Comparison of an self-organizing migration algorithm with simulated annealing and differential evolution for automated waveform tuning

L. Nolle\textsuperscript{a,}\textsuperscript{*}, I. Zelinka\textsuperscript{b}, A.A. Hopgood\textsuperscript{a}, A. Goodyear\textsuperscript{c}

\textsuperscript{a}School of Computing and Informatics, Nottingham Trent University, Burton Street, Nottingham NG1 4BU, UK
\textsuperscript{b}Institute of Information Technologies, Faculty of Technology, Tomas Bata University, Mostni 5139, Zlin, Czech Republic
\textsuperscript{c}Oxford Research Unit, The Open University, Boars Hill, Oxford OX1 5HR, UK

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Abstract

In this article, the performance of a self-organizing migration algorithm (SOMA), a new stochastic optimization algorithm, has been compared with simulated annealing (SA) and differential evolution (DE) for an engineering application. This application is the automated deduction of 14 Fourier terms in a radio-frequency (RF) waveform to tune a Langmuir probe. Langmuir probes are diagnostic tools used to determine the ion density and the electron energy distribution in plasma processes. RF plasmas are inherently non-linear, and many harmonics of the driving fundamental can be generated in the plasma. RF components across the ion sheath formed around the probe distort the measurements made. To improve the quality of the measurements, these RF components can be removed by an active-compensation method. In this research, this was achieved by applying an RF signal to the probe tip that matches both the phase and amplitude of the RF signal generated from the plasma. Here, seven harmonics are used to generate the waveform applied to the probe tip. Therefore, 14 mutually interacting parameters (seven phases and seven amplitudes) had to be tuned on-line. In previous work SA and DE were applied successfully to this problem, and hence were chosen to be compared with the performance of SOMA. In this application domain, SOMA was found to outperform SA and DE.

Keywords: Langmuir probes; Active compensation; RF plasma; Optimization; Simulated annealing; Differential evolution; Self-organising migration algorithm

1. Introduction

In recent years, a broad class of optimization algorithms has been developed for stochastic optimization, i.e. for optimizing systems where the functional relationship between the independent input variables $x$ and output (objective function) $y$ of a system $S$ is not known. Using stochastic optimization algorithms such as genetic algorithms (GAs) \cite{1}, simulated annealing (SA) \cite{2,3} and differential evolution (DE) \cite{4}, a system is confronted with a random input vector and its response is measured. This response is then used by the optimization algorithm to tune the input vector in such a way that the system produces a better output. This procedure is repeated until the desired output, i.e. target value, is finally reached. One of these optimization algorithms is the self-organizing migration algorithm (SOMA) \cite{5}, which was used in this research and compared with SA and DE.

Many optimization algorithms have been developed and studied extensively over recent years. However, these studies were mostly carried out on artificial test functions or simulations rather than on real systems. Optimization algorithms for engineering applications have different demands compared with artificial test functions, because they might work on real systems, are often confronted with noisy and incomplete data, and they must be both effective and efficient. One of these engineering applications is the automated tuning of a Langmuir probe system for radio-frequency (RF) driven discharge plasmas \cite{6}.

Low pressure radio-frequency driven discharge plasmas that are not in thermal equilibrium are widely used in the material processing industry for etching, deposition and surface treatment, e.g. in the semiconductor industry \cite{7}. 
In order to achieve the best quality products, it is essential for users of such plasmas to have tight control over the plasma and hence appropriate diagnostic tools are beneficial for closed-loop control. Tighter tolerances and higher throughput place greater emphasis on accurate diagnostic feedback as surface processing demands increase to atomic scale resolution.

In this work, a self-organizing migrating algorithm was used for on-line control of an actively compensated Langmuir probe, as can be used as a diagnostic measurement system for industrial RF driven plasma systems. Its performance is compared in this research with simulated annealing [2,3] and differential evolution (DE) [4].

2. Problem domain: low-temperature plasma systems

Artificially produced plasmas are typically generated through the application of electrical energy to a gas. Under normal conditions gases do not conduct electrically with almost all electrons being bound to atoms or molecules. If, however, electrons are introduced and given enough energy by an external power source, then they have the potential for collision with gas atoms or surfaces to release more electrons, which themselves may release other electrons. The resulting electrical breakdown is known as an avalanche effect. The ionized gas or so-formed plasma becomes partially conducting.

