AIR FORCE TECHNOLOGY, OHIO, USA

VIRTUALLY OPTIMIZING METASURFACE TOPOLOGY WITH A GENETIC ALGORITHM

An optimization algorithm inspired by natural selection is used to determine the best design configuration for the metasurface of an optical antenna.

by SARAH FIELDS

Often in engineering, we look to the natural world to find inspiration for new ways to approach our design problems. Whether we are taking inspiration from fluid flow around wings to inform a system for cooling devices, studying slug slime to invent better medical adhesives, or designing the nose of a bullet train to resemble the beak of a bird, nature holds the key to even the most elusive design solutions.

At its essence, optimization involves minimizing a loss function by systematically selecting input values from within a set of parameters governing the system under study. It is unsurprising that even in the mathematics-dense world of the optimization of electromagnetic metasurfaces, nature has something to say.

Bryan Adomanis of the Air Force Institute of Technology (AFIT) was interested in creating a pixelated grid antenna that would function as a 3D Huygens source; that is, a 3D, metal, nanoparticle-based optical antenna capable of propagating only in a specified direction while maintaining the desired amplitude and phase delay. In the development of such an antenna, the geometry of the metasurface is the primary driver of the electromagnetic response. As such, by optimizing the geometry of a "blank slate" — this grid of 3D pixels (voxels) — it is possible to find the best design, which would possess a high forward scattering and minimal backscattering.

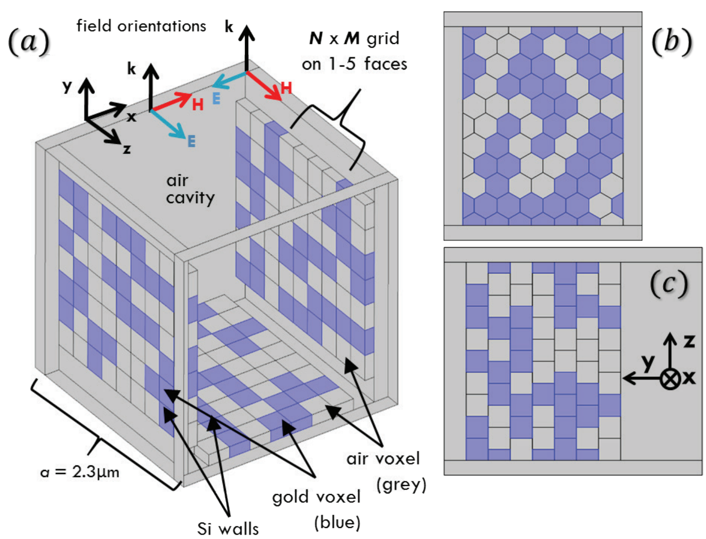

FIGURE 1. Sample voxel and cavity geometries, which can be used for the genetic algorithm.

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The challenge in designing this antenna is the large design space: A voxel can exist as either gold or air, and there are so many possible geometrical configurations for the antenna that it was unclear how to identify the best design. For even the lowest-resolution design, 2^{40} (over 1 trillion) unique models could be generated (Figure 1). Gold and air voxels (cubes) are represented in blue and gray, respectively. Using a genetic algorithm (GA) routine, the COMSOL® software finds the best solution, or arrangement of voxels, in about 2000–4000 models. Also, there was no identifiable correlation among patterns of geometry and performance (transmittance and phase), and as such, no function to minimize. Therefore, a COMSOL model was implemented to efficiently solve these highly nonanalytical models.

Essentially, this pixelated grid antenna is a scattering unit cell, where the walls can be populated with dielectric and metal as needed. In selecting the best geometry for metal, nanoparticle-based antenna out of nearly one trillion possible configurations, a routine inspired by biological reproduction and natural selection was the answer.

