Stability considerations and efficient computing in chiral materials electromagnetic simulations

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Abstract- A solution for the computational efficiency/accuracy compromise is searched for the electromagnetic simulation of a hexachiral honeycomb. Convergence stability is investigated for the frequency and time domain solvers, and an optimum solution (FDTD analysis in parametric studies with frequency simulation as a permanent reference) is found.

I. Introduction

In the high frequency range (GHz) the cost of the measurement is high enough (both in terms of devices and cost of highly qualified labor force) to justify extensive use of pre-measurement computer simulation.

We intend to analyze a fiber reinforced polymer [2] prototype, developed in the framework of the CHISMACOMB FP6 EU project by the Italcompany (figure 1). This auxetic material was developed primarily for his mechanical and thermal properties, but his EMC shielding properties are also of great importance in order to obtain a low cost, low weight, multifunctional material (aeronautics [1], medicine, construction etc.). The structure is a hexachiral honeycomb, each of the equally spaced cylinders being connected with strings to 6 of his neighbors.

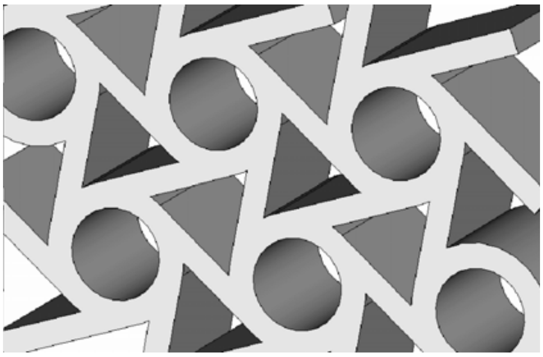


Figure 1. Hexachiral honeycomb

As is often the case when a structure is analyzed for the first time, no previous literature results are available, so a question arises: how can we trust that a particular software gives accurate results? This paper will explain the steps taken to ensure that accurate results are found.

II. Convergence stability analysis

The software product used for the electromagnetic simulation was CST Microwave Studio, which is capable to perform both frequency and FDTD simulations. This dual capability offers the possibility to verify the results obtained by one method of computation with another.

In order to limit the dimensions of the model, the periodicity of the structure has been investigated, a rectangular unit cell containing 4 cylinders was placed between electric walls (both walls on x directions) and magnetic walls (y direction walls) in order to investigate the interaction with a normal incident plane wave. In order to verify the boundary conditions setup a three layer Jaumann microwave absorber was investigated in the same test setup. The results were found to be identical to those mentioned in the literature [3].

The adaptive meshing facility of the software was used, the mesh cell size being decreased to increase the theoretical accuracy of the solution.

A. Frequency domain analysis

The CST Microwave Studio frequency domain solver solves the problem for a single frequency at a time, and for a number of adaptively chosen frequency samples in the course of a frequency sweep. For each frequency sample, the linear equation system will be solved by an iterative (e.g. conjugate gradient) or sparse direct solver.

Results obtained through frequency analysis are plotted in figure 2. Seven adaptive passes were performed, the number of mesh cells increasing from 2145 to 149,328. As we see, from the 5^{th} pass, no noticeably difference between the results is found, so in this case we have a good convergence to a solution.

