



SHAPE Pilot ENTARES Engineering: Electromagnetic simulation for large model using HPC

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Abstract

We have started the extension of the electromagnetic software CAPITOLE developed at ENTARES Engineering to HPC machines. This has been possible with the aid of the SHAPE pilot project, which has provided us with some expertise and computation hours at Marenostrum III. Two numerical methods have been addressed to solve the resulting dense MoM linear system, MSCBD and MLACA. A new implementation based on asynchronous tasks has been performed for the direct method MSCBD. Dependencies between tasks need to be well defined before moving to a runtime scheduling such as STARPU. As for the iterative method MLACA, a hybrid MPI-OpenMP parallelization has been done with excellent results. So far, electromagnetic models up to 6 Million unknowns have been properly solved.

1 Introduction

With the improvement of computing resources in the last decades, electromagnetic simulation has become a very important tool in several industrial domains, such as aeronautics, space or automotive. This growth has also pointed out some new challenges and requirements. One of the biggest encountered challenges is the solution of problems with larger frequencies and model dimensions, which rapidly leads to linear systems with millions of unknowns. The solution of these systems calls for special numerical techniques which are able to highly reduce the numerical effort and complexity of the solution as well as the necessary used memory. These techniques are usually based both in physical and mathematical properties. However, there is a certain point where these methods are not enough and we need to add some more gain. There it enters the era of parallelization and HPC systems. Parallel codes can extremely reduce computational times if they have a good scalability with the number of cores. Getting to an efficient and optimized parallel code requires some expertise and resources which are hard to reach for a SME.

In this context, the European projects which have recently appeared to bring closer HPC systems and SMEs have been of preponderous importance for us. Firstly, it was the French project HPC-PME and then the present SHAPE pilot project. They have allowed us to jump from a personal computer version of our software CAPITOLE-EM to a HPC version, still under development, CAPITOLE-HPC. We have reached the solution of very large electromagnetic problems otherwise unaffordable.

This whitepaper is organized as follows: Section 2 briefly presents the SME ENTARES Engineering and its relation with the SHAPE pilot project and its goals. Section 3 mainly describes the activity done during the duration of the project including some interesting numerical results. It also contains a state of the art on the use of the Method of Moments for electromagnetic simulation in order to put everything in context. Section 4 states

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the sort of cooperation which has been present between the company and PRACE people and resources. Section 5 summarizes which have been the benefits from the project for ENTARES. Section 6 gives some guidelines about the direction that the SME is taking for the future as well as a constructive discussion about strong points of the project and things which could be improved from our perspective. Finally, a short conclusion with some final remarks can be found.

2 SME : ENTARES Engineering

ENTARES Engineering is a French SME, subsidiary of Nexio Group, developing an electromagnetic simulation software called CAPITOLE (see Figure 1) to study the electromagnetic behavior of any product during the design process, before the manufacturing phase.

Among the different applications of the software, the solver can be used to design an antenna and study its performances. Furthermore, it can help to optimize the placement of an antenna on its supporting structure (such as a car, an airplane, etc. see Figure 2). It might be used as well to analyze interferences between equipment to meet EMC (ElectroMagnetic Compatibility) standards.

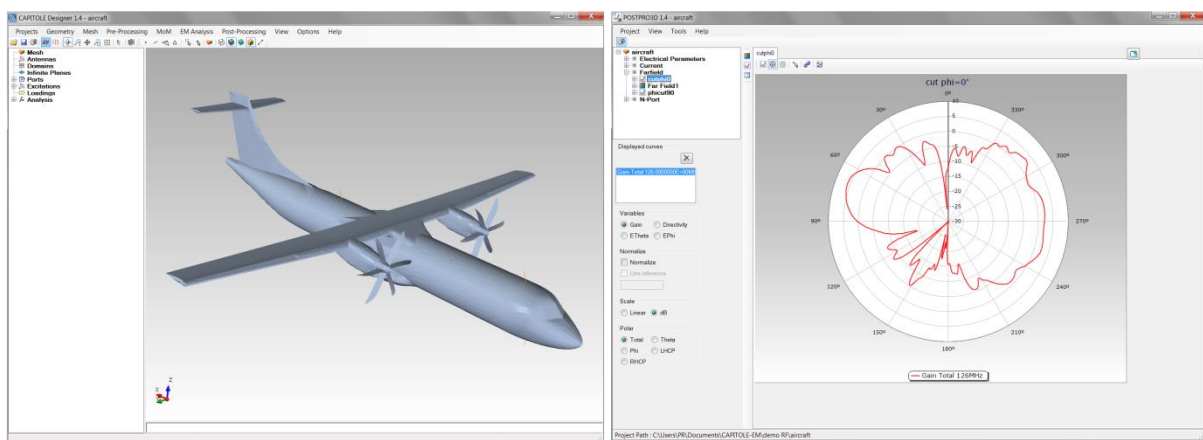


Figure 1 A couple of snapshots from the CAPITOLE-HPC user interface. On the left we have CAPITOLE-DESIGNER used to define the object, discretization and simulation parameters. On the right, POSTPRO3D which shows the different demanded results from the simulation such currents, near field, radiation pattern...

