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Comparison of Different Optimization Techniques in Electron Lens Design

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***Abstract*— To design electron lens systems, applying a fully automated optimization routine has not yet been feasible, especially for the case where the optimization has many free variables of the lens system, such as all parameters that define the geometry of the lens electrodes and the voltage of each electrode. Hence, the study of the implementation of different optimization procedures has not yet been possible either. In one of our previous studies, we have proposed to use the so-called Second Order Electrode Method (SOEM) which performs the electrostatic field calculations in a very short time by the approximations of the field near the optical axis. There, using SOEM in field calculation, a Genetic Algorithm (GA) was successfully implemented to optimize the electron lens systems. One of the questions that has not been studied and answered in the literature yet, is whether the GA is the most suitable option among different optimization techniques for the design/optimization of electron lens systems. In this paper, by implementing the SOEM technique as the field calculation method, different optimization procedures are implemented and their performances are compared. For this study, a typical six electrode lens system is employed. The implemented optimization techniques include calculus-based local optimization ('Fmin') and metaheuristic methods such as GA, Particle Swarm Optimization (PSO), and Simulated Annealing (SA). The results demonstrate that the population-based global optimization techniques like GA and PSO significantly outperform single-based local optimization methods such as 'Fmin' and SA. Additionally, PSO shows slightly better performance than GA, although it cannot be concluded that PSO will always outperform GA for every electron lens design problem. Furthermore, in the comparison between the two single-based optimization techniques, the metaheuristic approach (SA) outperforms the calculus-based one ('Fmin'). Hence, we recommend implementing metaheuristic, global, population-based optimization techniques like GA and PSO for the optimization electron lens systems.**

Keywords—Electron Electrostatic Lens Design, Global Optimization, Local Optimization, Meta-heuristic based Optimization Algorithms, Genetic Algorithms, Particle Swarm Optimization , Simulated Annealing, SOEM (Second Order Electrode Method)

I. INTRODUCTION

Design and optimization of electron lens systems are yet a laborious work for electron-optical designers. In such lens system optimization, the objective function is to obtain the correct focus position while to minimize of lens aberrations. To calculate these, the electric field of the lens system, which is generally calculated by accurate methods such as the Finite Element Method (FEM) [1] have to be derived. To perform the electron lens system optimization while voltages and all geometries of the electrodes are free parameters of the optimization, thousands of systems need to be evaluated [2, 3]. Using the existing accurate field calculation methods such as FEM (60 seconds per system evaluation on a modern PC), a fully automated optimization becomes impractical in a feasible time [2, 3]. Due to the problem mentioned above, to our knowledge, there is not yet a fully automated optimization routine which performs the optimization of a multi electrode-lens system, having all its geometric dimensions as free parameters. Therefore, studying the performance of different optimization techniques for electron lens system design has not been also studied either. Previously, the authors have presented an optimization technique [2, 3] based on a fast but approximate so-called Second Order Electrode Method (SOME) (proposed by Adrianse on 1988) [4, 5] to calculate the electric fields around the optical axis (0.4 second per system evaluation on the same PC) while implementing a Genetic Algorithms (GA) [6, 7]. Now, having such an automated and fast routine developed, we decided to use that to perform the above mentioned study on comparison of the performance of different optimization techniques for the electron lens design optimization. In our previous studies on electrostatic lens system design optimization, it was demonstrated that in optimization of electrostatic lens systems, a global optimization is needed [8]. Our case-study is a highly-nonlinear complex optimization problem [3, 8]. In many papers it has been shown that for such optimization problems the meta-heuristic optimization techniques can be the most suitable choice. However, which one of the meta-heuristic technique provides the best result in our case-study? This question will be answered in this paper. In addition, a comparison with a calculus-based local optimization is presented here to show the difference between the performance of a local optimization compared to a global one.

