NOVEL ALGORITHM FOR GEOMETRICAL OPTIMIZATION OF FLOW CHANNELS

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Abstract. The paper proposes a novel algorithm developed for the geometrical optimization of various flow channels. Mainly, such optimization aims at decreasing the total pressure losses in the channel, but the present algorithm may be used with trivial modification for any optimization criterion. The concept of the proposed algorithm is using an approach consisting in a combination of Factorial Design of Experiments (FDoE) and Artificial Neural Networks (ANN) to evaluate the effect of the flow channel geometry on the aerodynamic parameter defining the objective of the optimization. The training and testing sets for the development of the ANN will be obtained through simple CFD Reynolds Averaged Numerical Simulations (RANS) of the flow in geometries selected by means of the previously performed FFDoE. These numerical simulations will be carried out as "experiments" able to provide values for the aerodynamic objective. Finally, the aerodynamic objective of choice will be optimized by means of a Genetic Algorithm (GA). The GA results may be, in the end, validated through detailed, time accurate, Large Eddy Simulations (LES).

Keywords: aerodynamic optimization, artificial neural networks, design of experiments.

1. INTRODUCTION

The advantage of the proposed approach rather than carrying out expensive CFD simulation for a series of geometrical configurations resides in the significantly decreased design time, which will not only significantly reduce the design costs, but it will also allow for a more detailed exploration of an extended design space, thus providing a better likelihood of identifying an solution closer to the absolute optimum. Instead,.

The most important advantage the GA has over other optimization methods is the fact that at any time step the GA provides an entire population of potential solutions, compared to just one in the case of simulated annealing, for instance, which increases the algorithm flexibility and allows its automatic redirection towards the sought optimum even if, at a certain point, it may happen to evolve in the wrong direction.

Also significant for the selection of the optimization approach is the fact that in typical optimization problems in gas turbine engine design, a significant number of the possible geometrical parameters combinations lead to an ill defined geometry. In other words, the definition domain of the optimization function is not simply connected. A GA algorithm is flexible enough to quickly discard such ill defined individuals (they are tagged "born dead" at the conception stage and a new reproduction operation is carried out to produce a "healthy" child). Moreover, for this type of problems, the use of both classical, deterministic, optimization approaches, such as the gradient method, as well as alternate Monte Carlo optimization methods (like simulated annealing) is at least impractical, if not plainly impossible, as the likelihood of the algorithm becoming stuck in a restricted region of the objective function definition domain is very high.

2. ALGORITHM DESCRIPTION

2.1. Design space definition

First of all, the starting geometry that needs to be modified is parameterized and discretized into a set of computational cells. The design space will then be defined by the set of operational parameters and their corresponding ranges of values, which is also known as the matrix of the full factorial experiment. Ideally, in order to fully understand the effect of each individual factor and correlations between different factors on the performance of the system, it would be necessary to solve all the cases of the matrix. The main problem is that the number of possible combinations, given by Eq. 1, is quite large, and it is clear that, for more than 2 or 3 parameters, it becomes unfeasible to run all cases from the design space. Therefore, it is necessary to use a statistical tool that allows the simplification of the design exploration. This selection matrix must be chosen in such a way that its results will provide information about the most important features of the problem, while using only a fraction of the effort in terms of experimental runs and resources.

2.2. The Fractional Factorial Design of Experience approach

The FDoE approach is proposed to be used for the definition and selection of the points in the multi-dimensional design space of the engine air intake that will be used for the ANN training. A FDoE is, generally, a method to determine the effects of multiple input variables simultaneously on one, or more, responses. In the approach proposed here, the responses are the aerodynamic objectives listed in the topic call, while the input variables are the geometrical parameters that may be expected to have a significant impact on them, as well as the mass flow rate through the engine air intake, and the flight velocity and altitude. The most important advantage of the FDoE approach is that it can be used to find both main effects from each independent variable, as well as the interaction effects, when the correlated effect of several variables determines the response (Bourgeois et al., 2006). This feature is critical for the goal of the proposed project, as the various geometrical parameters of the engine air intake design are expected to be strongly correlated in determining the flow through the inlet, and hence, the aerodynamic objectives of the topic call.

Since FDoE deals with discrete values of the input variables, the continuous input variables that this proposal deals with will have to be discretized, by defining a variation interval for each, and by selecting a discretization mesh for each such interval.

If all the possible combinations of the input variables are considered, as in the case of a Full FDoE, than the number of experiments, Ne, or, in this case, CFD simulations to be conducted is:

$$N_E = N_L^{N_V} \quad (1)$$

where N_L is the number of distinct values the input variables may take, or "levels", and N_V is the number of input variables.

