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ORIGINAL ARTICLE

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The integration of design of experiments, surrogate modeling and optimization for thermoscience research

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Abstract This paper presents an integrated approach for the solution of complex optimization problems in thermoscience research. The cited approach is based on the design of computational experiments (DOE), surrogate modeling, and optimization. The DOE/surrogate modeling techniques under consideration include: A-optimal/classical linear regression, Latin hypercube/artificial neural networks, and Latin hypercube/Sugeno-type fuzzy models. These techniques are coupled with both local (modified Newton's method) and global (genetic algorithms) optimization methods. The proposed approach proved to be an effective, efficient and robust modeling and optimization tool in the context of a case study, and holds promise for use in larger scale optimization problems in thermoscience research.

Keywords Surrogate modeling · DOE · Optimization · Soft computing

Nomenclature

ANN	Artificial neural network
C	Characteristic length (m)
CAD	Computer-aided design
Cl	Cluster
CLR	Classical linear regression
CVD	Chemical vapor deposition
DOE	Design of experiments
$F(.)$	Activation function
FM	Fuzzy model
K	Heat spreader conductivity (W/mK)
$L(.)$	Logistic function
P	Power dissipation (W)
SM	Surrogate modeling
T	Maximum temperature on the heat source (°C)
V	Weight matrix associated with the input layer of an artificial neural network
W	Weight matrix associated with the hidden layer of an artificial neural network
h	Heat transfer coefficient (W/m^2 K)
k	Substrate conductivity (W/mK)
max	Maximum error (°C)
min	Minimum error (°C)
mse	Mean square error (°C)
$\vec{x}$	Vector of design variable values

Greek symbols

δ	Dimensionless parameter used in the perturbed version of the case study
$\mu(.)$	Membership value of the argument to a given cluster

Subscripts

I	Number of cluster

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1 Introduction

The optimal design of complex systems in thermoscience research has been limited by the fact that accurate numerical simulations associated with models for some of its most significant problems remain too resource intensive to be efficiently incorporated in traditional engineering optimal design efforts. As an example, consider the optimal design of electronic systems under continuously reduced design cycles with increasing power dissipation needs and restrictions regarding weight and power consumption.

In order to address this problem, for optimization purposes, the construction of lower fidelity models or surrogate models that could be used instead of the original (computationally expensive) one has been suggested [1, 2]. Issues critical to this approach include: (1) sampling the design space for screening and surrogate modeling construction using the accurate numerical model, (2) constructing and validating the surrogate model, and (3) using optimization approaches. If these issues are properly addressed, surrogate model-based optimization becomes an effective and efficient tool for complex system design.

There are a variety of alternatives for these different issues, for example, for issue (1) Latin hypercube sampling, fractional design, and A-optimal and D-optimal sampling; issue (2) classical nonlinear regression, artificial neural network (ANN) models, and fuzzy models; and issue (3) local gradient-based methods (e.g., modified Newton's method), local direct search methods (e.g., downhill simplex method) and global search (e.g., genetic algorithms) optimization methods. A number of authors have focused their attention on particular methods or issues. For example, Bernardo et al. [3] address the optimization of integrated circuit design using sequential experimentation, the modeling of CAD simulator outputs as realizations of stochastic processes, and an adaptive random search algorithm for optimization purposes. Xie et al. [4], proposed a gradient-based optimization procedure that incorporates Taguchi experimental designs and fuzzy surrogate models; their strategy has been applied to the optimization of a vertical CVD process. Yesilyurt and Patera [2] present a Bayesian-validated statistical framework for the construction and validation of surrogates from computer models and illustrate their methodology with the optimization of eddy-promoter heat exchangers. Yesilyurt et al. [5] have expanded their methodology to consider noisy computer simulations and have applied it to the problem of predicting the effective conductivity of a random fibrous composite material. Osio and Amon [6] developed an adaptive engineering design methodology based on Bayesian surrogates for the efficient use of computer simulations of physical models, and evaluated its performance with the assistance of a known analytical function and a thermal design problem of an embedded electronic chip configuration.