First, a brief recap of different types of the meta-heuristic optimizations and the reason why it is hard to predict in advance which type is the best choice for our case-study, is presented. In section II the optimization problem is defined. Section III presents a brief introduction of the most well-known meta-heuristic optimization techniques that are going to be compared in our case-study. In IV the results of the implementation and comparison are provided and the conclusion is presented in V.

More than 50 years have passed since the time when the mathematical foundations of Metaheuristic-based optimization algorithms (hereafter called MA) [9-11] were introduced by the pioneers of this work who include Holland [12], Schwefel [13], Foget et al. [14] and Rechenberg [15]. MA includes many different algorithms, the most common of which are from different categories of population-based and single–based are Genetic Algorithm (GA) [16], Particle Swarm Optimization (PSO) [17] and Simulated Annealing (SA) [18]. From the beginning, the practitioners of this field had questions on how to select the optimization algorithm type. “Is there any specific type of optimization algorithm which outperforms the others?”, and “Can we predict a specific optimization algorithm which can achieve the best performance out of the choice of algorithms for a defined optimization problem?”

In all these years, despite considerable efforts performed by the researchers in this field, it has been discovered that finding the type of optimization algorithm which is best in different optimization problems, is neither a problem that can be generalized, nor one easy to predict before running the optimization [19]. It is represented as “No Free Lunch” (NLF) theory in optimization [20].

In other words, a specific type of MA which outperforms the other types in one optimization problem may not do so in another problem with a different objective function landscape. Having the information from the objective function landscape will help to select the most appropriate type of MA. However, knowing the objective function landscape in advance, before running the optimization, is a challenge as it requires the optimization to be run first. Hence, it became a dilemma how to select the most appropriate algorithm among MAs for a specific optimization problem. One way to find this is to run the optimization for different problems, in a variety of MAs, to ascertain the situations at which the optimization achieves the best result. Here, our work is to perform such study in electron optics, for optimization of electrostatic lens systems, which to the best of our knowledge does not yet exist.

II. Optimization Parameters

For this case study we selected an example of an electrostatic lens with 6 lens electrodes to perform the comparison analysis of the above-mentioned different optimization techniques. A cross-section of the round lens is shown in Fig 1.

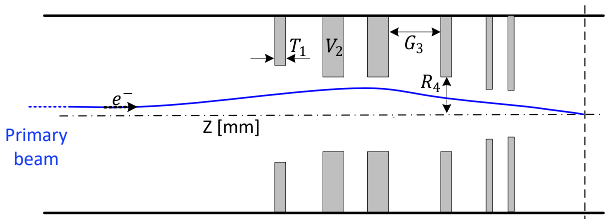

Fig. 1. A 2D illustration of a typical multi-electrode lens systems with 6 electrodes.

The free variables for the optimization are the thicknesses (T_i), Radii (R_i)and voltages (V_i) of each electrode, and the gaps between the electrodes (G_i). There are 23 free variables in total. The electrostatic lens system, as any imaging system, suffers from aberrations. The smaller the aberrations, the higher the resolution of the image and therefore the higher the quality of the lens system. The aberrations can be calculated by aberration integrals, using the electric field on axis and a first order (aberration-free) trajectory. These aberrations can be combined into a contribution to the spot size when the lens is used to image an electron source on a sample as is conducted in a scanning electron microscope. Hence, the objective function for the optimization problem is the spot size at the image side.

It is presumed in our case study that the lens only suffers from spherical and chromatic aberrations. The spot size (presented by D_s in equation 1) can be calculated using the equation below [21].

$$D_s^2 = (0.18\, C_s\, \alpha^3\,)^2 + \,(0.6\, C_c\, \alpha\, \tfrac{\Delta U}{U})^2 \qquad (1)$$

Where C_c and C_s represent chromatic and spherical aberration coefficients, respectively. α (the half opening angle of the beam) is taken as 10 milliradian. U and ΔU (the acceleration energy and the energy spread of the electron source) are chosen here to be 1 kV and 1 eV, respectively. This optimization problem’s constraint is to have the image at a fixed position X_C (at 15mm from the surface of the first electrode) and a maximum allowable electric field between sequential electrodes to prevent discharges. X_C is also a function of the electric field and can be calculated using ray-tracing. Our case-study used MATLAB as the programing language. To calculate the objective function and image position (i.e. D_s and X_C), the field calculation is performed by SOEM and our ray-tracing codes use the paraxial approximation. A PC with an Intel (R) Xeon (R) W-2123 CPU @3.60 GHz and 32 GB of RAM was used to perform the computational work related to this study.

