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NUMERICAL AND EXPERIMENTAL METHODS IN HEAT TRANSFER

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EXPERIMENTAL METHODS IN CONVECTION HEAT TRANSFER

CALIBRATION, ERROR ANALYSIS, AND MODELING OF HEAT FLUX SENSORS

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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 showed to be an effective, efficient, and robust, modeling and optimization tool in the context of a case study, and holds promise to be useful in larger scale optimization problems in thermoscience research.

NOMENCLATURE

ANN	Artificial neural networks
L_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 (^{o}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^2K)
k	Substrate conductivity (W/mK)
max	Maximum error (^{o}C)
min	Minimum error (^{o}C)
mse	Mean square error (^{o}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

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 (Gaston and Walton, 1994, Yesilyurt and Patera, 1995). Critical issues to this approach include: i) sampling of the design space for screening and surrogate modeling construction, using the accurate numerical model, ii) construction and validation of the surrogate model, and iii) optimization approaches. If these issues are properly addressed, surrogate model based optimization becomes and effective and efficient tool for complex system design.

There are a variety of alternatives for these different issues, for example, regarding issue i) Latin Hypercube Sampling, Fractional Design, and, A-Optimal and D-Optimal sampling; issue ii) Classical Non-Linear Regression, Artificial Neural Network Models, and, Fuzzy Models; and issue iii) Local Gradient based (e.g. Modified Newton's Method), Local Direct Search Methods (e.g. Downhill Simplex Method) and Global Search (e.g. Genetic Algorithms) optimization methods. Different authors have focused their attention on particular methods or issues. For example, Bernardo et al. (1992) 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. (1994), 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 (1995), presented 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. (1996) 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 (1996) developed an adaptive engineering design methodology based on Bayesian surrogates for the efficient use of computer simulations of physical models, and evaluate 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 Analysis, Latin Hypercube/ Artificial Neural Networks, 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 (Egan and Amon, 1996). The evaluation considers modeling (mean square error, maximum and minimum error) and optimization criteria.

PROBLEM DEFINITION

In general, the problem of interest, 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 involves the numerical solution of a thermofluid field problem. As a result each objective function evaluation requires the solution of a set of non-linear 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 of interest, the superposition principle does not apply and can not be used to simplify the search for optimal solutions.

Some representative examples:

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? (Yesilyurt and Patera, 1995).

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 where 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; see, for example, Balanchandran and Gero (1984), Keeney and Raiffa (1993), and Queipo et al. (1998).

SOLUTION METHODOLOGY

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

Main constituents

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

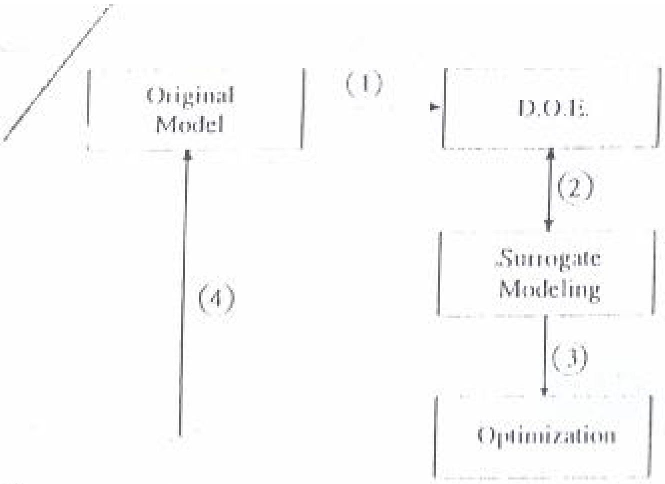

FIGURE 1: SCHEMATIC OF THE PROPOSED SOLUTION METHODOLOGY

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 model and *testing data*, for evaluating the prediction ability of the constructed models. ...se data are used in the construction and validation of the su... gate 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 are provided by Rao (1973), Mitchel (1974) and McKay et al.(1979).

Surrogate Modeling (SM). This module constructs lower fide... ...asy 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 classical linear regression, and latin hypercube sampling with, artificial neural networks (ANN) and fuzzy modeling approaches. Hecht-Nielsen (1989), among others, provide 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 Takági and Sugeno (1985) and Sugeno and Kang (1988).

