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Combining Iterative Heuristic Optimization and Uncertainty Analysis methods for Robust Parameter Design

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In the last years, several works have pointed out that products and processes lack quality because of performance inconsistency, often produced by parameters that are uncontrollable in the manufacturing process or the product usage. Robust design methods are aimed at finding product/process designs that are less sensitive to parameter variations. Robust design of computer simulations requires a high number of runs, making it prohibitive for time-consuming simulations. This work presents a novel methodology for robust design, which integrates an iterative heuristic optimization method with uncertainty analysis to achieve effective variability reductions, exploring a large parameter domain with an accessible number of simulations. To prove the effectiveness of this methodology, the robust design of a 0.15μm CMOS device is shown.

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Keywords: Robust design; Computer simulations; Uncertainty analysis; Heuristic optimization; Response surface modeling

1 Introduction

In the last years, several works have pointed out that products and processes lack quality because of performance inconsistency, often produced by parameter variations in the manufacturing process or the product usage that are not fully controllable (Nair 1992). Robust design methods are aimed at finding product/process designs that are less sensitive to parameter variations. Computer simulations are extensively used for designing new products, since they allow less expensive and shorter design cycles (Koehler and Owen 1996). Since the actual relationship between parameters and responses is usually complex and not known algebraically, the simulation process can be considered a black box that gives values for the simulation responses for any combination of the input parameter values.

Robust parameter design methods have successfully been applied to computer simulations (Yu 1998). Robust design of a system or process is formulated as an optimization problem, in which the objective function considers both obtaining desire response values and the minimization of the responses' variability. These two criteria are usually measured by computing the mean and the variance of the simulation responses. They can be obtained using the Monte Carlo method (Mavris and Roth 1997, Tarim et al. 2001, Chen 2003) or using Taylor expansion (Kim et al. 2002).

Some of the existent approaches (Hadjihassan et al. 2002) approximate the function which represents the simulation using polynomial models, limiting the validity of their methodologies to small parameter domains, since polynomial models can assure fitting to the real surface of the response only in small domains.

The goal of this work was to find a robust design method that allows reducing the number of simulations required and, at the same time, allows exploring a large parameter domain. As a consequence, a novel approach is introduced, which combines an iterative heuristic optimization method and uncertainty analysis for robust parameter design. The iterative heuristic method makes possible to cover large parameter domains while the uncertainty analysis allows obtaining the mean and the variance of the simulation responses with a smaller amount of simulations.

Computer simulations can be deterministic or stochastic. In deterministic simulations, each time the simulation is run using the same input parameter values, the same response values are obtained. Stochastic simulations involve stochastic processes and consider the variability of the system or process being modeled, so each time the simulation is run using the same input parameter values, different response values might be obtained (Koehler and Owen 1996). This work is focused on deterministic simulations.

To prove the effectiveness of the proposed method, it was applied to obtain the robust design of a 0.15μm CMOS device using computer simulations. Robust design has already been used to design semiconductors in previous works (Tarim et al. 2001, Hadjihassan et al. 2002). This is an area in which the research in simulation based robust design is important because of the cost of manufacturing real wafers and the increasing complexity and variability of the processes due to the continuous size reduction. The results of this work show considerable reductions in the variance of the responses, giving a manufactured product with smaller probabilities of being rejected in a quality test.

Chapter 2 describes the formulation of the robust design optimization problem. Chapter 3 presents the proposed method for solving the optimization problem. Chapter 4 shows the case study. Finally, in chapter 5, the main conclusions of this work are presented and future challenges are described.

2 Formulation of the Robust Design Optimization Problem

As mentioned before, the simulation model is treated as a black box, where m simulation responses (represented by the vector $\vec{r}$) depend on n simulation parameters (represented by the vector $\vec{p}$), and the relationship between them ($\vec{F}$) is only known implicitly (equation (1)).

$$\vec{r} = \vec{F}(\vec{p}) \quad (1)$$

Usually, there is a trade-off between reducing variability of those simulation responses and achieving design requirements. The objective function used to represent this compromise is a performance measure (PM) that is equal to the expected value of the quadratic quality loss function (L) proposed by Taguchi (Joseph 2004) (see equations (2)--(3)). This performance measure has a direct relationship with one of Taguchi's SN ratios (Nair 1992).

$$L(r) = c(r - T_r)^2 \quad (2)$$

$PM = E[L(r)] = c((\mu_r - T_r)^2 + \sigma_r^2)$ (3)

Where r is a scalar response of a deterministic computer simulation; c is a cost-related constant; T_r is the target for r; and, μ_r and σ_r^2 are the mean and the variance of r, respectively.

