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# Simulation Data Management for Adaptive Design Of Experiment

A literature review

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Recent evolutions of computer-aided product development and massive integration of numerical simulations to the design process require new methodologies to decrease the computational costs. Numerical design of experiments is used to improve quality of products by taking into account uncertainties in product development. But, this method can be time-consuming and involves a high computational cost. This paper presents a literature review of design of experiments methodology to identify potential improvements for simulation process shortening. By means of metamodelling and adaptive design of experiments, the computational cost of each simulation and the number of required experiment can be reduced. However, methods involved are still time-consuming to be set up.

Index Terms— Adaptive Design of Experiment, Numerical Model, Robust Design, Product Development Process.

#### I. INTRODUCTION

Nowadays, competitiveness and efficiency of companies must be continuously improved to face worldwide competitors. Their processes and products must be continuously optimised with Quality, Cost and Time (QCT) objectives. As simulation is integrated to the product development process and is used to reach QCT objectives, the simulation process must reach these objectives too.

By means of recent advances in computing, numerical simulations are required to: (1) understand the product behaviour, (2) optimise the product, (3) explore several solutions, and (4) validate the product. Numerical Design of Experiments (DoE) is more and more used [1] to fulfil these 4 objectives by planning several runs of a numerical model for different configurations. It can also increase product robustness and quality by taking into account product related uncertainties. Nevertheless, DoE can imply numerous runs of a costly numerical model. Thus, such a DoE can increase the cost and the time of the simulation process.

The paper proposes a research survey which focuses on two subjects: (1) reduction of the number of experiments and Julien LE DUIGOU

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(2) reduction of computational cost of each run. First, Section 2 presents numerical DoE and methods used to reduce cost and time of simulation process. Second, Section 3 focuses on adaptive DoE, used to reduce the number of experiments. Finally, we conclude with the main advantages and drawbacks of the different approaches to find a potential solution improving them.

#### II. NUMERICAL DESIGN OF EXPERIMENTS

#### A. Simulation Process

Numerical simulation is a set of computations representing the behaviour of a system subjected to a physical phenomenon. It aims predicting the response of a system subjected to its environment without any physical experiment. It can be sum up to 3 main steps. This representation can be found from several sources [2]–[4]. These three steps are, most of the time, embedded in Computer-Aided-Engineering systems.

The first step is the modelling (pre-processing): the physical problem is translated into mathematical equations. As an example, the Finite-Element (FE) method is the most well-known modelling method used in mechanical engineering. This step is critical because modelling assumptions are made [5]. The complete model involves a modelling of a phenomenon, a system and its environment. Then, the problem is discretised with respect to its dimensions (spatial, time and other parameters). Finally, solving algorithm parameters are set.

The second step is the solving: equations are formulated from the previously discretised model and solved by the solver software according to chosen algorithms. This step can be improved by optimising the used methods [6]. Usually, FE models may be solved in several hours or even more. Thus, loops on this step (iterations or DoE) may require an extremely high computational cost, without certainty about results correctness.

The last step consists in checking results and model validity (post-processing), and storing relevant data.

#### B. Classic design of experiments

Numerical DoE is a set of numerical experiments defined to assess the numerical model for different configurations, specifications or solutions. This method consists in exploring a design space, to improve product robustness and quality. It is used for sensitivity analysis, product optimisation or design exploration. A DoE is defined by a number n of factors of different types (qualitative, discrete or continuous) and their p levels. Thus, a DoE involves generally n\*p experiments.

As a numerical DoE is applied to a numerical model, each experiment involves an evaluation of the FE model, and thus computational cost depends on two parameters. First, a run of a FE model may require a huge amount of computational resources to be performed. Second, a DoE involving a large number of runs (i.e. experiments) will increase drastically the needed resources. Thus, an optimal strategy is to choose the most efficient DoE and to use a method for reducing the computational cost of each run. An efficient DoE should minimise the number of runs and optimize the space-covering of the runs, according to the objective (exploration, product optimisation...).