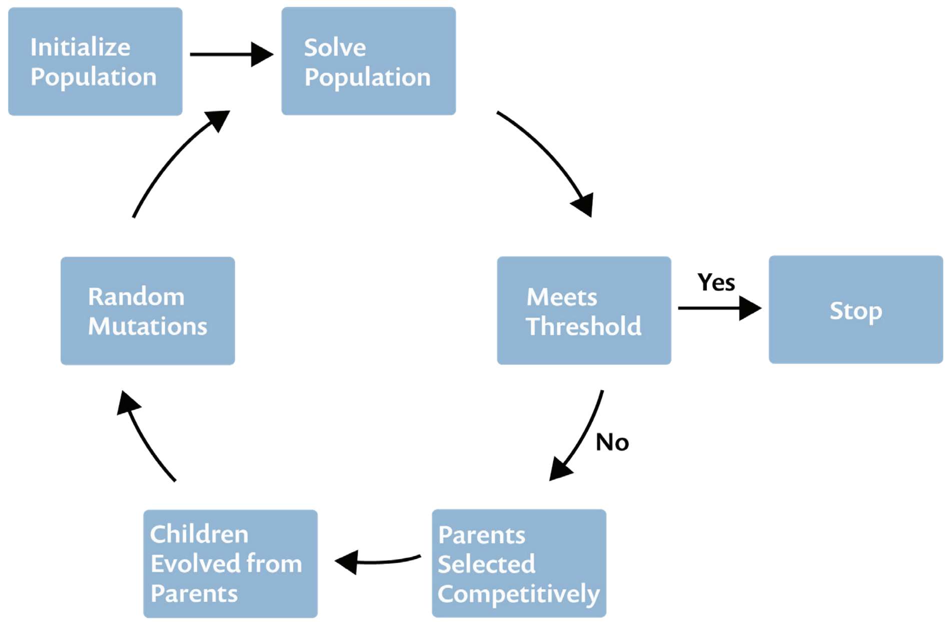

FIGURE 2. Genetic algorithm solution steps.

⇨ GENETIC ALGORITHM ROUTINE

"Due to the nonlinear nature of the problem and the large parameter space, other optimization methods were insufficient — They were either too computationally intensive, or could not be trusted to find the global minimum. In this context, genetic algorithms get the job done," Adomanis explains.

In a genetic algorithm (Figure 2), a design parameter, what can be thought of as the gene, exists within a group of design parameters, or the chromosome. Each group of design parameters represents a unique design, or what can be thought of as the individual, with all unique designs forming a total population. The fitness of each individual in the population is scored, which informs the likelihood of the individual becoming a parent to an individual in the next generation.

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In his implementation of a genetic algorithm, Adomanis initializes the population with individuals representing different voxel arrangements or antenna designs. He used MATLAB® to create the population, generated its binary representation or "mask," which enters the GA routine for each set of unique parameters; and feed it to the COMSOL model.

He then used multiphysics simulation to evaluate the fitness of each individual, or unique design, within the population, or set of unique designs. An individual is fit when a fitness threshold representing the desired scattering is met. After the fitness of the individuals, or unique models, in the population, or set of unique models, is computed, individuals who do not meet the threshold are removed from the routine. The next generation of models, or "children," is then populated

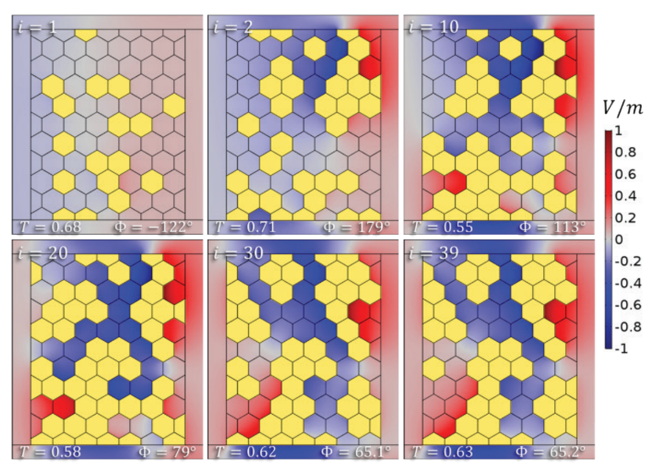

FIGURE 3. Simulation results showing the magnetic field (scaled in terms of V/m) resulting from the optical antenna in intermediate steps of optimization. As the topology forms, so do strong magnetic modes.