Optimization. The optimization procedures should identify the vector of variables, $\vec{x}$, that minimize the objective function, $f(\vec{x})$, 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) op... ...ation procedures are considered in the context of this work. A ...ssion on the subject of genetic algorithms as adaptive search procedures for global optimization, can be found in the books by Holland (1975) and Goldberg (1989), for an introduction to Genetic Algorithms in the context of thermoscience research, see for example, Queipo et al. (1994)

Algorithm of execution

With reference to Figure 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).

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 Artificial Neural Network and Fuzzy models (Sugeno type) were generated with the assistance of the Stuttgart Neural Network Simulator (SNNS), available through 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 (1985) 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 anonymous ftp at the machine cs.ucsd.edu in the pub/GAucsd directory.

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 (Egan and Amon, 1996). With reference to Figure 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 since the materials are considered to be polymer composites (conductive filler and polymer). The dimension of the chip is 25x25x6 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.

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

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	29.5	270.4	9.1	0.012
Latin H./ANN	1.0	116.7	401.0	10.0	0.012	1.0	88.48	400.0	9.95	0.012
Latin H./FM	1.0	14.7	401.0	10.0	0.012	1.0	114.2	260.0	10.0	0.012

TABLE 4: OPTIMAL SUGGESTED VALUES IN THE DESIGN SPACE UNDER ALTERNATIVE DOE/SURROGATE AND OPTIMIZATION 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	1.51	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

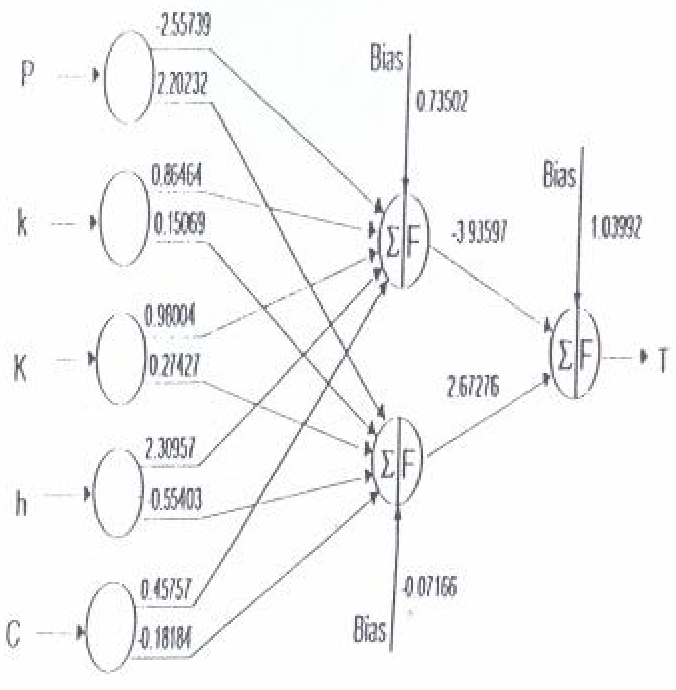

FIGURE 5: ARTIFICIAL NEURAL NETWORK MODEL (CASE STUDY/PERTURBED VERSION)

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 Figure 5.

$$T = 0.29 + 0.63P - 0.41h - 0.39Ph + 0.25h^2 - 0.03C^2 + 0.12P^2 \tag{3}$$

$$\begin{aligned} R_1 &: if\ \vec{x} \in C_1\ then\ T_1 = 1.18 - 0.26P - 0.70h \\ R_2 &: if\ \vec{x} \in C_2\ then\ T_2 = 0.48 + 1.00P - 0.60h - 0.27C \\ R_3 &: if\ \vec{x} \in C_3\ then\ T_3 = 0.49P \\ R_4 &: if\ \vec{x} \in C_4\ then\ T_4 = 1.00P - 0.26h \end{aligned} \tag{4}$$

As shown by Table 4, all the DOE/surrogate modeling techniques adjusted reasonable 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 a 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 classical linear regression model ($Y = X\beta + \epsilon$) 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.

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/Classical Linear Regression, Latin Hypercube/Artificial Neural Networks, and Latin Hypercube/Sugeno-type Fuzzy Models; coupled with local (modified Newton's method) and global (Genetic Algorithms) optimization methods.

The cited approach showed to be an effective, efficient, and robust strategy in the context of a model for the 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 to be useful in larger scale nonlinear optimization problems in thermoscience research.

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