This study presents an integrated approach for the solution of complex optimization problems in thermoscience research with different alternatives for surrogate model-based optimization. Specifically, A-optimal/classical linear regression (CLR) analysis, Latin hypercube/ANN, and Latin hypercube/fuzzy model (Sugeno type). These alternatives are coupled with local (modified Newton's method) and global (genetic algorithms) optimization methods. Their relative performance is evaluated using a case study that considers a model for the problem of finding the optimal thermal design of an embedded electronic configuration, a manufacturing alternative for portable and handheld electronic systems [7–8]. The evaluation considers modeling (mean square error, maximum and minimum error) and optimization criteria.

2 Problem definition

In general, the problem under consideration can be stated as follows: What is the set of boundary conditions, initial conditions or parameter values associated with a thermofluid field problem, denoted by $\vec{x}$ so that a given vector of objective functions, $\vec{f}(\vec{x})$, is minimized?

In thermoscience research, the cited optimization problem has in general, some special features, namely:

Time consuming and limited number of objective function evaluations The objective function evaluations usually involve the numerical solution of a thermofluid field problem. As a result, each objective function evaluation requires the solution of a set of nonlinear partial differential equations which, in general, are computationally demanding and require a significant amount of computer time. Considering the time constraints imposed by most analysis/design environments, in particular those associated with the electronic industry, the possible number of objective function evaluations to be conducted in thermoscience research optimization problems are seriously constrained.

Large design space and nonlinear solution space The problem at hand is typically an inverse problem. Consequently, the design space is rather large, with the added difficulty that due to the nonlinear nature of the problem under consideration, the superposition principle does not apply and cannot be used to simplify the search for optimal solutions.

Some representative examples are:

Eddy-promoter heat exchangers For a given thermofluid configuration, what is the eddy-promoter placement and radius, which minimize pumping power and eddy-promoter volume, and maintain a temporally and spatially average bottom-wall heat flux not significantly lower than a given nominal value? [2]

Industrial furnace design What should be the burner placement and characteristics, furnace geometry and material properties, which minimize the difference between the expected temperatures and heat fluxes in the furnace and those provided by the design?

Thermal design of electronic systems For a given thermofluid configuration, what set of parameters (e.g., material properties, and geometric characteristics), would provide the minimum operating temperatures, subject to electrical, manufacturing, and cost constraints?

Here, attention is given to the special case in which the problem involves a single objective function and simple bound restrictions on the design variables. The extensions to account for multiple objectives and restrictions are available in the literature [9–11].

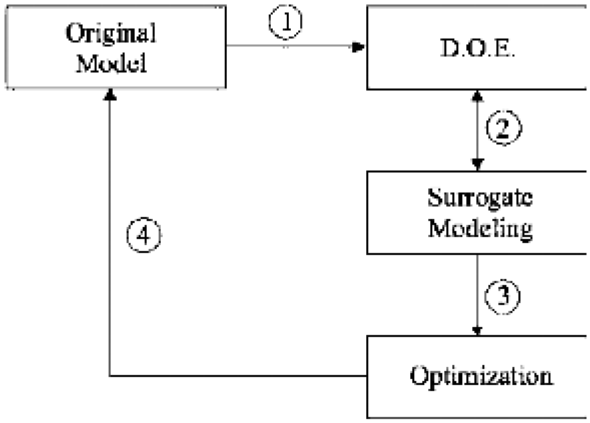

Fig. 1 A schematic representation of the proposed solution methodology

3 Solution methodology

This section provides a description of the proposed solution methodology (see Fig. 1), in terms of its main constituents, algorithm of execution, and implementation.