DoE were initially used for physical experiments. Classic DoE were largely studied [7]–[12]. This kind of DOE requires repeated experiments to take into account measure uncertainty. It includes very expensive Full-Factorial design and Fractional-Factorial design, which is a cheaper version as some interactions between several parameters are neglected. It includes also central-composite and Box-Behnken design, limited for 3 or 5 levels, and Doehlert design, involving a more uniform distribution of experiments. All of these designs are based on a pre-selected regression model: they are model-dependent. But, in simulation process, each experiment is made by a deterministic solver. Thus, repeated experiments involved by these DoE are useless. Space-filling designs are more appropriate. This category is based on different criteria, which can be combined, to improve the uniformity of experiment distribution in the design-space. Distance criteria, as maximin and minimax criteria, aim to avoid too closed samples. They are easy to set up but limited for low dimensionality. Other criteria are based on the minimisation discrepancy, i.e. the difference between a uniform sampling and the sampling of interest. Lowdiscrepancy-sequences-based-designs includes, amongst others, uniform design, Halton, Faure or Sobol' sequences designs. However, the distribution uniformity decreases with problem dimensionality. Low-discrepancy designs are based on these DoE and on stochastic algorithms, which minimise the discrepancy. These algorithms improve the distribution uniformity of low-discrepancy-sequences-based-designs, but are largely more costly. Maximal entropy design exists also. It maximises the amount of information in the distribution of experiments. A repulsion criterion is used for Strauss DoE, to maximise the uniformity. Latin Hypercube Sampling (LHS) and orthogonal arrays are built on constraints on projection of experiments on design-space axis. They are largely used as they are simple to build and to be used. The adaptive WSP algorithm [9] was developed to build a space-filling design able to deal with high-dimensional problems (number of parameters >20) and experimental constraints. It is also able to increase the density of experiments in particular zones of interest.

Model-oriented designs can be used to obtain an optimal design [13], [14]. Several optimal designs exist, depending on the optimised criterion used to define each assessment: D-optimal, A-optimal, I and M-optimal [13], etc. If the model is linear in its parameters, these optimal designs are model-independent, otherwise not. However, the choice of the criterion is objective-dependent. A criterion for optimal design is proposed [1], as combination of a criterion to "identify the design region in which system performance is optimised" and design criteria "on the prediction error of the true output". Others criteria for this kind of DoE exist [15]. The authors give an assessment of these criteria for sensitivity analysis.

The selection of a DoE method for a specific problem depends on the uniformity of the distribution, and the filling of design space. Moreover, it is also linked on the objectives and the constraints of DOE. DoE types are numerous, related to different applications and properties (see [1] for additional details on DoE properties). Thus, selection of DoE method may be a very time-consuming process. A design comparison chart was developed to help designers in their choices, but it is non-exhaustive[16]. Thus, there still exists a need for classification and comparison of DoE methods, in order to support designers' decisions. In order to decrease the computational cost, by reducing the number of runs, several methods have been developed, such as adaptive DoE and surrogate modelling. Moreover, the choice of a specific DoE method will depend on the selected metamodel.

#### C. Metamodels

Metamodeling, or Surrogate modelling, consists in replacing the costly FE model by a simpler model, as an analytical function, to approximate a specific response with a lower computational cost. Metamodels are used in many fields and a large amount of works was found related to this method. Applications for structural mechanics [17], Computed Fluid dynamics [18], electromagnetics [19], [20], or forming process [21], [22] can be mentioned. Furthermore, metamodels are used to faster fulfil FE models objectives faster, as model approximation, design space exploration, sensitivity analysis [23] and optimisation [7].

Three steps are required to define a metamodel: (1) the metamodel type selection, (2) the training and (3) the validation.

