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Rapid Design of Wide-Area Heterogeneous Electromagnetic Metasurfaces beyond the Unit-Cell Approximation

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Abstract—We propose a novel numerical approach for the optimal design of wide-area heterogeneous electromagnetic metasurfaces beyond the conventionally used unit-cell approximation. The proposed method exploits the combination of Rigorous Coupled Wave Analysis (RCWA) and global optimization techniques (two evolutionary algorithms namely the Genetic Algorithm (GA) and a modified form of the Artificial Bee Colony (ABC with memetic search phase method) are considered). As a specific example, we consider the design of beam deflectors using all-dielectric nanoantennae for operation in the visible wavelength region; beam deflectors can serve as building blocks for other more complicated devices like metalenses. Compared to previous reports using local optimization approaches, our approach improves device efficiency; transmission efficiency is especially improved for wide deflection angle beam deflectors. The ABC method with memetic search phase is also an improvement over the more commonly used GA as it reaches similar efficiency levels with a 35% reduction in computation time. The method described here is of interest for the rapid design of a wide variety of electromagnetic metasurfaces irrespective of their operational wavelength.

1. INTRODUCTION

Metasurface [1–3, 5] is the two-dimensional analogue of metamaterial. It is a spatially heterogeneous array of nanoscale resonant elements (called meta-atoms) that can, in general, alter the amplitude, phase, spectrum and polarization values of an incident wave-front in a very short propagation distance and with sub-wavelength resolution in the transverse plane [5]. Being a structured surface, it can be fabricated easily in relation to the metamaterial. Additionally, it reduces the insertion losses and provides compactness.

The metasurface is a frequency agnostic concept and is finding applications across the electromagnetic spectrum in different tasks. In the optical and infrared frequency regions, they are of interest in connection with integrated photonics. Although this concept [6] has been initially explored in connection with plasmonic materials [3, 4], attention has now turned towards all-dielectric metasurfaces [7–10]. Such high refractive index dielectric nanoantenna arrays can also be considered as two dimensional high-index contrast subwavelength diffraction gratings; various optical wavefront manipulation possibilities have been demonstrated with these so called HCTA (high contrast transmit arrays) [11–13]. In the microwave region, low-profile transmitarrays are also of interest for a variety of applications [14]. Metasurfaces can achieve phase and polarization control simultaneously and are of interest in achieving millimeter wave beam-shaping lenses [14, 15] and carpet-cloaks [16].

The constituent elements of a metasurface, the meta-atoms, are subwavelength resonators while the transverse extent of the metasurface can be several orders of magnitude larger than the operating wavelength (in other words, useful metasurfaces will be electrical large in the transverse plane). For

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heterogeneous metasurfaces, this means that the number of free parameters in the design of the metasurface can exceed 10^9 [17]. This structure is not easily amenable for analysis, synthesis and optimization tasks. Conventionally, the so-called unit-cell approximation [18] has been adopted [17] in the design of heterogeneous metasurfaces, whereby each constituent meta-atom is designed as if it was part of an infinite periodic lattice. This unit-cell approach has also been extensively used in reflectarray design in the microwave domain and it has been reported that it leads to discrepancies when experiments are compared with the simulated designs [18]. The unit cell approximation has several limitations; chiefly, it tends to be inadequate in the presence of strong phase gradients, interactions between neighboring pillars, and oblique incidence angles. These constraints become important for instance in the case of a focusing lens [14, 15, 17, 19].

In this paper, we propose an approach whereby spatial order is applied on an extended cell, which includes several individual resonator elements. This technique is similar to the Extended Local Periodicity (ELP) approach [18] proposed for reflectarray design. Specifically, we focus our attention to a beam deflector element which is a commonly used structure for benchmarking metasurfaces design strategies [17, 19, 20] as the transmission efficiencies can be compared across designs. The beam deflector element changes the direction of an normally incident plane wave by giving it a predesigned inclination with respect to the normal. Although a simple element, the beam deflector, in addition to being an important element in itself, can be combined to produced metasurfaces with more advanced functionality like high numerical aperture and multi-wavelength focusing lenses and holograms [17, 20–22]. The beam deflector elements considered in this paper do not use the local phase approach [20] which is based on the unit-cell approximation but move beyond this by considering an extended unit-cell consisting of a larger number of nanoantenna.