2.1. Radio-frequency driven plasmas

The use of RF rather than DC has developed for a number of reasons including efficiency and compatibility with systems in which direct electrical contact with the plasma is not feasible. In the case of industrial RF-powered plasmas, an RF generator is used as the external power source, usually operating at 13.56 MHz or a harmonic of this frequency. This frequency is assigned for industrial, non-telecommunications use. For materials processing, the RF power is either inductively or capacitively coupled into a gas, usually contained in a vacuum vessel with a gas flow control system. Fig. 1 shows a typical configuration for a capacitively coupled system using electrodes.

A main application of RF-powered plasmas is to produce a flux of energetic positive ions, which impinge continuously over a large area of work piece, e.g. for etching or deposition. By its nature the plasma medium is quasineutral. In order that this quasineutrality is obeyed, a plasma sheath forms between the plasma and the bounding surfaces, resulting in a plasma potential that tends to be positive relative to the surfaces. The plasma sheath prevents electrons that have greater mobility than the larger positive ions, from leaving the plasma at a greater rate than the ions. Ions generated in the plasma bulk through ionisation are accelerated across the plasma sheath to the chamber walls and work piece where they are used for surface modification.

2.2. Langmuir probes

Langmuir probes [8], developed in 1924 by Langmuir are one of the oldest probes used to obtain information about low-pressure plasma properties. They consist of small metallic electrodes that are inserted into the plasma bulk. By applying a positive or negative DC potential to the probe relative to the plasma, either an ion or an electron current can be drawn from the plasma. The form of this current with applied DC voltage is used to determine plasma properties such as charged particle densities and the electron energy distribution function. These measured quantities can be related to processing conditions at the surface of the work piece.

The region of space-charge (the sheath) that forms around a probe immersed in a plasma has a highly non-linear electrical characteristic. In RF-generated plasmas, this is a major issue as the excitation process leads to the space potential in the plasma having RF components. As a result, harmonic components of the RF potential across this layer give rise to serious distortion of the probe’s measured DC signal. In order to achieve accurate measurements, the harmonic components across the probe sheath have to be eliminated.

2.3. Active compensation in RF-driven plasmas

To eliminate the time variation of RF potential difference between the probe and the plasma, the probe potential is made to follow that of the plasma [6]. This can be achieved by superimposing a synchronous waveform of appropriate amplitude and phase onto the probe tip. Because plasmas are inherently non-linear, they can generate many harmonics of the exciting fundamental. As a consequence, the RF signal necessary for satisfactory compensation has not only to
match the amplitude and the phase of the exciting RF fundamental, but it has also to match the complex waveform of the harmonics generated in the plasma.

Conveniently, the electrostatic probe generates a useful control signal that indicates the degree of uncompensated RF voltage across the probe sheath. In the presence of a plasma, and without any deliberate biasing of the probe, the isolated electrostatic probe tip adopts a ‘floating potential’, at which it draws zero net current. The effect of inadequate compensation on a probe in an RF plasma is to drive the floating DC potential of the probe less positive than it would be in a perfectly matched situation. Thus, optimal tuning is identical with the probe adopting the most positive potential possible. This ‘floating potential’ of the probe is also referred to here as its DC bias. This DC bias was used in an automated control system as a feedback parameter for compensation of the harmonics at the Langmuir probe tip.

2.4. Automated control system

During previous work, an additive synthesizer (harmonic box) with seven harmonics has been developed [9] to generate the appropriate waveforms for compensation of a Langmuir probe system attached to a Gaseous Electronics Conference (GEC) standard reference plasma reactor [10]. Fig. 2 shows the schematics of the control system for waveform tuning.