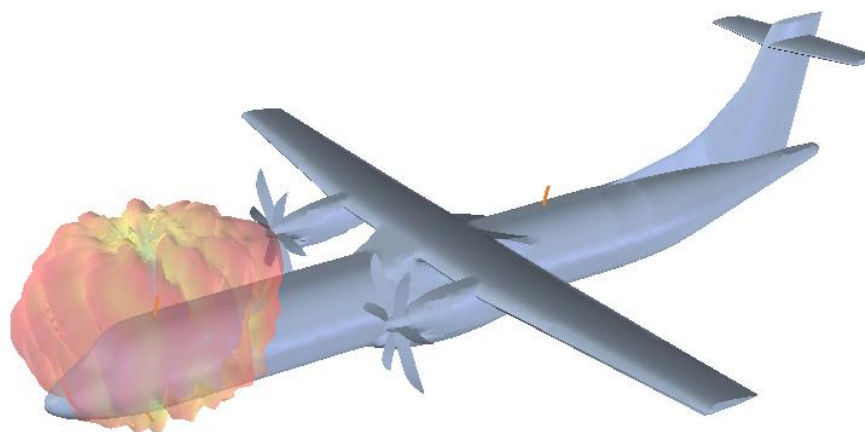


Figure 2 Classical set-up for an antenna placement problem. Several position configurations are analyzed obtaining the radiation pattern and input impedance in the presence of the plane.

This project is in the framework of the SHAPE pilot program for which ENTARES Engineering is supported by GENCI. The project aims to improve the parallel efficiency of an electromagnetic solver based on the concept of compressed low-rank matrix.

ENTARES started developing a new version of its electromagnetic simulation software for HPC computers a year ago. A couple of different solvers have been developed, a direct one and an iterative one. Although the direct solver requires more memory and computational time than the iterative method with a lower scalability, it still has its advantages and is somehow complementary. The goal of the project was to improve the efficiency of both solvers in order to propose a flexible solution for electromagnetic simulations.

Electromagnetic simulation is more and more used these days, due to the increase of communicating devices such as mobile phones, modems, etc. Therefore, it becomes necessary for large industrial companies to study the effects of interferences between pieces of equipment as well as to improve the performances of the transmitting and receiving systems or antennas.

3 Activity done

3.1 State of the art and description of the problem

Figure 3 schematically summarizes the global procedure from the Maxwell equations governing any electromagnetic (EM) system to the possible outputs interesting for industry. In particular, we have chosen the Method of Moments (MoM) [1], being one of the more powerful methods for the solution of various EM antenna and scattering problems for its accuracy and robustness. The application of some boundary conditions (BC) leads us from the differential Maxwell equation to an integral equation. These boundary conditions are usually surface integral equations for Perfect Electric Conductors (PEC) and volumetric in the presence of dielectric materials. In particular for a PEC object, as shown in the figure, an extended possibility is the use of the Electric Field Integral Equation.

After discretization of the object with some set of basis functions and testing with the same functions (Galerkin) we arrive to the so called MoM linear system. These basis functions are defined over triangles (RWG for Rao-Wilton-Glisson) for the surface case and over tetrahedrons (SWG for Schaubert-Wilton-Glisson) in the volumetric case. We want to solve the system in order to obtain the equivalent currents J . Almost any interesting parameter of the system can be easily obtained from these currents. For instance, we could compute the electromagnetic field at some points in space, the input impedance or the radiation pattern of an antenna, amongst others.

