

# Sequential Designs for Complex Computer Experiments with an Application to a Nuclear Fusion Model<sup>1)</sup>

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## Abstract

Data-adaptive sequential suboptimal designs for very complex computer simulation codes are considered based on a spatial prediction model. These designs are constructed for two simulators of the computational nuclear fusion devices model. The difficulty of constructing the optimal designs due to the irregular design region, and its alternatives are also discussed with some computational algorithms for obtaining the designs.

## 1. Introduction

Computer simulation is widely used for prediction of the behavior of complex system, where analytical solutions are difficult or impossible to obtain for system study. Advances in computing facilities allow programming very complex simulation codes. The time and effort needed to develop simulation models and to experiment with them has always been a major concern. Thus one aim of applying statistical methodologies to simulation has been to reduce the time spent in simulation life cycle and to help the simulationist and end user at various phases of simulation studies.

One feature of a computer simulation experiment, different from a physical experiment, is that the output is often deterministic - the response is observed without measurement error. There is of course stochastic simulations in which random errors are involved in the responses. Moreover simulation codes are often computationally very expensive to run. Thus a careful selection of inputs and an efficient analysis of its outputs are necessary. This is a statistical design and analysis problem for a complex and deterministic simulation experiments. In this paper, we mostly concentrate on the sequential construction of efficient statistical designs for computationally very expensive computer experiments, based on a spatial linear model.

The research described here was motivated by a nuclear fusion research which needs to

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estimate the universal constants in the simulation code. There is a very complex computer simulation code known as **BALDUR** (Singer et. al., 1988) which was implemented based on a comprehensive mathematical model for the nuclear fusion devices (called tokamaks). This simulation code is computationally very expensive, and a single run of the code requires about five minutes of CPU time on a super-computer (**CRAY-Y/MP**).

One of the simple measures of energy efficiency in tokamak is the global energy confinement time. The theoretically-based confinement model may be written as (Kaye and Goldston, 1985):

$$\tau_E = f(\underline{c}^*, P, I, N, B),$$

where  $f$  is a known function which is calculated by a simulation code (called **BALDUR**),  $P$  is the input total power,  $I$  is the plasma current,  $B$  is the electron density, is the magnetic field and  $\underline{c}^* = (c_1^*, c_2^*, c_3^*, c_4^*)$  are the adjustable parameters determining energy transfer known as drift waves, rippling, resistive ballooning and critical value of  $\eta_i$ , respectively. There is also a large experimental database of results from nuclear fusion reactor. The experimental data were taken from the database collected by S. Kaye for two tokamaks: 32 observations from **ASDEX** tokamak in Germany and 42 observations from **PDX** tokamak in Princeton.

A probably well known design for deterministic computer experiments is Latin-hypercube design (LHD) which was introduced by McKay, Beckman and Conover (1979). They illustrated that LHD is better than random sampling for computer experiments, and this property was theoretically proved by Stein (1987), and Owen (1994). Another interesting designs are minimax and maximin distance designs by Johnson, Moore and Ylvisaker (1990), and maximum entropy design by Shewry and Wynn (1987).

We model the response of computer simulation code as the realization of a stochastic process, which has been successfully used in design and analysis of computer experiments (Sacks, Welch, Mitchell and Wynn, 1989). Based on this model, an initial optimal design is constructed, and it is then sequentially updated. The spatial model to approximate the complex simulation code and the basic ideas of sequential (**IMSE** and **MMSE**) optimal designs are discussed in the next section. In Section 3, the procedure of constructing the actual sequential optimal designs for the **BALDUR** code are presented. Finally, Section 4 contains discussion and future research.

