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SEQUENTIAL DESIGNS FOR SIMULATION EXPERIMENTS: NONLINEAR REGRESSION METAMODELING

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ABSTRACT
In this paper we propose a method to select an experimental design for estimating nonlinear simulation metamodels. Through a careful selection of design points, the method provides better fitting results than equally spaced point selection, with the same simulation effort. This method accounts for the input/output function of the simulation model, possibly a mathematical function nonlinear in the parameters. In spite of the fact that the paper concentrates on nonlinear regression metamodels, the method may be applied to other type of metamodels. The procedure is easy to construct (so, it is attractive to be used in practice) and focus on simulations scenarios in sub-regions where the input/output behavior has more interest. This procedure is illustrated with an application to a automobile parts factory. Finally, we draw some conclusions.area.

KEY WORDS
metamodels; nonlinear regression; simulation; design of experiments.

1 Introduction

Although the simulation model is simpler than the real system, the interpretation of the large amounts of data produced by the simulation model can become quite difficult. The construction of a simple mathematical function can expose, more clearly than the simulation model, the fundamental nature of the system input-output relationships. A *metamodel* [1], a model of the simulation model, can be very useful in answering 'what if' questions. It uses fewer computer resources, when compared with the computer simulation model itself, and it can be used for verifying and validating of the simulation model as well.

The general linear model has had a preferential treatment by some simulation researchers [2, 3]. However, the intensively studied polynomial form of the general linear regression model is unable to make a global fit to curves of arbitrary shape. Moreover, in real-life systems the nonlinearity is common [4] and the approximation using polynomials becomes unrealistic, for instance, in problems involving queuing systems [5]. An alternative way of providing a better and more realistic global fit may be the use of *nonlinear* metamodels; for example, nonlinear regression metamodels [6, 7], Kriging metamodels [8], and neural nets [9]. Even when a linear metamodel works well, a nonlinear metamodel may be useful, in order to clarify the meaning of the model parameters.

Nonlinear metamodels frequently fit their data well and often with a fewer metamodel parameters. However, selecting an efficient design, selecting the type of the metamodel, fitting the metamodel, and interpreting the resulting nonlinear metamodel may be an important challenge.

One of the main difficulties associated with optimal experimental designs for nonlinear models is its dependency on the true values of the underlying unknown parameters of the model [10, 11]. This type of experimental designs require strong *a priori* assumptions on the selection of the metamodel's type and on the nature of the response (for example, white noise) [12]. As a result, when the input/output relation is seriously in doubt, this type of designs may be completely inappropriate. Khuri and Cornell [13], section 8.5.4, introduce a criterion for the choice of a design for nonlinear models that does not depend on the initial values of the parameters. This approach is based on the Lagrange interpolation, by a polynomial of a certain degree, combined with the D-optimality and, as we referred above, the approximation using polynomials may be unrealistic.

However, simulation experiments are implemented sequentially; except possibly when parallel computers are used, but this kind of procedure is not typical [12]. In addition, sequential designs require fewer runs than fixed sample designs (i.e. they are more efficients). This characteristic is most critical when we are deal with expensive simulations. Recently, in the Kriging metamodeling context, both Kleijnen and van Beers [8] and Sasena et al. [14] developed sequential designs. Our method is sequential and the design points are chosen so as to ensure an approximate uniform response behavior. As a result, it concentrates on inputs in sub-regions where the input/output behavior has more interest. In our example, we select a larger number of designs points where the arc-tangent metamodel varies more rapidly. Also, we select a few number of design points on the relatively flat parts of the metamodel.

This paper is organized as follows. Section 2 introduces nonlinear regression metamodels and some notation.

Section 3 explains our sequential method. Section 4 describes an example concerning a automobile parts factory. which is studied using the proposed method. Finally, Section 5 stated conclusions.