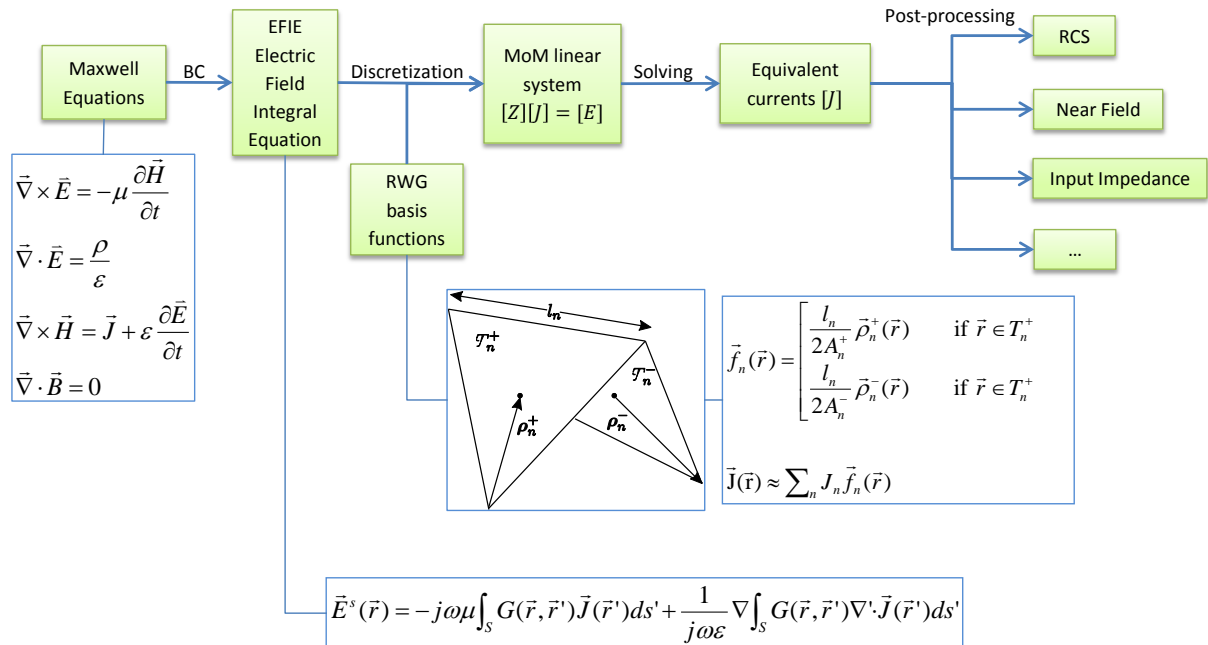


Figure 3 Schematic diagram summarizing the Method of Moments, which transforms Maxwell equations ruling the electromagnetic properties on the object to a linear system. Once the system has been solved any interesting parameter can be easily obtained from the resulting equivalent currents.

The main drawback of the MoM is the costly construction, storage, and solution considering the unavoidable dense linear system. As a consequence, a wide range of fast methods [2] have been developed for accelerating the iterative solution of the electromagnetic integral equations discretized by Method of Moments (MoM) [1]. Most of them are based on multilevel subdomain decomposition and require a computational cost per iteration of order $N \log N$ or $N \log(2N)$. One of these methods is the Multilevel Fast Multipole Algorithm (MLFMA) [3]. The MLFMA has been widely used in the last years to solve very large electromagnetic problems due to its excellent computational efficiency.

The main drawback of the MLFMA is the dependence of its formulation on the problem Green's function or integration kernel. Notwithstanding, other general purpose methods have been developed. For instance, the Multilevel Matrix Decomposition Algorithm (MDA-SVD) [4], exploits the compressibility of MoM submatrices corresponding to well separated sub-scatterers by using equivalent surface basis/testing functions cleverly distributed that radiate and receive the same fields as the original basis/testing functions. Another fast solver, the Adaptive Integral Method (AIM) [5] replaces the actual basis and testing functions with a regular volumetric grid, that again radiates and receives the same fields as the original discretization, in order to efficiently compute the integral equations convolution using the FFT algorithm.

However, all the aforementioned methods rely on the appropriate selection of elements with an equivalent physical behavior, either multipoles or equivalent surface or volume basis/testing functions. Hence the interest of purely algebraic methods, whose formulation is still independent of the problem Green's function and operate solely with some of the impedance matrix elements, such as the IE-QR Algorithm, the IES3 and the Adaptive Cross Approximation (ACA) [6]. Unfortunately, these algebraic methods present an asymptotic computational time and memory requirement not as good as that of the above-mentioned methods. The recently developed multilevel version of the ACA (MLACA) [7] overcomes this computational complexity.

These new iterative algorithms have enormously extended the range of problems that MoM can manage. The maximum affordable number of unknowns used to be limited to a few thousands. Now problems with hundreds of thousands or even millions of unknowns are within reach, depending on the available computational resources.

Based on the previous, one might be tempted to conclude that direct solution of the MoM matrix equation, through Gaussian elimination or LU decomposition, has become obsolete. This is not entirely the case, for the following number of reasons:

- First of all, the fast algorithms are very efficient for electrically large structures, while the direct solution is faster for small and medium size problems, depending on the computational resources and on the specifics of the problem. The turning point may be of the order of a few thousand unknowns.
- Furthermore, iterative solution methods for matrix equations yield the solution to the linear system for only one independent vector (excitation vector) at a time. Consequently, the computational effort is proportional to the number of independent vectors. By contrast, the bulk of the effort in LU decomposition, which is the generation of the L and U factors of the impedance matrix, needs to be done only once for as many independent vectors as needed.
- Finally, the convergence rate of iterative methods can vary in an unpredictable way. It is related to the matrix condition number, which is notoriously bad for the EFIE in large problems. The only remedy is the use of a good preconditioner with a relatively large number of non-zero elements, but the construction of such a preconditioner becomes the bottleneck of the computation.

Therefore, the introduction of an accelerated direct solver such as the MultiScale Block Decomposition method (MSCBD) [8] is of much interest.

3.2 Asynchronous MSCBD

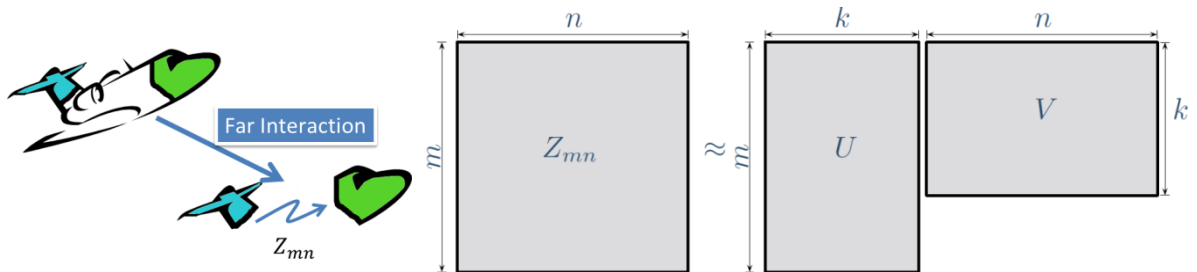


Figure 4 Compressibility of a far interaction matrix Z_{mn} as a product of two matrices U and V where $k \ll m, n$. It is obtained with the ACA+SVD technique.

