USING MATLAB AND COMSOL MULTIPHYSICS FOR HOMOGENISATION OF COMPOSITE MATERIALS

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Abstract

The aim of this paper is to introduce a method for creating a homogenous substitute material for composite materials using optimisation algorithms. Composite materials are modern construction materials used, for example, in aircraft construction. However, numerical modelling of these materials is, due to its multi-layer structure, very difficult to compute. This multi-layer structure and loss materials of the composite model are represented, in the numerical simulators, as a very fine grid, resulting in an extremely high density of cells and making the simulation time much longer and the calculation much more complex. When modelling tests for aircraft electromagnetic resistance to lightning, and for other high-intensity electromagnetic fields, the intension was to replace the composite material with a homogenous substitute material having equivalent behaviour to that of the composite material in an electromagnetic field. This homogenous substitute material is then represented by much less detailed grid then the original composite, thus reducing computing time and hardware demands. The main point of the analysed inversion task, referred to below, was to find a frequency flowchart for complex permittivity of this substitute material, where the transmission characteristics are the same as those of the composite material. To solve this inversion task, optimizing algorithms in the MATLAB environment were used. When evaluating a criteria function of the optimizing algorithm, a 2D model of the substitute homogenous dielectric was produced using the Comsol Multiphysics program. Then, also using this program, the distribution of electromagnetic field was calculated for each actual value of complex permittivity calculated by MATLAB.

1. Introduction

The demands on the reduction of the weight and the fuel consumption of today's airplanes enforce designers to replace the fully metallic skin of airplanes by composite materials. Therefore, a very strong research effort is focused on the development of new analytical and numerical techniques for the modeling of these structures in order to efficiently determine their scattering parameters.

Dealing with a numerical characterization of composite materials, conventional or hybrid finite-difference time-domain (FDTD) methods are usually used [1], [2]. Due to the relatively complicated structure of the composite materials, CPU-time demands of such an analysis might be relatively high.

In order to solve this problem, global optimization methods are originally applied to identify such a frequency dependency of the complex permittivity of a homogeneous dielectric layer, which exhibits similar frequency responses of scattering parameters as the composite material.

Section 2 of the paper describes a numerical analysis of the composite material in CST Microwave Studio using FDTD which determines scattering parameters of the material. Two models of the composite materials with a different degree of details were created. The first model consists of a metallic grid covered by homogeneous dielectrics. In the second model, the dielectric cover is reinforced by carbon fibers.

Section 3 of the paper describes the specific settings of the used global optimization methods and discusses differences between the single-objective approach and the multi-objective approach to the global optimization. We used the following global optimization methods: Genetic Algorithms (GA), Differential Evolution (DE), Particle Swarm Optimization (PSO) and Niched-Pareto Genetic Algorithms (NPGA). The methods have been implemented in MATLAB.

Section 4 of the paper describes the principle of replacing the composite material by a homogeneous substitute. The proposed approach is based on the exploitation of COMSOL Multiphysics for solving the inverse task using global optimization methods and the 2D model of the analyzed structure (a compact

dielectric layer). The frequency-dependent relative permittivity and loss factor of the substituting layer are the output of the optimization. These frequency dependent parameters are imported into CST Microwave Studio. In CST, the reflection and the transmission of the equivalent layer are calculated and compared with the original composite material. Section 5 concludes the paper.

2. Modeling of composite materials

Numerical models of the investigated composite material inside a rectangular waveguide were developed in CST Microwave Studio. The waveguide was excited by the transversally electric wave TE_{10} which can model a linearly polarized vertical wave illuminating the layer. The waveguide was terminated by an absorbing layer in order to suppress the reflected wave. Frequency response of the reflection coefficient S_{11} and the transmission coefficient S_{21} are computed for the modeled composite material.