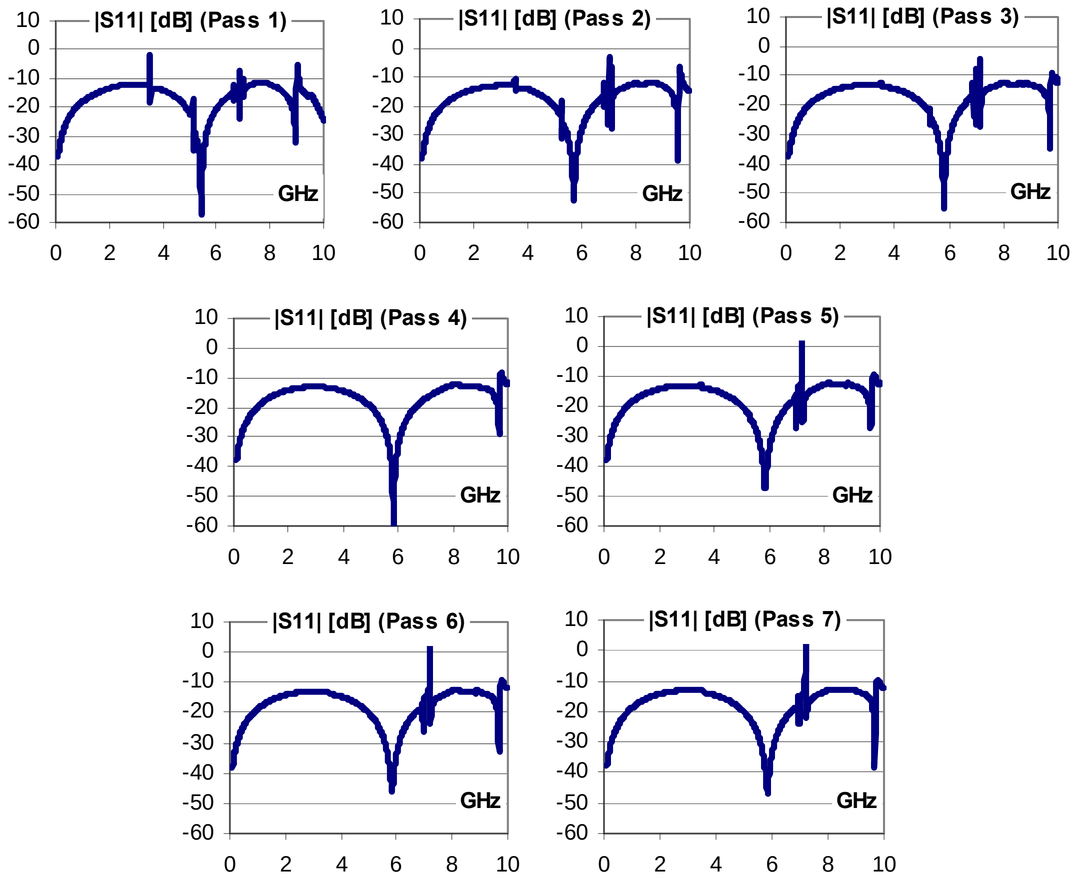


Figure 2. $|S_{11}|$ versus frequency (passes 1 to 7, frequency domain analysis)

B. Time domain analysis

The CST Microwave Studio time domain solver calculates the development of fields through time at discrete locations and at discrete time samples. It calculates the transmission of energy between various ports and/or open space of the investigated structure.

The fields are calculated step by step through time by the so called "Leap Frog" updating scheme. It is proven, that this method remains stable if the step width for the integration does not overcome a known limit. This value of the maximum usable time step is directly related to the minimum mesh step width used in the discretization of the structure. So, the denser the chosen grid, the smaller the usable time step width.

Results obtained through FDTD analysis are plotted in figure 3. Ten adaptive passes were performed, the number of mesh cells increasing from 2145 to 338,496. In this case, from the 5^{th} pass, it is clear that a solution cannot be found, all values being annulled (up to a small value ~10^{-5} which can be attributed to round off errors).