The control software selects set-points for the harmonic generator and sets the parameters, i.e. seven amplitudes and seven phases, using 14 digital–analogue (D/A) converters. The harmonic generator, which is synchronized with the main RF power generator, generates the required waveform which is applied to the Langmuir probe. The probe’s floating potential (DC bias) is used as a fitness-measure, i.e. the higher the DC bias the better the compensation. The DC bias is read on-line via a DC buffer and a A/D converter by the computer system. Depending on the optimization algorithm used in the system, the software then calculates a new set-point based on the actual measure of the fitness. It can be seen that all the fitness evaluations are actually measurements rather than simulation results. This implies time restrictions on the search process.

The 14 input parameters interact to some degree due to the technical realization of the synthesizer hardware and the nature of the problem. For example, the slightest departure from an ideal sinusoidal shape in one of the channels introduces harmonics itself. In practice, even after careful electronic design, it is found that there is a weak but significant coupling between amplitude control and phase and vice versa. Small variations in the 14 parameters caused by these interactions could lead to a large deviation from optimum tuning and hence the probe measurement itself. As a consequence of this, the number of points in the discrete search space has to be calculated as follows

\[ n = \left(2^b\right)^p \]  

where

- \( n \) number of points in search space
- \( b \) resolution per channel in bits
- \( p \) number of parameters to be optimized

The D/A and A/D converters used in this project had a resolution of 12 bits and the dimensionality of the search space was 14. Hence, the search space consisted of \( n \approx 3.7 \times 10^{50} \) search points. Due to the system time constant, mapping out the entire search space would take approximately \( 10^{41} \) years with the plasma system used. Hence, mapping out the entire search space was not a practical option.

In previous work, SA [9,11] and DE [12] were used successfully to tune the Langmuir probe. Their performance was compared with the performance of SOMA in this work.

3. Experimental method

All experiments were carried out at the Open University, Oxford Research Unit, UK. Fig. 3 shows the experimental set-up. A digital oscilloscope was used to measure the actual waveforms found by the three-optimization algorithms. The control software ran on a PC under the Linux operating system. The algorithms used for this experiments were written in C++ and integrated with the existing Langmuir probe control system.
3.1. Simulated annealing

Simulated annealing (SA) is a robust general optimisation method that was first introduced by Kirkpatrick et al. [2], based on the work of Metropolis et al. [3]. It simulates the annealing of a metal, in which the metal is heated-up to a temperature near its melting point and then slowly cooled to allow the particles to move towards an optimum energy state. This results in a more uniform crystalline structure and so the process allows some control over the microstructure. SA has been demonstrated to be robust and capable of dealing with noisy and incomplete real-world data. This makes SA suitable for engineering applications.

Simulated annealing is a variation of the hill-climbing algorithm. Both start off from a randomly selected point within the search space. Unlike in hill-climbing, if the fitness of a new candidate solution is less than the fitness of the current solution, the new candidate solution is automatically rejected. Instead it becomes the current solution with a certain transition probability $p(T)$. This transition probability depends on the change in fitness $\Delta E$ and the temperature $T$. Here, ‘temperature’ is an abstract control parameter for the algorithm rather than a real physical measure. The algorithm starts with a high temperature, which is subsequently reduced slowly, usually in steps. On each step, the temperature must be held constant for an appropriate period of time (i.e. number of iterations) in order to allow the algorithm to settle into a ‘thermal equilibrium’, i.e. a balanced state. If this time is too short, the algorithm is likely to converge to a local minimum. The combination of temperature steps and cooling times is known as the annealing schedule, which is usually selected empirically.

3.2. Differential evolution

Differential evolution [4] is a population-based optimization method that works on real-number coded individuals. For each individual $\xi_{i,G}$ in the current generation $G$, DE generates a new trial individual $\xi'_{i,G}$ by adding the weighted difference between two randomly selected individuals $\xi_{r1,G}$ and $\xi_{r2,G}$ to a third randomly selected individual $\xi_{r3,G}$. The resulting individual $\xi'_{i,G}$ is crossed-over with the original individual $\xi_{i,G}$. The fitness of the resulting individual, referred to as perturbated vector $\tilde{u}_{i,G+1}$, is then compared with the fitness of $\tilde{x}_{i,G}$. If the fitness of $\tilde{u}_{i,G+1}$ is greater than the fitness of $\tilde{x}_{i,G}$, $\tilde{x}_{i,G}$ is replaced with $\tilde{u}_{i,G+1}$; otherwise $\tilde{x}_{i,G}$ remains in the population as $\tilde{x}_{i,G+1}$.