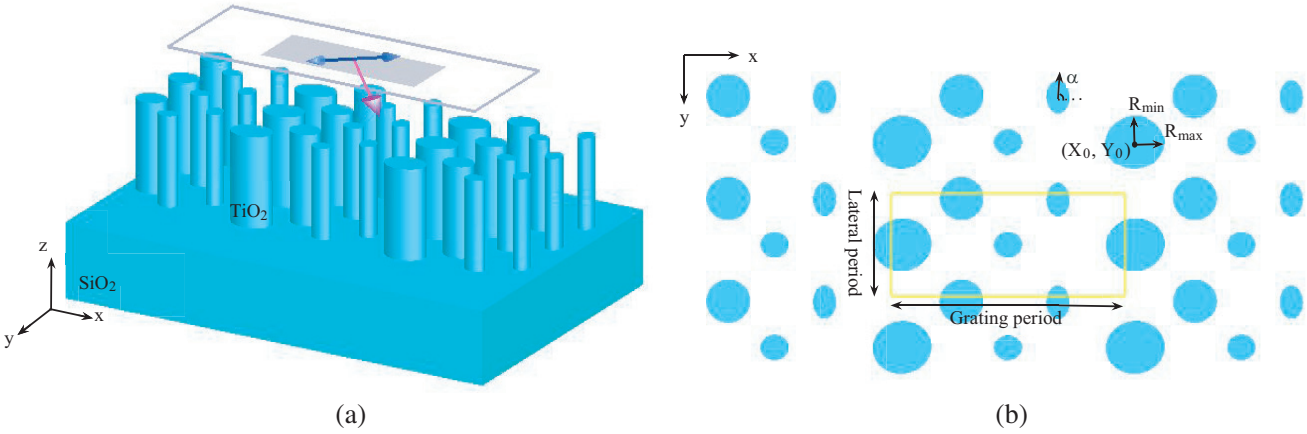
The main contribution of this article is that it presents a systematic investigation of global optimization methods for the design of the extended unit-cells. In comparison to the beam deflector synthesis method reported by Byrnes et al. [17] which uses local optimization methods, our method which relies on global optimization methods, as the Genetic Algorithm and Artificial Bee Colony, shows significant improvement in efficiency by not getting stuck at local optima. In comparison to [20] which has studied the application of Genetic Algorithm (GA) to the beam deflector design problem, we have explored unit-cells which do not restrict the design to a rectangular lattice and cylindrical elements. Additionally, our Artificial Bee Colony method is seen to outperform GA method in speed by cutting the convergence time by 35%.

The paper is organized as follows. Following this introduction, in Section 2, we describe the beam deflector geometry and optimization algorithms in detail. In Section 3, we discuss how to phrase the optimization problem in terms of the GA and Memetic ABC algorithms and suggest how to best choose the hyperparameters of these algorithms. The performance figures for the designs and comparisons with previously published reports are presented in Section 4 before concluding the paper in Section 5.

2. SPECIFICATION OF THE OPTIMIZATION PROBLEM

As discussed earlier, the beam deflector geometry is a canonical element in the design of a wide variety of metasurfaces. The system considered here can be directly compared with the geometry reported in Byrnes et al. [17] where a wide-area focusing lens was designed using beam-deflectors as motifs. Specifically, this required beam deflectors with deflection angles varying in the range 20 to 70 degrees. Figure 1 shows the geometry of such a beam-deflector with rectangular shaped extended unit-cells. Here TiO_2 nanoantennae are arranged in a hexagonal lattice within the unit-cells on a fused silica substrate. We have kept the overall dimensions of the extended unit-cells for any particular deflection angle exactly equal to those in Byrnes et al. [17] so that our designs can serve as a drop-in replacements with higher efficiencies.