Parameter values are considered to have bound constraints, shaping a rectangular parameter domain. In this case, constraints are related to the parameters' mean since their variances are considered to be constant.

Thus, the formulation of the nominal-the-best problem, using a weighted sum of the responses' PM, is the following (weights w_j replace the c constant):

$$
\begin{aligned}
&\text{Minimize:} \\
&\quad \sum_{j=1}^{m} w_j PM_j \\
&\quad \text{where } PM_j = (\mu_{r_j} - T_{r_j})^2 + \sigma_{r_j}^2 \\
&\text{subject to:} \qquad\qquad\qquad\qquad (4) \\
&\quad l_i \le \mu_{p_i} \le u_i, \quad i = 1, \ldots, n \\
&\quad \sigma_{p_i}^2 = vo_{p_i}, \quad i = 1, \ldots, n \\
&\quad r_j = F_j(\vec{p}), \quad j = 1, \ldots, m
\end{aligned}
$$

Where the mean and the variance of the response r_j (μ_{r_j}, $\sigma_{r_j}^2$) are computed by means of an Uncertainty Analysis process (see section 3.2) based on the responses of the deterministic computer simulation, which is represented by the function $\vec{F}(\vec{p})$; μ_{p_i}, $\sigma_{p_i}^2$ are the mean and the variance of the parameter p_i; l_i and u_i are the lower and upper bounds of the mean of the parameter p_i; vo_{p_i} is the constant variance of the parameter p_i; and T_{r_j} is the target for response r_j.

Alternatively, it is possible to use the following objective functions, respectively, for smaller-the-better and larger-the-better problems:

$$PM_{STB} = \mu_r + \sigma_r^2 \quad (5)$$

$$PM_{LTB} = -\mu_r + \sigma_r^2 \quad (6)$$

3 Solving the Robust Design Optimization Problem

The proposed methodology for solving the robust design optimization problem is a combination of an Iterative Heuristic method based on Response Surface Models (IHRSM) and Uncertainty Analysis (UA). IHRSM is the optimization strategy used to solve the problem shown in the previous section. UA allows obtaining the mean and the variance of the simulation responses for a given parameters' variability.

The interaction between IHRSM and UA is a three level structure, as shown in Figure 1. IHRSM gives UA the set of experiments (DOE) that it requires as part of the optimization process. In this case, the DOE is formed by different combination of the parameters' mean and variance. As a result, UA returns the responses' mean and variance.

[Insert Figure 1 about here]

Similarly, UA evaluates different parameter combinations by running multiple times the simulation process, obtaining different response values. Those values are then used to compute the responses' mean and variance. Each evaluation made by IHRSM requires an UA process. The following three sections describe these two processes and the complete algorithm.

3.1 Iterative Heuristic Method Based on Response Surface Models (IHRSM)

Figure 2 shows an optimization scheme based on computer simulations. An optimization strategy generates values for the simulation parameters. Simulations are run and their responses are used as feedback for the optimization search process. The optimization strategy repeats the interaction with the simulation model until some stopping criterion is triggered, providing the best solution found.

[Insert Figure 2 about here]

Methods based on Response Surface Modeling (RSM) approximate the real response surfaces by a series of deterministic polynomial models that can be optimized using standard mathematical optimization methods (Myers and Montgomery 2002). The process usually begins with linear models. After reaching the neighborhood of an optimum, polynomials of greater order are used. Compared with most of the search methods based on gradients, RSM is an efficient method in terms of the number of required computer simulations. Nevertheless, for complex functions, with sharp edges or flat valleys, it does not provide good results.

