Algorithmic Design of Nanophotonic Structures

Eric Johlin
Department of Mechanical and Materials Engineering
University of Western Ontario, London, ON, Canada
Email: ejohlin@uwo.ca

***Abstract*—Algorithmic design holds promise of dramatically improving the efficiency of nanophotonic components. Herein we explore two aspects related to the configuration of evolutionary algorithms, as well as the design of new structures to enhance absorption and emission directivity of perovskite nanocrystals.**

I. Introduction

DESIGN of nanophotonic structures, particularly those with fully 3D geometries, has proven challenging due to the necessity of considering the wave nature of light in their operation. While traditional intuitive design has allowed for the use of micron-scale features by working within a ray-optics approximation, *e.g.* in solid-immersion lenses [1], these structures are far from ideal. Algorithmic design (AD) works to address this by permitting the inclusion of complex nanophotonic effects in the design, through fully considering the wave nature of light while determining the structures. This is done by utilizing iterative simulations to converge on the geometry of a component, with the algorithm having full control over the structure, and thereby precluding the need for initial guesses or user intuition. A number of approaches have been demonstrated for 2D nanophotonic structure design, including inverse design [2], genetic and evolutionary algorithms [3], [4], and machine learning [5].

We have recently demonstrated the use of an evolutionary algorithm to design a 3D nanophotonic lens (nanolens) for nanowire emitters [6]. These structures realized a performance in directive lensing 3 times greater than optimally positioned spherical solid immersion lenses of the same size, and showed nearly uniform performance over a wide bandwidth (more than 200 nm).

In this work, we explore two aspects of the configuration of the design algorithm used in creating nanophotonic structures, and then leveraging these results, design a new high-performance nanolens for nanoscale point-source emitters and absorbers.

II. Design by Evolutionary Algorithms

Along with select examples of inverse design [7], evolutionary algorithms (EAs) are one of the few AD techniques that have been demonstrated for fully 3D structures. For the discussions herein we use "3D" to refer to structures with varying heights, and the allowance of overhanging structures (*i.e.* multiple layers at a single point on a substrate), while "2.5D" refers to structures that can have variable heights, but no overhangs, and "2D" as those with a single, uniform height.

The EA investigated herein is shown schematically in Fig. 1 – the design process beings by generating a population of 30 random pixel arrays, with constraints on the minimum feature size. These arrays are then used to create 3D structures (either through rotation or extrusion of the array), which are then simulated using a finite-difference time-domain (FDTD) technique. The results of the simulations give the fitness of each structure (*e.g.* the absorption within a structured nanoparticle), which is used to determine the 6 best performing geometries from the pool of 30 structures. These 6 structures are used as the "parents" for the future generations, with a small chance of being purged after each generation ends. For each subsequent generation, a set of 30 new structures are created through one of three options: breeding two previous high-performing structures, mutating single high-performing structures, or introducing new random structures. This process continues until there is little change in the highest performance over multiple generations, and the design is considered converged.

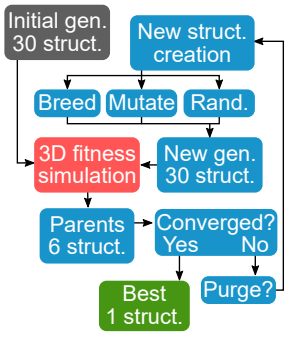

Fig. 1. Diagram of the evolutionary design process. The evolutionary algorithm is depicted in blue. The starting structures (grey) are fully random, with a minimum feature size. Fitness of each structure is evaluated through full 3D FDTD calculations (red), and once the algorithm has converged on a maximum fitness value, the final structure is returned (green).

III. Influence of Symmetry

The convergence of the design process depends on a number of factors – the number of parents and individuals per generation influence the convergence rate and robustness, but the boundary conditions of the problem also have a strong impact. We explore the influence of these conditions next. In Fig. 2 we show the resulting structures from two EA design processes with the goal of optimizing the absorption cross section of a gallium arsenide (GaAs) nanoparticle. For this simple example a 2D system is investigated (and so absorption *length* is used as the fitness metric), with 570 nm wavelength plane wave of excitation coming from the top of the figure. The particles are constrained by a 600 nm $\times$ 600 nm bounding box, but can be any shape (permitted by a 40×40 array of pixels). In the first case, there is no symmetry requirement, with any arbitrary shape permitted (free of constraints). The second design is mirror-plane symmetric, to reflect the symmetry in the oscillations of the incident electric field.

We find that when the two differently constrained EA designs are run to convergence (with multiple design runs), two interesting results appear: First, there is a similarity in

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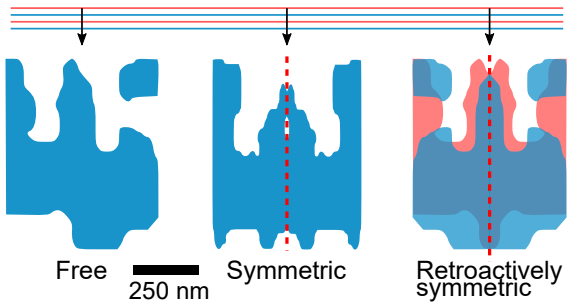

Fig. 2. Comparison of absorbing GaAs nanoparticles under plane-wave illumination designed by the EA, with varying symmetry conditions: no symmetry imposed (free), symmetric mirror plane, and forced symmetry applied retroactively to the free structure. Absorption lengths of the 2D structures are indicated.

the design between the two cases; out of all of the possible configurations, both the symmetric and free simulation result in structures with 3 lobes on the front facing the plane-wave, followed by a solid, wide region in the middle, and smaller protrusions at the trailing end. Second, the symmetric structure achieves an absorption length of 1.0 μm, while the constraint-free structure, despite the larger freedom in design, achieves a smaller 0.8 μm absorption length. This suggests that it is not *despite* the reduction in design space that the symmetric structure is able to achieve a higher performance than the free structure, but more likely *by virtue* of the strategic reduction of space the algorithm must search.

