics of large mixed memory computers (distributed clusters of shared-memory nodes).

A three stage parallelization strategy has been considered for the FMM-FFT. It is determined by the following key points: a distribution of *k*-space samples among processors to account for the far-field interactions taking advantage from its independence; a distribution of oct-tree groups for near-field interactions; a distribution of unknowns for the iterative solver. This strategy leads to optimal load balancing and data locality, while it minimizes the memory footprint and communication requirements.

Regarding the parallelization strategy considered for the nested FMM-FFT, it implies the following stages: for the far interactions, a mixed approach is applied by distributing by groups at the finest level and distributing by field samples at the coarsest level. For the near interactions, a well-balanced partition of work by groups at the finest level is applied. Finally, the iterative solver is distributed by equal number of unknowns per processor. The use of a two-level scheme to obtain the far interactions requires the interpolation/anterpolation of outcoming/incoming fields across the two levels. On the other hand, the different partition of work, by groups and by fields, implies inter-node communications during the MVP. The MPI library provides an efficient management of all the required the communications.

Regarding the MLFMA-FFT method we use a parallelization strategy based on distributing the MLFMA between nodes (solved internally by OpenMP). The rest of parallelization strategy is simmilar to FMM-FFT.

Figure 2 makes a comparison between the scalability behavior of both the FMM-FFT and the nested FMM-FFT methods. It can be seen that the additional communications required during the MVP in the nested algorithm due to the interpolation/anterpolation of fields has a reduced impact on the scalability.

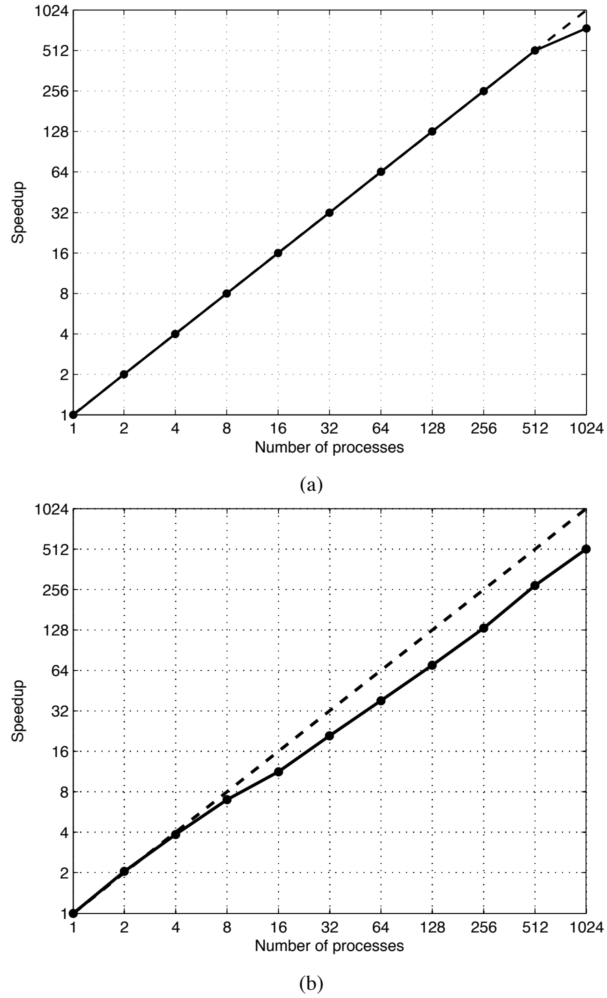

Fig. 2. PEC sphere problem with 10 million unknowns. (a) Parallel speed-up for the FMM-FFT algorithm. (b) Parallel speed-up for the nested FMM-FFT algorithm.