Heuristic methods represent the last developments in the field of direct search methods, those that only require values of the objective function represented by the simulation model (and not the analytical representation of the function). Most of these techniques balance exploration with search space covering, being efficient search strategies (Moré and Wright 1993).

The method used in this work, the Iterative Heuristic method based on Response Surface Models (IHRSM), is a novel combination of methods. From response surface models, it takes advantage of its mathematical basis and the low number of simulations required for the optimization process. From the heuristic methods, it takes its capacity to define dynamic mechanisms to cover all the search space and to escape from local optima. It provides an iterative approach to optimize problems whose parameter domains are not sufficiently small so as to use the traditional methods based on response surfaces.

This method was developed by Sepúlveda (Integrated Systems Engineering 2003) for the optimization of computer simulations in the scope of Technology Computer-Aided Design (TCAD). The work described in this paper is the first effort to apply this approach to the robust design problem.

The optimization problem can be defined as the minimization of a weighted ($\vec{w}$) sum of the simulation responses (equation (7)) subject to parameter bound constrains ($\vec{l}$ and $\vec{u}$).

$$\min \sum_{j=1}^{m} w_j F_j(\vec{p}) \qquad (7)$$
$$l_i \le p_i \le u_i \quad \forall i = 1,\ldots,n$$

The iterative optimization method explores a new region (Figure 3a) of the parameter domain called region of interest (roi), at each iteration. Within this region, an optimization based on RSM is performed. An RSM is a quadratic model that approximates the real response in a reduced small region of the parameter domain (equation (8)).

$$RSM_j^{roi}(\vec{p}) = \vec{p}^T Q_j^{roi} \vec{p} + \vec{p}^T \vec{d}_j^{roi} + c_j^{roi} \cong F_j(\vec{p}) \qquad \forall j = 1,\ldots,m \quad (8)$$

RSM models are created based on a sample of the region of interest. The sample is created using a technique called design of experiments (Montgomery 2000), which is aimed at selecting a representative, but small, set of points of the region of interest. Some statistics, such as the adjust coefficient of determination (R^2_{adj}), allow to measure the RSM models accuracy. When the accuracy of the models is good enough, they can be used for finding a local optimum inside the region of interest. The optimization problem can then be reformulated as shown in equation (9).

$$\min \sum_{j=1}^{m} w_j \cdot RSM_j^{roi}(\vec{p}) \qquad (9)$$
$$l_i^{roi} \le p_i^{roi} \le u_i^{roi} \quad \forall i = 1,\ldots,n$$

The optimization method implemented to solve this general constrained nonlinear problem is based on the well-known sequential quadratic programming (SQP) approach (Bazaraa et al. 1993, Fletcher 2000). It solves the nonlinear problem using an iterative approach. At each iteration, the problem is approximated by a quadratic problem, which is easier to solve. The quadratic problem is solved using the Newton (or quasi-Newton) method to directly find a solution to the Karush–Kuhn–Tucker (KKT) conditions of the original problem. The subproblem solved at each iteration is a minimization of a quadratic approximation to the Lagrangian function, optimized over a linear approximation of the constraints.

The optimum found using the RSM models is also simulated. If the optimum is confirmed (the objective function for that particular parameter setting is better than any other solution found up to that moment), it is assumed the RSM models might also be representative for a slightly larger local domain. The region of interest is therefore enlarged (Figure 3b) and the optimization process is repeated in the new region using the same RSM models that were created for the smaller region (no extra simulation is required). If the new solution is better than the best solution found previously, the expansion of the region of interest is repeated until no further improvement is obtained (Figure 3c). At that point, the region of interest is calculated again, and the local iterative process is restarted from the best solution found up to that moment (Figure 3d).

[Insert Figure 3 about here]

In order to bring to an end the iterative process, a set of stopping criteria is defined. These criteria consider the quality of the solution, computer resources usage, and the proximity to a local optimum. The heuristic process converges to a good local optimum, but, like in any other heuristic, it is not possible to guarantee the global optimum has been found.

3.2 Uncertainty Analysis

Uncertainty Analysis (UA) is a statistical analysis that allows measuring responses' variability due to parameters' variability. It obtains the two first moments (mean and variance) of the responses' probability distribution.