A plane wave is normally incident from the substrate side and upon leaving the beam deflector emerges at an angle (θ in the x-z plane) that is decided by the design (vice-versa a light wave incident at this angle from the free-space side emerges at normal incidence). The period of the beam deflector unit-cell in the x direction is called the grating period (G. P.) and the period in the y direction is called



(a) (b)

Figure 1. (a) Three dimensional schematic of a beam deflector made of extended unit-cells containing TiO_2 nano elliptical antennae on fused silica substrate. (b) Design parameters of the extended unit-cell. The yellow line shows the boundaries of the extended unit-cell.

the lateral period (L. P.). These periods are given by:

$$\begin{aligned} G.P. &= \lambda_0 / \sin\theta, \\ L.P. &= \Phi f \tan\theta, \end{aligned} \tag{1}$$

where, λ_0 is the free space wavelength of source light and θ the angle of incidence or the desired deflection angle. Φ is the angular width of unit cell in y direction and is decided by the lateral width and the desired focal length. Throughout the paper we consider the lateral period as 400 nm as in [17]. As seen in Equation (2), a beam deflector with a larger deflection angle requires a larger period.

Within each extended unit-cell, we consider elliptically shaped nanoantennae each with freely choosable values of the following 5 parameters: major and minor axes $r_{\max}$ and $r_{\min}$ respectively, the x and y coordinate of the center of the ellipse in the cell coordinate system x_0 and y_0, respectively, and the orientation angle of the major axis α. In each unit cell, the number of nanoantennae N can be calculated by:

$$N \leq G.P./d_{\min}, \tag{2}$$

where $d_{\min}$ is the minimum diameter of nano structure and can be decided based on the fabrication constraints. Here we impose the condition that the minimum feature size of the entire shape should not be lower than 100 nm.

The optimization problem can now be stated as:

$$\begin{aligned} &\underset{s}{\text{maximize}} \quad 0.5\left(\eta^1(s) + \eta^2(s)\right) \\ &\text{subject to} \quad f_i(s) \leq b_i, \quad i = 1, \ldots, m, \end{aligned} \tag{3}$$

where s is a $5N$ sized vector describing the extended unit cell (i.e., $s = [r^i_{\max}, r^i_{\min}, x^i_0, y^i_0, \alpha^i]$ and $i = 1 \ldots N$); η^1 and η^2 describe the first order beam efficiency of the designed grating for x and y polarized normally incident beams, respectively (the first order is made to coincide with the desired angle θ). The number that is optimized is the ratio of power diffracted into the +1 order beam to that of the incident beam power (averaged over the two possible orthogonal polarizations of the normally incident input beam). Fabrication techniques impose several constraints on realizable designs, which could be incorporated through the various functions f_i that describe constraints imposed on the values that the vector s or its elements can take (for instance, these constraints could require that the ratio of the major and the minor axes be limited to 5).

In order to calculate the first order efficiency of a particular extended unit-cell, we use the rigorous coupled wave analysis (RCWA) approach [23] using the open-source S^4 application. S^4 combines the S-matrix approach with the RCWA method. Full-wave simulations are performed using the commercial software program COMSOL Multiphysics using the Finite Element Method on the finally obtained optimal vectors to verify the obtained efficiency figures.

3. OPTIMIZATION VIA GENETIC ALGORITHM AND ME-ABC ALGORITHM

Due to the relatively large number of free parameters and stringent fabrication related constraints required to design efficient metasurface scanning over the full parameter space is not feasible. Stochastic optimization methods are more appropriate to improve the efficiency and are expected to perform better than simpler gradient descent based approaches. In order to optimize the polarization averaged first order diffraction efficiency we employed two techniques: Genetic algorithm and hybrid ABC algorithm with memetic search phase.

3.1. Genetic Algorithm

Genetic Search is a very popular method used in electromagnetic problems having a large multidimensional unknown search space [24]. We have employed genetic algorithm with three common parameters: selection, crossover and mutation. Additionally, we have set upper and lower bounds for the radii and position of nanoantennae in the beam deflector. Radius values of ellipses are limited between 50 nm and 125 nm and the minimum distance between two antennae centres is set to 100 nm.