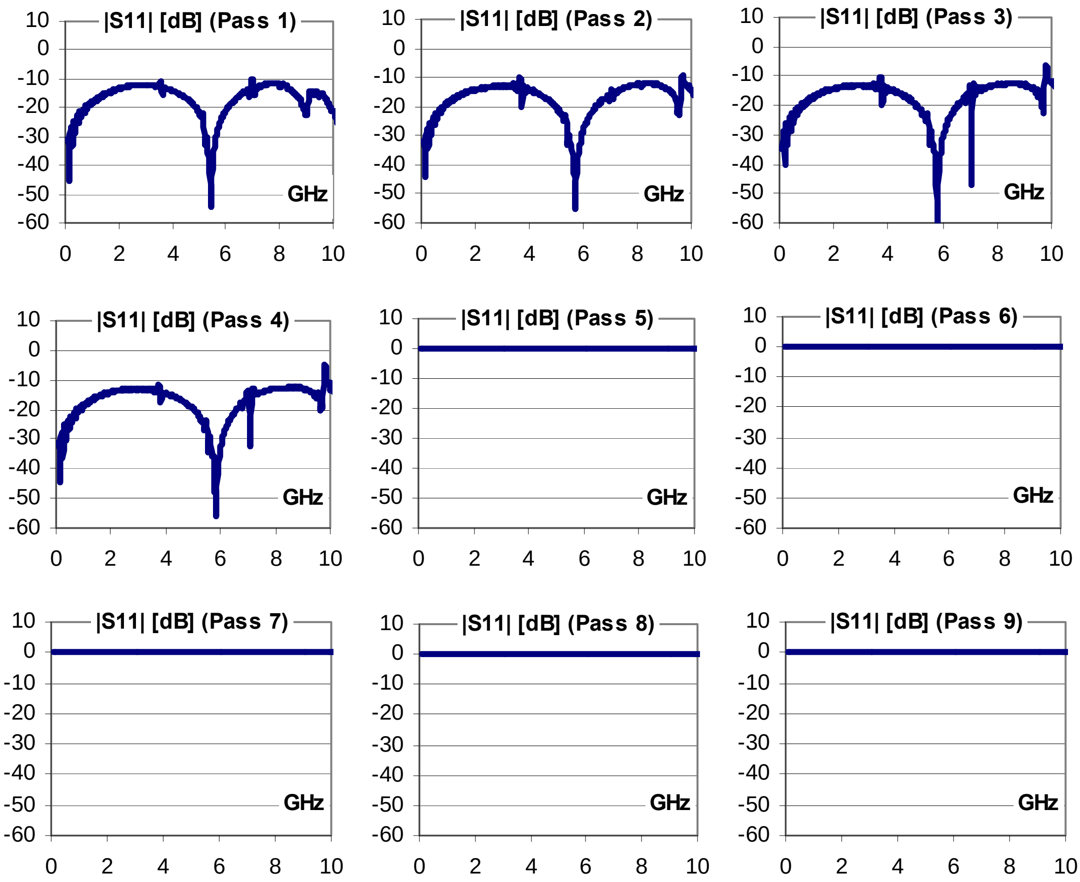


Figure 3. $|S_{11}|$ versus frequency (passes 1 to 9, time domain analysis)

Both analysis (frequency and time domain) were performed with hexahedral meshing, the CST proprietary technology **Perfect Boundary Approximation®** (PBA) is used for the spatial discretization of the structure. The simulated structure and the electromagnetic fields are mapped to hexagonal mesh. PBA allows a very good approximation of even curved surfaces within the cubic mesh cells [4].

III. Computational efficiency

As figures 2,3 show, at a glance, the frequency domain solver offers better results so it would be the solver to choose in this case. However computational efficiency is to be taken into account in order to have real time solutions.

A. Solver time

A first thing to consider is the time needed to perform the computations. Figure 4 shows the time consumed to achieve the solution. For the reference, all previous computations were made on an IBM compatible computer, with Intel Core2 E6400@2.13GHz processor, 2GB RAM, only one of the two separate processing cores being used by the solver.

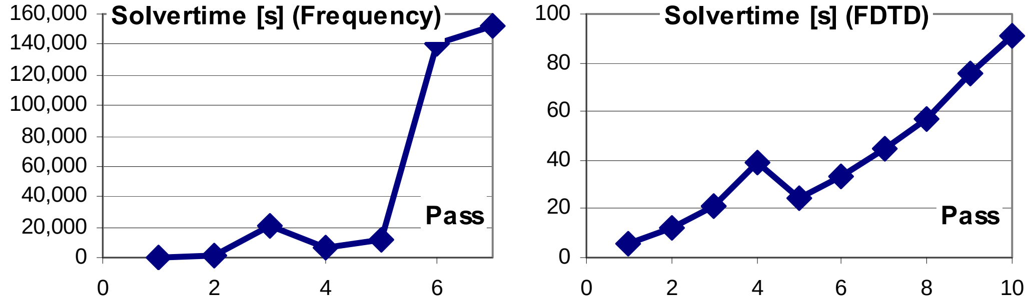


Figure 4. Solver time versus passes – frequency (left) and time (right) domain solvers

The first thing to consider is the tremendous difference between the two solvers. The 7th pass frequency solver used 152,068 seconds (e.g. 42 h, 11 m, 53 s) to achieve the solution whereas the 10th pass time domain solver only needed 91 s. When multiple analysis are to be performed (like in [5] where parametric studies involved more than 100 different analysis) the time consumed has a critical importance.

B. Number of mesh cells

Another important parameter is the number of mesh cell used for the discretization of the structure. This number closely relates with the amount of memory used in computations. This is also a critical parameter, when the physical memory limit is reached and the virtual (e.g. HDD storage) memory comes to use, a major performance decrease is witnessed.