The selection of the parameter values to be simulated is called Stochastic Design of Experiments (SDOE) and it is performed using a technique called probabilistic collocation (Tatang 1994). This technique uses the roots of orthogonal polynomials as values to be experimented, which represent the regions with higher probability of occurrence. The SDOE allows building a stochastic RSM (SRSM) that approximates the real function better in those regions more likely to happen.

Some empirical benchmarks (Tatang et al. 1997) have shown that this approach is potentially a factor of 25 to 60 faster than the pure Monte Carlo method. A more computationally demanding simulation process may result in a larger factor.

To determine the polynomial function used to approximate a response, a sequence of polynomials $\{H_i^0(p_i), ..., H_i^N(p_i)\}$, of orders $0, ..., N$ is created for each parameter p_i. These polynomials are constructed to be mutually orthogonal using the probability density function $f_i(p_i)$ as a weight function, meeting the following functional orthogonally condition:

$$\int_{a_i}^{b_i} f_i(p_i) H_i^s(p_i) H_i^t(p_i) dp_i = C_i \delta_{s,t} \quad \forall\ s,t \in \{0,...,N\} \quad (10)$$

Where $\delta_{s,t}$ is the Kronecker delta, C_i is a positive constant and the interval of integration is the domain of the corresponding probability density function.

The approximation function is constructed as a weighted sum of some of the products of orthogonal polynomials. The equation below is an example of a stochastic RSM with only first-order and second-order orthogonal polynomials.

$$\begin{aligned} \hat{Y}(p_a, p_b) &= A_{0,0} + A_{1,0} H_a^1(p_a) + A_{0,1} H_b^1(p_b) \\ &+ A_{2,0} H_a^2(p_a) + A_{1,1} H_a^1(p_a) H_b^1(p_b) + A_{0,2} H_b^2(p_b) \\ &+ A_{2,1} H_a^2(p_a) H_b^1(p_b) + A_{1,2} H_a^1(p_a) H_b^2(p_b) \\ &+ A_{2,2} H_a^2(p_a) H_b^2(p_b) \end{aligned} \quad (11)$$

The weights ($A_{s,t}$) are determined by least squares, using the results of a family of simulations. The set of parameter values is given by the zeros of selected orthogonal polynomials.

The mean and the variance are obtained from the SRSM using the Monte Carlo method. A larger number of parameter values are randomly generated based on the probability distribution of each parameter. The different parameter settings are evaluated using the

SRSM, generating a large number of response values that are used to compute the responses' mean and variance.

3.3 The Complete Algorithm

For robust design, the optimization strategy solves a problem where the parameters are the mean and the variance of the simulation parameters (μ_{p_i}, $\sigma^2_{p_i}$), and the responses are functions of the mean and the variance of the simulation responses (μ_{r_j}, $\sigma^2_{r_j}$); see the formulation of the nominal-the-best problem in equation (3).

Figure 4 shows a simplified diagram of the algorithm, including the steps for IHRSM and UA. For more details on each step of IHRSM and UA, see sections 3.1 and 3.2 (respectively).

[Insert Figure 4 about here]

4 Case Study

To prove the effectiveness of the proposed method, it was applied to obtain a robust design of a 0.15μm CMOS (Complementary Metal Oxide Semiconductor) device using computer simulations.

4.1 Simulation

The simulation process used to test the performance of the methodology is the simulation of an N-type device of a 0.15μm CMOS device. The simulated FET (Field Effect Transistor) device has a gate length of 180nm. Simulations are run using a TCAD software package, which was developed by ISE AG (Integrated Systems Engineering AG). It simulates the manufacturing process and the electrical behavior of the manufactured device, and then extracts parameters from the IV curves (current versus voltage graphs) of the device.

The parameters considered for the robust design were selected through a screening analysis. Two parameters where selected as the most relevant with respect to their influence on the responses. The parameters discarded showed negligible influence on the responses. Table 1 shows a description of these parameters and their probability distributions. GATE_OX_TH is the thickness of the silicon oxide layer that isolates the gate of the device. BF2_IMPL_DOSE is the dose for the last well implantation step. The mean of these parameters was varied between the lower and upper bounds shown in Table 2.