III. Challenging numerical results

The outstanding results obtained using the FMM-FFT and the nested FMM-FFT approaches are those corresponding to the 150 and 500 millions of unknowns challenges mentioned in previous sections. Both results were performed using the HPC supercomputer Finis Terrae, installed in the Supercomputing Centre of Galicia (CESGA). Finis Terrae consists of 142 cc-NUMA HP Integrity rx7640 with 8 dual core Intel Itanium 2 Montvale processors at 1.6 GHz with 18 MB L3 cache and 128 GB of memory, and two Integrity Superdome nodes, one of them with 128 cores and 1,024 GB of memory, and the other with 128 processors (single core) and 384 GB of memory. Besides, there are two special nodes with 4 cores and 4GB of memory for testing and development purposes. Altogether, they sum more than 2,500 cores and 19,000 GB of memory, being one of the computers with the best ratio memory/processor in the world. The nodes are interconnected through a high efficiency Infiniband network (4xDDR), and the operating system is Linux SLES 10. The data storage system consists of 22 nodes with 96 cores for management, 390 TB in disks and 1 PB in Robot Tape Library. The Intel C++ Compiler version 11.0.069, and Intel MPI version 3.2.0.011 for internode communications have been used. For matrix/vector linear algebra operations we have employed the Intel Cluster MKL version 10.0.2.018.

Regarding the electromagnetic formulation, the examples have been addressed with an Electric Field Integral Equation (EFIE) based Method of Moments formulation, in which the well-known Rao-Wilton-Glisson (RWG) basis functions [10] have been applied both in the discretization of the geometry and the Galerkin's testing procedure. No preconditioning has been considered and the iterative solver has been GMRES [11].

The geometries considered in the simulations were PEC spheres. The main configuration parameters of both methods and the technical data corresponding to the results are gathered in Table I. Even in this case where there is a significant difference between the number of unknowns solved, it is clear than the total memory saving obtained when using the nested FMM-FFT algorithm is important.

TABLE I
TECHNICAL DATA FOR THE SOLUTION OF ELECTROMAGNETIC PROBLEMS OF 150 AND 500 MILLIONS OF UNKNOWNS OBTAINED WITH THE FMM-FFT AND THE NESTED FMM-FFT METHODS, RESPECTIVELY.

	FMM-FFT	Nested FMM-FFT
Sphere diameter	400λ	728.36λ
Frequency	300 MHz	300 MHz
Num. of unknowns	150, 039, 552	500, 159, 232
Groups dimensions (fine / coarse level)	2λ	0.5λ / 4λ
Num. of nodes / processors per node	64 / 16	64 / 16
Min. / max. peak memory in node	76.3 GB / 84.7 GB	89.2 GB / 99.9 GB
Total memory	5.4 TB	6 TB
Num. of iterations / GMRES restart	11 / 10	10 / 10
Setup / solution time	66 min / 5 h	5 h / 26 h

From the obtained distribution of the surface current density, the bistatic radar cross section (RCS) was computed. An excellent agreement between the numerical results and the analytical solution provided by the Mie series was obtained in both cases. The solution corresponding to the 0.5 billions of unknowns problem is shown in Figure 3 in order to illustrate this concordance.

The MLFMA-FFT simulations were carried out using the LUSITANIA supercomputer, installed in the Centro Extremeño de Investigación, Innovacióon Tecnológica y Supercomputación (CénitS). Lusitania is made up of 2 HP Integrity SuperDome SX2000 nodes with 64 dual core Itanium2 Montvale processors at 1.6 GHz (18 MB cache). The 79 GHz radar cross section (RCS) analysis of a car (CITROEN C3) using the MLFMA-FFT has been carried out. The 77-81 GHz frequency band has been designed for the automotive collision warning future Short Range Radars (SRR). For this reason, modeling

