An assessment by a commercial software of the accuracy of electromagnetic finite element simulators in the presence of metamaterials

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April 11, 2008

Structured abstract

Purpose
To deduce additional information on the accuracy of finite element simulators for electromagnetic problems involving effective models of metamaterials.

Design - methodology - approach
The objective is achieved by solving, with a well known commercial simulator, many different configurations of two types of electromagnetic problems: a free-space scattering by a sphere and a waveguide discontinuity problem. Such problems are known to be able to point out the difficulty of numerical simulators. On the other hand, they are representative of two important classes of problems and can provide indications on what can happen in other cases.

Findings
This analysis confirms that the numerical errors can be important just in close proximity of the interface between metamaterials and standard media. Small values of loss tangents can be sufficient to obtain very accurate results. When this is not the case, adaptive mesh generators should not be used. For more uniform meshes the results are satisfactory, with sufficiently fine meshes. This is not necessary when the magnitude of the real parts of the effective dielectric permittivity of a metamaterial and of the adjacent standard media are significantly different.

Research limitations - implications
The results are obtained by considering problems of two types. There is no guarantee that all our deductions apply to other models.

Practical implications
To design practical devices involving metamaterials reliable electromagnetic simulators are necessary. The reported results seem to indicate that it is possible to adopt some countermeasures against the possible lack of accuracy of finite element simulators in the presence of effective models of metamaterials.

Originality - value
For the first time, to the best of authors’ knowledge, an extensive analysis on the accuracy of finite element simulators for critical problems involving metamaterials has been carried out. Some simple suggestions to improve their reliability in these cases are provided.

Paper type
Research paper.

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1 Introduction

The recent advent of metamaterials (Ziolkowski and Engheta, 2003), (Itoh and Oliner, 2005) have opened new possibilities for the development of innovative microwave components (Engheta and Ziolkowski, 2005), (Alù et al., 2007).

Due to the huge difficulty in predicting the practical effects of the presence of metamaterials and standard media, at least when the geometric configuration is not trivial or canonical, the role of numerical simulators have become fundamental (Kärkkäinen, 2003), (Ziolkowski and Heyman, 2001), (Caloz et al., 2001). Clearly, in the above statement it is implicitly assumed that numerical simulators provide reliable results even in the presence of metamaterials, but this assumption is not at all trivial.

As a matter of fact, two different approaches to the numerical simulations of electromagnetic problems involving metamaterials are used: the first one considers all the inhomogeneities of the macroscopic materials (Moss et al., 2002) while in the second approach all metamaterials are dealt with as effective media (Caloz et al., 2001).

Since in the first approach any simulator has to deal just with standard “double positive” materials (Ziolkowski and Engheta, 2003), the already available results on the performances of numerical methods apply and the results obtained by using this approach are known in advance to be reliable (see, for example, (Monk, 2003)). The drawback of this approach is that, as a consequence of the very fine grids required by this approach in order to take account of all the inhomogeneities, so far it is computationally extremely difficult to obtain numerical simulations of components of practical interest. This is one of the reasons why the second approach has been proposed and, since then, used very often. As a matter of fact, in order to obtain system level electromagnetic simulations, it is useful to consider metamaterials as media characterized by effective constitutive parameters (Ziolkowski and Engheta, 2003). In this way the extremely fine grids required by the first approach are not necessary anymore. Unfortunately, when such an approach was first proposed, it was not known that this choice would have prevented the application of all results of reliability of the numerical approximations.

Nowadays, on the contrary, some aspects related to the lack or the availability of convergence results in the presence of effective models of metamaterials have been clarified. For example, it is now known that some problems involving particular configurations of effective models of metamaterials and standard media are ill-posed (Shatrov, 2007), (Raffetto, 2007), (Oliveri and Raffetto, 2008); that the usual proofs of convergence in infinite precision arithmetics of the numerical approximations do not hold true (Monk, 2003), and that the linear algebraic system of equations usually solved by time-harmonic numerical methods can be ill-conditioned (Cevini et al., 2007), (Cevini et al., 2006).