2 The Nonlinear Regression Metamodel

To represent the simulation model, the following nonlinear regression model in the unknown parameters $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_m)^T$ is proposed as a metamodel

$$Y_{ij} = f(X_i, \boldsymbol{\theta}) + \epsilon_{ij}, \quad i = 1, \ldots, n, \quad j = 1, \ldots, r. \quad (1)$$

ϵ_{ij} represents the inaccuracy of the model and f is an unknown function simpler than ϕ (ϵ_{ij} includes both the effects of the inadequacy of f as a representation of ϕ, and the intrinsic effects encountered in any stochastic simulation model). We assume that $\mathrm{E}[\epsilon_{ij}] = 0$ and $\mathrm{Var}[\epsilon_{ij}] = \sigma_i^2$, $\sigma_i > 0$. The simulation model defines a statistical population of observations. The elements of the population correspond to all possible random number streams that drive the simulation at $\mathbf{S}$. That is, in theory the population has an infinite dimension and, hence, we can assume the classical hypothesis $\epsilon_{ij} \sim \mathrm{N}\left(0, \sigma_i^2\right)$. The variable X_i may be the same as the simulation variable S_h, or a transformation of one or more variables S_s.

The factor settings for the i-th simulation configuration ($i = 1, \ldots, n$), named scenario, are specified by the design point X_i, where the set of such points constitutes the experimental design. For each scenario, r independent replications of the simulation model are carried out and the simulation experiment yields r observations Y_{ij} ($j = 1, \ldots, r$). The variance of Y_{ij} is estimated by

$$\hat{\sigma}_i^2 = \sum_{j=1}^{r} (Y_{ij} - \bar{Y}_{i.})^2 / [r(r-1)], \qquad i = 1, \ldots, n, \quad (2)$$

where $\bar{Y}_{i.} = \sum_{j=1}^{r} Y_{ij}/r$, $i = 1, \ldots, n$.

Under the hypothesis that the ϵ_{ij} are independent and normally distributed, $\epsilon_{ij} \sim \mathrm{N}\left(0, \sigma_i^2\right)$, and some further regularity conditions, it is shown that the nonlinear least squares estimator of $\boldsymbol{\theta}$ ($\hat{\boldsymbol{\theta}}$) satisfies

$$\hat{\boldsymbol{\theta}} \approx \boldsymbol{\theta}^* + [\mathbf{F}^T \boldsymbol{\Sigma}^{-1} \mathbf{F}]^{-1} \mathbf{F}^T \boldsymbol{\Sigma}^{-1} [\bar{\mathbf{Y}} - \mathbf{f}], \quad (3)$$

and is asymptotically normally distributed as $N = nr \to \infty$, that is

$$\hat{\boldsymbol{\theta}} \sim \mathrm{N}_m \left(\mathbf{0}, \frac{1}{r} [\mathbf{F}^T \boldsymbol{\Sigma}^{-1} \mathbf{F}]^{-1} \right). \quad (4)$$

where $\boldsymbol{\theta}^*$ is the exact value of $\boldsymbol{\theta}$, $\mathbf{f} = \mathbf{f}(\boldsymbol{\theta}^*) = (f(X_1, \boldsymbol{\theta}^*), \ldots, f(X_n, \boldsymbol{\theta}^*))^T$, $\mathbf{F} = \mathbf{F}(\boldsymbol{\theta}^*)$ is the Jacobian matrix of $\mathbf{f}$, evaluated at $\boldsymbol{\theta}^*$ and $\bar{\mathbf{Y}} = (\bar{Y}_{1.}, \ldots, \bar{Y}_{n.})^T$. $\boldsymbol{\Sigma}$ is the diagonal matrix $\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_1^2, \ldots, \sigma_n^2)$. In order to simplify the notation, we omit in our notation that $\mathbf{f}$ and $\mathbf{F}$ are evaluated at $\boldsymbol{\theta}^*$.

In general, we do not know $\boldsymbol{\Sigma}$ and so, it must be replaced by $\hat{\boldsymbol{\Sigma}} = \mathrm{diag}[\hat{\sigma}_1^2, \ldots, \hat{\sigma}_n^2]$; as a result, we have the estimated generalized nonlinear least squares estimator. The verification of these results is shown in [15].

3 Sequential Design Strategy

The metamodel described in 2 describes the relation between the input and the response. In order to obtain a good metamodel fit the data collected from the simulation executions should provide a good description of that relation. The selection of the input values, or experimental design, used to construct the metamodel is very important. A good choice of input values is critical in providing a good fit, since a poor choice may require many additional inputs [11].