3.1 Main constituents

3.1.1 Design of computational experiments (DOE)

The purpose of this component is to make an efficient and representative sampling of the design/solution space. At the points in the design space selected by this component, the computationally expensive and time consuming original model (in contrast to the surrogate model to be discussed shortly) is executed, and the corresponding objective function values are calculated. The collected data is divided into two parts: *Training data*, for constructing the models, and *Testing data*, for evaluating the prediction ability of the constructed models. These data are used in the construction and validation of the surrogate models. In this paper, random sampling, Latin hypercube, and A-optimal sampling approaches are used within the context of different surrogate modeling techniques and stages of the solution methodology. A detailed discussion on the subject of DOE and these sampling schemes is provided by Rao [12], Mitchel [13] and McKay et al. [14].

3.1.2 Surrogate modeling (SM)

This module constructs lower fidelity, easy to evaluate yet effective surrogate models from the data collected during the DOE stage of the solution methodology. After proper validation of their prediction capabilities, these surrogate models are used in the context of optimization processes. The DOE strategies recently mentioned are coupled with surrogate modeling approaches, namely, A-optimal sampling with CLR, and Latin hypercube sampling with ANN and fuzzy modeling approaches. Hecht-Nielsen [15], among others, provides a good introduction to the area of function approximation using ANN. The modeling of Sugeno-type fuzzy systems (the ones considered in this work) is discussed in detail by Takagi and Sugeno [16] and Sugeno and Kang [17].

3.1.3 Optimization

The optimization procedures should identify the vector of variables, $\vec{x}$, that minimizes the objective function, $\vec{f}(\vec{x})$, using a surrogate model. The corresponding objective function value is calculated using the original model with the variables suggested by the optimization module. Both local gradient-based (modified Newton's method) and global (Genetic Algorithms) optimization procedures are considered in the context of this work. A discussion on the subject of genetic algorithms as adaptive search procedures for global optimization can be found in the books by Holland [18] and Goldberg [19]; for an introduction to Genetic Algorithms in the context of thermoscience research see, for example, Queipo et al. [20].

3.2 Algorithm of execution

With reference to Fig. 1, in stage 1 of the solution methodology, the original model is evaluated at selected values of the design variables, as specified by an appropriate DOE/surrogate modeling alternative. With the collected data, the surrogate model is constructed and validated (stage 2); if necessary, additional sampling points are introduced within the context of the previous stage. In stage 3, the validated surrogate model is introduced in an optimization loop; then, the objective function value corresponding to the solution obtained by the optimization procedure is calculated using the original model (stage 4).

3.3 Implementation

The solution methodology is implemented using a combination of both commercial and academic software. The statistical analysis system (SAS), specifically the procedures OPTEX and REG were used for the design of A-optimal data sets and the development of the linear regression model, respectively. The ANN and Fuzzy Models (Sugeno type) were generated with the assistance of the Stuttgart neural network simulator (SNNS), available through an anonymous ftp at the machine ftp.informatik.uni-stuttgart.de in the directory/pub/SNNS, and the Software for Inducing Fuzzy Models (SIFM), respectively. The SIFM computer code was developed by two of the authors (NQ; CA) using Matlab, and implements a modified version of an algorithm proposed by Wang and Langary [21] for the induction of rules from examples. The optimization procedures for gradient-based (modified Newton's method) and global search (Genetic Algorithms) methods were provided by Matlab (CONSTR procedure), and the GAucsd system, respectively. The GAucsd system is available from an anonymous ftp at the machine cs.ucsd.edu in the pub/GAucsd directory.

4 Case study

The proposed solution methodology is illustrated using a model for the problem of finding the optimal thermal design of embedded electronic components of wearable computers [7]. With reference to Figs. 2 and 3, the model seeks to find the set of design variables: chip power level (*P*), substrate conductivity (*k*), heat spreader conductivity (*K*), heat transfer coefficient (*h*), and characteristic length (*C*), that will minimize the maximum temperature in the heat source (*T*), modeling an electronic component. Note that the substrate and heat spreader conductivities are assumed to be continuous variables as the materials are considered to be polymer composites (conductive filler and polymer). The dimension of the chip is 25×25×6 mm^3, the package thickness is 20 mm, and the heat spreader thickness is 2 mm. Table 1 provides the interval of interest for each of the design variables.