However, some results related to or on the reliability of numerical simulators have been recently obtained. In the presence of lossy effective models of metamaterials and standard media, time-harmonic electromagnetic boundary value problems are well-posed and, for the finite element method, the convergence of the approximation is proved (Fernandes and Raffetto, 2005), (Raffetto, 2004). Moreover, well-posedness results have been obtained (Dhia et al., 2007) for problems involving lossless standard media and metamaterials characterized by effective constitutive parameters sufficiently different from the particular cases indicated above (implying ill-posedness).

The above considerations point out that our knowledge on the capability of numerical simulators to provide reliable results for time-harmonic electromagnetic boundary value problems involving effective models of metamaterials is far from being satisfactory.

In this paper we try to shed more light on this topic. In particular, we try to provide some more information on the cases which can be pathological for numerical simulators and on the cases which are not. This is done by using a well known commercial simulator, COMSOL Multiphysics, whose performances are well recognized to be satisfactory in the presence of standard materials. The same
simulator was exploited in (Oliveri and Raffetto, 2008), where a single problem was considered as an example of what can go wrong when effective models of metamaterials are involved.

Our analysis is carried out by considering two canonical problems: the plane wave scattering by a sphere in free space and a discontinuity problem in a rectangular waveguide by a planar slab. These problems have been chosen since, on the one hand, they can be solved analytically, thus allowing an evaluation of the errors of the numerical approximations, and, on the other hand, they have been shown to be able to point out the difficulties of numerical simulators (Cevini et al., 2007), (Oliveri and Raffetto, 2008). Such problems could be sufficiently representative to provide indications on what can happen in other cases.

Many dielectric configurations are considered. In particular, several real and imaginary parts of the effective constitutive parameters are analyzed in order to increase our confidence of having found the pathological dielectric configurations. Moreover, one of the targets of this activity is to provide some indications on the effects of perturbations of pathological dielectric configurations on the performances of numerical simulators.

Different grids are used for each case considered, in order to evaluate the convergence or the lack of convergence of the approximate solutions to the analytical ones.

This analysis confirms that in any case the numerical errors can be important just in close proximity of the interface between metamaterials and standard media.

The results are satisfactory when the magnitude of the real parts of the effective dielectric permittivity of a metamaterial and of the adjacent standard media are different by a factor bigger than or equal to two, independently of any other effect. The same conclusion is obtained by considering the magnetic permeability, even though, in this case, the errors are not controlled in the same satisfactory way.

No other “critical” configurations has been found, in addition to the one already known (Raffetto, 2007), (Oliveri and Raffetto, 2008). For all dielectric configurations the results remain satisfactory, even though with a progressive deterioration of the performances as the configuration becomes closer and closer to the critical one, provided that the adaptive mesh generator is disabled. When it is exploited, impressive errors can affect the numerical solution (see also (Oliveri and Raffetto, 2008)).

Finally, the effects of losses are known to be important (Fernandes and Raffetto, 2005), (Raffetto, 2004). Here we show that electric and magnetic loss tangents as low as one hundredth are sufficient to avoid the worst instabilities. The introduction of losses seems to be the best remedy for the lack of accuracy in the worst situations.

This paper is organized as follows. In Section 2 the numerical models considered in this analysis are defined, together with the error figures used to provide indications on the accuracy of the results obtained. Then, before concluding the paper, in Section 3 we show and discuss the numerical results obtained by using COMSOL Multiphysics.

## 2 Models considered and error figures

The two models considered in this paper have been previously considered in (Oliveri and Raffetto, 2008) and (Cevini et al., 2007).

In the waveguide discontinuity problem several dielectric configurations are numerically analyzed but the problem geometry is exactly the same as the one studied in (Oliveri and Raffetto, 2008). In particular, a rectangular waveguide (width 0.02 m, height 0.01 m) is loaded by three different materials as shown in Figure 1. Near the two ports, in the regions characterized by $z \in (0, 0.03)$ and $z \in (0.09, 0.12)$, $\varepsilon_r = 1 - j0.1$ and $\mu_r = 1 - j0.1$. In the region $z \in (0.03, 0.06)$ we have $\varepsilon_r = 1$ and $\mu_r = 1$. Finally, for $z \in (0.06, 0.09)$ the medium is a double negative metamaterials characterized by effective constitutive parameters $\varepsilon_r$ and $\mu_r$ as described below. The two ports are matched for the propagation of the fundamental mode and on the port at $z = 0$ a unit amplitude TE$_{10}$ mode is impinging at $f = 11.25$ GHz.