The value of the reflection coefficient and the transmission coefficient serve as a reference (desired) value for the optimization methods. The structure is discretized by the hexahedral mesh cells (30 cells per wavelength) for the time domain solver and the tetrahedral mesh cells (4 cells per wavelength) for the frequency domain solver. The analysis is computed in the frequency range from 7 GHz to 40 GHz.
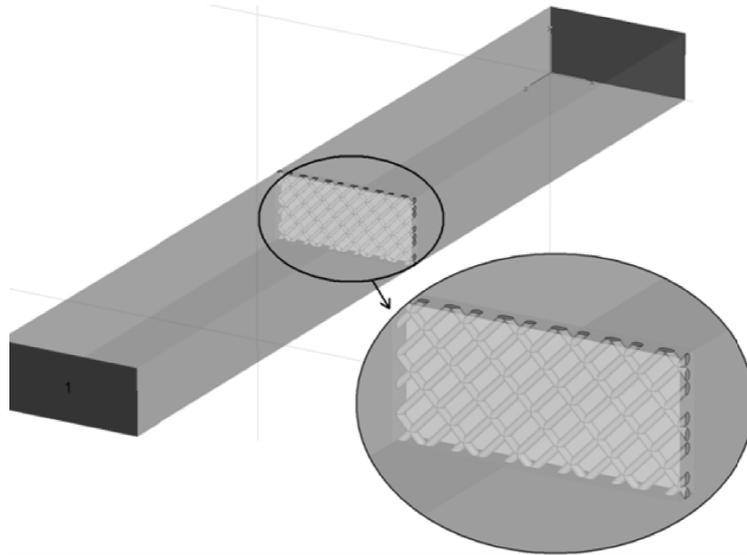

Figure 1: Simple three dimensional model of composite layer.
Simulated in CST Microwave Studio.

2.1. Three dimensional composite layer without carbon fiber reinforcement

The simple three-dimensional model of the composite material is created by a lossy metallic grid (copper grid). The grid is made from the wire of the diameter 0.3 mm. Cells of the grid are of the dimensions 3.0 mm × 1.5 mm. The grid is rotated for 45 degrees. The metallic grid is covered by the lossy dielectrics Taconic RF-35 from both sides. The relative permittivity of the dielectrics is 3.5, and tan δ = 0.0018. The thickness of the dielectric layer is 1mm on both sides (see Figure 1).

The waveguide constrains the lowest frequency of the simulation. For the waveguide R100, the critical frequency is 6.55 GHz. Figure 2 shows that the investigated composite material totally reflects the incident electromagnetic energy since 6.5 GHz. Since about 20 GHz, the composite layer starts to transmit the energy due to the wavelength comparable to the size of cells of the metallic grid.