In the case of the present paper, if a number of 5 levels is chosen for the discretization of the input variables definition intervals, and assuming a conservative number of 10 input variables, the number of CFD simulations required for a Full FDoE is close to a million, which is quite outside the project timeframe and budget. To avoid this, but maintaining the information regarding the influence of the input parameters and their interactions upon the aerodynamic objectives, a Fractional FDoE (FFDoE) will be applied. The resolution of the FFDoE is defined as the ability to separate main effects and low-order interactions (Box et al.). The most important fractional designs are those of resolution III, IV, and V. Resolutions below III are not useful and resolutions above V are wasteful in that the expanded experimentation has no practical benefit in most cases (Box et al.).

To further refine the methodology, and to avoid missing geometrical parameters that may be significant for the aerodynamic objectives of the topic call, the FFDoE will be carried out in two stages.

In the first stage, an exhaustive list of possible geometrical parameters defining the engine air intake geometry will be considered as factors, and a Resolution III FFDoE will be carried out. In terms of accuracy, a Resolution III FFDoE will be able to estimate the main effects, which may be confounded with two-factor interactions (Box et al.). The result analysis of the first stage FFDoE will, however, be able to identify the factors that are not significant for the aerodynamic objectives of the project. For the second stage FFDoE, these factors will be eliminated and a Resolution IV FFDoE will be carried out. In terms of accuracy, a Resolution IV FFDoE will be able to estimate the main effects of each input variable (or factor), unconfounded by two-factor interactions and to estimate two-factor interaction effects, even though these may be confounded with other two-factor interactions (Box et al.).

2.2. The Artificial Neural Networks method

However, FFDoE can only provide relative values8, and to achieve actual numerical values more intricate methods are needed. The approach proposed here is based on ANN. Thus, the CFD evaluated values of the aerodynamic objectives, together with the geometrical parameters used to obtain them, will be used to train and test a set of ANN, one for each aerodynamic objective and for each considered flight velocity, which will be able to predict their values for any combination of input variables.

In general terms, an ANN is a system modelled after the structure of the human brain. Its basic component, called processing element (PE), and analogous to the biological neuron, is a non - linear element that receives a number of inputs (representing the dendrites of its cellular counterpart), as shown in Fig. 1.

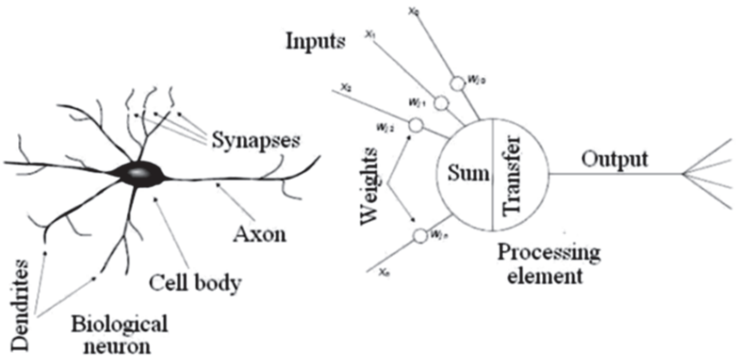


Fig. 1. Schematic representation of the analogy between a biological neuron and an ANN processing element (Porumbel, 2007)

Each input connection has a corresponding weight that modifies the contribution of each input signal to the total PE input. The result of this weighted summation is then processed through the application of a transfer function, and the information is passed along either to another PE or to the ANN output.

The processing elements that form a neural network are organized into groups called layers and are linked to some or all of the neighbouring neurons with various degrees of connectivity representing the strength of the connection. The different layers of the ANN are serially inter-connected, the first layer accepting the input from the external environment and the last one is producing the ANN output. By adjusting the values of these strength coefficients through a process called network training or learning, the network is able to generate an output that is consistent with the expected, known, result.

Once the training phase is completed, the ANN can be further applied for similar problems with satisfactory accuracy to predict the results for unknown problems, meaning a new set of input parameters, in a manner similar to the functioning of the human brain and termed recalling.

The method that is proposed to be used in this project is based on the perceptron concept proposed by Rosenblatt (1962), and employs the back – propagation learning technique. The perceptron was initially developed as a pattern classification system aimed at optical pattern recognition, capable of limited learning and generalization and possessing a great deal of robustness and plasticity.

The back-propagation technique (Parker, 1985) assumes that any error appearing in the output has to be assigned to all processing elements and connections, and the responsibility for the error is affixed by propagating it backwards through the existing connections to the previous PE layer, until reaching the input layer. This is carried out using a transfer function and with the goal of minimizing a global function describing the error between the desired output and the network output.