In the free space electromagnetic scattering problem a sphere of double negative metamaterial of radius 0.2 m and effective constitutive parameters $\varepsilon_r$ and $\mu_r$ as described below, is illuminated
Figure 1: Geometry of the waveguide discontinuity problem.

by a unit amplitude plane wave characterized by $E_{\text{inc}} = \mathbf{x} e^{-j2\pi f \sqrt{\varepsilon_0 \mu_0} z}$, $f = 300$ MHz. The are two planes of even and odd symmetry for the electric field in this problem and we have reduced our model by considering a perfect magnetic conductor on the plane $y = 0$ and a perfect electric conductor on the plane $x = 0$. The domain of numerical investigation is bounded by other planes at a distance of 0.5 m from the sphere. On these planes a (inhomogeneous) free space impedance boundary condition is implemented. These boundaries introduces an approximation which, however, is always very satisfactory when the scatterer is made up of a standard media, even when it is much denser than the metamaterials we are going to consider. Figure 2 shows the details of the geometry of the problem.

Two grids are used for each class of models: the “finer” and the “extra fine” meshes for the waveguide discontinuity problem and the “fine” and the “finer” grids for the electromagnetic scattering problem. In the waveguide problem the “finer” mesh has 400 nodes, 1265 elements, 708 faces and 9684 degrees of freedom, whereas with the “extra fine” mesh we have 1477 nodes, 6015 elements, 1920 faces and 42546 degrees of freedom. In the scattering problem the “fine” mesh has 1910 nodes, 8927 elements, 1668 faces and 57168 degrees of freedom, whereas the “finer” has 5345 nodes, 26925 elements, 3422 faces and 172520 degrees of freedom. In all cases (but one; see the corresponding comment in Section 3) the adaptive mesher has been disabled to prevent the use of the simulator in the most critical conditions.

The two problems of interest can be solved analytically. This feature is crucial for our analysis. Since an electric field formulation is always adopted, for a given subregion $\Omega$ of the domain of numerical investigation, we define an average relative error as follows:

$$\text{Average relative error} = \frac{1}{\text{volume}(\Omega)} \int_{\Omega} \frac{|E_{\text{COMSOL}} - E_{\text{analytic}}|}{|E_{\text{analytic}}|} dV,$$

where $E_{\text{COMSOL}}$ and $E_{\text{analytic}}$ are the electric field calculated by the numerical simulator or analytically, respectively.

In this numerical study we have analyzed the effects of 441 different metamaterials for both problems. In particular, the imaginary parts of the relative dielectric permittivity $\varepsilon_r$ and magnetic permeability $\mu_r$ of the double negative metamaterial involved in both problems assume, independently, the values 0, $-0.01$ or $-0.1$, whereas the corresponding real parts have values belonging to $\{-2, -1.75, -1.5, -1.25, -1, -0.75, -0.5\}$. 
All results presented in this work have been calculated by choosing UMFPACK as the direct solver of the algebraic system of linear equations generated by COMSOL Multiphysics.

3 Numerical results

In the first phase of our analysis we have considered the results obtained in the whole domain of numerical investigation. In all cases the results are completely satisfactory at some distance from the interfaces between the lossless double positive media and the double negative metamaterial involved. Figure 3 shows some examples of what can be observed along the waveguide axis. The relative error can have significant values only near the indicated interface. The same happens in all electromagnetic scattering models considered, as shown in Figure 4. Since this effect is also theoretically expected (Oliveri and Raffetto, 2008), in the following we focus our attention on subregions containing the indicated interface. In particular, the relative error in (1) will be calculated by using \( \Omega = \{(x, y, z) \in \mathbb{R} | x \in (0.02, 0.022), y \in (0, 0.01), z \in (0.055, 0.065)\} \) for the waveguide problem and \( \Omega = \{(x, y, z) \in \mathbb{R} | x \in (0.005, 0.405), y \in (0.005, 0.405), z \in (-0.4, 0.4)\} \) for the scattering problem.