## 2. A statistical model and optimal designs for simulation data

### 2.1 A Gaussian spatial linear model

We use a spatial regression model which treats the response  $y(\underline{x})$  as a realization of a

random function superimposed on a regression model,

$$y(\underline{x}) = \sum_{j=1}^k \beta_j f_j(\underline{x}) + Z(\underline{x}) + \varepsilon, \tag{2.1}$$

where  $f$ 's are known functions and  $\beta$ 's are unknown regression coefficients. Here the random process  $Z(\cdot)$  representing the systematic departure from the assumed linear model is assumed to be a Gaussian process with mean zero and covariance  $cov(\underline{t}, \underline{u}) = \sigma^2 R(\underline{t}, \underline{u})$  between  $Z(\underline{t})$  and  $Z(\underline{u})$ , for  $\underline{t} = (t_1, \dots, t_d)$ ,  $\underline{u} = (u_1, \dots, u_d)$ , where  $d$  is the dimension of  $\underline{t}$  and  $\underline{u}$ ,  $\sigma^2$  is the process variance (a scale factor) and  $R(\underline{t}, \underline{u})$  is the correlation function. The measurement errors  $\varepsilon$  are assumed to be uncorrelated, mean zero normal random variables with constant variance  $\sigma_\varepsilon^2$ , and assumed to be independent of  $Z$ . See Cressie (1990) or Ripley (1981) for details of this spatial linear model, and Sacks, Welch, Mitchell and Wynn (1989), and Currin, Mitchell, Morris and Ylvisaker (1991) for its application to design and analysis of computer experiments.

Some possible choices of correlation function are from the power exponential family which is given by

$$R(\underline{t}, \underline{u}) = \exp\left[-\sum_{i=1}^d \theta_i |t_i - u_i|^2\right] \tag{2.2}$$

where  $\underline{\theta} \geq 0$ . The non-negative parameter  $\underline{\theta}$  determines the covariance structure of  $Z$ : small  $\underline{\theta}$  reflects large correlations between nearby observations while large  $\underline{\theta}$  reflects small nearby correlations (see Sim, Park, and Bai, 1994 for an illustration of this effect).

Once a correlation function and its parameters in (2.2) are specified, one can optimally predict  $y(\underline{x})$  based on the model (2.1) using the observations  $y(\underline{y})$ . Now define the times  $n \times n$  matrix  $V$  by

$$V = [R(s_i, s_j)]_{\substack{1 \leq i \leq n \\ 1 \leq j \leq n}} + \gamma^2 I, \tag{2.3}$$

where  $\gamma^2 = \sigma_\varepsilon^2 / \sigma^2$ , and a  $n \times k$  matrix  $F$  be so called a design matrix, where  $(s_1, \dots, s_n)$  are the design sites. For any prediction site  $x$ , the  $n \times 1$  vector  $\underline{v}_x$  and  $k \times 1$  vector  $\underline{f}_x$  are defined by  $\underline{v}_x' = [R(s_1, x), \dots, R(s_n, x)]$ ,  $\underline{f}_x' = [f_1(x), \dots, f_k(x)]$ , respectively. Here  $\underline{v}_x$  is a correlation vector between design sites and a prediction site  $x$ . Then the best linear unbiased predictor (BLUP) of  $y(x)$  given the observation vector  $\underline{y}$  is (see Ripley, 1981, pp. 44-58)

$$\begin{aligned} \hat{y}(x) &= [\underline{v}_x', \underline{f}_x'] \begin{bmatrix} V & F \\ F' & 0 \end{bmatrix}^{-1} \begin{bmatrix} \underline{y} \\ 0 \end{bmatrix} \\ &= \underline{f}_x' \underline{\hat{\beta}} + \underline{v}_x' V^{-1} (\underline{y} - F \underline{\hat{\beta}}), \end{aligned}$$

where  $\hat{\beta} = (F'V^{-1}F)^{-1}F'V^{-1}y$  is the generalized least squares estimator of  $\beta$ . The normalized mean squared error of the prediction of  $y(x)$  is

$$\begin{aligned} mse(x) &= E_{\theta}[\hat{y}(x) - y(x)]^2 / \sigma^2 \\ &= R(x, x) - [\underline{v}_x', \underline{f}_x'] \begin{bmatrix} V & F \\ F' & 0 \end{bmatrix}^{-1} \begin{bmatrix} \underline{v}_x \\ \underline{f}_x \end{bmatrix} \end{aligned} \quad (2.4)$$

