Genetic Algorithm For Geometry Optimization Of Optical Antennas

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Abstract: A genetic algorithm was programmed in Matlab and a link was performed with COMSOL Multiphysics to obtain the better geometry for an optical antenna (nanoantenna). The proposed computational model demonstrated that nanoantenna geometries does not feature a conventional macroscopical antenna geometry, such as those utilized for the radiofrequency range. In addition to the final geometry obtained, many other useful data and graphical information were obtained with COMSOL Multiphysics software.

Keywords: Genetic Algorithm, Geometry Optimization, Optical Antennas.

1. Introduction

Evolutionary algorithm research attempts to imitate nature, where all living organisms exist in a given environment. These organisms possess specific genetic material, which contains information about each organism and allows them to transfer some of their characteristics to new generations via reproduction. The other organism involved in reproduction also transfers some of its characteristics. These characteristics are encoded in genes stored in chromosomes, which together constitute the genetic material known as a genotype. Genes are modified during the characteristic transfer process as a consequence of the crossover between maternal and paternal chromosomes. Mutation may also occur, altering the information contained within the genes of a given chromosome. Although the newly created individual possesses the information of its parents, the combination of two different organisms makes the individual unique. This organism begins life in an environment that is not significantly different from that of its parents. The new organism develops in a manner that allows it to survive and transfer its genome, permitting the species to persist in a given environment. An individual that cannot adapt to its environment will struggle to survive and transfer its genes to new generations.

These ideas can be modified and used for optimization problem solutions. An analog of this process can be implemented based on numerical calculations, assuming that the environment is defined based on known values and characteristics. The population of individuals constitutes potential solutions to the given problem, such that the solution already exists within the environment [1-6].

An adequate mathematical function must be chosen to define the fitness of any given individual representing how well adapted they are to their environment. Individuals will exchange genetic materials and mutations will occur during the genetic crossover process. Thus, an optimal solution will be created that best suits a given environment.

In this work, a genetic algorithm (GA) is applied to obtain the geometry that optimally concentrates the electromagnetic field of a dipole–type nanoantenna at a resonance frequency of 500 THz, which can be varied based on the nanostructure dimensions. The nanoantenna radiation pattern was obtained via computational simulations and compared to a classical geometry dipole, demonstrating the achieved optimization.

2. Method

The electro-optical nanostructure characterization calculations are conducted using the COMSOL software package. The nanoantennas are analyzed using Matlab, which evaluates the goodness of fit between the algorithm results and optimal conditions. Iterative changes or adjustments are then made to optimize the solution, and the new proposed nanostructure is analyzed using COMSOL until convergent results are obtained.

Both the user interface and the genetic algorithm implementation were designed in Matlab (part of the Global Optimization Toolbox). The genetic algorithm performs the nanostructure analysis required to suggest a geometry that approaches the optimal design conditions, assuming a (two–dimensional) flat nanostructure. The solution space is constrained to dimensions near the optical wavelength for an antenna irradiated by a normal–incident electromagnetic wave. The main parameters required by the genetic algorithm, such as the dimensions of the simulation space (maximum size of the antenna), number of chromosomes (number of individuals to be analyzed), chromosome resolutions (quality), overlap between generations (mortality index), mutation rate (as a percentage) and mating rules, must be input by the user.

COMSOL's LiveLink™ for MATLAB® (henceforth referred to as LiveLink) [7] is a module that links COMSOL and Matlab in two modes. One allows calling MATLAB from COMSOL, whereas the other does the opposite. Each of these configurations has a specific applicability range that can be adapted to particular cases. As previously mentioned, MATLAB performs the geometry generation calculations and COMSOL runs the simulation and produces antenna response data for a given frequency. These data are then transferred to MATLAB and used to perform the necessary genetic algorithm adjustments. This process is repeated until a convergence value is reached. Thus, MATLAB controls the data flow within LiveLink.

Figure 1 illustrates the MATLAB and COMSOL processes, which together comprise the genetic algorithm.