The elliptical nanoantennae represent individuals in a generation. Each generation has some number of families N_f represented by beam deflectors with N_i number of individuals. The number of individuals in a family is given by Equation (2). The evolution usually starts from a population of randomly generated individuals that constitute potential metasurface designs. We are targeting to maximize the polarization averaged first order diffraction efficiency. For each generation, we choose a fraction f_t of the best performing beam deflectors and a fraction f_d of individuals randomly out of remaining $1 - f_t$ fraction of the lesser performers from the population based on diffraction efficiency. These individuals then act as parents for next generation so that we promote genetic diversity in addition to fitness. The Crossover step applied next is the process of taking more than one parent solutions and producing a child solution from them. The crossover operator given by P_c modifies the children generation by randomly mixing couples. After crossover, we mutate radii, position and angle of nano-ellipses by some amount given by mutation probability P_m. The pseudocode for the GA used here is shown below.

We have used traditional Grid search method for tuning of hyper parameters of the GA such as f_t, f_d, P_c, P_m and N_f. It was found that values of 0.15 and 0.10 was best suited for f_t and f_d respectively. The procedure followed in the grid search method is demonstrated in Figure 2. It shows how different population size, mutation rates and crossover rates affect the convergence of the efficiency function. Population diversity is crucial to the genetic algorithms ability to continue fruitful exploration without getting stuck at local maxima. The size of the population N_f dictates the available diversity. While a large value will lead to good diversity it will also increase the computational time. We observe that 300

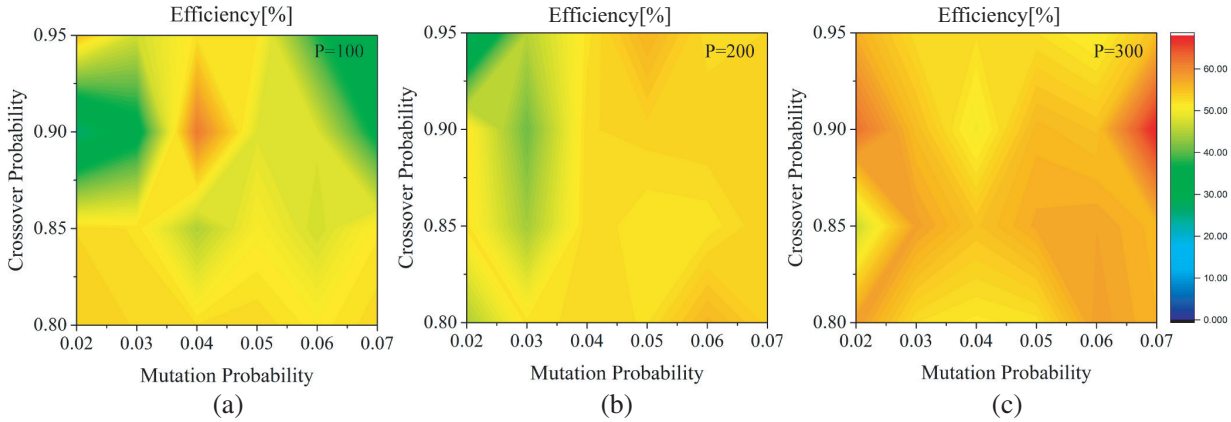


Figure 2. Selection of hyperparameters for properly tuning of GA algorithm via grid-search. (a)–(c) diffraction efficiency for 70 degree beam deflector as a function of mutation and crossover probability for population sizes of (a) 100, (b) 200 and (c) 300.

Algorithm 1 Genetic Search Method

```
Generate initial population of size N_f;
Evaluate initial population according to fitness criteria;
while Termination criteria meets do
    Select the best fit individuals for reproduction;
    Perform crossover operation given by probability P_c;
    Perform mutation operation given by probability P_m;
    Evaluate fitness of new individuals;
    Replace the worst individuals of population by best new individuals;
Report the best family achieved
```

families in each generation is sufficient to produce good fitness. The crossover rate P_c and mutation rate P_m are both continuous variables within $[0, 1]$. These two values are important for controlling the balance between exploration and exploitation. Table 1 summarizes a good set of values of all the hyperparameters for the GA used in this problem.

