Particle swarm optimization and evolutionary methods for plasmonic biomedical applications

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Abstract—In this paper the Evolutionary Method (EM) and the Particle Swarm Optimization (PSO), which are based on competitiveness and collaborative algorithms respectively, are investigated for plasmonic design. Actually, plasmonics represents a rapidly expanding interdisciplinary field with numerous devices for physical, biological and medicine applications. In this study, four EM and PSO algorithms are tested in two different plasmonic applications: design of surface plasmon resonance (SPR) based biosensors and optimization of hollow nanospheres used in curative purposes (cancer photothermal therapy). Specific problems—in addition of being multimodal and having different topologies— are related to plasmonic design; therefore the most efficient optimization method should be determined through a comparative study. Results of simulations enable also to characterize the optimization methods and depict in which case they are more efficient.

Keywords - particle swarm optimization; evolutionary method; biomedical; multimodal

I. INTRODUCTION

The biomedical applications of surface plasmon resonance (SPR) of metal nanostructures, taking advantage of the acute interaction between light and metallic objects, are of growing interest. For instance, the first successes of cancer treatment using nanoparticle-based photothermal therapy (PTT) (the illumination of the nanostructure induces an elevation of temperature which is used to burn the cancer cells) are encouraging for more investigations in this field to ensure efficient heat conversion. Biosensors, another SPR application, have also an increasing expansion since the success in the nanofabrication engineering control [1]. They have many applications like detection of molecules responsible for some diseases due to changes in optical properties once these molecules are present in the biosensor surroundings.

This breakthrough is due to many experimental costly studies devoted to applications of plasmonic resonance (e.g. the fabrication process of the SPR biosensors in nanometer scale is complex and costly). Some of these studies were devoted to optimization of the related devices (e.g. shape, size and illumination condition) to enhance their efficiency [2]. In addition to cost and time consuming, experiences deal only with some samples of nanodevices (not optimized) [3], [4]. Hence theoretical studies are required to depict the specificity of these problems. Moreover, finding adequate optimization algorithms could meet the need of enhancing these devices with minimal computational efforts mainly as some biomedical devices are complex (e.g. models where numerical discretization is required) and deriving a unique model could take several days.

Therefore in this study, we focus on two different applications of plasmonic resonance which are plane biosensors and cancer PTT by gold hollow nanospheres. The purpose is to determine the specificity of each of these problems (the topology of the fitness function) and to find the most efficient algorithm to be used in plasmonic field. The meta-heuristics used in this study are the Evolutionary Method (EM) which is based on competitiveness and the Particle Swarm Optimization (PSO) which is based on a collaborative search algorithm. Some modifications of these conventional methods were proposed [5], [6] to get faster convergence and are tested in this study as well as the standard PSO [7] and the adaptive PSO (APSO) [8].

This paper is organized as follows: the second section gives a brief overview of the four methods used in this study. In the third section, the SPR plane biosensor will be presented and results of simulations will be reported and discussed. In the fourth section, similarly the optimization of hollow nanospheres will be achieved. Finally, concluding remarks will be given.

II. OPTIMIZATION USING EVOLUTIONARY METHOD AND PARTICLE SWARM OPTIMIZATION

In this section brief overviews of the four methods used for plasmonic design are given. In this study, the target is to maximize the electromagnetic absorption (responsible for heat damage of cancer cells) of hollow nanospheres and to minimize the reflectance of SPR plane biosensor. The purpose of the optimization is to find as quickly as possible the best decision variables (to be detailed in the following sections) to reach the target in each case. A classical test of efficiency of the optimization methods consists in repeating several realizations of the optimizations. Thousand realizations in each case are done with a maximum of only 1000 function evaluations allowed within the objective of finding the optimization method that ensures fast convergence for further time-consuming application. Let us note that the same parametric setting of the optimization methods is used in both applications.
A. Evolutionary method: ANUHEM

Evolutionary Methods were first introduced by Schwefel in 1995 [9] and applied to the resolution of inverse problem in near-field optics [10]. The evolutionary method investigated in this study is a modified evolutionary method: the Adaptive Non Uniform Hyper Ellistist Evolutionary Method (ANUHEM) [6]. The evolutionary scheme consists basically of four steps: initialization, recombination, mutation and selection. A first population of parameters $x_i(1)$, $(i = 1...\mu)$, with $\mu$ “parents”, is randomly generated and their fitness is evaluated and then begins the evolutionary loop on generation (or step) $t$:

1) **Recombination** (or crossover); randomly extracted elements of the initial population are combined together to lead to a secondary population of $\lambda$ elements. The quality of each element (inverse value of the fitness function in case of minimization problem) is used to weight each element, leading to a barycentric approach.