For the purpose of the work proposed here, two types of transfer functions will be tested: the sigmoid function, defined by Eq. 2 (Porumbel, 2007) and the hyperbolic tangent function, given by Eq. 3 (Porumbel, 2007), but any differentiable function may serve the error back-propagation purpose (Neuralware, 2001).

$$f(z) = \frac{1.0}{1.0 - e^{-z}} \tag{2}$$

$$f(z) = \frac{e^{z} - e^{-z}}{e^{z} + e^{-z}} \tag{3}$$

Previous studies (Porumbel, 2007, Kapoor et al., 2001, Kapoor et al. 2002, Porumbel et al., 2104) have shown that the accuracy of the results predicted by the ANN is strongly affected by several requirements that need to be met:

- The initial training data set must cover the entire space that will be explored during the GA optimization.
- A validation data set is needed to determine the post-training network accuracy. This set of points must not have been used for the initial training in order to correctly assess the ANN validity. For this, the number of available RANS CFD simulations will be split in two sets: one for ANN training, containing two thirds of the available points, and the other for ANN testing.
- The best input / output range from the standpoint of ANN accuracy is in the interval [-1;1]. For this reason, all the data sets must be transformed first through a standardization procedure into a standard, zero mean and unity variance set and next through a normalization procedure into an [–1,1] interval.
- Finally, a logarithmic transformation (similar to a histogram redistribution) must applied on the

data set in order to smooth out the sudden changes in the response values that may affect ANN accuracy.

The typical back-propagation ANN architecture consists of an input layer, several, intermediate, hidden layers, and an output layer. Previous work (Neuralware, 2001) indicates that 3 hidden layers are sufficient for solving a problem with any degree of complexity.

So far there exists no established methodology or guiding principle for determining the optimum network structure and the ANN optimization still remains a trial and error procedure for each problem at hand.

The number of PEs in each layer is determined as follows:

- In the input layer, the number of PE must be equal to the number of factors in the FFDoE, i.e. the number of input variables (geometrical parameters).
- In the hidden layers, the number of PEs will be decided by trying to maximize the ANN accuracy, through a trial and error procedure. As a recommendation based on a multitude of trials performed by the researchers in the consortium 10,16, the total number of PE's in the hidden layers should be about the same as the number of PE's in the input layers, distributed decreasingly between the hidden layers.
- In the output layer, there should be 1 PE, corresponding to one of the aerodynamic objectives listed in the topic call.

Once trained, the ANN will provide the correlation coefficients able to model the variation of the aerodynamic objectives as functions of the input variables for any of the test cases required in the topic call. Those correlation coefficients will be computed off - line, stored in the form of weights and biases and read by the optimization algorithm at its initialization. A set of ANN will be developed for each of the flight cases required in the call topic.

2.3. The Genetic Algorithm optimization

The proposed optimization algorithm is GA. The GA evolution as an optimization algorithm is based on the so-called Monte Carlo (MC) methods (Shonkwiler and Mendvil, 2009). Generally, MC methods are computer algorithms that make vital use of random numbers and are usually used for problems of a complexity that renders the use of deterministic algorithms. The reasons can be because such a solution does not exist, or because a deterministic approach will require an extremely long solution time, or because the accuracy of the input data is highly uncertain (Cuciumita, 2011). In the case of the problem at hand, since a CFD solution for the flow inside the engine air intake is achievable, the use of deterministic algorithms is possible. However, this will be very costly in terms of computational resources, and the use of MC optimization algorithms is proposed instead. According to the definition given by a pioneer researcher in the field (Fermi et al., 1965), MC methods are techniques of performing computer mathematical experiments for simulating complex physical systems that allow quantitative modelling.

Generally, an MC method has four steps (Cuciumita, 2011):

- A problem variables definition domain is determined.
- Random values for these variables are generated inside their respective definition domain using Probability Distribution Functions (PDF) corresponding to the physical characteristics of the simulated system.
- A deterministic algorithm is applied on these values, and the state of the system is evaluated for each considered random variables combination.
- The results are analyzed.

As the MC methods were applied in more and more domains, they started being combined with the so-called Markov Chains (MkC) (Shonkwiler and Mendvil, 2009), which are defined as mathematical systems, usually discrete, having a finite, or at least enumerable number of states between which they may commute from a discrete computational step (usually in time) to the next. The state of the system at the next step only depends on the current state of the system, and not on the earlier states (Shonkwiler and Mendvil, 2009). A MkC applied for MC methods bears the name of "Markov Chain Monte Carlo" (MkCMC). They extend the idea of unique probabilistic experiment with a result in the known space, to a series of experiments carried out over a given solution space, one for each time step. The state of the MkCMC after a sufficiently large number of steps is called an "equilibrium distribution" (Shonkwiler and Mendvil, 2009).