Table 1. Hyperparameters chosen for the GA and MeABC method.

GA Parameters		Me-ABC Parameter	
Parameters	Value	Parameters	Value
No. of Families	300	No. of Food Sources	25
No. of Individuals in a Family	2–4	No. of Onlooker Bees	25
Mutation Probability, P_r	0.07	No. of Employed Bees	25
Crossover Probability, P_c	0.90	No. of Scout Bees	1
No. of Generations	50	No. of iterations before bee is tired	200

3.2. ABC Algorithm with Memetic Search Phase

Artificial bee colony (ABC) optimization algorithm is a relatively new population based probabilistic approach for global optimization based on the concept of swarm intelligence [25]. ABC has outperformed many other nature inspired optimization algorithms prompting our interest in it for metasurface design. Memetic algorithms (MA) is another growing area of research in evolutionary computation. It is inspired by Darwin's principle of evolution and Dawkin's notation of a "meme" [26]. The ABC algorithm has achieved excellent results when solving continuous and combinatorial optimization problems [27]. To achieve the benefits of both algorithm, ABC is hybridized with Memetic Algorithm [28, 29].

In the ABC algorithm [25], the search of a parameter space is accomplished by a set of honey bees called the swarm containing three types of bees: employed bees, onlooker bees, and scout bees. Consider an objective function $f_i(s)$ which evaluates some performance metric of an extended unit-cell represented by $s = [r^i_{\max}, r^i_{\min}, x^i_0, y^i_0, \alpha^i]$ (here s is a vector of $5N$ geometrical parameters and N is number of ellipses on a beam deflector). Each beam deflector is represented by a food source s in the swarm and it is generated as follows [28]:

$$s_{ij} = s_{\min j} + rand[0, 1](s_{\max j} - s_{\min j}), \tag{4}$$

where function rand $[0, 1]$ returns a random value between 0 and 1, and $s_{\max j}$ and $s_{\min j}$ represent maximum and minimum limits of the candidate solution s_i. The swarm will now navigate this parameter space and converge to an optimal geometry. The parameter space is considered a region of space where food sources are located; those regions of this parameter space that exhibits a high value of the function f are considered to be richer food sources. The solution search equation of the original ABC algorithm is significantly influenced by a random quantity which helps in exploration at the expense of exploitation of the search space; there is a significant chance of skipping true solutions due to the large step sizes that

are often used. In order to balance between diversity and convergence capability of the ABC (in other words between exploration and exploitation), a new local search phase is integrated with the basic ABC to exploit the search space identified by the best individual in the swarm. The addition of a memetic search phase to the ABC algorithm results in the the memetic ABC (MeABC) algorithm wherein the step size required to update the best solution is controlled by a Golden Section Search (GSS) approach. The MeABC has an enhanced exploitation capability in comparison to the bare ABC Artificial bee colony algorithm [28, 29].

In employed bee step, current solutions are changed by employed bees based on their individual experience. If the fitness of latest solution is better than previous solution, then the employed bees update their position to new solution. The employed bees in ABC algorithm use the following equation in order to improve self solution [29]:

$$v_{ij} = s_{ij} + \Phi_{ij}(s_{ij} - s_{kj}), \quad k \neq i, \tag{5}$$

where v_{ij} is the updated food, s_i the old food, and s_{kj} a random food from hive. Here $k \in I, 2, \ldots, s_N$ and $j \in I, 2, \ldots, N$ are haphazardly chosen indices, and Φ_{ij} is a random number in range $[-1, 1]$. Onlooker bees in the hive expect information of fresh solutions and their position. In the next step, onlooker bees inspect the available information and pick a solution with a probability given by

$$P_i = \frac{fit_i}{\sum_{j=1}^{n} fit_i}, \tag{6}$$

where fit_i is i^{th} solution in the swarm. If the position of a food source is not updated for a given cycle, it is considered to be abandoned. In the scout bee step, the bee whose food source has been deserted becomes a scout bee, and the deserted food source is replaced by a haphazardly chosen food source within the search space. Scout bees are agents for global food search; they replace a food source by another randomly chosen food source which is generated by the equation

$$s_{ij} = s_{\min j} + rand[0, 1](s_{\max j} - s_{\min j}), \quad j \in 1, 2 \ldots N, \tag{7}$$

where $s_{\min j}$ and $s_{\max j}$ are the bounds of s_{ij} in the jth direction.