The selection of a good experimental design must address a number of issues, since the response may be affected by other factors, besides the selected input values. These factors introduce effects that can be referred as unsystematic (random error or noise) and as systematic (bias). Observing the response multiples times at the same inputs, or replication, allows the estimation of the magnitude and distribution of random error, and the sample means of the replicated responses have smaller variances than the individual responses. The bias originates from a rare sequence of events, introduced by initial conditions, until the system achieves statistical equilibrium and can be managed by ignoring the response during this warm up period.

A careful choice of an experimental design may better expose the relation between the input and the response. For instance, a bad experimental design may suggest a linear relation between the input and the response while the response is in fact nonlinear. The detection of such nonlinearities is important and can be achieved with a larger number of input values or, better still, a careful selection of input values. Also, designs should be easy to construct if they are to be used in practice [12].

3.1 Choosing an experimental design

The experimental region of an experimental design corresponds to the values of the inputs to wish the metamodel is useful. A point in this region of interest is a specific input value. The experimental design must choose a set of n pilot design points, i.e., combinations of input variables and parameters of the simulation model. These points must be different from each other and must belong to a predefined domain region to explore. The points are chosen to efficiently investigate the relationship between the design factors and the responses. Assuming that the interesting features of the metamodel can belong any part of the experimental region then the design should be based on a selection of evenly distributed points throughout the region. Whenever some parts of experimental region exhibit more interesting characteristics, the design should include more points to explore these parts. These space-filling designs, or hybrid variations of evenly distributed and space-filling designs, may provide a better metamodel fit since a more detailed information of the relation between the input and the response. Some special cases, where the metamodel belongs to a previously known input/output class, it is pos-

sible to achieve an optimal design based on specific criteria formulation [11].

The proposed approach is a sequential hybrid design where a set evenly distributed points throughout the experimental region is complemented with a space-filling criteria based on a measure of distance between the response of two consecutive points.

3.2 Executing the simulation runs

In a stochastic simulation, for each execution of the simulation program, the initial conditions must be specified. In general, these conditions represent very uncommon system states as, for example, all queues being empty. As a consequence, the simulation program begins with a sequence of events that may have a low probability of occurring. So, the simulation output can be contaminated with an initial bias (see [16, Section 9.5]). To control the initial bias, that can be the greatest source of error in the estimation of the metamodel parameters, an initial data deletion is performed. This is equivalent to forget a portion of the initial results while the system is not in statistical equilibrium (warm up period). However, the initial data deletion selection involves a compromise, since in a small deletion the bias can still affect the result, while a large one may produce a large variance and it is not efficient. A good bias detection is important in the context of the independent replications method, because usually many runs are needed.

The sequential method proposed to collect the simulation results consists of four steps and uses Welch's procedure to eliminate the initial bias [16].

For each of these design points, execute r long pilot replications, each replication with L observations (L should be large when compared with the roughly guessed truncation point). It is convenient to choose $r > 9$ to obtain acceptable estimates of the variance (2) in each design point [17].

3.3 Determine Welch's window for each point

For each design point i, calculate and graphically represent the sequence of means $\bar{\mu}_i(k, W)$ such that

$$\bar{\mu}_i(k, W) = (r(2W+1))^{-1} \sum_{s=-W}^{W} \sum_{l=1}^{r} Z_{il}(k+s),$$

if $k \geq W+1$, and

$$\bar{\mu}_i(k, W) = (r(2j-1))^{-1} \sum_{s=-(j-1)}^{j-1} \sum_{l=1}^{r} Z_{il}(k+s),$$

if $k < W+1$, for different values of Welch's window, W, with $W \leq \lfloor k/2 \rfloor$. If the response is the average time in the system, then $Z_{il}(k)$ represents the time in the system for the k-th customer in replication l of the design point i. Select the smallest value W that corresponds to a sufficiently regular graphical representation and choose the k value, k_0, from the moment that the sequence $\{\bar{\mu}_i(k, W) : k = 1, \ldots, L-W\}$ seems to have converged, that is, choose the truncation point k_0.

If there exists some design point for which it is not possible to find a satisfactory W, then we consider $r = r + 10$ replications and repeat the process. Otherwise, for each replication of the ith experimental point, ignore the observations until the corresponding truncation point and collect the remaining simulation results $\{(X_{i.}, Y_{ij}, \hat{\sigma}_i) : i = 1, \ldots, n, j = 1, \ldots, r\}$, where

$$Y_{ij} = \frac{1}{K - k_0} \sum_{s=k_0+1}^{K} Z_{ij}(s), \qquad K = \lceil 100k_0/15 \rceil \leq L\,; \tag{5}$$

approximately 85% of the observations are collected.