At the root of the MSCBD direct method resides the Adaptive Cross Approximation (ACA) compression technique and a block subdivision of the object. The physical properties of the electromagnetic interaction

indicates that the interaction between distant blocks (far interaction) has a much reduced number of degrees of freedom than the actual number of unknowns. We might exploit this property to compress the far interaction matrix by the use of a singular value decomposition (SVD). However, an SVD needs to compute all the elements of the matrix and is very expensive in terms of computational time leading to too high computational complexity. The appearance of the ACA algorithm in 2000 overcomes this problem (see Figure 4). In a completely algebraic manner it is able to directly arrive to the compressed version of the far interaction matrix as a product of two matrices, where $k \ll m, n$. One only needs to compute some column and rows of the original matrix and has a computational complexity much smaller than the SVD.

The whole matrix is then subdivided in a hierarchical manner in near and far interactions. Far interactions are compressed by the ACA and near interactions are either subdivided to the next level or directly computed if they are at the finest level of the tree subdivision. Figure 5 shows an example of this sort of hierarchical low-rank matrix compression. The gray color of the different blocks indicates the actual number of degrees of freedom and we can see that they are very limited. The factorization phase of the MSCBD deals with these sort of subdivision recompressing the new blocks to finally arrive to a compressed decomposition similar to the original one.

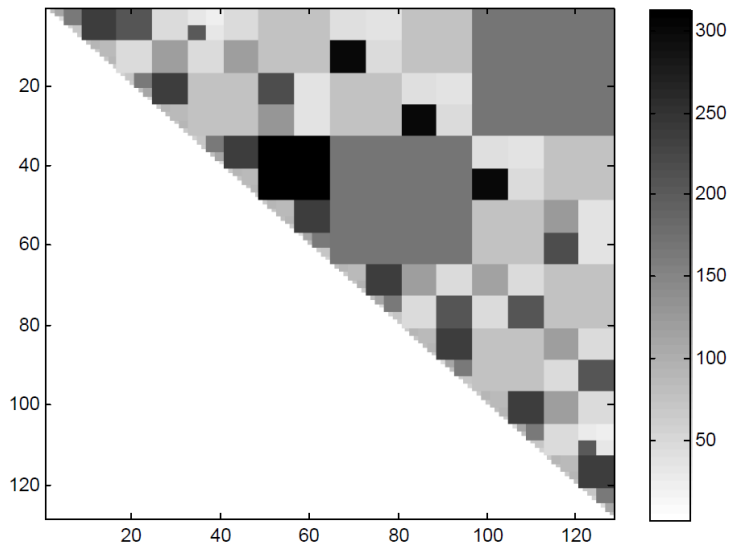


Figure 5 Aspect of hierarchical matrix decomposition. Blocks are never stored as full matrices but as compressed ones. The gray tone indicates the number of degrees of freedom of each subblock.

Before the SHAPE Pilot project we had an OpenMP implementation of the MSCBD algorithm. The build matrix step was quite scalable. However, the factorization phase had a poor scalability rate. To improve this scalability we have decided to use a runtime scheduling technique such as STAR-PU [9] based on asynchronous tasks which have certain dependencies. During the SHAPE project we have implemented a new version based on asynchronous tasks defining all the different dependencies between tasks. It remains, though, to include the runtime scheduling. The main problem is STARPU does not have a fortran interface, which we did not have the time to code.

3.3 MLACA – Hybrid MPI-OpenMP implementation

The MLACA is a multilevel version of the ACA algorithm to compress far interaction matrices. The new compressed matrix is a product of several blocked sparse matrices instead of two matrices. Figure 6 shows an example of this compressed form ($L=4$ levels) where the gray parts are the blocks different from zero. The same hierarchical subdivision as in the MSCBD is performed but the compressed blocks are compressed with MLACA instead of ACA. The advantage is the gain in computational complexity and memory.

This matrix is then used within an iterative algorithm to reach the solution. We have chosen to use a deflated GMRES [10]. The EFIE-MoM matrix is usually ill-conditioned, mainly with the complexity of the discretized object or at low frequencies. Therefore, it is necessary to use a good preconditioner to have an acceptable convergence rate. We have chosen to use a MUMPS [11] solution applied to the near field matrix (sparse) as a preconditioner.

We have implemented a hybrid MPI-OpenMP version which has a fairly good scalability. However, it is still interesting to further look into it. Next section shows some results on that, and give some guidelines on the things which could be optimized.