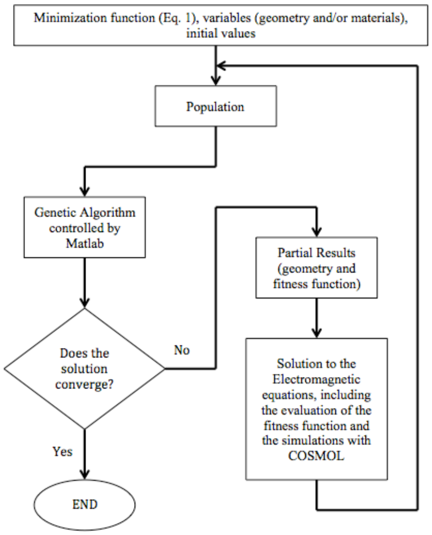

Figure 1. Flow diagram of the application process, noting the links between the COMSOL and MATLAB software packages.

The Bézier curve control points, which are modeled as chromosomes, are used to obtain the optimized geometry of the dipole–type nanoantenna. A total of 10 lines are set, including 4 with two Bézier control points, 4 with only one and 2 straight lines with no control points. The lines with no control points represent the section where the electromagnetic field is applied to the nanoantenna. The algorithm execution stops if the average loss in the electric field is zero or if the iterative limit is reached, which is based on the number of generations [8].

The fitness function [9] is shown in Equation (1). The optimized fitness function calculates the minimum loss (optimization function) of the electromagnetic field at a frequency of 500 THz and is a parameter that COMSOL submits to Matlab, which then evaluates it using the genetic algorithm function.

$$F_{Fitness} = \min\left(\frac{1}{2}\operatorname{Re}\left(J_{tot} \bullet E_{tot}\right)\right) \qquad (1)$$

Where J_{tot} is the total electric current density over the whole geometry shown in Equation 2.

$$J_{tot} = \sigma E \qquad (2)$$

σ is the electrical conductivity and E_{tot} is the electric field over the whole geometry shown in Equation (3).

$$E_{tot} = \left(\mu_0 \int \left(J + \varepsilon_0 \frac{\partial E}{\partial t}\right) \partial a\right) \qquad (3)$$

The refractive index in the optical regime of operation in the nanostructured materials (metamaterials) becomes a function of frequency [10].

A geometric model with 12 Bézier curve control points, plus 11 fixed points which represents the geometry limits (noting the first point is also the last one to have a closed geometry) is found during the first iteration, based on steady–state initial conditions, 100 chromosomes, a 50% intergeneration overlap and a 1% mutation rate. In addition, a single crossover point was used, which can occur between any pair of segments in the chromosome with equal probability. Figure 2 shows the superposition of the geometry as it evolves. Figure 3 plots the electric field power loss as it approaches zero. Values after the fourth population generation, which rapidly decrease from 1.3e^-7 nW/m2 to 8e^-15 nW/m2, cannot be detected due to scale limitations.

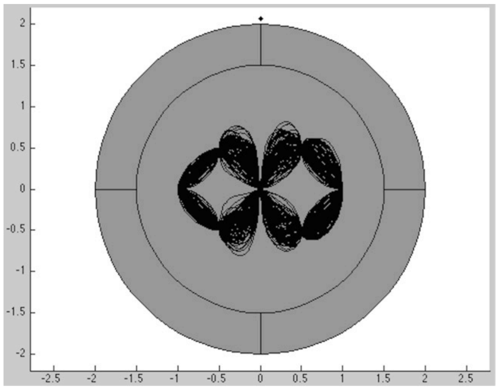

Figure 2. Lines demonstrating the geometry modification process due to mutations when applying the genetic algorithm.

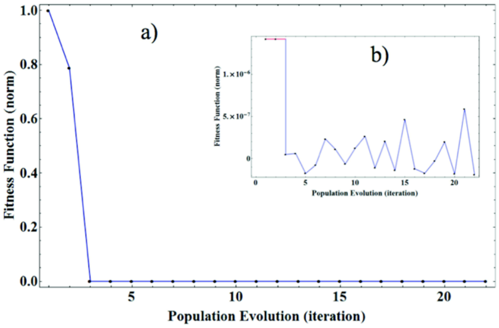

Figure 3. (a) Plot showing the trend toward zero of the electromagnetic field loss after each new population generation. (b) Data trends for a zoomed portion of the main plot.

The geometry obtained at the end of the genetic algorithm execution is shown in Figure 4(a). Figure 4(b) illustrates the data point at which the maximum optical energy absorption-emission is obtained in the terahertz range.

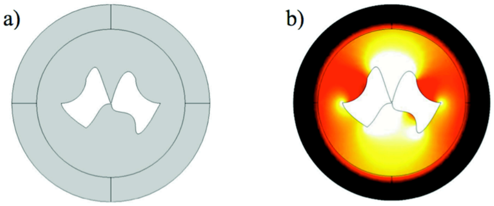

Figure 4. (a) Geometry obtained after the genetic algorithm optimization function application. (b) Finite–element method simulation of the nanostructure electromagnetic radiation pattern.