One of the most important and interesting domains where MkCMC can be applied is optimization (Shonkwiler and Mendvil, 2009). Formally, an optimization problem consists in determining, in a given definition domain, the vector x for which a given function, *f(x)*, named the "objective function", reaches its global optimum within its value domain. Among the best known and used MC optimization methods are the Simulated Annealing and the GA.

GA is an optimization method that simulate the evolution and the biological adaptation of living organisms. The principle behind a GA is, similar to the case of living organisms, that through the repeated application of the selective reproduction mechanisms included in the algorithm, the potential solutions population approaches an optimum.

Thus, GA is a MkC (Shonkwiler and Mendvil, 2009) consisting in a series of populations over the objective function definition domain. In the case of this proposal, the objective function is an expression of the aerodynamic objectives listed in the topic call, each of them being evaluated as a function of the input variables through the weights and biases provided by the ANN at the previous step. At a given time step, such a population is termed a "generation". The population is generally formed by a number of individuals characterized by a certain so-called "genetic code", or "chromosome", and they are, practically representations (usually binary) of the associated MkC state at the current time step (Cuciumita, 2011). The initial population is generated by a random combination of the state vectors over the possible state spaces.

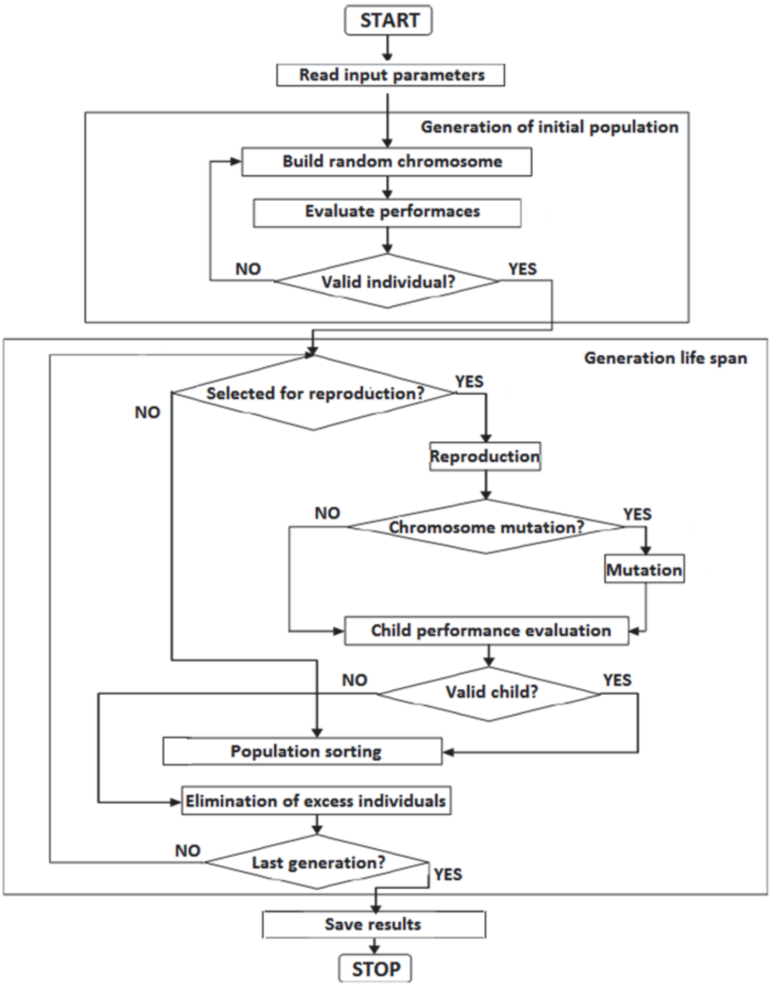
The individuals are subject to the action three operators: genetic recombination, mutation, and selection (Shonkwiler and Mendvil, 2009). The mutation is a unary operator, the genetic recombination is a binary operator, and the selection is a multidimensional operator. The MkC associated to a GA must always be irreducible and non-periodic, such that its equilibrium distribution exists and is unique (Shonkwiler and Mendvil, 2009). In the order of their GA application, the three operators can be briefly described as follows (Cuciumita, 2011):

- Genetic recombination (or reproduction) operates on two randomly selected individuals from the current generation population, termed as "parents". The selection is made based on a given PDF. The result of the operation is a third individual, the so-called "child", whose genetic code is a combination of the parental chromosomes. The purpose of the operation is to diversify the current generation population by creating new state vectors that can further optimize, step by step, the objective function.
- Mutation operates, with a given probability, on the children, at the time of their conception, by randomly modifying their chromosome. The role of the mutation is to avoid the algorithm to get stuck in local optima, by creating completely new children, different from both parents.
- Selection operates on the entire population of a generation, and decides which of the composing individuals survives to the next generation. The selection is made through the evaluation of the objective function, saving only the individuals (and, implicitly, their genetic codes), which are the closest to the sought optimum.