Memetic phase is designed on the golden grid/section search criteria. Basically we choose a negative value of a (that is some value on the left of the X-axis for that dimension of the best food) and equal but positive value of b (that is some value on the right of the X-axis) [26]. The values a and b dictate how wide the memetic search should be. The current best food lies exactly in the middle initially. The memetic search starts by determining whether a better food is on the Left of the current best food (i.e., more towards a) or to the right (i.e., more towards b). Similar to a binary search algorithm it updates the values of a and b and gradually zeroes in on the better solution around the current best. If it finds a better food source, it updates the best food else the search fails. This process is carried out until the difference between a and b (absolute value of the difference) is greater than the set value of epsilon; epsilon being the stopping criteria of memetic search phase. In MeABC algorithm, ABC algorithm behaves as a local search algorithm in which only the best individual of the current swarm updates itself in its neighbourhood while in memetic search phase the step size required to update the best individual in the current swarm is controlled by the golden section search (GSS) approach. GSS processes the interval $[a = -0.75, b = 0.75]$ and generates two intermediate points:

$$\begin{aligned} F_1 &= b - (b - a) \times \Psi, \\ F_2 &= a + (b - a) \times \Psi, \end{aligned} \tag{8}$$

where Ψ is the golden ratio. Memetic ABC algorithm has three steps similar to the ABC algorithm, and one more step, the memetic phase, is added for updating the location of an individual. It changes position [29] given by the equation

$$s_{ij} = s_i + \Phi_i(s_i - s_k) + \Psi(s_{best} - s_i), \tag{9}$$

where Φ_i is a random number in the interval $[0, D]$, and D is a positive constant. The pseudo code for the Memetic ABC algorithm that we have employed is given below.

From Equation (4), it can be observed that the step size consists of a random component Φ, and thus a proper balance is not possible manually [29] (Φ is a random component that decides direction

Algorithm 2 MeABC Algorithm

```
Generate an initial population of food sources using Equation (2);
Evaluate initial population according to fitness criteria;
while Termination criteria meets do
    Deploy employed bee searches to find new food searches in the neighbourhood using Equation (5);
    Calculate Probability P for each food source using Equation (6);
    Send onlooker bee to food source depending upon P;
    Evaluate fitness of each new food source;
    if any employed bee becomes scout bee then
        Send scout bee to a randomly generated food source;
    Employ memetic search phase;
    Memorize the best food source achieved so far;
Report the best food source achieved
```

and step size of an individual). Memetic search phase (MSP) improves the exploitation capability [30] considerably. We have used MSP to fine tune the value of Φ dynamically and iteratively using the Golden Section Search strategy. The range of Φ_{ij} is set to $[a, b]$ where $a = -0.75$ and $b = 0.75$; a and b dictate how wide the memetic search should be. To tune the hyper parameters of MeABC algorithm like the swarm population and numbers of each kind of bees, we used a traditional grid search method. The hyperparameter values that were found to yield good results in terms of efficiency are summarized in Table 1.

4. RESULTS AND DISCUSSION

The above design methodology was applied to the design of a set of beam deflecting metasurfaces operating at 580 nm wavelength. The extended unit cells are rectangular shaped, but within it the fill fraction is maximized by adopting a hexagonal grid. The elliptically shaped nanoantenna is made of TiO_2 and sits atop a fused silica substrate. The refractive index of $n(TiO_2) = 2.37$ at 580 nm and the nanoantenna height is kept at $h = 550$ nm.

Table 2. Optimal geometrical parameters of the extended unit-cells and their first order polarization-averaged diffraction efficiencies [%] at 580 nm wavelength.