According to the results obtained by [8, 11] and the resulting geometry in Figure 4(b), the geometries obtained by the genetic algorithms represent improvements over the classical or conventional radiofrequency antenna geometries. These geometries were obtained at a reduced computer costs and over a shorter processing time compared with traditional analytical processes or trying a wide classical RF geometries one by one.

3. Results

Many studies use analogies between nanostructure geometries and conventional radiofrequency macroscopic antenna geometries based on the assumption that their behaviors can be extrapolated to optical frequencies. However, the proposed computational model demonstrated that nanoantenna geometries require further study. The nanoantenna shape analyzed in this study does not feature a conventional geometry, such as those utilized for the radiofrequency range. Figure 5 shows a comparison between the classical dipole (a), the dipole generated by the algorithm after the first iteration (b) and the final geometry, which is based on the lowest electromagnetic field loss at the dipole center (c).

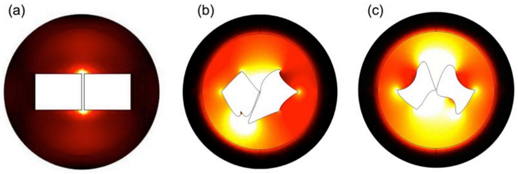

Figure 5. Electromagnetic field concentration comparison according to the geometry. Panel (a) shows a classical dipole; (b) shows the first iteration of the genetic algorithm; and (c) shows the final geometry, which is based on the maximum electromagnetic field concentration at the center of the nanostructure.

Figure 6 compares the electromagnetic field intensities of the classical dipole and the geometry generated by the genetic algorithm. The results obtained via the genetic algorithm represent an optimal concentration, and both geometries encompass the same effective area. Compared to results obtained by [6], Fig. 6 shows an increase in the electromagnetic signal and the effective bandwidth, with the difference that the area remained the same; as an added advantage the GA design presented in this work is simpler than the one shown in figure 2a, therefore the fabrication process would also be simpler. The peaks of both plots represent the dipole resonance frequencies. From this figure 8, with an increase from 0.4 for non GA dipole to 0.93167 for GA dipole at resonant frequency in the antenna response (a difference about 0.536), we found that the geometries obtained by the genetic algorithm provided a 33% better result than the classic dipole geometry and being the bandwidth for non GA dipole about 39 THz (from 481 to 520 THz) and for the GA dipole about 48.7 THz (from 475.6 to 524.4 THz) it was increasing the bandwidth by 25%.

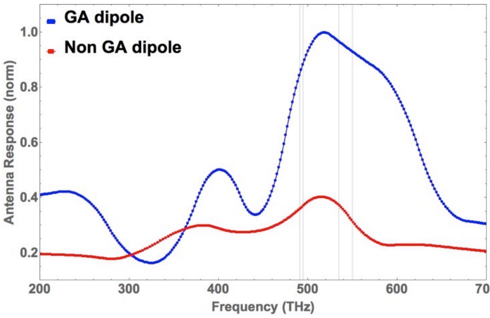

Figure 6. Electromagnetic field concentration comparison between the classical dipole geometry and that generated by the genetic algorithm.

4. Conclusions

The classical or conventional dipole–type antenna geometries (in the radiofrequency regime) do not encompass the maximum electromagnetic field concentration (in the optical regime). This is due to the intrinsic differences between electron and photon behaviors. In addition, many macroscopic antenna assumptions and simplifications are not applicable for nanoscale optical frequency regimes because the electromagnetic wavelength is comparable to or even shorter than the antenna dimensions. Thus, a new refractive index function [Equation (3)] is introduced that defines the electromagnetic field behavior at such frequencies.

The proposed alternative genetic algorithm was applied to improve dipole geometry while accounting for the nanoscopic scale properties of these structures. Our results demonstrate that the final nanoantenna shape is significantly different than the classical case in the context of providing the optimal electromagnetic field concentration.

The results of this study will be used in future nanostructure fabrication and characterization studies using two materials with different Seebeck coefficients (one positive and one negative). The materials will generate maximum heating in the region of interest, producing a direct electric current [11] that can be stored in batteries for subsequent use. This will contribute to the creation of renewable energy devices.

5. Acknowledgments

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