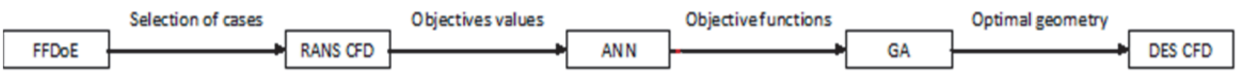
The most important advantage the GA has over the main rival MC optimization method, is the fact that at any time step the GA provides an entire population of potential solutions, compared to just one in the case of simulated annealing. This increases the algorithm flexibility and allows its automatic redirection towards the sought optimum even if, at a certain point, it may happen to evolve in the wrong direction (Shonkwiler and Mendvil, 2009).

Also, as an instance of irreducible MkC, the GA driven system will eventually pass through all possible states, hence through the global optimum as well, thanks to mutations (Shonkwiler and Mendvil, 2009). In different words, given an infinite number of generations, the probability of reaching the global optimum is 1 (Cuciumita, 2011). However, the time to reach this global optimum may be particularly long, and to avoid this, in practical applications, the successive restarts technique (Shonkwiler and Mendvil, 2009) is used, by which the current, assumed optimal, solution is saved and the algorithm is restarted with a new initial population. Previous studies of such a GA have shown that for a sufficiently large population (of the order of thousands of individuals), ten independent runs always lead to the globally optimal solution (Cuciumita et al, 2011).

Also significant for the selection of the optimization approach is the fact that in problems such as the one at hand, a significant number of the possible geometrical parameters combinations lead to an ill defined geometry. In other word, the definition domain of the optimization function is not simply connected. Another major advantage over most optimization approaches, is that a GA algorithm is flexible enough to quickly discard such ill defined individuals (they are tagged "born dead" at the conception stage and a new reproduction operation is carried out to produce a "healthy" child). Moreover, for this type of problems, the use of both classical, deterministic, optimization approaches, such as the gradient method, as well as alternate MC optimization methods (like simulated annealing) is at least impractical, if not plainly impossible (Cuciumita, 2011), as the likelihood of the algorithm becoming stuck in a restricted region of the objective function definition domain is very high (Cuciumita, 2011). A diagram of the proposed GA structure is presented in Fig. 2.



Fig, 2. Diagram of the proposed GA algorithm (Cuciumita, 2011).



Fig, 3. Diagram of the proposed workflow.

2.4. The numerical simulation validation

Finally, after the GA has provided an optimal solution, the optimization algorithm will be validated by means of detailed DES calculations aimed at verifying that the predicted engine air intake aerodynamic objectives values are indeed obtained. A diagram of the optimization workflow is presented in Fig. 3.

CFD flow calculations will be carried out in order to provide initial data for ANN training and within the developed workflow for 3D aerodynamic optimization process of the engine air intake, with and without considering the IBF. All the CFD simulations will be completed within the framework of the ANSYS Inc. simulation software. The flow calculations necessary for the ANN training will be carried out based on steady-state RANS formulation, while the flow predictions required for the validation of the developed workflow will be performed based on the DES approach. All the simulations part of the 3D aerodynamic optimization process of the engine air intake will be based on steady-state RANS calculations.

Within the CFD framework, the RANS formulations with the correspondent turbulence closures are very useful in particular for “fast-screening” of a large number of cases or set-ups. Simulating a large number of set-ups in a short period of time and identifying trends in the flow behavior when performing a parameter study are necessary processes within an ordinary design optimization process (Hirsch and Tartinville, 2009). Within the present project this advantage is maximized by integrating the RANS flow solver within the workflow for 3D optimization process which includes links between CAD, the mesh generator, the CFD solver and optimizer.

3. CONCLUSIONS AND FUTURE WORK

The paper presents a novel optimization algorithm based on a combination of Fractional Factorial Design of Experiments, Artificial Neural Networks, and Genetic Algorithms, validated through RANS / DES numerical simulations.

The presented algorithm will be used for the optimization of an aircraft engine air inlet within a European research program in the Cleansky 2 framework. The results from the optimization procedure will be presented in a future research paper.

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