#### 1) The metamodel type selection step

With the variety of existing metamodels, the selection of the best one may be difficult. A classification of these methods has been made by [24] and is presented here. First, statistical learning methods include Response Surface Methods (RSM) [25], and other polynomial approximations. These methods consist of an approximation of the model response by a polynomial function and to take into account relevant interactions between parameters. Polynomial Chaos is an evolution of these methods. The model response is defined as a stochastic vector and approximated by a linear combination of orthogonal polynomials [26]. Kriging [27], [28], is a linear estimation method, originally designed for geostatistics. It assumes a spatial-correlation between experimental points to interpolate the response, which is assumed to be a stochastic Gaussian process, between them. This method aims to minimize the variance of the estimation. Details on this method and its variants can be found in [29]. Multivariate Adaptive Regression Splines (MARS) method [30] is an upgrade of linear regression methods. It is defined as a linear combination of B-splines instead of linear functions, with algorithms to select relevant terms of the metamodel. Support Vector Regression can also be mentioned [29].



Fig. 1. The metamodel (2nd order polynomial) aims to predict the true function. [31]

The machine learning methods cover, amongst others, Artificial Neural Networks (ANN) and clustering techniques. Clustering techniques involve the clustering of the population of evaluation, generated by a DoE. For instance, for each cluster, only one assessment is executed and the others are done by another local metamodel, specific to each cluster. Artificial Neural Networks (ANN) such as Multilayer Perceptron Neural Networks (MLPNN), are nonlinear models. It can be represented by a series of nodes (activation functions), with weighted links between them, organized in different layers (input/activation functions/output). Thus, the response is approximated as a linear combination of these weighted non-linear activation functions. An activation function is active if its input is higher than a pre-defined threshold.

Finally, instance-based learning methods cover Radial Basis Functions (RBF) method, fitness inheritance methods and decision trees. RBF methods consist of a linear combination of functions approximation. This method can be represented as an ANN. More details on all of these methods can be found in [1], [7], [24], [29], [32], [33]. Table 1 summarize main properties of these metamodels.

TABLE I.	MAIN PROPERTIES	OF DIFFERENT	METAMODELS
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Metamodels	Advantages	Drawbacks
Polynomial regression	Simple Fast and cheap	Not adapted for highly non-linear response and high dimensional problems
Polynomial	More accurate	Not adapted for highly
Chaos	Fast and cheap	non-linear response
Kriging	Exact interpolation Integrated variance estimation	Costly for high dimension
ANN	Non-linear response supported	Very expensive Hard tuning
SVR	Fast and accurate Adapted to high- dimensional problems	Long training time

Metamodels are built on some assumptions as function continuities, shape and smoothness. If these assumptions are not valid, (e.g. in non-linear problems), multiple metamodels can be used together to deal with function discontinuities [29]. Different couples of DoE and metamodels were compared by [1] and authors highlight the strong dependency between both of them. Furthermore, they showed a need for a DoE and metamodel classification to help the user, regarding the objectives (e.g. optimisation, exploration, etc.). Metamodel selection is problem dependent and a universal method does not yet exist [24], [29], [34]. However, the SUMO Toolbox platform [35] integrates mathematical methods to select automatically the best metamodel. This solution replaces time lost in metamodel selection and tuning by increasing computational cost. An "automatic metamodel type selection framework" is proposed by [36] and explored the use of Evolutionary Model Selection (EMS) algorithm. EMS dynamically selects the best metamodel type and parameters. The same kind of algorithm is developed in [34]. However, as it is detailed further, it involves evolutionary algorithms drawbacks. Thus, as the selection is based on stochastic variables, the algorithm convergence is not guaranteed.