[Insert Table 1 about here]

[Insert Table 2 about here]

Table 3 shows the simulation responses with their default value (the value of the responses with the parameters at their central value, see Table 2). VT3 is the threshold voltage for the triode region (low drain current), VT5 is the threshold voltage for the pentode region (high drain current), and Ion is the saturation drain current.

[Insert Table 3 about here]

The design specifications selected for the device are expressed in the optimization criteria shown in Table 4.

[Insert Table 4 about here]

The weights w_j (see section 2) were set to 1 for the threshold voltages and 10^{-4} for the saturation current.

Then, the objective function for the robust design optimization is:

$$PM = (\mu_{VT3} - 0.5)^2 + \sigma_{VT3}^2 + \mu_{VT5} + \sigma_{VT5}^2 + 10^{-4}(-\mu_{Ion} + \sigma_{Ion}^2) \quad (12)$$

4.2 Results

Table 5 shows the results obtained using the proposed methodology, compared with the results of a standard deterministic optimization based on sequential quadratic programming (SQP) and RSM. The deterministic solution was also used as initial solution for IHRSM. The robust optimization results are substantially better than the values obtained with classical optimization methods, when considering their variability.

More than 300 simulations were required, consuming approximately 13.7 CPU days on a Pentium IV running Linux. The actual simulation time was about three days, since most of the simulations can be run in parallel. CPU time consumption without SRSM (using the Monte Carlo method directly) would have been almost one year (assuming the best case of benchmarks described in Tatang et al. (1997), 25 times slower).

[Insert Table 5 about here]

5 Conclusions

This work proposes an economic methodology for performing robust design based on deterministic computer simulations. The combination of a novel iterative heuristic optimization method based on response surface models (IHRSM) with an uncertainty analysis technique (UA) was introduced. This combination allows achieving effective reductions of variability of the simulation responses with a reasonable number of simulations. Thanks to the integration of these two methods, the methodology presents important advantages over previous approaches: reduces the number of simulations required and, at the same time, explores a larger parameter domain.

To study the performance and efficiency of the methodology, it was applied to the robust design of a semiconductor manufacturing process. These simulations took an average of 65.7 minutes on a standard personal computer. This fact makes the economization of simulations a priority. The approach showed great reductions of the variability, meeting design criteria, when compared with deterministic optimization methods based on sequential quadratic programming (SQP).

Each of the UA processes required by IHRSM involves several simulations. This appears to be a source of unnecessary consumption of resources. Future research can be done to find ad-hoc mathematical response surface models to avoid this problem and integrate IHRSM with UA more effectively.

6 Acknowledgements

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Biographies

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Table 1: Parameters' probability distribution.

Parameter	Distribution	Mean	Variance	Unit
GATE_OX_TH	Normal	5.0E+12	2.5E+23	$1/cm^2$
BF2_IMPL_DOSE	Normal	3	0.04	nm

Table 2: Domain of the parameters' mean.

Parameter	Lower	Central	Upper	Unit
GATE_OX_TH	3.5E+12	5.0E+12	6.5E+12	1/cm^2
BF2_IMPL_DOSE	2.4	3	3.6	nm

Table 3: Simulation responses and their default values.

Response	Value	Units
VT3	0.812	V
VT5	0.718	V
Ion	142	μA/μm

Table 4: Optimization criteria for a deterministic optimization.

Response	Criterion	Target	Units
VT3	close to	0.5	V
VT5	minimal		V
Ion	maximal		μA/μm

Table 5: Robust optimization and deterministic optimization results.