## 2.2 Minimum IMSE design

Of the many possible design criteria, we minimize the integrated mean squared error (IMSE) of prediction for a design  $S$ ,

$$IMSE_{\theta}(S) = \int_Q mse(x) d\mu(x), \quad (2.5)$$

where  $Q$  is the design region, and  $\mu$  is a "weight measure" which may be the empirical measure of uniformly distributed random points (see Section 3 and Figure 1), or of "semi-random" points (see Figure 3) which are crossproduct of uniform random samples on the set of allowed values ( $\underline{c}$ ) for the  $\underline{c}^*$  and values of  $P$ ,  $I$ ,  $N$  and  $B$  in the data base. Note that neither  $mse$  nor IMSE depend on the data  $y$  nor on the unknown parameters  $\beta$  and  $\sigma^2$ , but its are dependent on  $\theta$  and design  $S$ . This makes it possible to design an experiment (for a specified value of  $\theta$ ) before taking the data, i.e., to select the design sites  $S$  which minimize some criteria such as IMSE and maximum  $mse$  (MMSE) (see Sacks, Schiller and Welch, 1989). We always restrict the design points to lie in the prediction region. Since (2.1) is a spatial linear model, our optimal designs are basically the "spatial designs" which are extensively considered in Ripley (1981), and Sacks and Schiller (1988). Sacks, Schiller and Welch(1989) illustrated that minimum IMSE designs based on the model (2.1) is better than response surface designs based on classical regression model, and Welch, Yu, Kang and Sacks (1991) have applied the above method to a very large scale integrated circuit design problem. Sim, Park and Bai (1994) proposed minimum IMSE Latin-hypercube design which is selected to have minimum IMSE among all possible Latin-hypercube designs.

In our tokamak example, it is difficult to evaluate the integration (2.5) analytically over the design region  $Q$ , because  $Q$  is a nontrivial constrained region (see (3.2) or Figure 1). Initially we approximated (2.5) by Monte-Carlo method using a uniform measure on  $Q$ . Later we realized that we really cared about predictions at points ( $\underline{c}$ ,  $P$ ,  $I$ ,  $N$ ,  $B$ ) in data base. Therefore, we used the empirical measure of semi-random points (which are crossproduct of uniform random samples on the set of allowed values ( $\underline{c}$ ) for the  $\underline{c}^*$  and values of  $P$ ,  $I$ ,  $N$  and  $B$  in the data base) as the following manner:

**Step 1.** Construct  $m$  ( $m=1000$ , say)  $d$ -dimensional "semi-random" vectors (see Figure 3) as mentioned in the above, and denote them  $\underline{x}_j, j=1, \dots, m$ .

**Step 2.** Approximate the integral by

$$\int mse(x)d\mu(x) \approx \frac{1}{m} \sum_{j=1}^m mse(\underline{x}_j). \quad (2.6)$$

To minimize criterion (2.6) as a function of the  $n \times d$  design-point coordinates, we have mainly used Cox and Chang's algorithm (1989) to efficiently compute  $m$  MSE's and a quasi-Newton optimizer (Gill and Murray, 1972) in NAGLIB (1984). Because it is difficult to obtain the explicit form of first derivative of IMSE, the optimizer used finite difference approximation to the derivative. Computing time to minimize the criterion(2.6) is formidable since it involves  $n \times d$  dimensional global optimization problem ( $n = 10, d = 8$ , in our first example), even though we used Cox and Chang's efficient algorithm. This difficulty encourages some alternative design strategies. Thus a less slow global search plan on the construction of optimal design is given below.

Even though it is supposed that an optimal design is obtained by running the optimizer for a set of starting values, there is no guarantee that the design so obtained is a global minimizer of IMSE. To circumvent the above difficulty and not to waist computing time due to strange initial values, the following procedure was actually adopted in our example.

**Step 1.** Run the optimizer for  $k$  (2 or 3) different sets of random (or chosen by eyeballing) initial values.

**Step 2.** Stop at a moderate iteration limit and choose a design which has minimum of IMSE among those.

**Step 3.** Take the design selected at Step 2 as a starting design and run it.

The computing time is still formidable. A plan that may possibly achieve both time savings and globality is discussed in Section 4.