#### 2) The training step

The training step is managed by assessing the FE model with a DoE (as efficient as possible, see section 4.2) to determine metamodel parameters. Each metamodel is used with its fitting method, as, for instance, the least-square methods, which link the model and results obtained from FE model assessment. Some examples are described in [11]. The training step strongly depends on the number of assessments: not enough implies a low accuracy, but too much may lead to an overfitted model (learning by heart). This phenomenon means an inability to predict the behaviour beyond these first assessments. The analyst time, spent to tune metamodels parameters (and also optimisation algorithms), is also important [37]. This time may not be negligible for some of the considered metamodels, and must be taken into account with metamodeling time (DoE selection and training step) to obtain a more accurate computational cost.

#### *3)* The validation step

The validation is done by using another DoE to assess its predictive performance. The mostly used method consists in defining a DoE, using a partition (e.g. 20%) for the training and using the remaining partition (e.g. 80%) for validation. Several error measurements can be provided by statistical methods (e.g. RMSE, Leave-One-Out and Bootstrap methods [14]).

Metamodel usefulness for optimisation problems was discussed by [37]. They compared several metamodel-based optimisation and optimisation process without metamodels. They concluded that metamodeling does not always improve the optimisation efficiency. Metamodelling performance decreases with the complexity of the approximated function and depends also on allocated computational budget. However, the functions used during this test were perfectly known (analytical). It will not be the case for a real case study. Thus, the metamodel choice may be more difficult since its performance could be unpredictable.

The choice of the right metamodel is strongly linked to the function to approximate and to the available computational budget. It also depends on the DoE chosen. Recommendations about selection of some DoE and metamodels were given in [11], but are not complete. Also, a metamodel considering multiple parameters can be hard and long to be tuned. However, some algorithms were developed to automatically select and tune the metamodel. Metamodeling is not always the most efficient strategy, the choice of using or not metamodels is also important.

#### III. ADAPTIVE DESIGN OF EXPERIMENT

Adaptive DoE can be found in the literature with several names: metamodelling adaptive-recursive approach [37], sequential design [1], variable fidelity modelling [38] or

active learning [35]. Adaptive DoE is used to create iteratively a dedicated DoE for a specific problem, in order to maximise DoE efficiency. This method may fulfil several objectives as metamodel fitting, optimisation or design-space exploration. This method is based on 2 main steps: (1) searching for new experiments from an initial DoE and (2) selecting the best experiment to add to the initial DoE. A general view of this strategy is represented in figure 2. Definition of best experiment depends on the chosen infill criterion used for selection, which is linked to the study objective. Then, these steps are repeated until a convergence criterion is reached or until a maximum number of experiments is reached.



Fig.2. Adaptive DoE strategy for metamodelling. This process involves DoE, metamodels and metaheuristics to add new experiments (n.exp.) iteratively.

The main issue concerning the development of dynamically adaptive DoE is the choice of an infill criterion [29]. Many developments were made for optimisation problems. A typical framework for Surrogate Based Optimisation (SBO) involves an infill criterion chosen to intensify model assessment in order to find faster the global optimum of the objective function [18]. The authors used a combination of an adaptive updating method and a real-time updating performed by an evolutionary algorithm, to refine the DoE around optima. This method aims both to optimise the metamodel for fitting well with the objective function, and to obtain the optimum of the objective function. The SBO

framework is detailed and discussed in [29]. In the same approach, a particular SBO framework, the Efficient Global Optimisation (EGO), based on Kriging metamodel and Genetic Algorithm (GA) was used [39]. The infill criterion is the Expected Improvement (EI) criterion, which involves a measure of possible improvement. This criterion is largely used [12], [40]–[44]. The Particle Swarm Optimisation Intelligent Sampling (PSOIS) method, which combines a Particle Swarm Optimisation (PSO) method, used to add new experiments, and Adaptive RSM metamodel, can also be mentioned [22]. An algorithm (SOAKEA) combining Kriging metamodel and PSO algorithm for optimisation was also developed [45]. Another application can be found in [46], with a very specific metamodel and an elitist GA for forming applications. A taxonomy was presented to select the infill criteria related to the metamodel used, but only for polynomial metamodels and kriging [40].