Furthermore, we can compare these structures to retroactively forcing symmetry onto the symmetry-free design. This is shown as the 3rd structure in Fig. 2, with three possibilities – the blue structure (taken from the right half of the free structure), the red structure (from the left half), or the union of the two. Regardless of the method of enforcing symmetry, the performance is lower, (< 0.65 μm). This is not entirely unexpected, as the length scales here cause the entire structure to respond to the electromagnetic oscillations (single features do not respond in isolation), but it is instructive to observe that combinations of different features from the retroactively symmetric structures can lead to the creation of new features approaching those on the highest performing symmetric design. This helps to explain the success of the breeding process used in the EA which operates in much the same manner.

IV. Design of Point-Source Nanolenses

The benefits of symmetry can be applied to fully 3D structures as well – in designing nanolenses to either tune absorption of an unpolarized plane-wave (*e.g.* sunlight for nanoscale solar cells), or emission from unpolarized point source (*e.g.* photoluminescence from a nanocrystal), rotational symmetry is the equivalent to the mirror symmetry used the previous section. The EA discussed above is thus used to design a rotationally-symmetric, fully 3D nanolens for focusing 570 nm light onto (from) a 100 nm nanocube perovskite absorber (emitter).

The resulting nanolens is shown in Fig. 3 **a** and **b**. FDTD simulations indicate that such a lens will lead to a dramatic enhancement of the absorption cross section of the nanocube to 1.6 μm^2, and an emission directivity of 306.

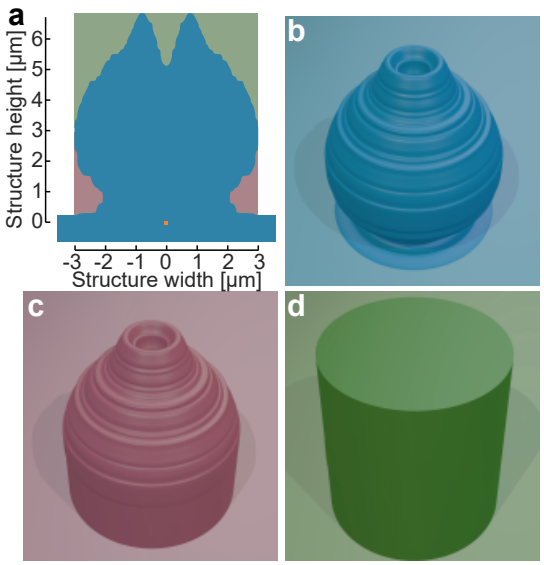

Fig. 3. **a** Diagram showing cross-sections of three levels of lens design dimensionality: full 3d (blue), 2.5D (red+blue), 2D (green+red+blue), with the nanocube shown at position [0,0] (small orange point). **b-d** Renderings of the three corresponding 3D, 2.5D and 2D nanolenses.

TABLE I
Lensing performance of the three nanolens dimensionalities

	3D	**2.5D**	**2D**
Directivity	306.8	232.1	21.4
Absorption cross section [μm^2]	1.61	1.21	0.11

We can furthermore analyze the benefits of the dimensionality of the fully 3D design by reducing the dimensions and inspecting the change in performance. The results are summarized in Table 1. We observe that by reducing the 3D structure to 2.5D (removing any overhanging features; allowing the structure to be fully described by a height map), the performance in both emission and absorption are reduced moderately. Reducing to a 2D structure has a much more significant influence, with directivity and the absorption cross section enhancement factor falling by more than an order of magnitude. This demonstrates the significant appeal of fully 3D algorithmic design of nanophotonic structures.

References

[1] V. Zwiller and G. Björk, "Improved light extraction from emitters in high refractive index materials using solid immersion lenses," *J. Appl. Phys.*, vol. 92, no. 2, pp. 660–665, 2002.

[2] J. Lu and J. Vučković, "Nanophotonic Computational Design," *Opt. Express*, vol. 21, no. 11, pp. 13 351–13 367, 2013.

[3] A. Mirzaei, A. E. Miroshnichenko, I. V. Shadrivov, and Y. S. Kivshar, "Superscattering of light optimized by a genetic algorithm," *Appl. Phys. Lett.*, vol. 105, p. 011109, 2014.

[4] P. R. Wiecha, A. Arbouet, C. Girard, A. Lecestre, G. Larrieu, and V. Paillard, "Evolutionary multi-objective optimization of colour pixels based on dielectric nanoantennas," *Nat. Nanotechnol.*, vol. 12, pp. 163–169, 2017.

[5] D. Liu, Y. Tan, E. Khoram, and Z. Yu, "Training Deep Neural Networks for the Inverse Design of Nanophotonic Structures," *ACS Photonics*, vol. 5, no. 4, pp. 1365–1369, 2018.

[6] E. Johlin, S. A. Mann, S. Kasture, A. F. Koenderink, and E. C. Garnett, "Broadband Highly Directive 3D Nanophotonic Lenses," *Nat. Commun.*, vol. 9, p. 4742, 2018.

[7] Y. Deng and J. G. Korvink, "Topology optimization for three-dimensional electromagnetic waves using an edge element-based finite-element method," *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 472, no. 2189, p. 20150835, 2016.