	Robust optimum	Deterministic optimum
Parameters		
$\mu_{GATE\_OX\_TH}$	2.56	2.09
$\mu_{BF2\_IMPL\_DOSE}$	3.5E+12	4.55E+12
Responses		
μ_{VT3}	0.633	0.483
σ^2_{VT3}	0.00222	0.0514
μ_{VT5}	0.544	0.412
σ^2_{VT5}	0.00218	0.0377
μ_{Ion}	252.7	238.0
σ^2_{Ion}	1 327.7	13 624.0
Goal function	0.67	1.84

Figure captions

Figure 1. Interaction between IHRSM, UA and computer simulations

Figure 2. Optimization of Computer Simulations

Figure 3. Iterative search process. (a) RSM-based optimization from an initial solution on the region of interest. (b) Optimization on a larger region with the same RSM used in (a). (c) Enlargement of the region of interest with no improvement. (d) Optimization on a new region of interest starting from the best solution found

Figure 4. Simplified algorithm

Figure 1

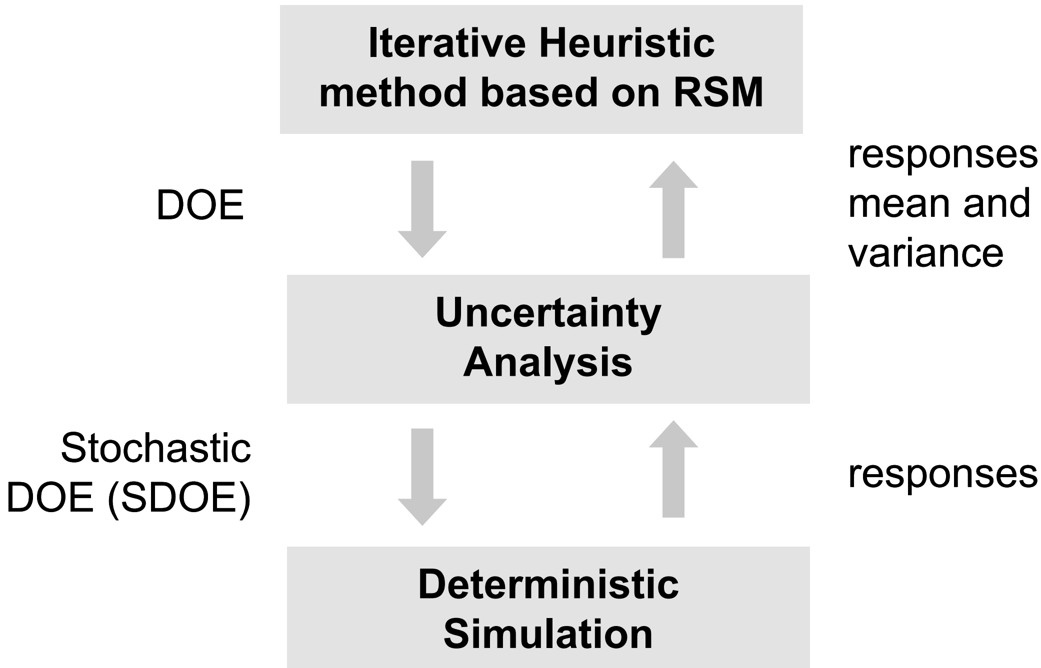

Iterative Heuristic method based on RSM
DOE
responses' mean and variance
Uncertainty Analysis
Stochastic DOE (SDOE)
responses
Deterministic Simulation