4.1 Original version

This version of the case study corresponds to the problem under consideration as previously described. It provides the opportunity to evaluate the performance of the proposed solution methodology considering the influence of these variables on the temperature of the chip and the optimal design is known.

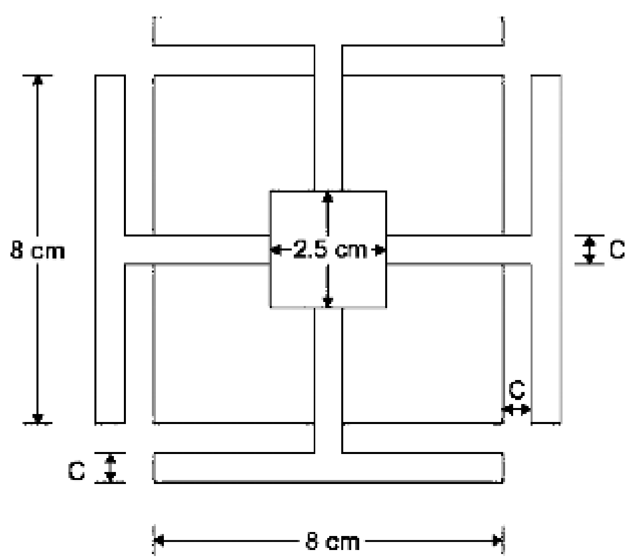

Fig. 2 A schematic representation of middle plane of an embedded chip configuration (case study)

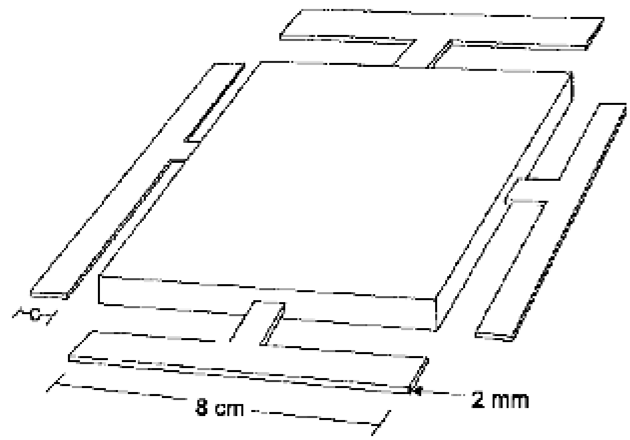

Fig. 3 A perspective of an embedded chip configuration (case study)

Table 1 Embedded chip case study: design variables and ranges

Design variable	Low level	High level	Units
P	1.0	3.0	*W*
k	14.7	116	W/mK
K	237.0	401.0	W/mK
h	5.0	10.0	W/m^2K
C	0.007	0.012	*m*

4.2 Perturbed version

To evaluate the robustness of the different alternatives for surrogate model-based optimization, a variation of the case study that includes a sinusoidal nonlinear perturbation is also considered. This version establishes that the temperature of the heat source, modeling an electronic component, is equal to that provided by the *original version* (*T*) plus an additional term in degrees Celsius equal to $\delta \cdot e^{-(11\delta - T)/2\delta} \cdot \sin\left(\frac{T^2}{10\delta}\right)$.

The perturbation is a sine wave with changing amplitude and period for increasing values of *T*. Throughout the study the parameter δ was assumed to be equal to 5, which represents a perturbation of up to 15% of the temperature values expected for the original version.

For the purpose of this work, the simulations necessary for predicting the temperature on the heat source and the construction of the surrogate models were calculated using a thermal resistive network approach. In a real design environment, the cited simulations would be conducted using numerical approaches (e.g., finite differences, finite elements, spectral methods, etc.) for solving the conservation equations. The thermal resistive network was formulated using the information provided by the geometry of the embedded chip configuration under study, and the values specified for the design variables [7].