Differential evolution is robust, fast, and effective with global optimization ability. It does not require that the objective function is differentiable, and it works with noisy, epistatic and time-dependent objective functions.

3.3. SOMA

SOMA is a stochastic optimization algorithm that is modelled on the social behaviour of co-operating individuals [5]. It was chosen because it has been proven that the algorithm has the ability to converge towards the global optimum [5,13].

SOMA works on a population of candidate solutions in loops called migration loops. Fig. 4 shows pseudo code of the algorithm. The population is initialized randomly distributed over the search space at the beginning of the search. In each loop, the population is evaluated and the solution with the highest fitness becomes the leader $L$ (Fig. 5). Apart from the leader, in one migration loop, all individuals will traverse the input space in the direction of the leader (Fig. 6).

An individual will travel a certain distance (called the path length) towards the leader in $n$ steps of defined length. If the path length is chosen to be greater than one, then the individual will overshoot the leader. This path is perturbed randomly.
3.3.1. Perturbation

Mutation, the random perturbation of individuals, is an important operation for evolutionary strategies (ES). It ensures the diversity amongst the individuals and it also provides the means to restore lost information in a population. Mutation is different in SOMA compared with other ES strategies. SOMA uses a parameter called PRT to achieve perturbation. This parameter has the same effect for SOMA as mutation has for GA. It is defined in the range \([0,1]\) and is used to create a perturbation vector (PRT vector) as follows:

\[
\text{if } \text{rnd}_j < \text{PRT} \text{ then } \text{PRT}_j = 1 \text{ else } 0, \quad j = 1, K, n_{\text{param}}
\]

The novelty of this approach is that the PRT vector is created before an individual starts its journey over the search space. The PRT vector defines the final movement of an active individual in search space.

The randomly generated binary perturbation vector controls the allowed dimensions for an individual. If an element of the perturbation vector is set to zero, then the individual is not allowed to change its position in the corresponding dimension.

Fig. 7 shows an example of a candidate solution Individual \(I\) that would make a number of steps towards Leader \(L\) without perturbation. With the perturbation vector \([0,1]\) it is only allowed to move in \(y\) direction.

3.3.2. Generating new candidate solutions

In standard ES the Crossover operator usually creates new individuals based on information from the previous generation. Geometrically speaking, new positions are selected from an \(N\) dimensional hyper-plane. In SOMA,
which is based on the simulation of cooperative behaviour of intelligent beings, sequences of new positions in the \( N \)-dimensional hyperplane are generated. They can be thought of as a series of new individuals obtained by the special crossover operation. This crossover operation determines the behaviour of SOMA. The movement of an individual is thus given as follows:

\[
\vec{r} = \vec{r}_0 + m \vec{t} \vec{PRT}\text{ vector}
\]  

where

- \( \vec{r} \) new candidate solution
- \( \vec{r}_0 \) original individual
- \( m \) difference between leader and start position of individual
- \( \vec{t} \) \&lt; 0, path length\[
\]

- \( PRT\text{ vector} \) control vector for perturbation

It can be observed from Eq. (3) that the PRT vector causes an individual to move toward the leading individual (the one with the best fitness) in \( N - k \) dimensional space. If all \( N \) elements of the PRT vector are set to 1 then the second terms on the right-hand side of Eq. (3) equal 0. This means those parameters of an individual that are related to 0 in the PRT vector are ‘frozen’, i.e. not changed during the search. The number of frozen parameters, \( k \), is simply the number of dimensions that are not taking part in the actual search process. Therefore, the search process takes place in an \( N - k \) dimensional subspace.

4. Experimental settings

In order to make the results comparable with results from previous research [9,11], the same plasma parameters were selected for the experiments: argon gas was used at a pressure of 100 m Torr and a flow rate of 9.5 sccm. The plasma was produced using a power output from the RF generator of 50 W.

