6-7

Theory and Implementation of a New Interpolation Method Based on Random Sampling.

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Abstract.

A new method of interpolation is presented. It is argued that the method eliminates all bias concerning the functional structure of the interpolated result. The method is integrated in a TCAD framework and was applied to several design problems in device engineering.

Introduction.

For a design problem with many interacting design variables or input factors it is advisable to exploit design of experiment (DOE) methods in order to efficiently scan the design space for the optimal setting of the input factors. TCAD frameworks are supplied with DOE software, since for device design computer experiments can be very CPU intensive. A single experiment may require a full 2D or 3D process simulation followed by a full device characterization. Consequently, scanning the design space means in practice selecting a limited set of points in this space according to the DOE plan and fitting a model of the responses (response surface) based on the experimental values. These methods have all been based on the assumption of the existence of a suitable analytic function in which a number of parameters has to be determined from the experiments. Since computer experiments have a deterministic nature, interpolation techniques are better suited than fitting techniques.

A typical method for modeling response surfaces uses Taylor polynomials. An alternative strategy has been proposed by Sachs et al. [1], using Gaussian functions, being the realization of a stochastic process. This interpolation method is inspired on the description of random variables, but nevertheless remains fully deterministic.

The mere fact that one selects some analytic function, causes a large amount of bias to enter the "solution" and the ignorance concerning the non-experimented points does not justify the inclusion of such presuppositions. In this paper we will follow a completely opposite way of reasoning. The *only* bias that we force into our solution will be that the responses are continuous functions of the input factors. There are not made any presuppositions concerning the functional relation between the factors and responses: on the contrary, we assume that *all* functional relations have an a priori probability to occur.

One Factor and One Response.

In order to explain the new method it is most convenient to consider one input factor and one response. Suppose the design window is [a,b] and let us assume that one experiment has been performed at $x = x_1$ with outcome R_1. The question that we are concerned with, is how to relate the outcome of this experiment to unexplored values of x. For that purpose we subdivide [a,b] using a grid with cell size Δx. Since no furhter experiments are performed for $x_i \neq x_1$, the response R_i can take any value. In Fig.1 a possible realization is shown. Highly irregular patterns are not a priori excluded although this is in conflict with a response being a smoothly varying function of the input. Whenever such a regularity claim exists it should be made explicit. A possible way to include regularity is by introducing correlation of the responses of neighbouring cells. The *least-biased* conditional probability for the response R_{i+1} given the response R_i is

$$P(R_{i+1}|R_i) = C_i \exp\left(-\frac{|R_{i+1} - R_i|^2}{\sigma_{i+1}}\right)$$

Continuity of the response function is realized by having $\sigma_{i+1} \propto (x_{i+1} - x_i)$ or $\sigma_{i+1} = \Delta x_{i+1}/\beta_{i+1}$, since if $\Delta x \to 0$ then $P(R_{i+1}|R_i) \to \delta(R_{i+1} - R_i)$. In fact, the probability that the responses $R_1, R_2, ...R_n$ are realized for the cells $x_1, x_2, ...x_n$ is

$$p(R_1; R_2; ...R_n) = \prod_{i=1}^{n-1} P(R_{i+1}|R_i) = C \exp\left(-\sum_{i=1}^{n-1} \beta_{i+1} \frac{(R_{i+1} - R_i)^2}{\Delta x_{i+1}}\right)$$

We can imagine such a realization as a path. Before any experiment is performed we cannot exclude any realization from our considerations; consequently all paths must be included if we want to make an estimate for

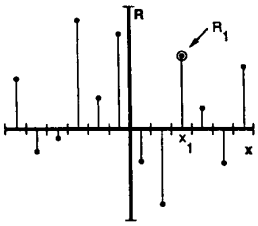

Figure 1: Possible realization of cell responses.

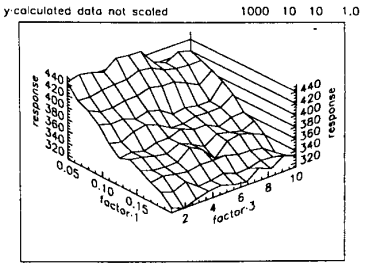

Figure 2. Expectation value of response with average over 1000 samples.

a response. By identifying the interpolated value as the expectation value of the response R_i for cell x_i (r_i), it is given by

$$r_i =< R_i >= \frac{\sum_{allpaths} R_i p(R_1; R_2; ...R_n)}{\sum_{allpaths} p(R_1; R_2; ...R_n)}$$

In the limit $\Delta x \rightarrow 0$, both numerator and denominator become Feynman path integrals [2]. The denominator can be interpreted as the partition function of a continuous statistical system. There exists a wide variety of numerical techniques for exploring such systems. For the realization of this new statistical interpolation technique we have implemented the Metropolis algorithm [3] for the random (Monte-Carlo) sampling of the equivalent statistical system.

NORMAN/DEBORA.

The NORMAN/DEBORA TCAD system [4] is an environment for efficiently planning and performing a series of simulation experiments. The scheduling and sequencing is done automatically (NORMAN). A non-linearly constrained optimizer (DEBORA) is included, which enables one to find optimal settings for the design parameters. Insight in the design problem is provided by construction of the response surfaces from the experimented points. The system has now been extended with the MOCCASIN module (Monte-Carlo Controlled Algorithm for Statistical INterpolation), which realizes the above ideas for an arbitrary number of input factors and responses, and which allows for the construction of the response surfaces without referring to an a priori selected analytic function. Moreover, the resulting interpolation will pass through the experimented values. It should be emphasized that by enlarging the set of experiments the event space of possible outcomes schrinks. In this way the "inverse temperature", β is determined. As an illustration of the statistical interpolation method we have applied the method to construct the response surface for the stress in a bump soldering of a multichip module as a function of the input factors , being the width (factor.1) and the radius (factor.2) of the solder. In Fig.2 the response surface is shown. The experimental plan corresponds is a CCF design. This least-biased interpolation is obtained by using a 10 $\times$10 grid and 1000 Metropolis sweeps.

Conclusions.

A new interpolation technique is presented. The method avoids all bias concerning presupposed analytic functions. The method has been implemented into a TCAD framework by developing a Metropolis algorithm in an an arbitrary number of dimensions. It is in particular very suitable for design problems where non-linear dependences are dominant and hints for appropriate factor or response transformations are lacking.

References.

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