5 Results and discussion

This section presents and discusses the results of applying the proposed solution methodology to the original (with known optimal solutions) and perturbed versions of the selected case study. The different alternatives of DOE and surrogate modeling, that is, A-optimal/CLR, Latin hypercube/ANN, and Latin hypercube/fuzzy models, are evaluated in terms of their: (1) mean square error, and maximum and minimum error over training and validation data sets, and (2) robustness, when addressing variations (nonlinear perturbations) of the case study under consideration. The optimization procedures were evaluated in terms of their suggested minimum objective function values. Note that the number of objective function evaluations to reach the optimum value was not included as a performance criterion because the optimization procedures are conducted coupled with the surrogate (easy to evaluate model) instead of the computationally expensive and time consuming one.

5.1 Preliminary considerations

The number of numerical simulations conducted using the original model, for the case study under consideration was limited to 30 as in Osio and Amon [6]. The data used for the construction of the surrogate models reported in this study is available through ftp at the machine vibora.ica.luz.ve in the directory pub/WAM98.

Each experimental design was repeated under three different random seeds. The reported results for the corresponding modeling techniques were those associated with the median.

The A-optimal designs were generated through an exchange-type algorithm starting with a larger Latin hypercube design.

The testing phase was conducted using a random sampling of size equal to 10,000 in order to fully test the prediction ability of the DOE/surrogate modeling alternatives.

The linear regression model was assumed to be quadratic, including main effects, two-factors, and quadratic factors. The coefficients in the regression model were considered to be significant when a t-test gave a confidence level of 95%.

The optimum number of artificial neurons in the hidden layer was found to be two (2) versions of the case study. In addition, the training algorithm was the standard back propagation with initial values provided by the best solution obtained by Monte Carlo optimization. The data was linearly normalized so that it meets the requirements of the activation function (F).

The output of the ANN model is calculated according to the following expression:

$$T(\vec{x}) = L[W \times (L[V \times \vec{x}])]$$

wherein the letters V and W denote weight matrices associated with the input-hidden and hidden-output layers, and the letter $L(.)$ represents the logistic function. The vector $\vec{x}$ identifies a given vector of design variable values.

The number of clusters in the fuzzy model was set to four and the membership values of the input data given by the experimental designs to each of these clusters was specified using the Fuzzy C-means Algorithm [22]. The number of clusters was specified such that in each cluster, there were at least as many data points as the number of design variables plus one.

The fuzzy model output is calculated using the following expression:

$$T(\vec{x}) = \frac{\sum_{i=1}^{4} \mu_I(\vec{x}) \cdot T_i(\vec{x})}{\sum_{i=1}^{4} \mu(\vec{x})_I}$$

wherein, I identifies the cluster under consideration, μ_I (.) the membership value of a given vector of design variable values $\vec{x}$ to the cluster I, and $T_I(.)$ denotes the local output of the rule (R_I).

The Genetic Algorithm was set to run with a chromosome length of 50 bits (10 bits per design variable) and the genetic parameters, such as population size, crossover, and mutation rate, were set as suggested by the heuristics encoded in the program GAucsd. The local optimization procedure used a random value as the starting point.

5.2 Case study–original version

Table 2 presents a summary of the results obtained corresponding to the original version of the case study. All the modeling techniques provided an excellent approximation under the training and testing phases, with the mean square error (°C) and maximum error (°C) in the intervals [0.01, 0.57] and [0.19, 5.53], respectively. During the *training phase*, the Latin hypercube/ANN model exhibited the best performance with mse and maximum errors of 0.01 and 0.19°C, respectively; however, during the *testing* stage the best modeling performance was exhibited by the A-optimal/CLR model, followed by the Latin hypercube/ANN and

Table 2 Modeling and optimization performance of different doe/surrogate modeling strategies (case study/original version)

