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# Inverse Design of Three-Dimensional Nanoantennas for Metasurface Applications

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***Abstract*—Recent advances in manufacturing techniques have been made to match the demand for high performance optical devices. To this end, tremendous research activity has been focused on optical metasurfaces as they offer a unique potential to achieve disruptive designs when paired with innovative fabrication techniques and inverse design tools. However, most metasurface designs have revolved around canonical geometries. While these elements are relatively easy to fabricate, they represent only a small portion of the design space, and rarely offer peak performance in transmission, phase range or field of view. In this work, a Lazy Ant Colony Optimization (LACO) technique is applied in conjunction with a full-wave solver using the Periodic Finite Element Boundary Integral (PFEBI) method to reveal high performing three-dimensional nanoantenna designs with potential applications for a variety of optical devices.**

***Keywords—three-dimensional nanoantenna, lazy ant colony optimization, metasurface***

## I. Introduction

Phase-gradient metasurfaces are desirable for their low profile and ability to abruptly and anomalously refract light [1]. These metasurfaces typically consist of periodic arrays of sub-wavelength unit cells, which leverage the generalized Snell's law to introduce a spatial variation in phase distribution to shape the desired optical wavefront. So far, a large portion of work in this area has revolved around canonical unit cell geometries (*i.e.* patches, strips, split-ring resonators or angled and loaded dipoles) manufactured using conventional fabrication techniques [1]. Although these unit cell geometries are relatively simple to simulate, analyze and fabricate, they represent only a small portion of the design space. As the demand for high performance optics is matched by advances in manufacturing, access to new unexplored three-dimensional design spaces can be exploited. Instead of relying on canonical structures, stochastic combinatorial optimization techniques such as the Multi-Objective Lazy Ant Colony Optimization (MOLACO) algorithm [2] have previously been introduced as an effective method to discover high performance periodic structures in the microwave regime. Unlike the traditional Genetic Algorithm (GA), MOLACO inherently enforces contiguity in its components, making the approach more amenable for three-dimensional fabrication techniques. This approach was first used to optimize multi-band three-dimensional frequency selective structures (which are closely related to metasurfaces) with polarization independent performance over extreme fields of view (up to 80° with respect to the optical axis). A proof of concept was fabricated via additive manufacturing and silver plating, then characterized with a broadband focused beam measurement system [3]. Although dispersion and plasmonic behaviors are negligible at these frequencies, a similar approach can also be applied to discover high performance optical designs [4] for advanced three-dimensional nanofabrication techniques [5].

## II. Lazy Ant Colony Optimization

The original Ant System (AS) [6] is a stochastic combinatorial optimization technique which relies on an indirect communication mechanism between ants known as stigmergy. As ants forage for food, they modify their local environment by depositing pheromones along their traveled path. These pheromones influence future ants' decisions on which path to choose, and each path can be interpreted as geometry of a unit cell design. This behavior can be mathematically modeled with some probability that is proportional to the pheromone concentrations. Thus, the probability that an ant would select a path $j$ that is locally accessible in the $i^{th}$ ant's neighborhood $N_i$ at iteration $k$ is dependent on the pheromone concentration associated with that particular direction, $\tau_j$, and is given by:

$$p_{ij} = \frac{\tau_j(k)}{\sum_{j \in N_i} \tau_j(k)} \quad (1)$$

Pheromones are directly proportional to the quality or fitness of the solution and over time, gradually evaporate at a user-defined rate to balance exploration and exploitation. To further balance this, the Max-Min Ant System (MMAS) introduced in [7] limits the pheromone concentration associated with each path,

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guaranteeing a non-zero chance of exploring new paths. However, despite the vast number of improvements to the original AS, one underlying assumption remained consistent throughout its many derivatives—that ants travel *indefinitely* throughout the pre-defined design space. Although this is useful for space-filling designs, it offers little value to inverse design of nanoantennas in three-dimensional space. Unlike its predecessors, LACO includes a probability of termination, modeled as an imaginary pheromone concentration which acts like a fatigue factor—the greater the fatigue, the less likely the ant continues traveling:

$$\tau_{imag} = \left( {}^{l}/_{L} \right)^{EF} e^{\upsilon} \tag{2}$$

where $l$ represents the current number of segments traveled out of $L$ total segments possible, while $EF$ and $v$ are parameters chosen to manipulate the rate of fatigue, and therefore the termination behavior of the ant. As a result, a wide variety of unique and unintuitive design geometries can be discovered, and their performance evaluated.

## III. Nanoantenna Optimization

In this study, the inverse design of three-dimensional nanoantennas was performed across four high power computing nodes. Each computer represents a colony with 768 ants operating in parallel across 24 cores over 100 iterations for a total of 161 hours. Nanoantenna designs are optimized based on maximum co-polarized transmission and minimal phase deviation of s-polarized light for various incidence angles at a wavelength of $\lambda_0 = 5.5$ µm, using the following fitness function:

$$T_{fit} = \frac{\min(T_{SS})}{1+\Delta T_{SS}} - \Psi_{correct} \tag{3}$$

where angle independence is assumed, while $\Delta T_{ss}$ and $\Psi_{correct}$ represent the maximum deviations of the transmission magnitude and phase angle respectively. Each unit cell is evaluated using a custom full-wave solver that applies the PFEBI method to solve for complex transmission of s-polarized light. By optimizing transmission while simultaneously accounting for phase information to sort results, it is possible to canvas a wide range of designs with high transmission, a variety of phase options and enhanced fields of view in a single procedure. Individual elements can then be manually selected for a particular metasurface application, based on the specific transmission magnitude or phase contribution required. Similarly, reflective metasurface applications can also be discovered by evaluating reflection in place of transmission.

## IV. Conclusion

Although canonical structures are fundamental in developing a physical understanding of the behavior of metasurface elements, the increasing demand for high performance optics cannot be met alone with canonical structures and traditional fabrication techniques. Alternatively, advanced manufacturing techniques that leverage three-dimensional design spaces can be employed to discover new, unintuitive nanoantenna structures. In particular, this work applies a LACO algorithm with a full-wave PFEBI solver to discover high performing three-dimensional nanoantennas for advanced optical applications.

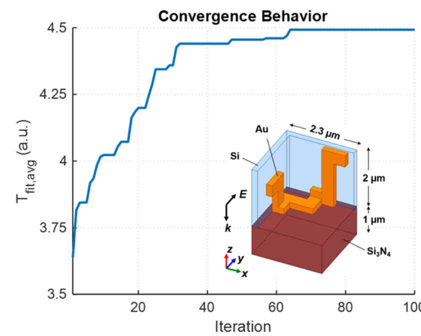


Fig. 1. Convergence behavior of MOLACO with an example unit cell (inset), where an individual ant represents the enclosed gold (Au) trace.

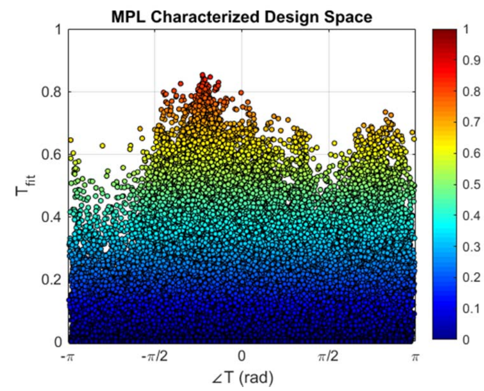


Fig. 2. Archive of designs discovered using LACO.

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