For metamodel fitting, a simple criterion consists in selecting the experiment related to the estimation which maximizes an error measurement between the FE model and the metamodel, such as variance of estimation provided by a Kriging metamodel [13], [14]. However, kriging metamodel is the only one to provide such a local information about the results accuracy, which is very convenient for adaptive methods. A class of infill criteria is related to contour approximation, which is close to metamodel fitting. Several criteria of this class were listed [12], based on the uncertainty of each experiment (margin uncertainty for a given trustregion or confidence intervals [47]). A margin indicator function can be defined to set a trust-region around the function (contour) to approximate. The goal is to select the closest experiment from the function. There exist also the margin probability function, and the expected feasibility function. A sub-class, called One-step-look-ahead criteria, includes the Weighted-IMSE [13] and Stepwise Uncertainty Reduction (SUR) [48] criteria. An EI-based criteria for contour estimation was developed [49].

TABLE II. SYNTHESIS OF COVERED ADAPTIVE METHODS

Metamodels	Criteria	Search method
Kriging	EI, T-IMSE[13], SUR [48], Expected Feasibility Function [12], [50], Augmented EI [41], bootstrapped EI [53], Maximal Variance	Metaheuristics, DoE
RSM	Re-sampling methods [51]	Metaheuristics, DoE
Polynomial Chaos	Trust-interval[52]	DoE
ANN	Maximal variance by Bootstrapp or Leave-One-Out methods [14]	DoE

These methods are summarized in Table II. A lot of papers aim to improve adaptive methods based on EI criterion and Kriging metamodel. Others criteria, which were not mentioned previously, were also developed [13], [41], [48], [50]. Concerning other kind of metamodels, just a few criteria were reviewed [51], [52]. However, some of these criteria could be applied to other metamodels.

Many adaptive methods are based on metaheuristics, in order to search for a new experiment. Metaheuristics are algorithms used to solve complex optimisation problems. A recent survey of these methods was published [54]. They are nature-inspired and based on stochastic components. These methods are largely used to create an adaptive DoE algorithm [18], [22], [39], [45], [46]. These methods were divided into two groups [54]: single-solution based metaheuristics (e.g. simulated annealing, Variable Neighbourhood Search, Tabu Search. etc.) and population-based metaheuristics. Population-based methods can be split up into two other subclasses: evolutionary computation methods (e.g. GA, cultural and coevolutionary methods, etc.) and Swarm intelligence methods (e.g. Ant colony, particle swarm, artificial immune systems, etc.) [54]–[57]. The first one covers genetic and evolution strategies, using selection, mutation, reproduction and recombination processes over a population of solution. The common stopping criterion is a maximum number of generations without significant improvement of the best individual. Several techniques to improve this algorithm exist (e.g. elitism and niching, local search). As an example of the second sub-class, particle swarm metaheuristics consists in a population of particles which explore the design space. To summarize, the swarm will follow best particles to optimal solutions. Thus, many optimal solutions can be found, as local optima as global optimum. Another assessment of several metaheuristics exists [58]. As for DoE and metamodels, selection and tuning are difficult. Methods were developed, as Adaptive metaheuristics and hyperheuristics to select and tune automatically metaheuristics [54]. Adaptive metaheuristics deal with time-consuming tuning task. The authors highlight a real need to develop a framework able to help users to compare, develop, combine and parallelize all of these metaheuristics algorithms. Hyperheuristics are designed to overcome the problem-dependent property of metaheuristics. It consists of a method to select automatically most appropriate metaheuristics to solve a specific problem, by using metaheuristics. It aims to be problem independent and used easily. Finally, hybrid optimisation methods are mentioned. They are based on a hybridization of different metaheuristics, different optimisation algorithms and techniques. However, several adaptive methods use a local search method (based on function derivatives) or a pre-defined sampling [14]. A combination of metaheuristics and local search methods is also possible [34].