In Figures 5 and 6 we show, respectively, the behaviour of the average relative error as a function of the real part of the effective relative dielectric permittivity \( \varepsilon_r \) or of the effective relative magnetic permeability \( \mu_r \) of the double negative metamaterial in the waveguide problem, for all cases considered. It is apparent that when \( \varepsilon_r = -2.0 \) or \( \varepsilon_r = -0.5 \) the results are satisfactory, independently of the values of all other parameters and of the “finer” or “extra fine” grid exploited. The same effect is present, even if in a less evident way, when \( \mu_r = -2.0 \) or \( \mu_r = -0.5 \) (see Figure 6).

By observing Figures 5 and 6 one can note that just one critical case has been observed, the already known (Oliveri and Raffetto, 2008), (Cevini et al., 2007) pathological configuration involving complementary media. When the “finer” mesh is used the result for this particular case is totally unacceptable but note that with the “extra fine” grid the error is not so big and could be tolerated. For other values of the effective relative dielectric permittivity \( \varepsilon_r \) or of the effective relative magnetic permeability \( \mu_r \) we can observe an intermediate behaviour between the two extreme cases so far considered. Starting from the satisfactory cases \( \varepsilon_r = -2.0, \varepsilon_r = -0.5, \varepsilon_r = -2.0 \) or \( \mu_r = -0.5 \),
Figure 3: Relative error along the axis of the waveguide \((x = 0.01 \text{ m}, y = 0.005 \text{ m})\) for different values of \(\varepsilon_{r2}\) and \(\mu_{r2}\) of the double negative metamaterial. All results are calculated by using the “extra fine” grid.

Figure 4: Relative error along a line of points through the sphere \((x = 0.005 \text{ m}, y = 0.005 \text{ m})\) for different values of \(\varepsilon_{r2}\) and \(\mu_{r2}\) of the double negative metamaterial. All results are calculated by using the “finer” grid.
Figure 5: Average relative error calculated in the waveguide discontinuity problem as a function of the real part of $\varepsilon_r^2$ only.

Figure 6: Average relative error calculated in the waveguide discontinuity problem as a function of the real part of $\mu_r^2$ only.
\(\mu_r^2 = -2.0\) or \(\mu_r^2 = -0.5\) there is a progressive deterioration of the accuracy of the numerical solution as the effective constitutive parameters \(\varepsilon_r^2\) and \(\mu_r^2\) approximate the pathological case indicated. In some cases particularly “close” to the critical one the error can be significant, even with the “extra fine” grid. See, for example, the average relative error calculated for the case \(\varepsilon_r^2 = -1.25, \mu_r^2 = -0.75\) (Figures 5 and 6).

In Figure 7 the average relative error as a function of the imaginary parts of \(\varepsilon_r^2\) and \(\mu_r^2\) is presented. For the adopted formulation a given value of the electric loss tangent guarantees a bigger reduction of the errors than the same value of the magnetic loss tangent, even though both can help in increasing the numerical accuracy. A value as low as 0.01 can give very good effects, according to the theoretical expectations (Fernandes and Raffetto, 2005), (Raffetto, 2004), and the results are completely satisfactory when the electric loss tangent is bigger than 0.01. These results can provide an indication for future research on how to introduce losses in the effective models of metamaterials, in order to improve the accuracy of the numerical results.

In order to give a statistical idea of the performances of the numerical simulator, in Figure 8 the relative frequency of the occurrence of a given value of the average relative error is shown. One can note that in almost all cases the average relative error is below 10% and that this happens in the 85.7% of the simulations performed when the “extra fine” mesh is used; another 11.1% of the simulations gives an average relative error in the range 10% − 20%.

The above considerations are qualitatively confirmed by the results obtained by solving the electromagnetic scattering problem, even though, in this case, the approximate boundary conditions enforced have an effect on the accuracy of the results, especially for strong scatterers.