The parameter settings for SA were chosen to be the same as in previous experiments [9]. The DE parameters were determined empirically based on suggestions described in [11]. Parameters for the SOMA algorithm were also set empirically, i.e. for each algorithm a number of tests with different parameter settings were carried out and the results were compared. The best settings were chosen, as shown in Table 1.

Finding the optimum parameter settings is not an easy task, and can be complicated by the plasma properties drifting over time, i.e. its behaviour is not constant. Plasma mode changes may also occur spontaneously if the plasma is being operated in an unstable regime, again leading to a change in plasma properties.

The experiments were designed so that, for all three algorithms, one optimization cycle took no longer than 4 min, which was a reasonable time period for use of such plasma diagnostic systems. Despite the fact that the search time was limited to 4 min, approx. 12,000 cost functions evaluation, i.e. DC bias measurements (see Fig. 2), satisfactory results were achieved in one optimization run.

5. Results

Each algorithm was applied 20 times in total. In order to compensate for drifts over time of the plasma,
the algorithms were applied alternating, i.e. an algorithm was applied once followed by runs of the other two algorithms before the first one was applied again. The experimental results can be seen in Figs. 8–20 for all three algorithms. Figs. 8–10 show a typical search run over time: the average fitness of the population in Analogue/Digital Converter (ADC) units, the best individual in the current generation and the standard deviation are shown. Figs. 11–13 show the average values of the Digital/Analogue Converters (DAC) and the deviation for all 14 parameters found by the algorithm and in Figs. 14–16 the average waveforms found by the algorithms are depicted. In Fig. 17, the average fitness values achieved and the standard deviations for all three algorithms are documented. From Fig. 18 it can be seen that there was a linear drift of plasma over time, which was observed during all experiments. Fig. 19 shows a comparison of efficiency of all three algorithms, i.e. frequency of which each algorithm outperformed the others.

From these results, it can be seen that SOMA has outperformed DE and SA not only by finding a greater average fitness, but also by having a standard deviation that is marginally smaller than DE and significantly smaller than SA.

6. Conclusion

Three stochastic optimization algorithms, SA, DE and SOMA, were used for online tuning of an actively compensated Langmuir probe system. These algorithms were selected because of the problem complexity. The experimental results demonstrate that, in general, all three algorithms were suitable for active compensation of
the RF-driven plasma probe. However, the results also show that SOMA and DE showed better performance compared with SA in this specific application. SOMA and DE performed almost three times better than SA. Bearing in mind that plasmas are highly non-linear dynamical systems with changing properties (see Fig. 18), then the results produced by SOMA and DE are encouraging.

One of the crucial points in science is reproducibility, i.e. the ability to achieve the same results for two identical experiments. In industrial applications like the one described in this paper, a high degree of reproducibility is needed. From Figs. 11–13 it is clear that SOMA and DE achieve greater reproducibility, i.e. smaller variations, than SA. Their precision was also greater than with SA.

The speed of the optimization process was not determined in this case by the computing power available, but by the time constants of the analogue equipment, e.g. the harmonic delivery hardware. SOMA and DE have shown similar speed performance in this specific application outperforming SA.
Figs. 19 and 20 clearly shows that the best results were obtained by the SOMA algorithm followed by DE. Results given for SA were significantly worse. The small difference between the performance of SOMA and DE shows that both algorithms are highly usable for ‘black-box’ optimization applications, like the tuning of the Langmuir probe.

Fig. 18 shows that the global extreme (and thus the whole fitness function landscape) was not static in time. During the above described experiments (which took almost 12 h of uninterrupted plasma operation), the plasma properties changed with time. This change was linear in behaviour. Changes to the condition of the plasma bounding surfaces, through particle bombardment effects and deposition on surfaces, are a possible reason for parameter drifts. Based on experiments, it can be stated that all three algorithms followed the global extreme position, or found a suboptimal solution, quite well.

Although only three algorithms were used for this experiments, the time needed for setting-up the experiments and the actual realization took slightly more than 2 weeks. The time needed for each experiment was about 4 min. This time can be reduced by using previous results, e.g. by using solutions from previous runs as starting points for new search runs. This modification should be considered for future experiments with active compensation in RF-driven plasmas where similar plasma processing conditions may be repeated.

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