Note that  $\sigma^2$  plays no role in this minimization, however the knowledge of  $\underline{\theta}$  and  $\gamma^2 = \sigma_{\varepsilon}^2 / \sigma^2$  is crucial. Because  $\underline{\theta}$  is generally not available for the initial design stage, a robustness study, described in Sacks, Schiller and Welch (1989), may be useful to choose  $\underline{\theta}$ . In our example, we used an rough estimate of  $\underline{\theta}$  based on a previous similar work and a prior information on  $\sigma_{\varepsilon}^2$  given by a BALDUR specialist at the initial design stage.

### 2.3 Minimum MMSE and sequential designs

As an alternative design criterion, we minimize the maximum mean squared error (MMSE) of prediction. This MMSE can be obtained, similarly as done in IMSE calculation because of irregularity of the design region, by the following formula,

$$MSE_{\max}(S) \approx \max_{\mathbf{x}_j \in Q} mse(\mathbf{x}_j),$$

where  $\mathbf{x}_j, j=1, \dots, m$ , are  $d$ -dimensional semi-random vectors. Comparisons of MMSE and IMSE for discrete designs were made by Sacks and Schiller (1988). MMSE is also used as a measure of accuracy of a given prediction model (see below and Section 3).

After collecting some observations based on the initial optimal design, we estimate parameters ( $\underline{\beta}$ ,  $\sigma^2$ ,  $\underline{\theta}$  and  $\gamma^2$ ) of the spatial linear models using the maximum likelihood estimation method (see Park and Cho, 1994, for details). Then we construct so called data-adaptive sequential optimal designs by the following procedure:

**Step 1.** Find an appropriate prediction model and estimates of parameters based on previous design ( $n_1$  points, say) by suitable analysis methods (for details, see Sim, Park and Bai, 1994).

**Step 2.** Check MMSE, and stop constructing the next stage design if MMSE is smaller than a preassigned target value. Otherwise, go to the next step.

**Step 3.** Use these model and estimates to choose the next stage optimal design ( $n_2$  points, say) under the condition that the previous design is given (i.e., update  $n_2$  more points to the previous design to make  $n_1 + n_2$  points). Then go to the Step 1.

In constructing the above sequential designs at the Step 3, the first  $n_1$  design points are fixed, and so the covariance matrix,  $mse$  and IMSE corresponding the first  $n_1$  points are not changed. This fact allows us to save much computer time by calculating IMSE for the new  $n_2$  points, and by updating it to the already calculated IMSE (for the first  $n_1$  points). For this purpose, we mainly used Cox and Chang's (1989) updating algorithm to save computing time. Their algorithm updates (partial) Cholesky and QR decompositions when new design points are added to the existing design. There, the linear model for the mean function in (2.1) is handled by a QR decomposition and the stochastic process ( $Z$ ) is handled by a Cholesky decomposition (see Cox and Chang (1989) for details of the algorithm).

When the obtained model is complicated, computing time for constructing the next stage optimal design is extremely expensive. In that case, a simple model is used to save CPU time instead of the best (complicated) model.

### 3. Sequential sub-optimal designs for nuclear fusion simulators

In this section, the actual data-adaptive sequential designs, discussed in the above section, for 2 tokamak (ASDEX and PDX) simulators are presented.

In running BALDUR code, we used  $c_1, c_2, c_3, c_4$  (parameters) and  $P, I, N$  and  $B$  (real variables) as input variables. Following the nuclear fusion specialist, we transform  $P, I, N$  and  $B$  to  $\log_{10}P, \log_{10}I, \log_{10}N$ , and  $\log_{10}B$  to define the input variables. Also  $\log_{10}\tau_E$  is used as a response  $y(\underline{x})$ .