III. Optimization Techniques Applied in Our Case-Study

The optimization procedures which are implemented here include four optimization techniques. The first one is taken from the category “Calculus-Based” which is a local optimization (called “Fmin” in MATLAB). The others are from the category of “Metaheuristics”. One is taken from the “Single-solution Based”, i.e. Simulated Annealing (SA). The two others are the most well-known optimization techniques from the “Population-Based” category namely, Genetic Algorithm (GA) and Particle Swarm Optimization (PSO).

A. *Calculus-Based local optimization*

The so-called “Fmin” in MATLAB, is a “Calculus-based optimization (CBO) technique. CBO uses the gradient (derivatives) of the objective function. This method is implemented on the objective function $f(X)$, starting from an initial point of X_0, taking the steps of δ_N, moving towards the direction of the negative gradient of the objective function to ultimately reach the local minimum of the function. If it is a maximization problem, the direction will be that of the positive gradient of the function to reach the maximum point. Note that in this method, the function $f(X)$ should be differentiable in all neighboring points which are progressively taken under search.

B. *Simulated Annealing (SA)*

Simulated annealing (SA) [22] is a single-solution based, meta-heuristic algorithm. This algorithm simulates the physical process of annealing in a material. Annealing means to heat up a substance to a specified level above a phase transition temperature, and then to lower the temperature gradually, in a specific way, to reach the minimum energy level of the system until the material crystalizes. This crystalized substance, with all its lattice atoms perfectly aligned, is an example of nature finding a beautiful optimum structure of a substance. If, however, the cooling process is performed too fast, the crystalized state will not be reached and the substance becomes an amorphous solid rather than a crystal. The way to achieving the minimum energy level and the crystalized state, is to carefully control the rate of temperature decrement.

In the mathematical optimization context, mimicking from the nature process, a trial point (electrostatic lens system parameters in our case-study optimization problem) is randomly generated based on a defined normal probability distribution within the specified ranges of the parameters. The distance between this trial point and the previous point is based on a probability distribution with a scale parameter depending on the current temperature. The temperature is a pre-defined value by the user. The algorithm then determines whether or not the new point is better than the previous point. If it is better, the previous point is replaced with the new point. If the new point is worse than the previous point, the algorithm may still select the new point based on a probability function. The algorithm lowers the temperature in every iteration. After a certain number of iterations the reannealing process is activated in which the temperature is increased again. The algorithm keeps exploring the landscape until a stopping criteria is reached.

C. Genetic Algoritms (GA)

Randomly created values of the parameters (elements,) called initial population, are the starting point for the GA , a population-solution based, meta-heuristic global optimization method, mimicking natural evolution. The parameter "population" defines the number of elements in each generation, denoted here by N_{pop}. In nature, the elements are the chromosomes of the organism. In electron lens design, the set of electron lens systems from which the lens design variables are determined, represents the elements.

The GA uses a variety of genetic operators namely Crossover, Mutation and Elitism, to gradually improve a set of elements in a so-called "generation" towards the next generation, having a better set of elements, regarding their objective function values. The algorithm proceeds until it satisfies the stopping criteria, which could be set as, for instance, a maximum computational run time, a specified value of objective function, or a maximum number of generations. In our case-study, reaching a specified computational time is chosen to end the process.

D. Particle Sawrm Optimization (PSO)

Particle swarm optimization (PSO) presented in 1995 [23], is another type of population-solution based, meta-heuristic global optimization method which mimics the intelligent collective behaviour of some animals in nature such as birds or flocks.