To be successful, all of these methods used to search for and select new experiments have to balance design-space exploration as exploitation (intensification) [29], [54]. The goal is to give accurate results without missing any optimum or falling into a local optimum. Each algorithm has a particular manner to achieve this equilibrium.

Adaptive DoE methods may involve metamodelling to reduce the computational cost and metaheuristics to search for new experiments. Many infill criteria exist to select the most efficient experiment and to sequentially add it to the DoE. This section has not covered all of these criteria, since they are very numerous. Although the EI criterion seems to be the most used, a clear assessment would be valuable to choose the most efficient criterion. The efficiency of adaptive DoE method strongly depends on metamodel, metaheuristics and While hyper-heuristics and criteria used. adaptive metaheuristics are being developed to shorten the simulation process, none of these methods are based on best-practices reusing. It could shorten the process by supporting decision by already known results, instead of run new computations. There exists a real need to develop methods able to compare, classify and select the right methods according to a specific problem. Thus, a capitalisation of successful combination of these elements could help designers to shorten especially preprocessing step of numerical simulation.

#### **IV. SYNTHESIS**

In this paper, we have presented two strategies used for reducing the computational cost of the simulation process. First, metamodelling methods reduce the computational cost of simulation. The main difficulty is the choice of the right DoE with the right metamodel. DoE and metamodels have to be chosen regarding to the objective of the case study and the type of response. A DoE has to be chosen regarding to its properties (uniformity, orthogonality, etc.). Concerning metamodels, some of them are able to deal with non-linear functions (e.g. ANN) but they are more costly, while others metamodels are lighter but only able to deal with polynomial functions (e.g. polynomial approximation). Since DoE and metamodels types are numerous, the selection of a specific couple DoE-metamodels can be hard. Moreover, tuning operation, consisting in selecting parameters for DoE (number of experiment) and metamodels can be a very timeconsuming task. Second, adaptive DOE for metamodelling reduce the number of experiments, by using metaheuristics to search for a new experiment and an infill criterion to select the best experiment found by the metaheuristics. As metamodelling, the selection of a specific set of methods (DoE, metamodel, metaheuristic, infill criterion) is also timeconsuming. Metaheuristics involves also some drawbacks such as computational cost (although they can parallelized) and some difficulty to predict its convergence.

These methods used to shorten the solving step need a long time to be selected and tuned. Metamodels, metaheuristics, infill criteria and DoE types are numerous, and a clear classification is needed to take into account the objective of the case study (optimisation, exploration, etc.) and the compatibility between all of these methods. Some methods are being developed for automatic choice and tuning, as optimisation methods (EMS, EGO) and hyper-heuristics. There is also a trend to hybridize different methods to obtain more efficient algorithms. But, these methods may also increase the computational cost to shorten the process.

#### V. CONCLUSION

Design of Experiments (DoE) methodology is commonly used to improve the product performances, quality and robustness. Numerical DoE are applied to simulation which may involve a huge computational cost. Thus, it is important to improve the method in order to decrease the DoE cost.

In this paper, two approaches were presented. First, metamodelling can shorten the solving step of the simulation process by replacing a FE model by a simple analytical function. Second, adaptive DoE can increase the efficiency of a DoE by choosing iteratively experiments during the solving process, based on previous results. This method involves an infill criterion to select and add the new experiment. This criterion depends on the objective of the case study (optimisation, metamodel fitting, etc.). It involves also specific methods to search for potentially added experiments. Metaheuristics were presented since they are able to propose multiple candidates at each iteration. But, metaheuristics are also difficult to be chosen and tuned.

Finally, these methods initially designed to shorten simulation process would increase it. Computational cost can also be increased. Selection and tuning of these algorithms can be long. Thus, a capitalization of simulation data, such as results and best practices could decrease simulation time by re-using previous results and assessments. By capitalizing results of simulation using these methods, a clear benchmark could be produced. Specific methods and parameters could be automatically proposed to support designers' decisions.

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