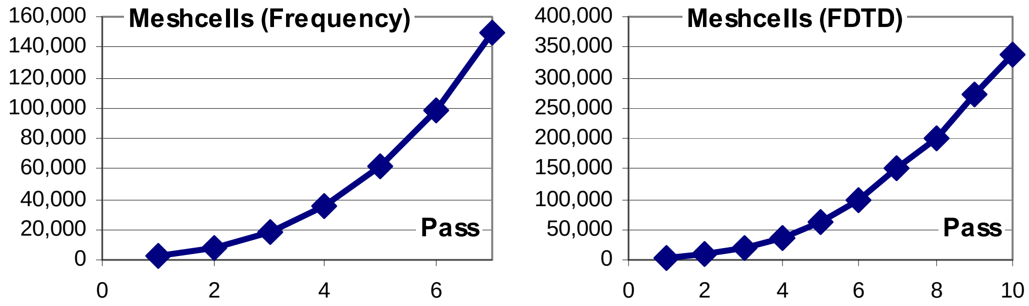


Figure 5. Number of mesh cell used for the discretization – frequency (left) and time (right) domain solvers

It's not only the mesh cells number who decides the memory occupation. Every algorithm has its own memory consumption particularities. Table 1 shows the actual figures, showing that the time domain algorithm is more memory efficient (even at 2 times more mesh cells, less memory is used e.g. 97MB vs. 865MB).

		Peak memory used (kB)		Free physical memory (kB)	
		Physical	Virtual	At begin	Minimum
Frequency solver 7th pass memory necessity	Matrices calc.	52800	47532	1197688	1170112
	Solver run total	694008	867164	1221852	95208
	Solver start	5588	2868	1221848	1221848
	Eq. system setup	212616	369464	1148788	564864
	Eq. system solve	694008	865984	993508	144780
FDTD solver 10th pass memory necessity	Matrices calc.	72716	67136	1399088	1338280
	Solver run total	97972	94064	1427024	1309240

Table 1. Memory consumption figures, frequency and time domain solvers

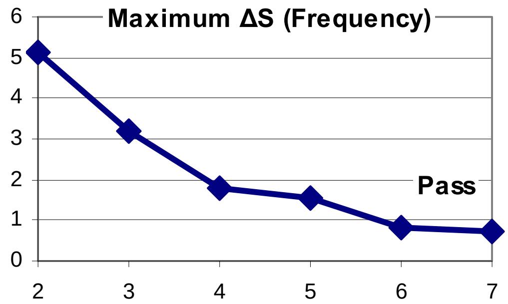
C. Convergence investigation

We compute the variation of the computed parameters between two consecutive passes as in equation (1).

$$\max \Delta S^k = \sqrt{\frac{\sum_i^N \left(|S_{11}|_i^k - |S_{11}|_i^{k-1}\right)^2}{N}} \qquad (1)$$

where k denotes the pass number, N the number of samples computed (e.g. 1000 in our case). With equation (1) we investigate the overall difference in S_{11} curves between two consecutive adaptive passes.

Figure 6 shows the variation through the adaptive process of the solution. The greatest value (17.5554 @ 5th pass for the FDTD solver) clearly shows the moment were the time domain solution diverges).



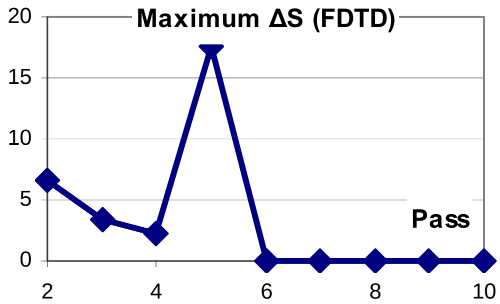


Figure 6. Convergence analysis (ΔS_{11} vs. adaptive passes)

IV. Conclusions

This paper shows that in the case of the chiral structure under test a choice must be made between speed and accuracy. The time domain solver clearly diverges by decreasing mesh cell size. The frequency domain solver has a good convergence to the solution but is very expensive in computation time (more than 42 hours for a single solution). The conclusion is that the 4th pass meshing for the FDTD solver offers the best compromise accuracy/time and was used for all parametric studies [5]. The accuracy is "good enough" to investigate the performance of the chiral material (figure 7), the frequency solver being permanently used as a accurate reference for the calculus.

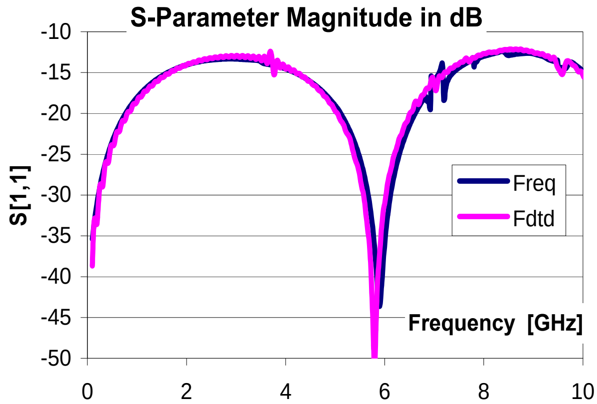


Figure 7. Comparison frequency/time domain solvers

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