2) **Mutation**: these elements are randomly mutated through a non-uniform law and evaluated. The non-uniform law is

$$NU(T, b, t) = 1 - (U^{(1-t/T)})^{b(t)}$$

where $U$ is the uniform law in $[0, 1]$, $t$ is the generation or step, $T$ is the maximum of allowed generations for the process, $b(t)$ is the adaptive term determining the degree of non-uniformity of the fitness function and given by the ratio of the standard deviation of the population to the standard deviation ($std$) of the fitness function $F$, and this, for each element of $x(t)$

$$b(t) = std(F(t))/std(x(t))$$

3) **Selection**: the $\mu$ best elements are selected.

4) The selected population replace the initial one (the new “parents”).

ANUHEM uses the non-uniform mutation that increases the search capability of the algorithm, and weighted recombination that enables faster convergence toward the best set of parameters, compared to other evolutionary scheme [6]. The exogenous parameters used for ANUHEM are $\mu = 5$, $\lambda = 25$ (typically $5 \leq \lambda/\mu \leq 7$ is the most efficient as discussed in [6, 9]) and $T = 40$ (as the maximum number of allowed evaluations is set to 1000 and $\lambda=25$ new elements are generated at each step).

B. Standard PSO

The PSO was first introduced by Kennedy and Eberhart in 1995 [7] and imitates the swarm behavior to search the best solution. This method is basically a cooperative method where vectors of variables $x(t)$ are randomly generated initially and considered as particles. The decision variables are therefore considered as particles of a swarm which communicate good positions to each other and adjust their own position $x(t)$ and velocity $V(t)$ based on these best positions as following:

$$V(t+1) = \omega V(t) + U_1 c_1(p(t) - x(t)) + U_2 c_2(g(t) - x(t))$$

$$x(t + 1) = x(t) + V(t + 1)$$

where $U_i (i = 1, 2)$ are independent random uniform variables between 0 and 1, $p(t)$ is the particle best position over previous generations at step $t$, $g(t)$ is the global best, $\omega$ is the inertial weight and $c_i (i = 1, 2)$ are the acceleration coefficients. Equation 3 is used to calculate the particle new velocity using its previous velocity and the distances between its current position and its own best found position i.e. its own best experience $p(t)$ and the swarm global best $g(t)$. Then the particle moves toward a new position following equation 4. The success of PSO strongly depends on values taken by $c_1$ and $c_2$. Initially, many PSO algorithms have used equal values for these parameters but recent work reports that it might be better to choose the cognitive parameter $c_1$ larger than the social parameter $c_2$, but with $c_1 + c_2 < 4$ [11]. For PSO, the population size is set to 20, $c_1 = 0.738$ and $c_2 = 1.51$ and $\omega$ is linearly decreased [12].

C. Adaptive PSO (APSO)

Zhan et al. outlined the necessity of updating the acceleration coefficients and the inertia weight at each step following the evolutionary state [8]. They estimate the evolutionary state at each step (exploration, exploitation, convergence or jumping out from a local optimum) using the previous state and the value taken by the “evolutionary factor” which is computed using distance between the best particle and other particles normalized by the maximal distance (see [8] for further details). Then based on this estimation, APSO updates the inertia weight and acceleration coefficients. The acceleration coefficients $c_1$ and $c_2$ are initialized to 2. Then $c_1$ keeps increasing during the exploration and exploitation and decreases during the convergence or jumping-out (following some specific rules), while $c_2$ performs the opposite behavior. This may help exploring the local optima during the exploration and exploitation phases and crowding around the global best in the other phases of the algorithm. Finally to avoid local optima, APSO performs elitist learning in the convergence state which will act on the globally best particle and to jump out of the likely local optima. APSO was efficiently applied to a set of test functions and an improvement of the convergence speed of this method was proposed in a previous study by decreasing the impact of the particles getting out of the domain of the physically acceptable parameters [13]. Similarly to the standard PSO, we set the population size to 20.

D. Adaptive non-uniform PSO (ANUPSO)

The ANUPSO [5] is introduced to exploit topological information gathered about the “slope” of the solution $b(t)$ (equation 2), i.e. the spreading/dispersion of the population with regards to their quality. Zhao et al. [14] explain how $b(t)$ determines the degree of non-uniformity: the diversity of parameters increases instead the average speed of the diversity decreases, when $b(t)$ increases. To exploit this information, the equations 3 and 4 are used to update position of particles, but a non-uniform law is used instead of the uniform law. This non uniform law is the law introduced by ANUHEM.
and given by equation 1. The acceleration coefficients are set to 10 to balance the cognitive and social velocities in equation 3 with non-uniform law, the inertia weight is given by

$$w(t) = \max_{b(t)}$$

and the population size is set to 20. This algorithm is considered as adaptive as the inertia weight and the accelerations are updated according to the slope of the solution. $b(t)$ can differ for each particle ($x(t)$) and therefore takes into account the “sensitivity” of the fitness function $F$ to different values of decision variables.