3.4 Selecting the design points

Consider an initial set of design points $\mathcal{X}^0$ from the experimental region R, $\mathcal{X}^0 = \{X_1, \ldots, X_n\} \subset R$, evenly spaced such that $X_i = X_1 + i(X_n - X_1)/(n-1)$, with $i = 1, 2, \ldots, n-1$. For each design point $X_{i.}$ execute r independent replications of the simulation model. From each simulation run, remove the initial bias, and evaluate the mean response value Y_{ij}. Compute the set of sample means of the replicated responses $\mathcal{Y}^0 = \{\bar{Y}_{1.}, \ldots, \bar{Y}_{n.}\}$.

Calculate the distances between consecutive points $\bar{Y}_{i.}$, that is, $d_i = |\bar{Y}_{i+1.} - \bar{Y}_{i.}|$, where $i = 1, \ldots, n-1$. Find $k = 1, \ldots, n-1$ such that $d_k \geq d_i$ for all $i = 1, \ldots, n-1$. The d_k represents the largest gap in the response in the experimental region and a new design point should be inserted to access the behavior of the input/output relation. If no information is previously available on the input/output relation, it is recommended to choose the middle point of the input values in the interval between X_i and X_{i+1}. The new ordered set of design points is now $\mathcal{X}^p = \mathcal{X}^{p-1} \cup \{(X_{k+1} + X_k)/2\}$ where $p = 1, 2, \ldots$ represents the p-th step in the sequential space-filling design strategy.

The number of steps in the space-filling design depends on the interesting features of the metamodel. The main objective of the proposed design strategy is to provide a better choice of design points. Therefor, the number of points is assumed to be previously determined. The past experience suggests that a balanced choice is to include half the points in the initial set, of evenly spaced design points, and determine the remaining points with the proposed space-filling design strategy. However, if the predefined number of points does not expose, with sufficient granularity, the interesting features of the metamodel, additional design points are to be chosen so as to ensure an uniform response behavior, in order to provide a more accurate fit of the metamodel.

4 Application to a Automobile Parts Factory

In this paper, a automobile parts factory is depicted. The factory contains two drills and a finishing area. Drilling time is triangularly distributed between 10 and 30 minutes, with a mode of 15 minutes. The time to perform the finishing operations has a uniform distribution on the interval $[2, 5]$ minutes and only one part can be finished at a time. The factory processes two types of parts. Type I and type II parts arrive according to a gamma$(2, \lambda)$ and gamma$(2, 20)$ distributions, respectively; following the notation of Law and Kelton [16], gamma(α, β) represents the gamma distribution with shape parameter $\alpha > 0$ and scale parameter $\beta > 0$ (the mean is given by $\alpha\beta$). After arriving, type I and type II parts take two and five minutes to be routed to the drill area, respectively. Both parts require the drilling and finishing operations and assume no time delays between these two operations. We assume that operators are always available if a machine is available. On the average, finishing operations have to be repeated 20 percent of the time. If a part has been routed through finishing twice but still needs to be refinished, it must be drilled again. The purpose of the simulation experiment is to express the average time in the system (response), Y, as a function of the mean time between arrivals of parts of type I (decision variable), $X = 2\lambda$.

Based on the proposed procedure described in the Section 3, we consider three distinct experimental designs with 19 design points each. The $fixed$ experimental design, uses only evenly spaced design points, $\mathcal{X}^0_{fixed} = \{0.5,\ 5,\ 10,\ 15,\ 20,\ 25,\ 30,\ 35,\ 40,\ 45,\ 50,\ 55,\ 60,\ 65,\ 70,\ 75,\ 80,\ 85,\ 90\}$. The $fill$ experimental design, starts only with two points $\mathcal{X}^0_{fill} = \{0.5, 90\}$ (corresponding to the experimental region limits) and determines all other design points with the space-filling proposed procedure. The $partial$ experimental design, starts with 10 evenly spaced design points $\mathcal{X}^0_{partial} = \{0.5,\ 10,\ 20,\ 30,\ 40,\ 50,\ 60,\ 70,\ 80,\ 90\}$ (approximately half the points in the experimental design) and uses the proposed space-filling procedure to determine the remaining design points. The $fixed$ as well as the $fill$ experimental designs are extreme situations of the proposed procedure, where the number of design points left to the space-filling procedure is minimum and maximum, respectively. The $fixed$ experimental design can also be used as a reference to measure the relative improvement of the proposed procedure when compared with the routinely used experimental designs.