Let  $\tau_E^*$  be a true (theoretical) energy confinement time. Then our observation  $\tau_E$  from BALDUR code is equal to  $(1 \pm \varepsilon) \tau_E^*$ , where  $\varepsilon$  is a random variable thought of as measurement error, because of the Monte-Carlo integration in BALDUR code. It is known that  $\text{var}(\varepsilon) \approx .0025$  from the previous experience. Then

$$\begin{aligned} \log_{10}\tau_E &= \log_{10}(1 \pm \varepsilon) \tau_E^* \\ &= \frac{1}{\log_e 10} (\log_e(1 \pm \varepsilon) + \log_e \tau_E^*) \\ &\approx \frac{1}{\log_e 10} (\pm \varepsilon + \log_e \tau_E^*) \end{aligned} \quad (3.1)$$

so that  $\sigma_\varepsilon^2$  for  $\log_{10}\tau_E$  is approximately equal to .0005.

As discussed in Section 2.3, we will stop constructing the next stage design if MMSE, calculated for a given prediction model, is smaller than a target value. Tokamak specialist allows 10% maximum prediction error for  $\tau_E$ . Then by the same calculation as (3.1), we obtain approximately .002 as a target value.

### 3.1 Sequential designs for ASDEX Tokamak simulator

The design region  $Q$  is as follows :

$$\begin{aligned} 0 \leq c_1, c_3 \leq 2, \quad 0 \leq c_2 \leq 5, \quad 1.0 \leq c_4 \leq 1.4, \\ .2 \leq P \leq 4, \quad .18 \leq I \leq .42, \quad .2 \leq N \leq 1.05, \quad 1.4 \leq B \leq 2.6 \end{aligned}$$

with additional constraints

$$\frac{N}{I} \leq 2.5, \quad 5.15625 \leq \frac{B}{I} \leq 8.25. \quad (3.2)$$

The upper bound of second constraint was changed, by examining the data base, to 11.3 (which is the maximum of  $B/I$  in the data base) after several sequential design steps. Actually  $c_4$  was set 1.0 by default until after we obtained 30 design points. The 2-dimensional projections of  $Q$  with new upper bounds are shown in Figure 1 in which 1000 random numbers generated over  $Q$  are plotted. Input variables are shifted and rescaled by, for example