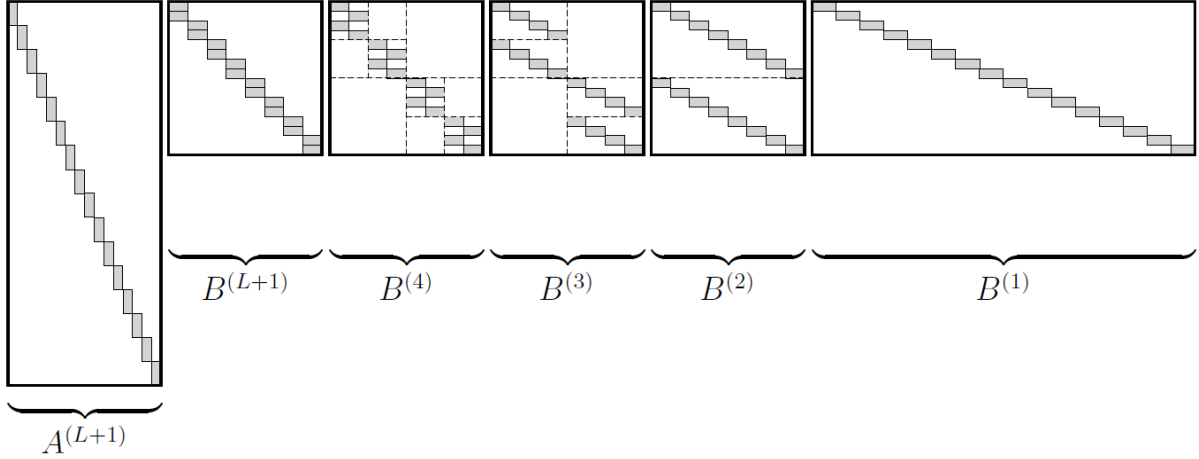


Figure 6 Multilevel MLACA compressed matrix decomposition as a product of several sparse matrices ($L=4$ levels). Only the gray blocks are different from zero.

3.4 Numerical Results and achieved performance

Without being exhaustive we pass to present some interesting numerical results. First of all, Figure 7 shows the electromagnetic simulation of an airplane at a frequency of 10 GHz. On the left, we have the computed equivalent currents in response to voltage generator localized on the top antenna. The object has been discretized with an average discretization size of $\lambda/10$, where λ corresponds to the wavelength, into 601678 unknowns. The length of the airplane is about 46λ . For the simulation we have used the MLACA algorithm with a total of 128 cores (8 MPI x 16 OMP). It took, in total, 14GB of memory for the MLACA matrix and 5.4GB for the MUMPS preconditioner. The matrix was computed in 1 minute whereas the GMRES solving iterations took 3 min. 51s. So the whole simulation was held in less than 5 minutes.

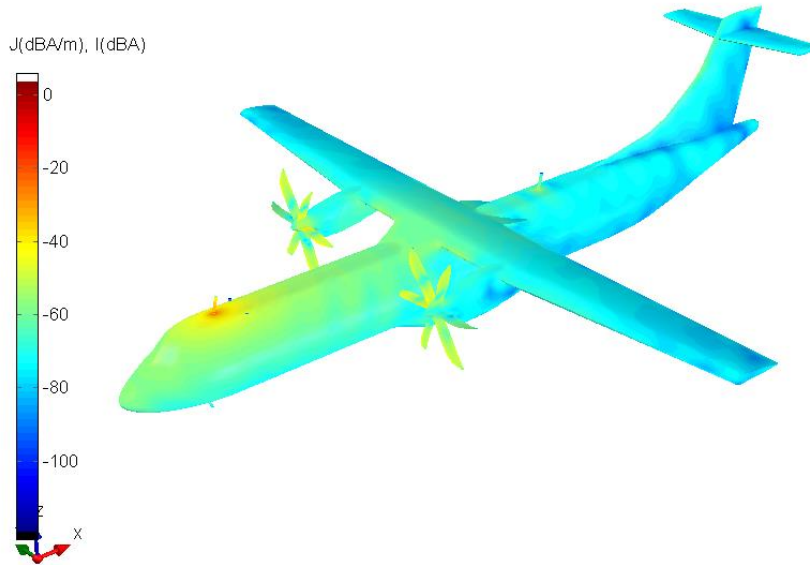


Figure 7 Equivalent currents on an airplane.

Figure 8 shows the scalability of the hybrid MPI-OpenMP implementation of the MLACA algorithm. The analyzed object is a sphere with 277000 unknowns. For each MPI process, 16 OpenMP threads are used when possible, considering that each computation node has 16 cores. It is clear that the build matrix step has a scalability close to the optimum. However, the performance is reduced due to the preconditioner computation (Facto at the figure) and the GMRES iterations. If we further analyze the results, we can see that at each iteration, a matrix-vector product and an application of the preconditioner are performed. Subdividing the time spent at each of those, it is observed that the scalability is mainly lost due to the preconditioner application.

Therefore, it deserves an insight analysis of the preconditioner step in order to further optimize our HPC code. Notwithstanding, a better parallel gain is expected for larger objects, being this sphere quite small to use 128 cores. We have used this model in order to have results with few number of cores at a relatively short time.