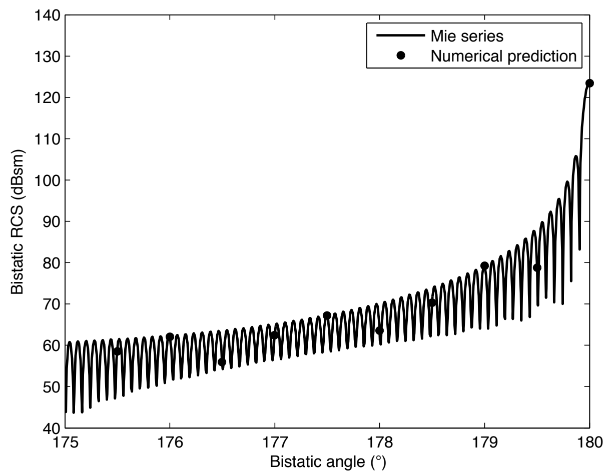

Fig. 3. Bistatic RCS of more than 0.5 billion of unknowns PEC sphere obtained with the nested FMM-FFT algorithm.

the electromagnetic behavior of a car at 79 GHz is of great interest for the automotive industry. The large size of the required analysis has made difficult to obtain suitable results up to now. Instead of resorting to asymptotic approaches with reduced accuracy, a reliable result can be achieved by means of the MLFMA-FFT method. This example has been performed employing the LUSITANIA supercomputer described above. A total of 1.6 TB of RAM and 2 HP Integrity SuperDome SX2000 nodes with 128 processors have been used. The model of the car is made up of 620 million unknowns. Both configuration and solution related data are gathered in Table 2. The 79 GHz bistatic RCS result is shown in Figure 4. A

TABLE II
TECHNICAL DATA FOR THE SOLUTION OF ELECTROMAGNETIC PROBLEM OF 620 MILLIONS OF UNKNOWNS OBTAINED WITH THE MLFMA-FFT ALGORITHM.

Frequency	79 GHz
Number of unknowns	620,739,632
Groups dimensions (fine / coarse level)	0.2λ / 12.5λ
Number of levels	7
Multipole terms	4/7/11/18/29/52/95
Number of total /non-empty groups (fine level)	16,841,845,020/31,201,960
Number of total /non-empty groups (coarse level)	66,600/7,848
Num. of nodes / processors per node	2 / 128
Min. / max. peak memory in node	816GB / 821GB
Total memory	1.6 TB
Num. of iterations / GMRES restart	5 / 50
Setup / solution time	3.65 / 43.2 h

front incidence ($\theta = 90^o$, $\phi = 270^o$) has been considered. Due to the rapid fluctuation of the RCS pattern with changing aspect angle, a window of 2^o has been selected to calculate the median value of the RCS in the backward direction, which results 0.34 dBsm. As far as we know, this is the largest electromagnetic problem solved until now.

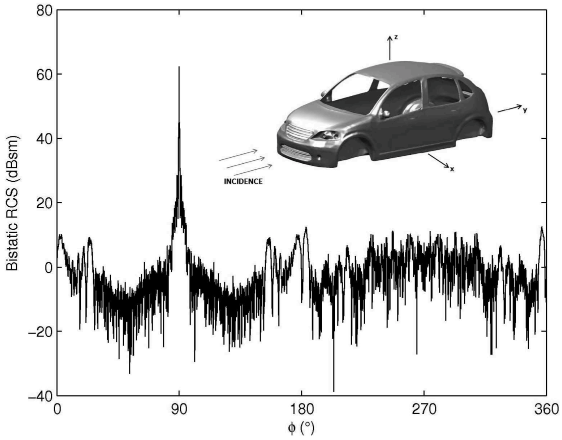

Fig. 4. Bistatic RCS of a 620 million unknowns car at 79 GHz.

IV. Conclusions

An efficient parallelization of the FMM-FFT algorithms has been implemented, exploiting its natural high scaling properties to benefit from the availability of massively distributed supercomputers. In order to accomplish the analysis of very large-scale scattering problems, a nested configuration of the method that improves the memory requirements has been also proposed. These efficient algorithms in addition with the computational resources provided by the supercomputers Lusitania and Finis Terrae, have allowed us to address the electromagnetic scattering of large problems involving hundred of millions of unknowns in the course of 2008 and 2009.

During 2010, we applied to the Spanish Government for the use of a ICTS center for the solution of a problem with more than one billion unknowns.

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