Using the time domain solver, the total time of the simulation was about 6 hours. Unfortunately, Figures 2 and 3 indicate inaccuracies of the simulation (scattering parameters overshoot over zero axis and oscillate). The accuracy of the simulation can be improved by narrowing the frequency range of the analysis, by reducing of the maximal frequency of the frequency range, by using locally refined meshes or by combining the approaches [6].
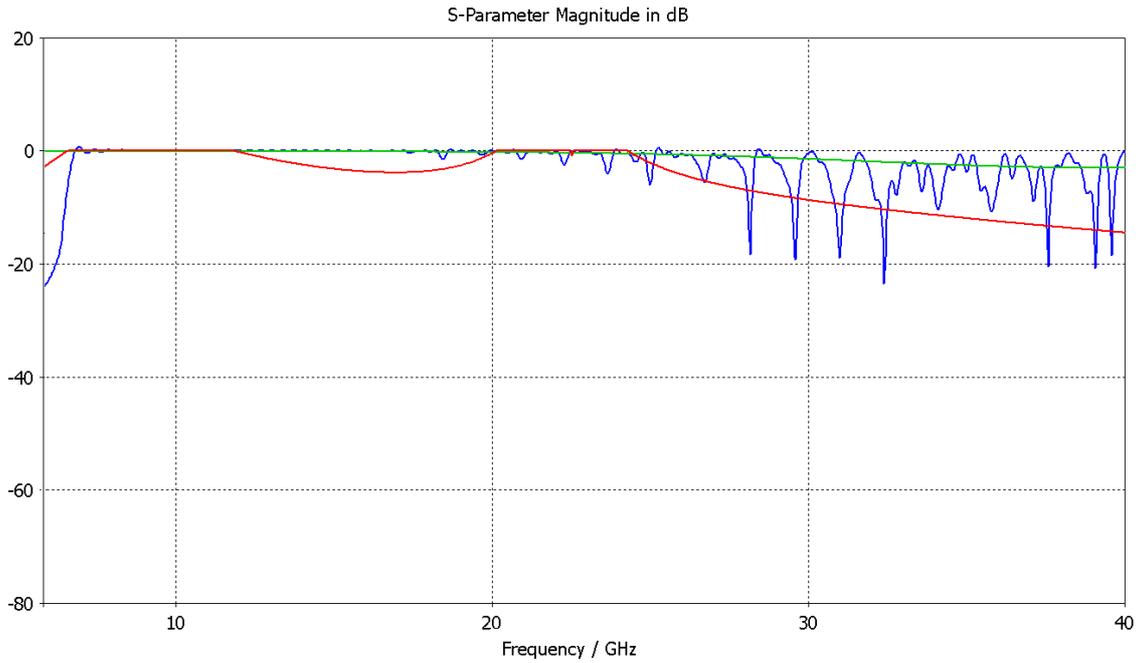
Figure 2: Reflection coefficient of the simple model of the composite material. Red line: frequency solver, green line: frequency domain with periodic boundary conditions, blue line: time domain solver. Simulated in CST Microwave Studio.
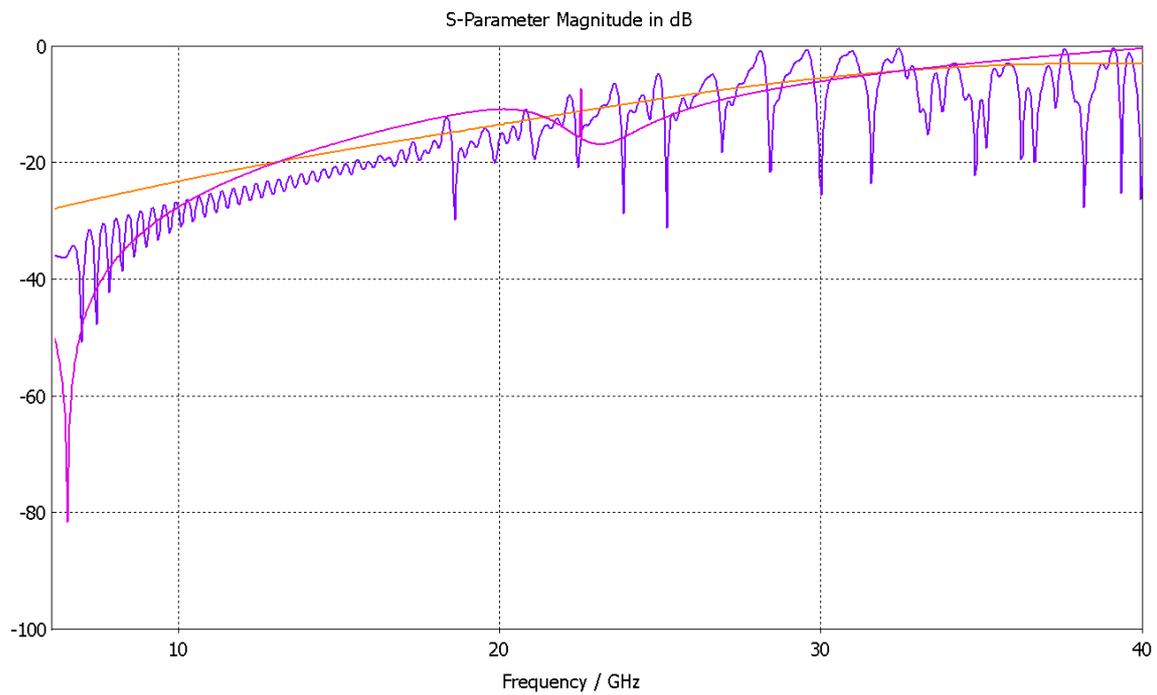

Figure 3: Transmission coefficient of simple model of composite material. Violet line: frequency solver, orange line: frequency domain with periodic boundary conditions, blue line: time domain solver. Simulated in CST Microwave Studio.