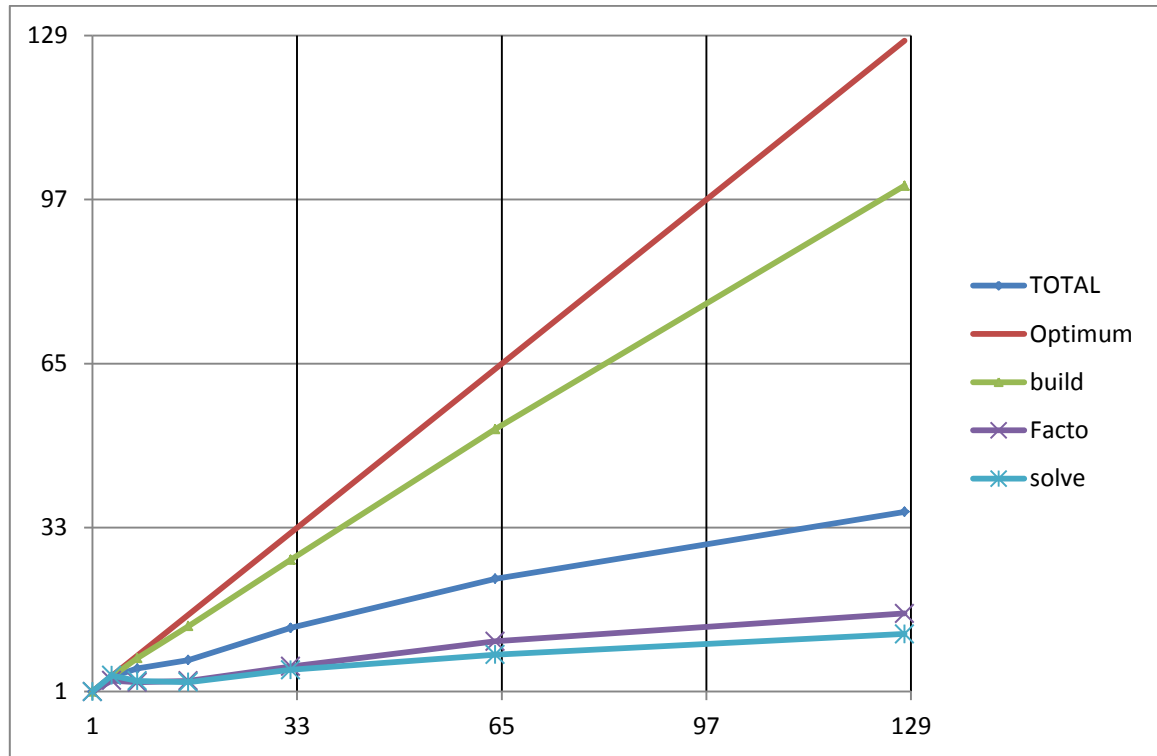


Figure 8 Scalability with the number of cores of the hybrid MPI-OpenMP implementation of the MLACA algorithm. It corresponds to the simulation of a sphere with 277000 unknowns.

Finally, we have performed the RCS (Radar Cross Section) simulation of three different PEC spheres with increasing sizes utilizing the MLACA algorithm. We have chosen the sphere because it has an analytical solution based on the MIE series. Therefore, we can assess the quality of the simulation, which is in excellent agreement with the exact solution. Figure 9 shows the different results. We can observe how with the growth of electrical size a faster variation appears at the RCS. For all the simulations a frequency of 300 MHz is used, an average discretization size of $\lambda/10$ and 128 cores (8MPI x 16OMP). The first sphere, at the top of the figure, has a diameter of 43λ and 2Million unknowns. The MLACA matrix took 58GB and was calculated in 10 minutes. The preconditioner took 28GB and the GMRES iterations lasted 15 minutes. So, in total the simulation was held in 25 minutes. The second sphere, at the middle, has a diameter of 60λ and 4Million unknowns. The MLACA matrix took 125GB and was calculated in 30 minutes. The preconditioner took 59GB and the GMRES iterations lasted 39 minutes. So, in total the simulation was held in 1hour 9 minutes. The third sphere, at the bottom, has a diameter of 74λ and 6Million unknowns. The MLACA matrix took 200GB and was calculated in 55 minutes. The preconditioner took 90GB and the GMRES iterations lasted 50 minutes. So, in total the simulation was held in 2hour 45 minutes.