In Figures 9 and 10 we show the same type of data as those shown in Figure 5 and 6, respectively. From Figure 9 it is apparent that the accuracy is satisfactory for \(\varepsilon_r^2 = -2.0\) or \(\varepsilon_r^2 = -0.5\), independently of the value of any other parameter. Moreover, when the “finer” mesh is used, the most critical cases seem to be with \(\varepsilon_r^2 = -1.25\) or \(\varepsilon_r^2 = -1.5\). The results in the expected most difficult situation \((\varepsilon_r^2 = -1.0, \mu_r^2 = -1.0)\) are very good. The reader should consider, however, that the “finer” mesh has many more degrees of freedom than it would be required if the scatterer was made up of a (not too dense) standard media.

The effect of the real part of \(\mu_r^2\), on the contrary, are less evident, as was the case for the
Figure 8: Statistics of the errors for the waveguide problem.

Figure 9: Average relative error calculated in the free-space scattering problem as a function of the real part of $\varepsilon_{r2}$ only.
waveguide discontinuity problem (see Figure 10).

As far as the effects of the imaginary parts of $\varepsilon_r^2$ and $\mu_r^2$ are of interest, the behaviour of the average relative error is provided in Figure 11. Also in this case the results obtained for the waveguide discontinuity problem are confirmed: the electric loss tangent has a more significant impact on the reliability of the results. Moreover, with values of $-\text{Im}(\varepsilon_r^2) \geq 0.01$ satisfactory results are obtained. In this case too, it is important to remember that finer meshes than it is usually done for standard media are here exploited.

Finally, in order to provide a statistical indication on the accuracy of the simulator, the histogram of the occurrences of the average relative error has been reported in Figure 12. In almost the 85% of the cases the error is below 10%. In this case, however, in a more significant percentage of the cases than before we obtain an average relative error greater that 20%.

All these results and comments are calculated and apply when the adaptive mesh generator is disabled. If this is not the case very bad performances can be obtained as a consequence of the fact that such generator refines the meshes near the interfaces and this can amplify the effects of the ill-conditioning and/or ill-posedness of the problem. A result for the waveguide discontinuity problem, with the adaptive mesh generator enabled, has been discussed in (Oliveri and Raffetto, 2008). In Figure 13 we report the result obtained along the line $x = 0.08432836$ m, $y = 0.006$ m for the free-space scattering problem. Starting from a “normal” mesh, two steps of adaptive refinement were performed and a final mesh with 8864 nodes, 45530 elements, 4434 faces and 277242 degrees of freedom was obtained. The analytical solution is provided for comparison. It can be noted that the error is totally unacceptable near the dielectric interface, in this case.

4 Conclusions

The purpose of this paper is to extend our knowledge on the capability of finite element simulators to provide reliable results when effective models of metamaterials are involved in the formulation of the electromagnetic problems of interest.

Our study has been carried out by solving many different models belonging to two classes of time-harmonic electromagnetic boundary value problems. All solutions are computed by using a
Figure 11: Average relative error calculated in the free-space scattering problem as a function of the imaginary parts of $\varepsilon_{r2}$ and $\mu_{r2}$.

Figure 12: Statistics of the errors for the free-space scattering problem.
Figure 13: Amplitude of $E_x$ along the line $x = 0.08432836$ m, $y = 0.006$ m. The analytical solution is provided for comparison. The mesh has been obtained by using the adaptive mesher.

well known commercial simulator.

The two classes of problems considered are known to be able to create a lot of difficulties to usually reliable numerical simulators and, for this reason, our results could provide indications on the accuracy of finite element simulators when other problems involving effective models of metamaterials are considered.

Our analysis confirms that the numerical errors can be significant just near the interfaces between metamaterials and standard media. Even small values of electric or magnetic loss tangents can be sufficient to obtain very accurate results. This effect could be exploited to modify critical models to obtain more accurate results. When the indicated interface involves losses media, adaptive mesher should not be used. For more uniform meshes the results can be, to some extent, satisfactory, but it is usually necessary to exploit much finer meshes than it is usually done when only standard media are involved. The adopted meshes may not be so fine when the magnitude of the real parts of the effective dielectric permittivity of a metamaterial and of the adjacent standard media are significantly different.

References