The use of the locally refined mesh (sub-griding) increases the total number of mesh cells in the model which can potentially increase numerical errors. When modeling composite materials, sub-griding was proven to be inadequate [1].

Accuracy of the numerical analysis can be partially improved by using frequency domain solver. Unfortunately, time demands of the frequency-domain model were much higher (about 16 hours). In the frequency domain, the analysis of the structure is performed at each frequency separately which is a problem in case of a wide frequency range. Finally, accuracy of the solution can be improved by applying periodic boundary conditions. The 3D model of the composite layer is created in free space by one unit cell, which contains one cell of the metallic grid (see Figure 4). Periodic boundary conditions are used at the side walls of the elementary cell. Thanks to the periodic boundary conditions, the composite layer is of an infinite size.
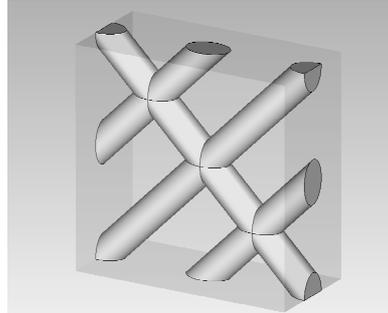

Figure 4: Elementary cell of the simple three dimensional model of the composite material. Simulated in CST Microwave Studio.

Lines corresponding to periodic boundary conditions in Figures 2 and 3 show that problems with overshooting zero axis were eliminated. The simulation time is about 15 seconds. Computational demands of this model are reasonable. Unfortunately, periodic boundary conditions can be applied in frequency domain only, and therefore, independent simulations have to be performed for each harmonics of interest.

2.2. Three dimensional composite with carbon fiber reinforcement

The second composite material to be modeled is of the same dimensions as the first material, but carbon fiber reinforcement was added into the dielectric walls. The material of the dielectric layers was changed from the Taconic RF-35 to the epoxy resin ($\varepsilon_r = 4$ and $\sigma = 0$ S/m). In between the reinforced dielectric walls, the metallic grid is embedded again.

Figure 5 shows the structure of the carbon fiber reinforcement of the composite material simulated in CST Microwave Studio. This structure can represent a real composite material. The carbon fiber layer is anisotropic. In this model, the conductivity of the carbon fiber is set to $\sigma = 10^4$ S/m in fiber axis (in y-axis here) and $\sigma = 50$ S/m in the direction across the fiber. The diameter of the fiber is 35 µm and the permittivity is $\varepsilon_r = 2$. Adding the carbon fiber, the shielding efficiency was increased (see Figure 6).
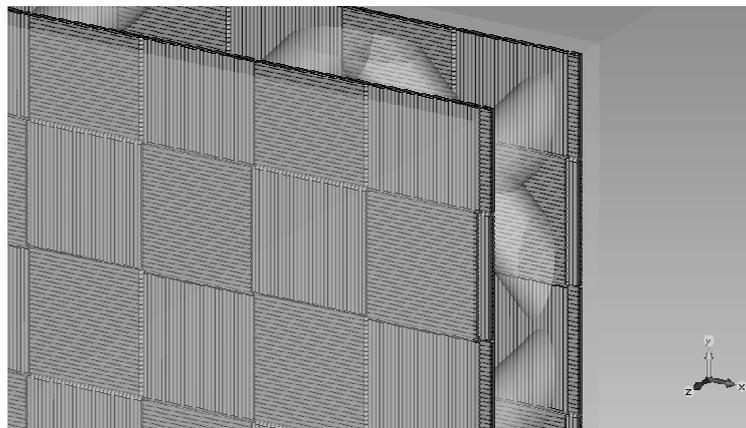

Figure 5: Detailed three dimensional model of composite material with carbon fiber reinforcement.

Simulated in CST Microwave Studio.