The algorithm starts by generating a set of initial particles (electrostatic lens systems parameters), and assigns a velocity (randomly selected from a range given by the user) to each particle. It evaluates the objective function for each particle and defines the best location and lowest objective function. It choses new velocities based on particle current velocity, the particle's individual best location and best location of all particles. It then updates the particle position (current position plus the velocity, while making sure the boundaries and constraints are fulfilled). The iteration continues until a stopping criteria is reached. When the defined stopping criteria is reached the algorithm will be ended. The stopping criteria can be determined by the user using different schemas. In this case-study, reaching a certain computational time is set as the stopping criteria.

IV. Results and Analysis

To compare the performance of the above-mentioned different optimization techniques, the minimum value of the Objective Function (OF) reached by the optimization procedures should be evaluated. However, to achieve a fair comparison, the run time is set to a constant value as the stopping criteria of the optimizations. In a previous study it is illustrated that a reasonable computation time could be around T= 1500 sec [7]. This value therefore is set as the stopping criteria of the optimizations.

It should be noted that for the local optimizations, such as "Fmin", the optimization routine may stop before this fixed time, due to the fact that a calculus-based optimization would stop when it reaches the minimum point at each base of attractions.

To perform the comparisons, as the first step, an analysis is performed among the four optimization routines running 10 times to achieve statistically-reliable results. The GA and PSO are run without initial data. However, SA and Fmin need to be assigned an initial data set to start. A random initial system is taken and given as the starting point of SA and Fmin. For some of the initial data, these two optimizations could not find any system which satisfied the constraints (the constraints are considered as part of the objective function). As the first step for these algorithms, an initial system is taken which could lead the SA and Fmin to reach an optimum system which has satisfied the constraints (this initial system is found by trial and error among different randomly created systems).

Figure 2 shows the minimum objective function values, averaged over 10 runs, achieved by the four different optimization techniques. The green bars represent the averaged minimum objective function values. The black thin bars inside the green bars represent the standard deviation in the averaged values for 10 runs.

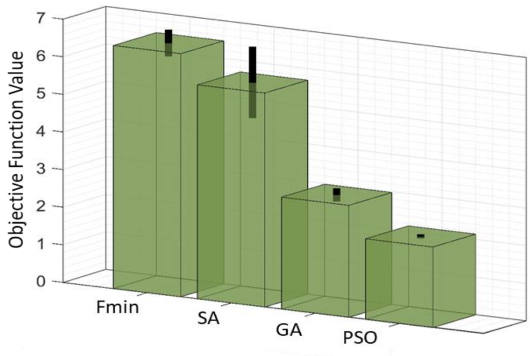

Fig.2. The comparison of the performance for four different Optimization techniques namely Fmin, SA, GA and PSO. The presented values are averaged over 10 runs.

Among the 10 runs, one example run (with the objective function value in the middle range) is depicted as the representative of all runs and illustrated in Figure 3. The y-axis shows the objective function value in the course of the runs. The x-axis presents the system evaluations. The blue, pink, red and green starts are representatives of runs related to the PSO, GA, Fmin and SA, respectively [24-26].

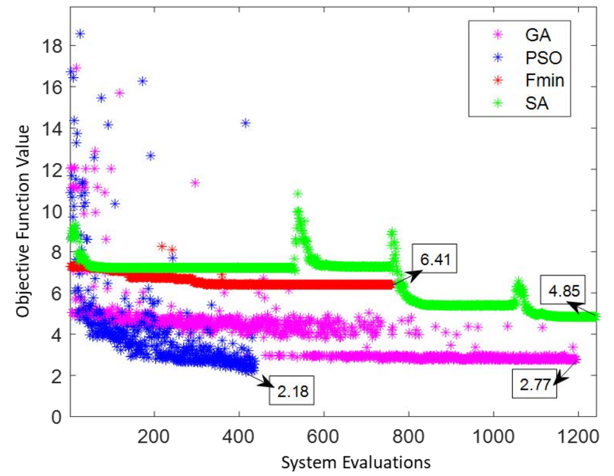

Fig. 3. Comparison of the progress in the four different Optimizations . The presented data is taken from one run among 10 runs as an example representative of different runs.