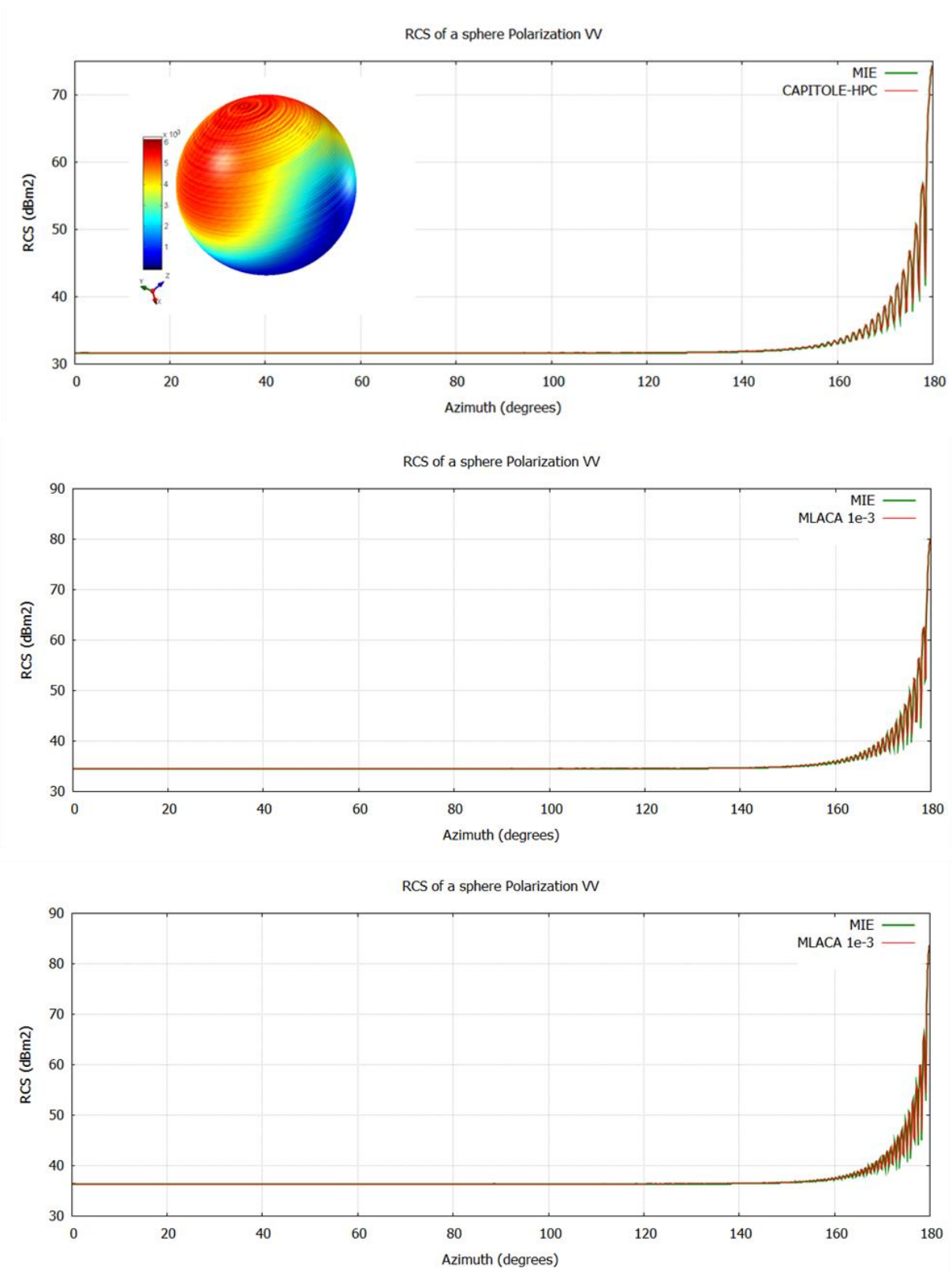


Figure 9 Bistatic RCS on three different PEC spheres with diameters 43λ at the top, 60λ in the middle and 74λ at the bottom. The number of unknowns is 2 Million, 4 Million and 6 Million, respectively. A comparison with the exact analytical result from the MIE series is also shown.

To end with the numerical results section we have included a schematic plot (Figure 10) summarizing the evolution of the performance we have got at ENTARES Engineering during the last years and the main reasons which has allowed this evolution. Thanks to parallelism and the introduction of the MLACA algorithm we have passed from the solution of a problem with 200000 unknowns in more than 4 hours in 2010 to the solution of a problem with 6Million unknowns in less than 2hours.

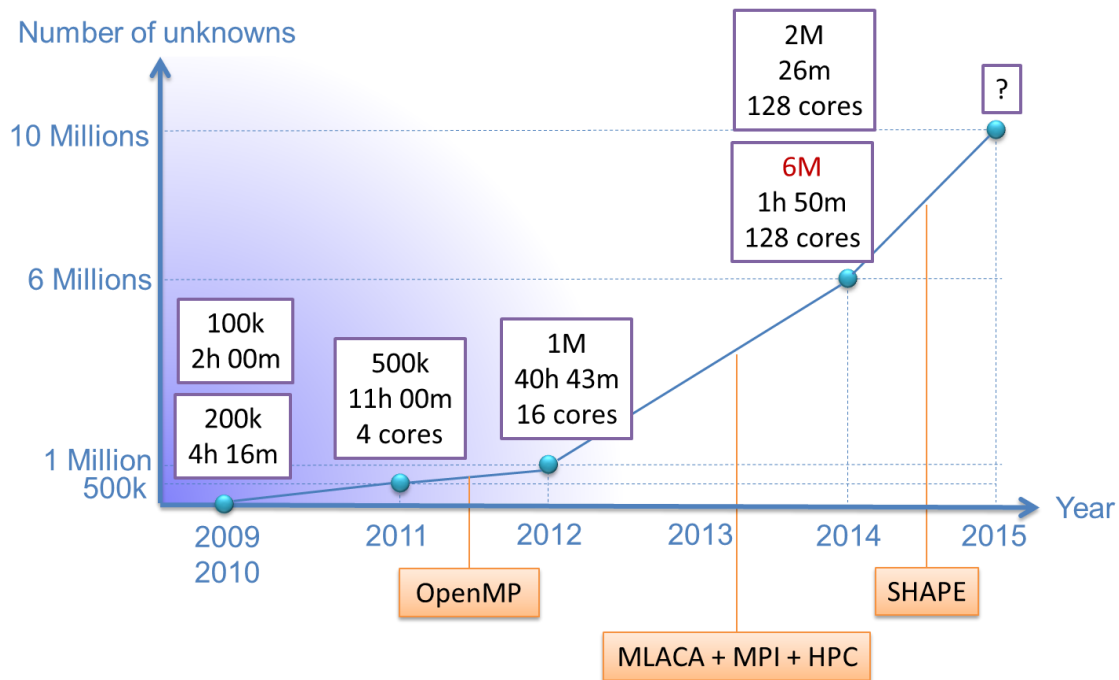


Figure 10 Influence of different techniques or European projects in the performance evolution of CAPITOLE over the last few years.