The reinforced model of the composite material is very accurate. The simulation time is about 7 hours (comparable to the previous model), but memory demands are huge. For simulating the reinforced model, we used the computational server with two processors Opteron 2384, 2.7 GHz with 4 cores and 32 GB RAM plus two processors Opteron 2352, 2.1 GHz with 4 cores and 16 GB RAM.
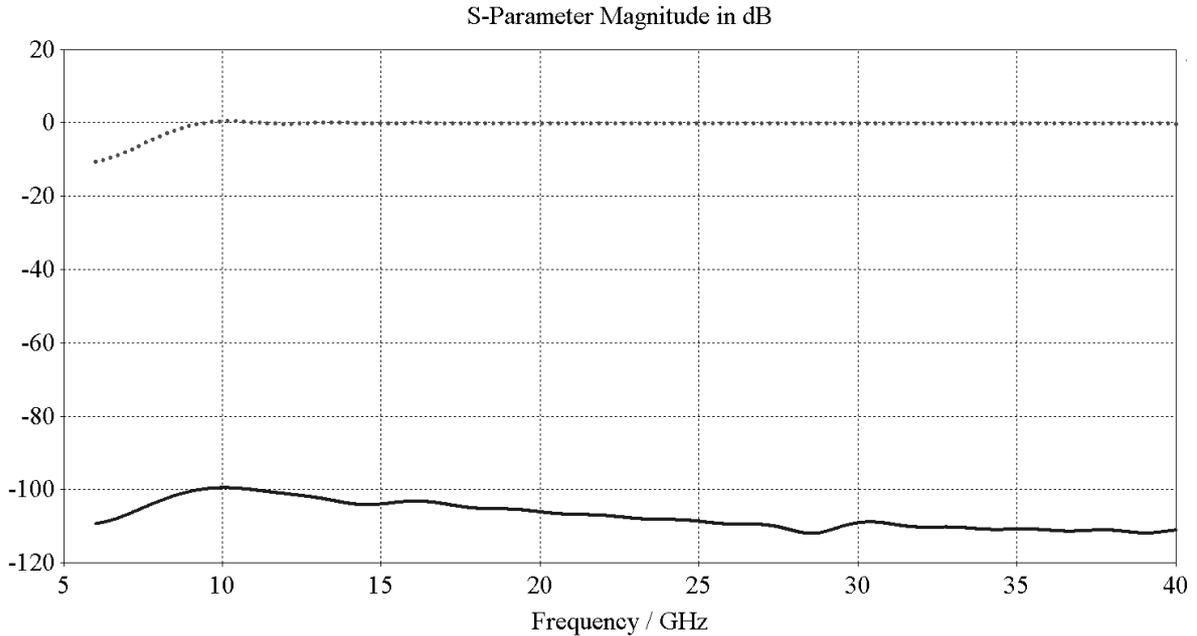

Figure 6: Transmission coefficients of 3D model of composite material with carbon fiber reinforcement. Dotted line is reflection coefficient, solid line is transmission coefficient. Simulated in CST Microwave Studio.

3.   Optimization methods

Four global optimization methods were used for the synthesis of composite materials analyzed in the previous section:

Differential Evolution (DE) is a new type of the stochastic, real-coded global optimization method based on the evolution strategy. Ken Price and Rainer Strom are authors of DE. For the implementation, the basic variant of DE was selected. The values of the control parameters were chosen considering recommendations published in [5]. The population consisted of 50 individuals; the weighting factor was 0.8, the crossover constant 0.5.

Genetic Algorithms (GA) are the stochastic global optimization methods based on the Darwinian Theory of the evolution of species. The implementation is based on the basic variant too. The values of the control parameters were chosen according to recommendations published in [3]. The population consisted of 50 individuals. Accuracy of coding was 0.001. Individuals for the next population were selected by the tournament. Probability of the multi-point crossover was set to 70 % and probability of the multi-point mutation was assumed to be 6 %. The elitist strategy was applied [3].

Particle Swarm Optimization (PSO) is the stochastic global optimization method too. The method is based on the principle of the behavior and intelligence of the swarm [4]. Dealing with the control parameters, the swarm consists of 50 agents, absorbing walls were implemented.

Niched-Pareto Genetic Algorithms (NPGA), by Horn et al., is a multi-objective GA based on the non-domination concept. NPGA uses the binary tournament selection. The population consisted of 50 individuals. The mutation probability is 6%, the crossover probability is 70%, accuracy of coding is 0.001.