DOE/surrogate modeling	Training			Testing			Optimization (T_{chip})	
	Mse	Max	Min	Mse	Max	Min	Local	Global
A-optimal/CLR	0.10	0.87	0.02	0.09	1.42	0.00	30.33	30.37
Latin hypercube/ANN	0.01	0.19	0.00	0.15	4.44	0.00	30.17	30.16
Latin hypercube/FM	0.15	0.92	0.03	0.57	5.53	0.00	29.79	29.93

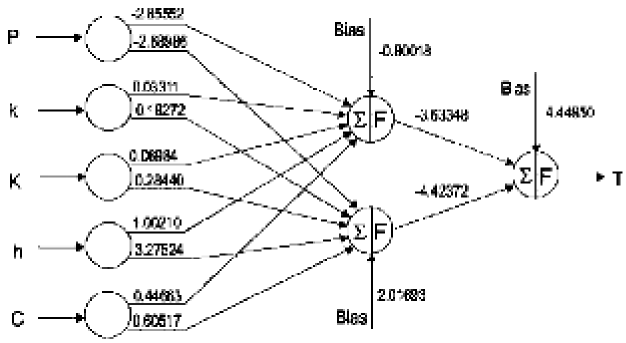

Fig. 4 Artificial neural network model (case study/original version)

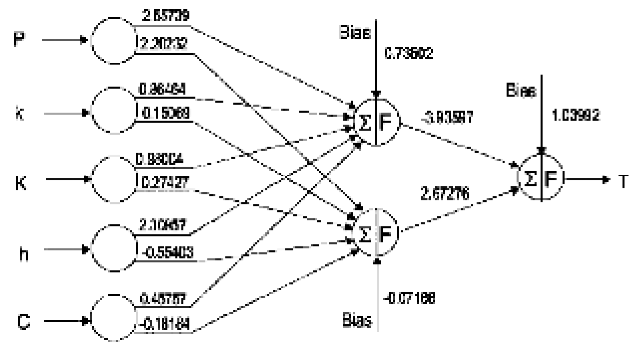

Fig. 5 Artificial neural network model (case study/perturbed version)

Latin hypercube/FM models. The A-optimal/CLR and the Latin hypercube/FM models are expressed by Eqs. 1 and 2, respectively. The Latin hypercube/ANN model is depicted in Fig. 4.

$$T = 0.30 + 0.77P - 0.40h - 0.06C - 0.39P \cdot h + 0.10P \cdot C + 0.25h^2 \quad (1)$$

$$\begin{cases} R_1: \text{ if } \vec{x} \in \text{Cl}_1 \text{ then } T_1 = 0.0 + 0.40P + 0.22k \\ R_2: \text{ if } \vec{x} \in \text{Cl}_2 \text{ then } T_2 = 0.13 + 0.82P + 0.08k - 0.25h \\ R_3: \text{ if } \vec{x} \in \text{Cl}_3 \text{ then } T_3 = 1.02 + 0.71P - 0.62k - 0.92h \\ R_4: \text{ if } \vec{x} \in \text{Cl}_4 \text{ then } T_4 = 0.36 + 0.06P - 0.18C \end{cases} \quad (2)$$

These differences at the modeling stage did not affect their suggested minimum objective function values under local or global optimization procedures. In all cases, the suggested values were set equal to approximately 30°C, that is, right at the known optimum value (29.73°C). However, this value was suggested as a result of different solutions found in the design space. Table 3 shows the solutions in the design space suggested as optimal under alternative modeling and optimization techniques. Note that the design variables, conductivity of the substrate (k) and conductivity of the heat spreader (K), as in Osio and Amon [6], do not seem to be significant in this particular case. This latter result would be suggested by a dimensional analysis.