	E1			E2			E3			E4			
D.A.	Rx	Ry	θ_r	Rx	Ry	θ_r	Rx	Ry	θ_r	Rx	Ry	θ_r	Eff.
20°	69.15	83.17	−9.6	50	50	0	50	50	0	162.2	89.14	0.01	83.8%
30°	111.14	85.63	175.7	50.04	50.06	175.16	95.99	134.80	88.66	-	-	-	79%
40°	93.25	101.76	78.36	50	50	0	-	-	-	-	-	-	78.6%
50°	58.09	77.46	179.99	50	50	0	-	-	-	-	-	-	81%
60°	106.21	79.77	−179.96	50	50	0	-	-	-	-	-	-	71.8%
70°	103	89.86	−177.76	50	50	0	-	-	-	-	-	-	65%

Figure 3(a) shows comparison of the polarization averaged efficiencies obtainable with all three methods viz: the local steepest gradient ascent [17], genetic algorithm, and ABC with memetic phase search (Table 2 lists the optimal parameters for all the beam deflectors). Firstly, note that all three curves indeed follow the well-known fact that efficiencies are nearly constant up to deflection angles of about 50 degrees but start to decay rapidly afterwards. While all three methods give nearly equal efficiencies in the initial angular range, the designs obtained with the global optimization methods significantly outperform at steeper angles.

Comparison of the convergence times using all three methods for three different beam deflectors