III. APPLICATION TO DESIGN OF SPR BIOSENSOR

A. Characterization of SPR biosensor

The operating principle of the SPR biosensors is based on the shift of the position of mathematical poles. This mathematical issue is in fact related to a critical change of the interaction between light and substrate that happens in presence of slight environment changes (the presence of substances to be detected by the sensor) [15]. Basically, a sudden absorption of light by metal layer of the biosensor occurs, for a given incidence angle of the illumination, leading to a device with high sensitivity to any change in the surrounding biological environment [16]. For instance, as shown by figure 1, the presence of biological molecules induces a shift of the minimal reflectance. This shift should be specific to each molecule to be detected if the biosensor is of high sensitivity.

To guarantee the sensitivity of the biosensor, a pronounced minimal reflectance (approximately zero) should be found. This problem depends on complex variables (permittivity of some components). Moreover, in general case, it could be a function of more than ten variables [17], [18]. As the number of variables increases, the need of defining an appropriate optimization method should be met.

The SPR biosensor, considered in this paper, is made of a glass prism and two metallic layers: a stick chromium layer with fixed thickness of 2 nanometers (nm) and a gold layer of thickness $e$ (see figure 2). The performance of the structure corresponds to a vanishing reflection i.e the light reflected by the biosensor once illuminated by light with incidence angle $\theta$. We denote by $R(e, \theta)$ the reflectance which represents the objective function to be minimized, explicated fully in [6], where $e$ (nm), $\theta$ (degrees) are the decision variables. The search space, governed by physical constraints [2], is $(e, \theta) \in [30.0, 70.0] \times [58, 89.5]$. The optical characteristics of the biosensor correspond to a monochromatic red light (wavelength of 670 nm).

B. Results and discussion

Table I summarizes the obtained results: success ratio and mean number of evaluations used as an indicator of the convergence speed. The success ratio is given by the percentage of realizations that succeed to reach an objective value of $R(e, \theta) = 10^{-4}$ (as mentioned previously one thousand realizations are carried).

The theoretical best solution (see table I) is determined through a double loop (scanning the considered search space). The theoretical model matches with experience as the results are in agreement with the experimental results obtained by
Neff et al. [2]. In their study, Neff et al. consider a Chromium layer with fixed thickness (2.5 nm) and find a pronounced minimum reflectance for illumination incidence $\theta = 68^\circ$ and for a gold layer thickness in the range of 50-60 nm. The purpose of this study is to set a benchmark for plasmonic field therefore the efficiency of optimization algorithms is discussed. A pronounced supremacy of APSO and ANUPSO could be concluded as both guarantee a success ratio of 100% and a fast convergence with only about 200 evaluations while finding the exact solution by a double loop requires 12800 evaluations (precision of 1 degree for $\theta$ and 0.1 nm for $e$). Therefore, finding adequate optimization scheme is important to minimize the computational effort (in this particular simple 2D problem the required number of evaluations is deceased by three orders of magnitude via APSO or ANUPSO).

Regarding the results obtained by the standard PSO and ANUHEM, the failure (success ratio < 100%) could be related to the topology of the optimized function. In fact, as shown by figure 3, the associated problem is multimodal (the map of the fitness function is non-convex) and these methods do not avoid local optima in all realizations. A further discussion of this issue will be carried in the next section, after testing these methods on the second SPR problem.

In addition to the topology, the number of parents $\mu$ may be so small that ANUHEM fails to find global optimum (lack of diversity). Therefore, $\mu$ is varied from 5 to 70 by step of 5 and the selection pressure $\lambda/\mu$ is varied from 1 to 7. As the best success ratio and the lowest number of evaluations are aimed at, we remove all the Pareto-dominated couple $(\mu, \lambda)$ i.e. for which a better success ratio and a lower number of evaluations are found using different values of $(\mu, \lambda)$. The retained solutions show that equal number of children and parents should be used $(\mu, \lambda)$ that differs from the results obtained for sphere function [9]. For instance, a success ratio of at least 99% with lower mean number of evaluations is obtained when $\mu=\lambda=60$ (success=99.7%, evaluations=511). Using this setting, the success ratio of ANUHEM is improved; however the method is slower than APSO and ANUPSO which may be explained by the topology of the problem.  