5.3 Case study–perturbed version

Equations 3 and 4 display the A-optimal/CLR, and Latin hypercube/FM surrogate models when the original case study is subject to an additive nonlinear perturbation, as discussed in a previous section. The corresponding Latin hypercube/ANN model is shown in Fig. 5.

$$T = 0.29 + 0.63P - 0.41h - 0.39P \cdot h + 0.25h^2 - 0.03C^2 + 0.12P^2 \quad (3)$$

$$\begin{cases} R_1: \text{ if } \vec{x} \in \text{Cl}_1 \text{ then } T_1 = 1.18 - 0.26P - 0.70h \\ R_2: \text{ if } \vec{x} \in \text{Cl}_2 \text{ then } T_2 = 0.48 + 1.00P - 0.60h - 0.27C \\ R_3: \text{ if } \vec{x} \in \text{Cl}_3 \text{ then } T_3 = 0.49P \\ R_4: \text{ if } \vec{x} \in \text{Cl}_4 \text{ then } T_4 = 1.00P - 0.26h \end{cases} \quad (4)$$

As shown in Table 4, all the DOE/surrogate modeling techniques adjusted reasonably well to the nonlinear perturbation, and exhibited a robust behavior considering the nature and size of the perturbation, and the fact that the sample size to construct them remained constant (30). During the *training* and *testing* phases, the A-optimal/CLR model exhibited the best performance with an mse of 0.48°C (1.51°C) and a maximum error of 1.83°C (6.59°C) during the training (testing) stage. This may be explained by the additive nature of the perturbation, which goes well with the structure of the CLR model ($Y = X \cdot \beta + \epsilon$) that provides the possibility to easily adjust to random-like perturbations. In design problems associated with significant nonlinear interactions among the design variables, not easily captured through simple factors, the ANN and FM modeling alternatives are expected to outperform the CLR approach.

The different optimization procedures also showed a robust behavior, providing suggested minimum objective function values within small fractions of the optimum value (29.37°C). The solutions in the design space provided by the different DOE/surrogate modeling and optimization techniques were not, in general, significantly altered by the nonlinear perturbation.

Table 3 Optimal suggested values in the design space under alternative doe/surrogate and optimization strategies (case study/original version)

DOE/surrogate modeling	Local optimization					Global optimization				
	P	k	K	h	C	P	k	K	h	C
A-optimal/CLR	1.0	19.5	348.3	9.0	0.012	1.0	29.50	270.4	9.10	0.012
Latin hypercube/ANN	1.0	116.7	401.0	10.0	0.012	1.0	88.48	400.0	9.95	0.012
Latin hypercube/FM	1.0	14.7	401.0	10.0	0.012	1.0	114.2	260.0	10.0	0.012

Table 4 Modeling and optimization performance of different doe/surrogate modeling strategies (case study/perturbed version)

DOE/surrogate modeling	Training			Testing			Optimization (T_{chip})	
	Mse	Max	Min	Mse	Max	Min	Local	Global
A-optimal/CLR	0.48	1.83	0.12	1.15	6.59	0.00	30.07	30.09
Latin hypercube/ANN	0.80	2.13	0.00	2.59	10.32	0.00	31.34	31.36
Latin hypercube/FM	1.11	2.57	0.11	2.25	8.79	0.00	29.43	29.68

6 Conclusions

This paper discussed an integrated approach for addressing complex optimization problems in thermoscience research. The approach incorporates a variety of DOE/Surrogate modeling and Optimization techniques. The DOE/Surrogate modeling techniques include: A-optimal/CLR, Latin hypercube/ANN, and Latin hypercube/Sugeno-type fuzzy models coupled with local (modified Newton's method) and global (genetic algorithms) optimization methods.

The proposed approach proved to be an effective, efficient, and robust strategy in the context of a model for the optimal thermal design of embedded electronics (case study). It provided surrogate models with excellent prediction capabilities and generated known optimal solutions (effectiveness), with a small number of objective function evaluations involving the original model (efficiency), and with good adjustment to additive random-like nonlinear perturbations (robustness).

The proposed integrated approach has the flexibility to tackle increasingly complex modeling and optimization problems, even with multimodal solution spaces. As a result, it holds promise for use in larger scale nonlinear optimization problems in thermoscience research.

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