Figure 2

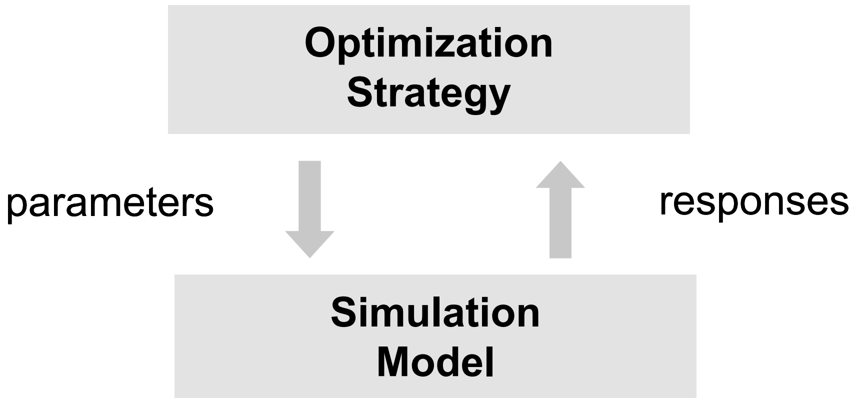

Optimization
Strategy
parameters
responses
Simulation
Model

Figure 3

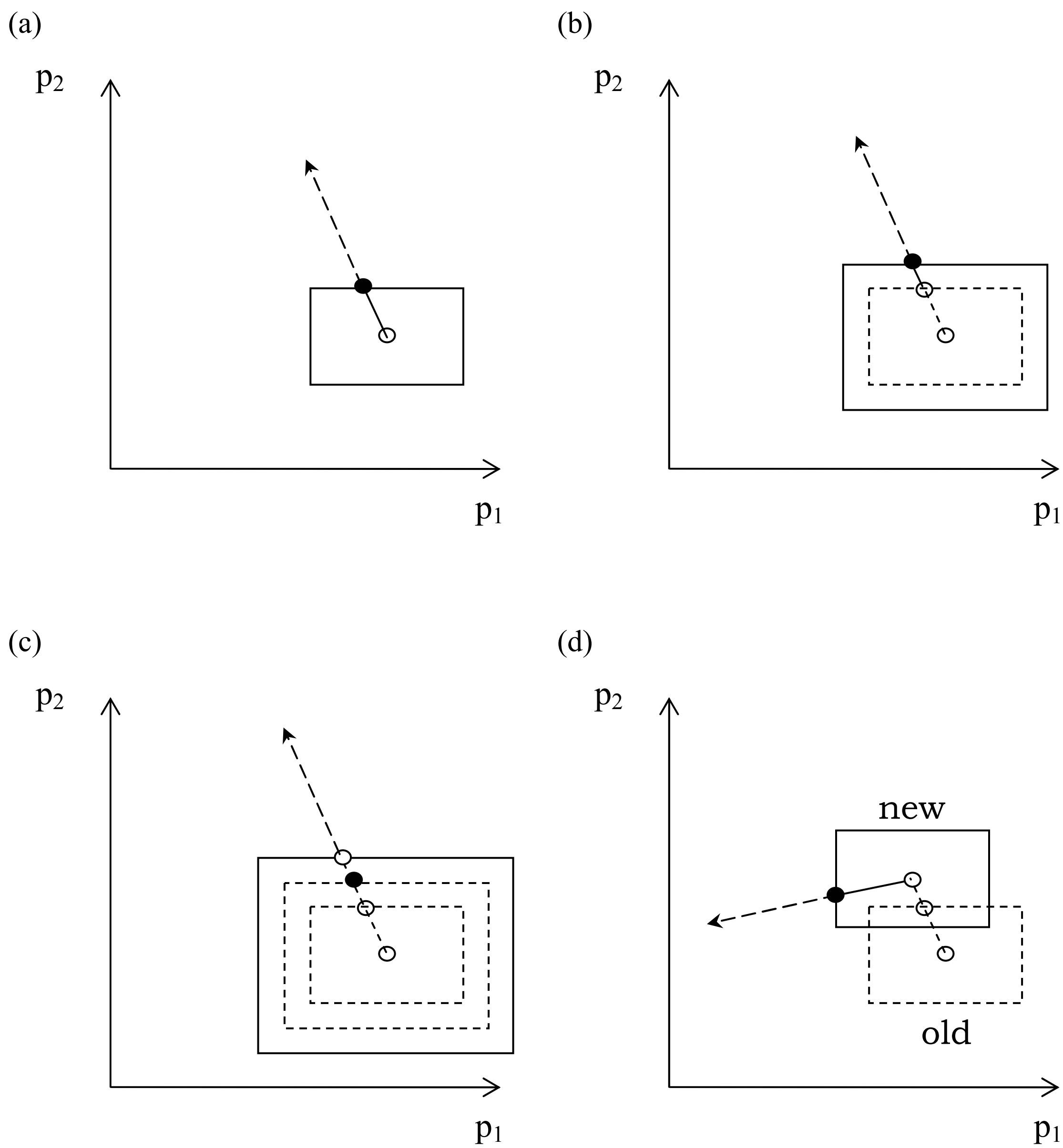
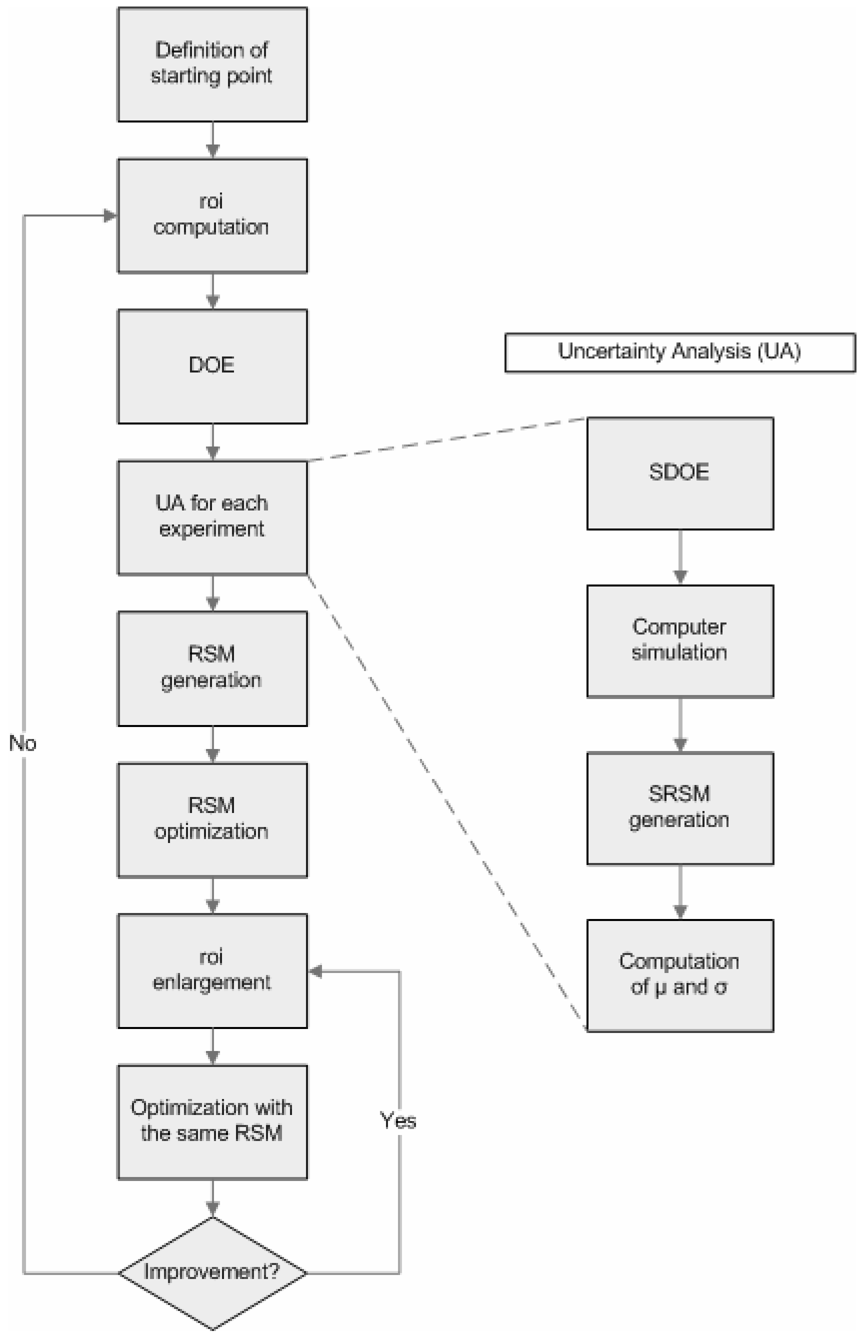


Figure 4


Definition of starting point
roi computation
DOE
UA for each experiment
RSM generation
RSM optimization
roi enlargement
Optimization with the same RSM
Improvement?
No
Yes
Uncertainty Analysis (UA)
SDOE
Computer simulation
SRSM generation
Computation of μ and σ