4. Principles of replacing composite materials

The synthesis is based on the full-wave simulation of the homogeneous equivalent in COMSOL Multiphysics and the variation of state variables of the equivalent by a global algorithm programmed in MATLAB. State variables are changed to the same frequency response of scattering parameters of the homogeneous equivalent and the original composite layer. The homogeneous equivalent is 2 mm thick and is placed into the waveguide R100 terminated by the perfectly matched layer.

The schematic of the global optimization implemented in MATLAB is depicted in Figure 7. Such a frequency response of the complex permittivity of the homogeneous material is searched in which the value of the transmission coefficient and the reflection coefficient of the equivalent model meet the actor during the reference reflection and the reference transmission of the 3D model of the multilayer composite material. These computed reference values can be replaced by the values obtained by measurement, if it is available.

In order to evaluate the fitness function, the COMSOL model was simulated to compute values of the reflection coefficient and the transmission one for the randomly generated complex permittivity. The dielectric constant could vary within the interval $\varepsilon_r = [1; 1000]$ and the loss tangent can change within the interval $\tan \delta = [0; 1000]$. For the entire frequency range, a single evaluation of the relative permittivity and a single evaluation of the loss tangent are required (see Table 1). The fitness function is of the form:

$$F_1(x) = \sum_{n=1}^{N} \left[S_{11,ref}(f_n) - S_{11,opt}(x, f_n) \right]^2 \tag{1}$$

$$F_2(x) = \sum_{n=1}^{N} \left[S_{21,ref}(f_n) - S_{21,opt}(x, f_n) \right]^2 \tag{2}$$

Here, $S_{11,ref}(f_n)$ is the computed value of the reflection coefficient of the realistic model of the composite material at the frequency f_n. Then, $s_{11,opt}(\mathbf{x}, f_n)$ is value of the reflection coefficient of the equivalent homogeneous material computed in COMSOL Multiphysics for the frequency f_n and for the vector of state variables $\mathbf{x} = [\varepsilon_r, \tan \delta]^T$.

The composite structure is analyzed for N frequencies. Similarly, $S_{21,ref}$ is the computed value of the transmission coefficient of the realistic model of the composite material at the frequency f_n and $s_{21,opt}(\mathbf{x}, f_n)$ is value of the transmission coefficient of the equivalent homogeneous material computed in Comsol Multiphysics for the frequency f_n and for the state vector $\mathbf{x} = [\varepsilon_r, \tan \delta]^T$.

For the single-objective solution, the fitness functions (1) and (2) are weighted by weighting coefficients w_1 and w_2 and summed:

$$F(x) = w_1 F_1(x) + w_2 F_2(x) \tag{3}$$

Figure 9 compares frequency responses of the reflection coefficient of three homogeneous substitutes synthesized by single-objective global optimization methods, one substitute synthesized by a multi-objective global optimization method and frequency responses for the original composite material. Substitutes synthesized by genetic algorithms in the single-objective form and the multi-objective form and the differential evolution exhibit a good agreement with the original composite material. For particle swarm optimization, such a good agreement was not achieved.