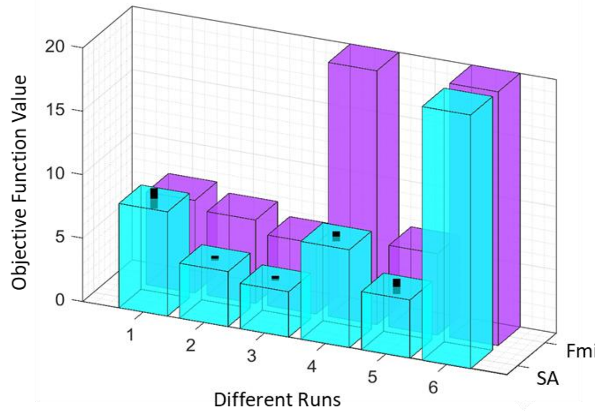

Fig. 4. Comparison of the performance of Fmin and SA. The presented values are averaged over 10 runs.

From Figure 2 and 3, it can be seen that the two optimizations GA and PSO clearly outperform the two others Fmin and SA. Moreover, the standard deviations for the former optimizations (GA and PSO) are much lower compared to the two latter ones (Fmin and SA). This is due to the nature of being meta-heuristic and also to starting and proceeding with populations and not only a single system. This provides a much higher chance of finding the area in the parameter landscape with lower values of the objective function. Due to this, in some literatures, SA is assumed as a local optimizer and not a global one.

Since for Fmin and SA, the results depend on the initial data (X0) which the optimization started with, these two optimizations are run with different initial data to achieve a statistically more reliable analysis. Six different initial data sets are randomly selected by the user and given as the starting points. The correspondent runs are called Try1 to Try6, respectively. Each "Try" is executed 10 times to provide statistically reliable results. The OF averaged over 10 runs and the standard deviations are given in the table below. For the Fmin, because it is based on the derivative of the function, the root finding is always the same and there is no standard deviation. It should also be noted that there are some situations that these two optimizations could not find any systems which have satisfied the constraints.

The data is visualized in figure 4. The blue (purple) bars represent the OF for 6 "Run"s related to the SA (Fmin). The black thin bars inside the blue bars are representative of the standard deviations for different runs.

As can be seen, the OF related to the SA are in most cases lower than the ones of Fmin. There is only one case (Run1) in which Fmin could perform better than SA. In all other runs SA could outperform the Fmin. This can be due to the metaheuristic nature of the SA which does not exist in the calculus-based optimization procedures such as Fmin. The metaheuristic nature causes the optimization to search more extensively the area which leads it not to trap in one local minimum related to that specific basin of attraction of the given starting point.

V. Conclusion

Different optimization techniques such as Fmin, SA, PSO and GA are implemented for electrostatic electron lens design on a typical lens system with six electrodes (23 free variables) to perform a study on the comparison of their performance. The extension of the electrodes to more complex designs is straightforward. In this study it is recognized that the GA and PSO outperform Fmin and SA. The reason can be that the former ones are population-based optimization techniques while the latter ones are single-based optimization ones. It is also seen that the PSO achieves better results than the GA. However, the difference between PSO and GA is not as much as the difference between population-based optimizations and single-based optimizations. It is hence advised to implement the meta-heuristic, global, population-based optimizations such as GA and PSO. It is not possible to conclude that PSO will outperform GA for every problem in electron lens design.

Moreover, from the comparison between two single-based optimization techniques, it is illustrated that the metaheuristic one (SA) outperforms the calculus-based one (Fmin). These two optimization methods work as a sort of local optimization which might not even find any system within the constraints and thus has limited use in electron lens design.

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