IV. APPLICATION TO OPTIMIZATION OF HOLLOW NANOSPHERES

A. Use of hollow nanosphere in photothermal therapy (PTT)

PTT in the visible region is suitable for shallow cancer (e.g. skin cancer) whereas for in vivo therapy of tumors under skin and deeply seated within tissue, near infrared (NIR) light is required because of its deep penetration. In the NIR, organic molecules have limited absorption [19], whereas gold nanoparticles absorb light millions of times stronger than the organic molecules. Almost all the absorbed light is converted to heat and consequently cancer cells embedded with nanoparticles are burned with minimal damage to the surroundings.

Most of gold nanoparticles have sizes that are too large or shapes that are too complex for biomedical applications. The right size and shape are needed for effective delivery to locations of interest for PTT. In addition, the spectral bandwidth of the surface plasmon absorption should ideally be narrow for a better match with the laser wavelength (illuminating light). The breakdown of the symmetry of nanostructures produces different modes and thus broad spectrum absorption. Therefore, in the ideal case, nanostructures with narrow but tunable absorption band, small size, and spherical shape are preferred [20], [21]. Hollow nanospheres (figure 4) guarantees such tunable resonance of plasmon absorption by adjusting their size parameters at different wavelength ranging from visible to near infrared [22]. In what follows, the purpose is to find the best set of inner radius $r$ and shell thickness $e$ to maximize the absorbed density of electromagnetic power $M$ [23], through a more efficient method than the basic double loop on these parameters.

B. Results, discussion and comparative analysis

The hollow particles can be made in sizes ranging from 10–12 nm in radius (outer radius) and 3 nm in shell thickness with a precision of 0.6 nm [22]. For this, we can consider hollow gold nanospheres and nanoshells having an inner radius within the range 10-50 nm and a metal thickness 3-30 nm which is an ideal range for biological applications that require small particles to be incorporated into living cells. Two different
The optimization of nanoparticles differs from the one of planar biosensor in terms of the mathematical properties of the model: different topologies are found even if the best parameters should correspond in both cases to a plasmon resonance. Therefore, the methods ANUPSO and ANUHEM exhibit different performances in each application. In the case of hollow nanospheres for PTT, the problem is also multimodal (see figure 5) but the global optima is localized within a tight space (like a deep well). In this case, the ANUHEM succeed to find the global optima driven by the deep slope of the global solution (as explained in the second section) and succeeds to avoid local optima. However, in the case of SPR biosensor, as shown by figure 3, the local optimum is localized on the boundary of the search area (figure 3 and has a more pronounced slope and therefore ANUHEM is sometimes trapped in this optimum (30% of the realizations/trials when \((\mu, \lambda)=(5,25)\) or needs more function evaluations for convergence (511 when \((\mu, \lambda)=(60,60)\)).

The failure of ANUPSO in optimizing the hollow nanosphere is related to the presence of deep well (figure4). In fact, once some particles are attracted to this well, the standard deviation of the fitness function \(\text{std}(M)\) gets high values, as well as \(b(t)\) (see equation 2). Consequently, the particles are monitored by big steps (velocity \(V\)) dispersing them in the search space which prevents the convergence. Therefore, some corrections need to be carried to avoid similar behavior of the method in presence of deep wells.

### V. Conclusions

In this study, two plasmonic 2D problems are addressed to be used as a benchmark study for future complex theoretical application in this field. The first application is the design of plane biosensor used to depict the presence of some molecules in a fluid. The second application is related with the photothermal therapy of cancer: optimizing size parameters of gold hollow nanospheres in two practical cases shallow cancer and deep cancer.

To optimize these two applications, we tested four methods involving one evolutionary method and three variations of particle swarm optimization. The success of the method induces a higher efficiency of the related devices. This means a biosensor able to detect specific molecules in its surroundings (a pronounced minimal reflectance and a pronounced shift). Regarding the nanoparticles used in photothermal therapy a higher efficiency implies a higher heat delivery to cancer cells that should necrosis rapidly in this case.
The different performances depicted of ANUHEM and ANUPSO are analyzed through a comparison of topologies of the two applications. It was found that the ANUHEM is very sensitive to the slope of fitness function and therefore such method could be drawn in failure if a deep local optimum is on the boundary of the search area. Nevertheless, ANUHEM succeeds to find the global optimum if adequate parametric setting is used for each plasmonic application. Regarding the ANUPSO, failure trials are explained by big steps (velocity V) dispersing the particles and preventing the convergence. This method, recently introduced, has encouraging results in the design of the Champagne Ardenne,” the “Conseil général de l’Aube” and 241818).

Results show that the standard PSO fails to avoid local optima: 15% to 30% of failure for the different cases (particles are trapped in local optima). Therefore, improved PSO like APSO (almost 100% of successful trials) is more recommended. For further applications, the APSO algorithm could be used efficiently to optimize more complex plasmonic structures—having more complex geometry or more parameters and for which function evaluations are much more time consuming—as it converges within few evaluations to the global optimum.

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