At each design point, we run Welch's procedure in order to determine the length of each simulation and the initial-data deletion. Welch's moving average is based on $r = 20$ replications of the simulation metamodel, where each replication contain 2000 observations. For example, at the design point $X_8 = 2\lambda_8 = 35$ of the $fixed$ experimental design, we delete 200 observations from the beginning of the run and we use only the next 1134 observations to estimate the response Y (the remaining 666 observations are ignored). We carry out $r = 20$ replications of each of the $n = 19$ design points; since $r > 9$ we obtain an appropriate estimate for $\hat{\sigma}_i, i = 1, \ldots, n$ [7].

To identify a curve that might fit the input/output relationship of the simulation model (computer program), we performed a visual check, observing the simulation results plots of each experimental design, in the Figure 1. Comparing the plots with graphical representations of known functional relationships, for example [18, pages 329, 338 and 340], a good candidate seams to be the arc-tangent function

$$y = \theta_1 + \theta_2 \text{arctg}(\theta_3 x + \theta_4)$$

Since the number of replications is equal for all design points and the populations are assumed to be normal, the variance heterogeneity is checked using the Hartley test [19, page 764]. We obtained

$$H = \frac{\max \hat{\sigma}_i^2}{\min \hat{\sigma}_i^2} = 705.4 > H(19, 19; 0.95) \approx 5.0,$$

so we assume that the errors have unequal variances. Thus we will use the method of nonlinear weighted least squares. The estimators were obtained using the Levenberg-Marquardt method implemented in MATLAB. This method is robust and works well when solving this type of problem. However, on large residual problems its linear convergence can be very slow and it may even not converge. When this happens we must choose a method that is adequate for large residual problems.

Table 1. Metamodel's estimated parameters for the experimental designs.

Design	$\hat{\theta}_1$	$\hat{\theta}_2$	$\hat{\theta}_3$	$\hat{\theta}_4$
$fixed$	115.748	−55.8394	0.917799	−30.2146
$partial$	116.052	−56.1696	0.872902	−29.2967
$fill$	116.139	−56.0346	0.854421	−28.6705

To check the validity of the remaining hypothesized metamodels, we observe a fairly close agreement between the PRESS and SSE values (see Table 2), so MSE is a reasonably valid indicator of the predictive capability of the model [19, page 345]. As a consequence, we conclude that the metamodel built with the $partial$ experimental design achieves the best predictive validity when compared with the metamodels based on the other experimental designs. In fact, a careful observation of the plots of the Figure 1 evidences large gaps in the representation of the input/output relation. While the $fixed$ experimental design originates a large output gap between the design points 30 and 35, the $fill$ experimental design exhibits large input gaps between points 0.5 and 22.875, and also between 45.25 and 90.

The elected experimental design produces a metamodel described by the arc-tangent function is depicted in Figure 2, with parameters described in Table1.

To gain more insight into the predictive validity of the $partial$ arc-tangent metamodel, we analyzed the results of