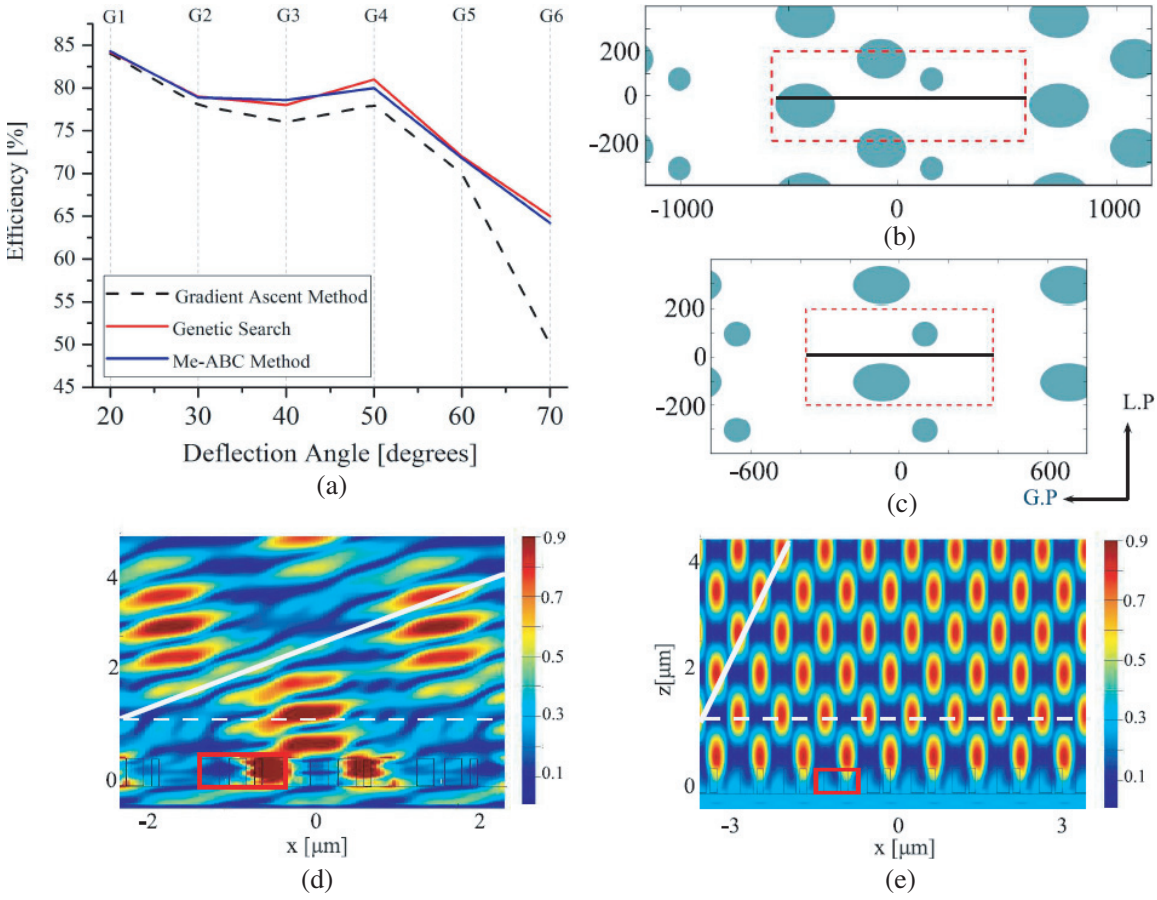


Figure 3. (a) Comparison of the polarization-averaged first order diffraction efficiencies for beam deflectors with bend angles ranging from 20 to 70 degrees designed via Gradient Ascent, Genetic and MeABC Approach. Top view of the optimal beam deflectors at deflection angles of (b) 30 degree and (c) 50 degrees (red lines delineate the extended unit-cell). Full-wave simulation based power transmission plots (d) and (e) shown for a x-z plane denoted by black line in the gratings (b) and (c) respectively.

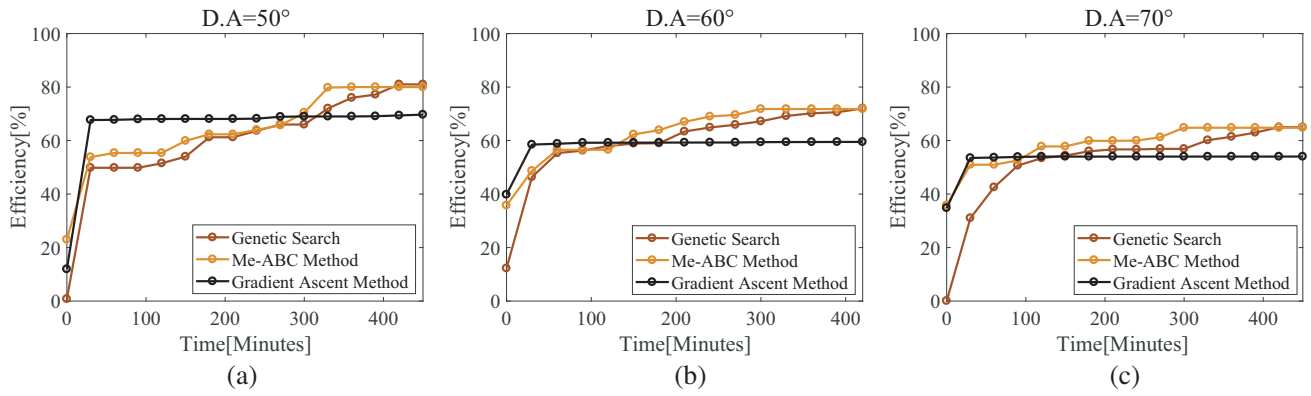


Figure 4. Comparison of convergence time needed to arrive at the optimal beam deflectors for gradient ascent, GA and MeABC methods. Three different deflection angles have been considered.

is shown in Figure 4. All runs were made on machine with the following configurations: Processor — Intel (R) Xeon(R) CPU E5-2650 V2@2.60 GHz; RAM — 32 GB; and, System Type — Windows 64 bit operating system. It is evident that the gradient ascent method gets stuck early on in a local optima

and never improves the overall efficiency. The global optimization techniques clearly avoid this problem. Furthermore, the time taken by the global search is not too much in comparison to the local methods. While the efficiencies achieved by GA and MeABC are almost similar, the MeABC approach converges to the final geometry in approximately 35% time compared to the GA approach.

5. CONCLUSION

We have presented two global optimization techniques based on nature inspired algorithms for the rapid design of all-dielectric metasurfaces and have applied them to the case of beam deflectors. Compared to local optimization methods like the gradient ascent algorithm, Genetic and Me-ABC algorithms provide higher deflection efficiencies. Up to 15% efficiency improvement is achieved for larger deflection angles. The MeABC method proposed by us is significantly faster than previously proposed gradient ascent algorithm [17]. It also outperforms the GA in terms of computation time.

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