Table 1: Comparison of optimization methods

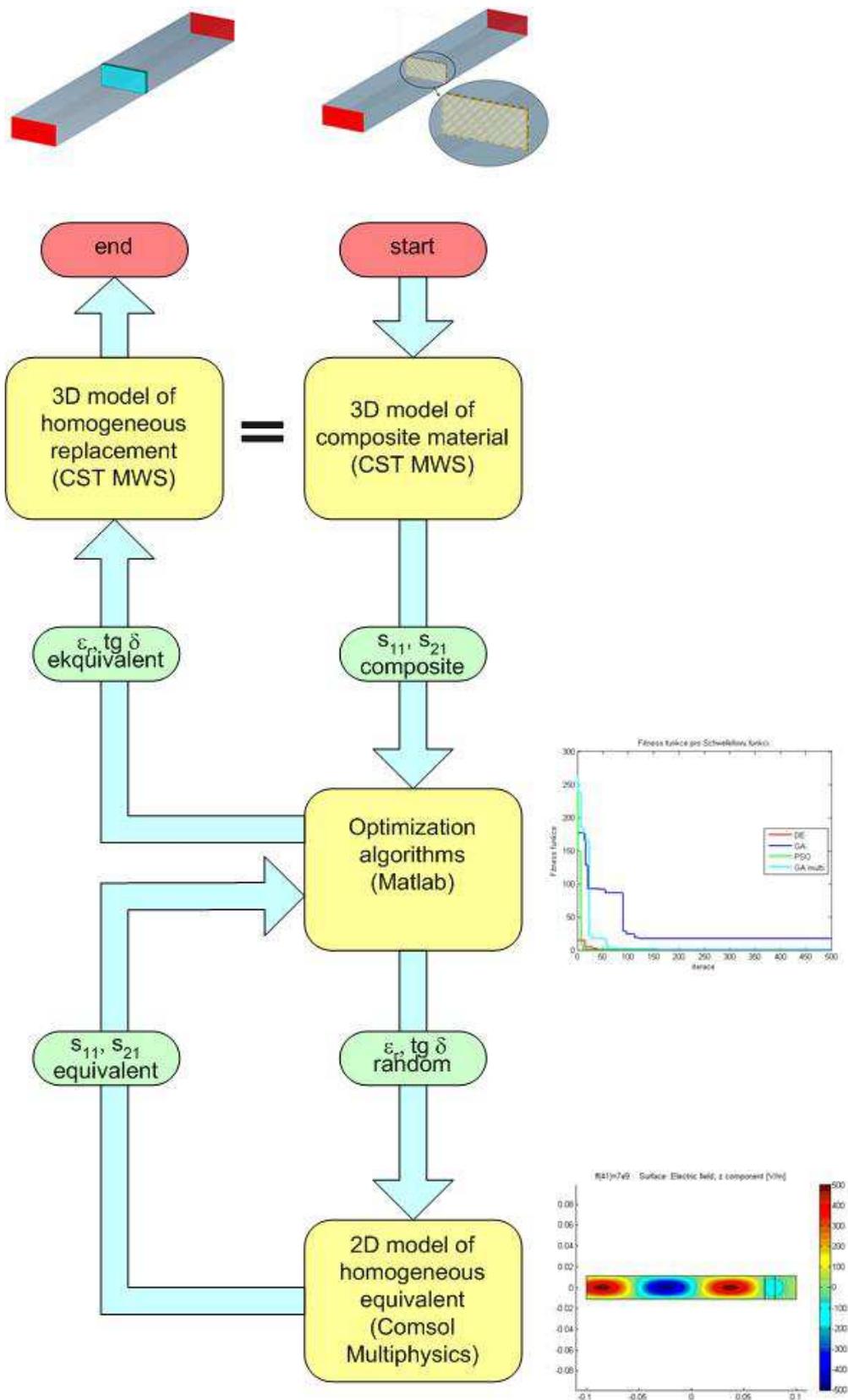| Optimization method	ε_r [-]	$\tan \delta$ [-]	time [s]
GA	36.64	549.34	44 940
DE	40.50	200.10	35 456
PSO	1000.00	0.62	29 073
NPGA	70.62	521.52	20 580

Figure 7: Flow chart of the synthesis of the homogeneous equivalent of the composite material.

For the multi-objective approach, the time of the simulation was half compared to the single-objective approach. In Table 1, results of the optimization process with the necessary CPU time are summarized. The paper describes the original approach to the substitution of the composite materials with