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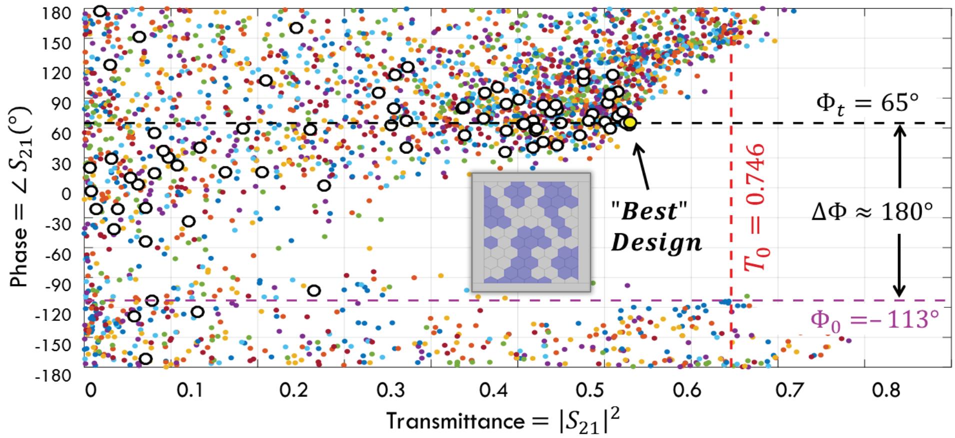

FIGURE 4. Plot of the transmittance, or the scattering parameter $|S_{21}|^2$, against the phase. Generations are distinguished with color.

from the unique models that met the fitness threshold and formed by "crossovers," where substrings of two binary representations are concatenated in a child, and "mutations," where a bit within the binary string is switched. Adomanis integrated MATLAB® with COMSOL Multiphysics® through the add-on product LiveLink™ *for* MATLAB®.

⇨ CONVERGING ON THE BEST DESIGN

To identify the best topology for the metasurface of the optical antenna, Adomanis needed to optimize the phase delay of a total field transmittance in a given direction while maintaining the amplitude. The electromagnetics modeling capabilities were used for this purpose, allowing him to set his GA routine to go through many sets of voxel configurations and compute the resulting electromagnetic radiation without needing to dive too far into the complexity of the physics. Figure 3 shows the magnetic field resulting from the antenna in various stages of optimization.

As the individuals of a generation are evaluated, parents are selected, the child generation populated, and the individuals of the child generation evaluated, the routine continues, and the population shifts toward the best design (Figure 4). Using the genetic algorithm routine, the COMSOL® software generated the best design in a few thousand models, compared to a parameter space of approximately one trillion possible designs.

With this routine, Adomanis could maximize transmittance at various phase values. Within 30 generations, the unique designs of the population began to meet his performance criteria (Figure 5).

Visualizing the performance in a multiobjective solution space allowed Adomanis to select a design based on the criteria that is most important for a specific application. In one design, he might prioritize the highest transmittance, while in another design, he might want to prioritize accuracy in the phase delay.

Adomanis was able to successfully generate the colocalized electric and magnetic dipoles from a pixelated grid that produces a total field only in the forward direction, with little backward scattering. By combining a GA routine an with electromagnetics simulation, he could generate an optical antenna that functions across the entire 2π phase space. An example is shown in Figure 5. "This work represents the first time that the topology of a pixelated grid antenna has been optimized with a genetic algorithm in 3D," Adomanis comments.

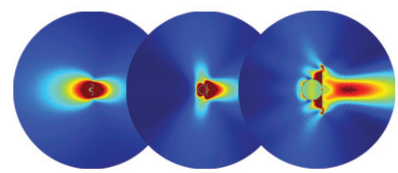

FIGURE 5. Genetic algorithm optimization of the geometry of an optical scatterer called the omega particle. The aim is to design a scatterer with, from left to right, maximum forward scattering and minimal backward scattering.

⇨ LEADING DESIGN BECOMES REALITY

After Adomanis determines the best design from the GA routine, his next challenge is creating a real-world prototype based on the optimized design. However, because the smallest features of the optical antennas are about 100 nanometers, a specialized, newly developed fabrication process was necessary to implement the concept.

Bryan Adomanis, Air Force Institute of Technology

To accomplish this, Adomanis is collaborating with a research team at Sandia National Laboratory that has the capability to print the antenna. He simply provides the group with the optimized pixelated grid that resulted in optimal scattering in his simulation. "We have high confidence that our design is working properly, since we have composed a properly functioning, full-scale simulated lens using the results of each individual element in that model." Adomanis concludes, "Being able to use COMSOL for computing the performance of the antenna was powerful, as we could focus on implementing the GA routine to optimize the design instead of the details of the electromagnetics computation of an arbitrary array of voxels." ❖