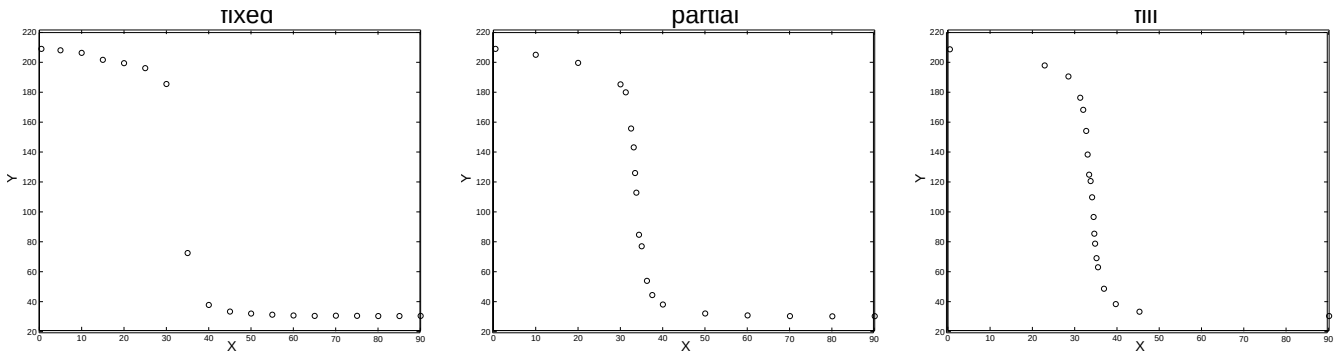

Figure 1. $fixed$, $partial$ and $fill$ experimental designs, with 19 design points.

Table 2. Metamodel's diagnostics.

Design	SSE	MSE	PRESS	SSE/PRESS
$fixed$	660.39	1.84983	667.779	0.988934
$partial$	502.456	1.40744	512.932	0.979577
$fill$	958.215	2.68408	968.237	0.98965

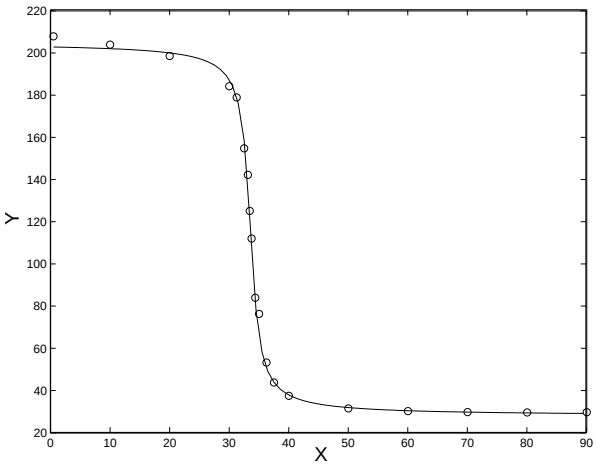

Figure 2. Plot of the elected metamodel and the $partial$ points.

double cross-validation [19, page 439]. We observe in Table 3 a good agreement between the estimated coefficients for both subsets. Also, the coefficients of determination are quite similar.

Table 3. Double cross-validation test.

$\hat{\theta}_1$	$\hat{\theta}_2$	$\hat{\theta}_3$	$\hat{\theta}_4$	R^2_{hui}	R^2_{val}
116.04	-56.117	0.8724	-29.256	0.9990	0.9988
115.98	-56.246	0.8919	-29.981	0.9988	0.9989

5 Conclusion

Metamodels can be used, as simulation model surrogates, to expose the fundamental nature of input/output relationships. Represented as a simple mathematical function, the metamodel can also be used for verifying and validating the original simulation model. Queuing systems, as many other real-life systems, exhibit a nonlinear behavior. Nonlinear regression metamodels provide a better and more realistic global fit than polynomials since they are able to fit curves of arbitrary shape.

In order to provide a good fit, the sample design points must be chosen to efficiently investigate the input/output relationship of the simulation model. A careful choice of an experimental design may better expose the relation between the input and the response, such as subtle nonlinearities of the simulation model. The design should be generic, in spite of the fact that the paper concentrates on nonlinear regression metamodels, and should be easy to construct if they are to be commonly used in practice.

The proposed approach is a sequential hybrid design where a set evenly distributed points throughout the experimental region is complemented with a space-filling criteria based on a measure of distance between the response of two consecutive points. The number of steps in the space-filling design depends on the interesting features of the metamodel. The main objective of the proposed design strategy is to provide a better choice of design points.

The application example is investigated using three distinct experimental designs that represent two extreme uses of the proposed procedure and a balanced approach. Using MSE as an indicator of the metamodel's predictive capability, as illustrated by the application example, we compare the three experimental designs, with the same number of design points. The balanced approach exhibit a better predictive capability, when compared with the extreme designs, one of which coincides with the ordinary evenly spaced design.

This paper exposes the fact that a careful choice of an experimental design can lead to better metamodels, with the same simulation effort, and proposes a sequential hybrid design that improves the predictive capability of the constructed nonlinear simulation metamodels.

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