metal lattice by homogeneous equivalents. The synthesis of equivalents is based on the exploitation of the global optimization methods.
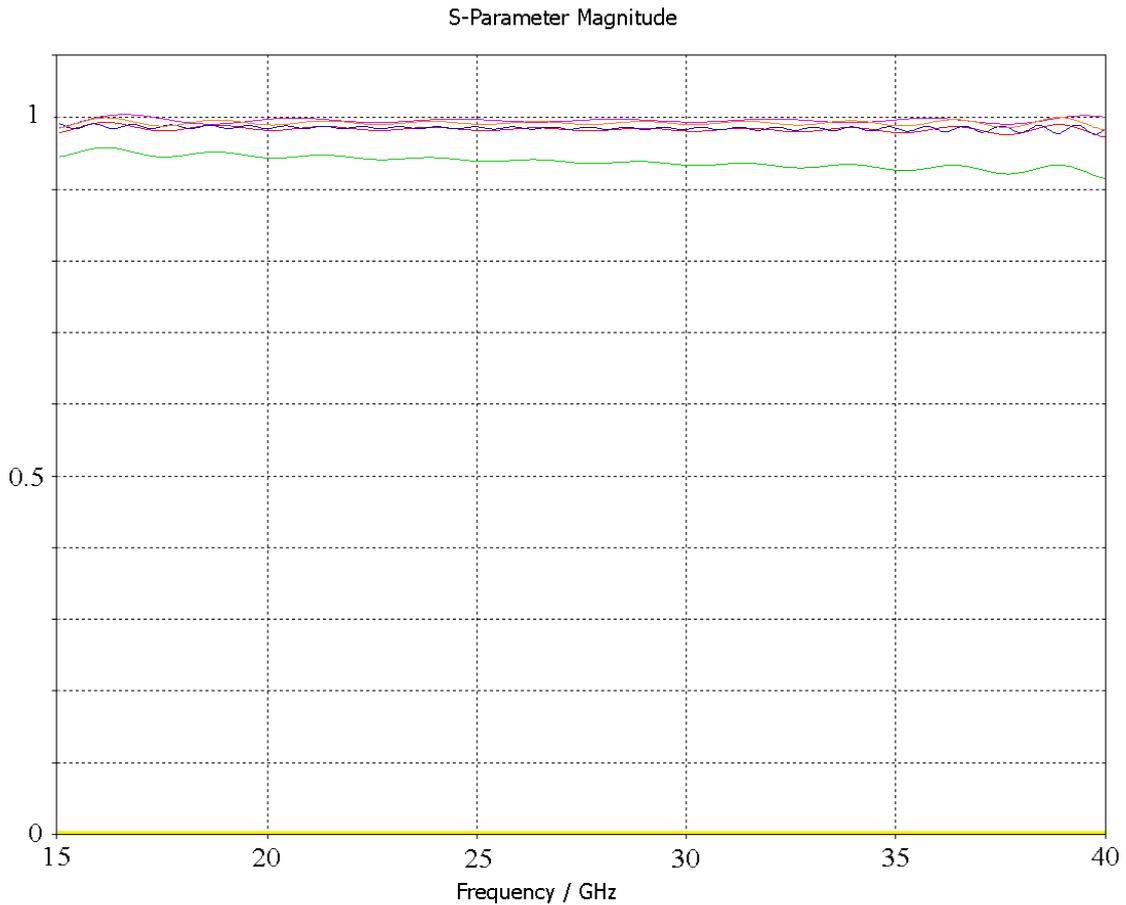

Figure 8: Reflection coefficients of replacements achieved by different optimization methods in comparison with originally reflection coefficients of composite material (blue line). (GA - orange, NPGA - violet, DE - red, PSO - green). Transmission coefficients are yellow. Simulated in CST Microwave Studio.

3. Conclusion

For the comparison, the single-objective optimization (reflection coefficient considered) and the multi-objective optimization (both the reflection coefficient and the transmission one) were tested. In order to compute the minima of objective functions, genetic algorithms, particle swarm optimization, differential evolution and Niched-Pareto genetic algorithm were applied. The synthesis was implemented considering numerical models of two different composite structures: the metallic lattice was covered by the homogeneous dielectrics in the first case, and by the dielectrics reinforced by carbon fibers in the second case.

First, the single-objective approach exhibits a very good functionality for all three evolutionary methods. Particle swarm optimization shows worse results than other methods, but the difference is smaller than 5%. Substitutes synthesized by GA and DE exhibit error smaller than 2%.

Second, the substitute synthesized by the multi-objective approach shows a very good agreement too. The error of the substitute synthesized by NPGA was smaller than 2%. The most significant advantage of the multi-objective approach is the speed of the simulation. Time needed to one simulation for NPGA was one half compared to single-objective approaches.

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