4 Benefits from SHAPE Pilot project

The cooperation between PRACE and ENTARES Engineering was composed of three parts:

- 200.000 core-hours on MARENOSTRUM at BSC, SPAIN
- 1 PRACE support expert, Nicolas Mignerey, GENCI, France
- Support of HPC Experts of INRIA Bordeaux, France

This project has helped us to continue to develop the HPC version of our program. The main work is to test on larger and larger models and optimize the computational time, scalability and the use of memory.

We had some interesting discussions with research teams from different laboratories specialized in HPC. (IRIT, INRIA, CALMIP) and it has been a very useful help for us. We use more and more libraries (like PT-SCOTCH, MUMPS, STAR-PU) already optimized for HPC machines which reduces the development time and increases performance.

Having access to a HPC machine is also very important for a SME. We need to perform plenty of tests and at the starting point it is impossible for us to buy a proper server.

The expected business impact is to commercialize the HPC version of the CAPITOLE software all over the world. We expect half of the sales of CAPITOLE in the future to be with the HPC version. We have observed an increasing demand to solve bigger models and an increase in the operating frequency of telecommunication devices.

5 Future plan and lessons learned

At first, we selected the CURIE machine of the TGCC for this project because its characteristics are adapted to our application but the access at TGCC was impossible due to security policies. TGCC authorizes only connection from enterprise networks (with static IP-addresses) and not from internet access providers which is usually the case for SME. A connection to a special network (like RENATER in France) is too expensive for an SME.

For this reason we have switched during the project to MARENOSTRUM III at BSC, which has finally been a success. We have a limitation due to available memory on each node. Our application is very demanding in terms of memory. We plan to over pass this limitation by an out-of-core implementation using hard disk instead of ram memory.

We had a meeting at Bordeaux with INRIA people at the beginning of the project to use the STAR-PU runtime in our program. The main problem is that the library has no interface in Fortran, what introduces an additional step in order to use it. We had not enough time to develop a Fortran interface during the project.

The idea is basically to continue with the development and optimization of the two methods, MSCBD and MLACA. We have done the important step of splitting the MSCBD into asynchronous tasks but it remains to include the use of STAR-PU to optimize the parallelization of these tasks. As for MLACA, a further analysis is necessary, including some HPC tools in order to find the main bottlenecks in the parallelization.

6 Conclusions

Overall, the SHAPE pilot project has been a success for us. It has allowed us to go a bit further in HPC electromagnetic simulations. Of course, there is still a long way to go but thanks to the project a SME like us has got access to valuable resources otherwise unaffordable. We pretend to continue in the same direction, trying to optimize the parallel execution of the different available solvers, both in computational time and memory usage and treatment. Our main goal is to achieve the electromagnetic simulation of larger objects which are of interest to several companies.

References

- [1] R. F. Harrington, *Field computation by moment methods*. New York: Macmillan, FL, Krieger, 1983.
- [2] W. C. Chew, J.-M. Jin, C.-C. Lu, E. Michielssen, and J. Song, "Fast solution methods in electromagnetics," *IEEE Trans. Antennas Propagat.*, vol. 45, no. 3, pp. 533–543, Mar. 1997.
- [3] J. Song, C.-C. Lu, and W. C. Chew, "Multilevel fast multipole algorithm for electromagnetic scattering by large complex objects," *IEEE Trans. Antennas Propagat.*, vol. 45, no. 10, pp. 1488–1493, Oct. 1997.
- [4] J. M. Rius, J. Parron, A. Heldring, J. M. Tamayo, and E. Ubeda, "Fast Iterative Solution of Integral Equations With Method of Moments and Matrix Decomposition Algorithm Singular Value Decomposition," *Antennas and Propagation, IEEE Transactions on*, vol. 56, no. 8, pp. 2314-2324, Aug. 2008.
- [5] E. Bleszynski, M. Bleszynski, and T. Jaroszewicz, "AIM: Adaptive integral method for solving large-scale electromagnetic scattering and radiation problems," *Radio Sci.*, vol. 31, no. 5, pp. 1225–1251, Sept./Oct. 1996.
- [6] M. Bebendorf, "Approximation of boundary element matrices," *Numer. Math.*, vol. 86, no. 4, pp. 565–589, 2000.
- [7] J. M. Tamayo, A. Heldring and J. M. Rius, "Multilevel Adaptive Cross Approximation (MLACA)," *Antennas and Propagation, IEEE Transactions on*, 2011, vol. 59, pp. 4600 -4608.
- [8] A. Heldring, J.M. Tamayo, E. Ubeda and J.M. Rius, "Accelerated Direct Solution of the Method-of-Moments Linear System," *Proceedings of the IEEE*, 2013, vol.101, pp. 364 -371.
- [9] Cédric Augonnet, Samuel Thibault, and Raymond Namyst. StarPU: a Runtime System for Scheduling Tasks over Accelerator-Based Multicore Machines. Technical Report 7240, INRIA, March 2010
- [10] Y. Saad et M.H. Schultz, « GMRES: A generalized minimal residual algorithm for solving nonsymmetric linear systems », *SIAM J. Sci. Stat. Comput.*, 7:856-869, 1986
- [11] Amestoy, P.R.; Duff, I.S.; l'Excellent, J.-Y. (2000). "Multifrontal parallel distributed symmetric and unsymmetric solvers". *Computer Methods in Applied Mechanics and Engineering* 184 (2–4): 501–520

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