$$x_8 = \frac{\log_{10}B - \log_{10}(2.6/1.4)}{\log_{10}(2.6)} - .5,$$

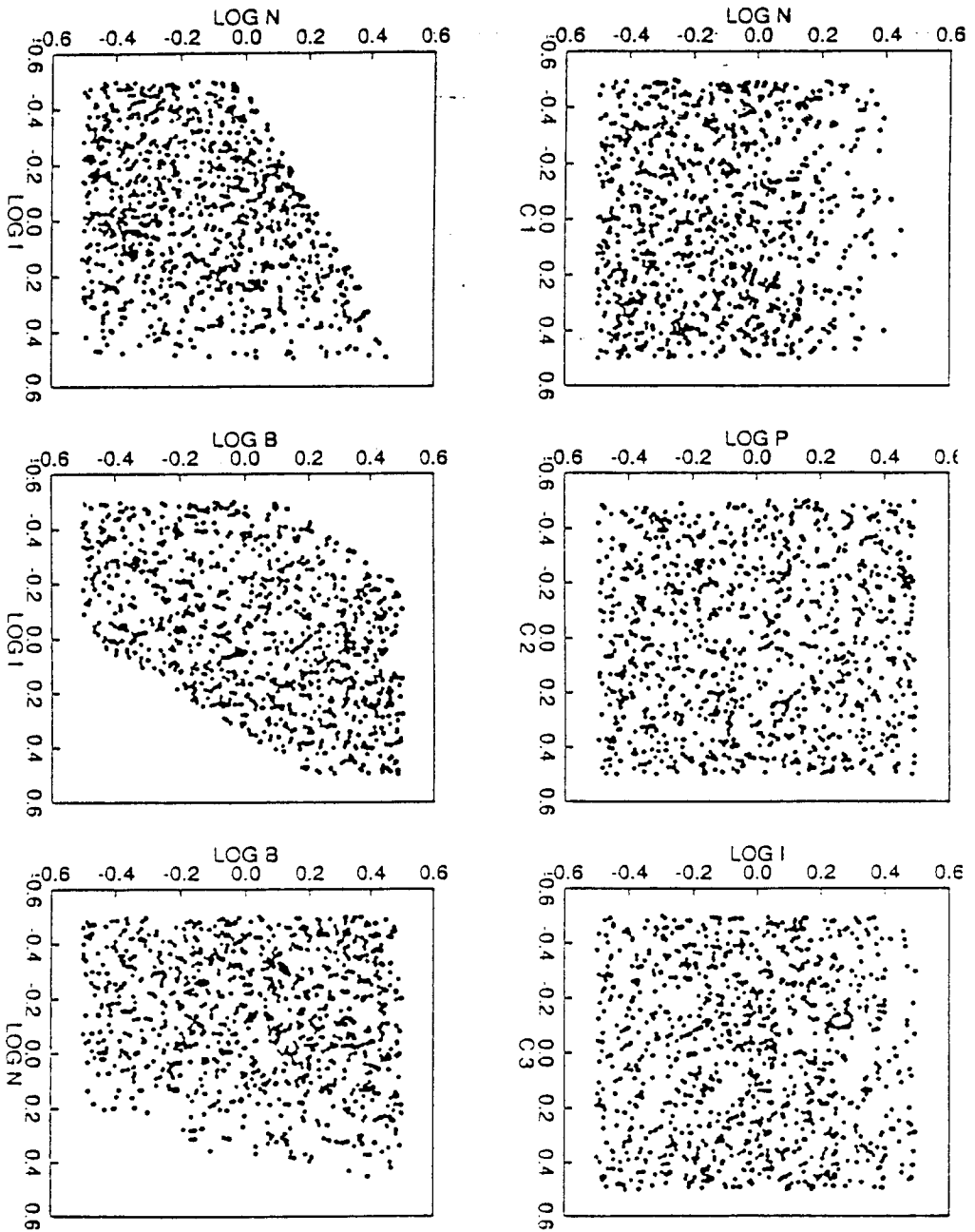


Figure 1. Two-dimensional plots of an irregular design region for ASDEX tokamak simulator.



so that the prediction region is in  $[-.5, .5]^d$  (i.e.,  $x_8 \in [-.5, .5]$ ), , where  $d$  is the number of input variables (here  $d = 8$ ).

### (1) Initial Design

We found initially 10 design points which minimize IMSE of the formula (2.6) that was computed using 1000 uniformly distributed random points over  $Q$ . We used a constant model ( $y(\underline{x}) = \beta + Z(\underline{x}) + \varepsilon$ ) and covariance function (2.2), with  $d=7$ , a common  $\theta = .5$  (all  $\theta_i$ 's are set to be equal),  $\sigma^2 = .1$  and  $\gamma^2 = .001$ . These values were obtained from some previous similar experiments. After running the BALDUR code 10 times, we collect 10  $\tau_E$ 's and computed the MLE using constant model:

$$\hat{\theta} = 0.13, \quad \hat{\sigma}^2 = 0.37, \quad \hat{\gamma}^2 \approx 0.0, \quad \hat{\beta} = -1.28 .$$

Next stage design was constructed by using these estimates in the same model.

### (2) The Second and Third Stage Designs

Based on the previous 10 design points and estimates under the constant model (with a common  $\theta$ ), 5 more design points and observations are obtained. Using these 15 data, 7 different  $\theta$  estimates are computed. Then using the above 7  $\hat{\theta}$ 's, still under constant model for the mean, we obtained 5 more sites to make 20 points. Because  $\hat{\theta}_2$  (corresponding  $c_2$ )  $\approx 0.0$ , only 6 variables (excluding  $c_2$ ) were used in the optimizer. Then we inserted 5 random points in  $[-.5, .5]$  for  $c_2$ . Two-dimensional plots of this design is shown at Figure 2.

We built a linear model based on 20 observations (see Park, 1991, for details of selecting a good model based on the cross validated mean squared residual), however the MMSE of the model is still large (around 0.0065). So we decided to obtain 10 more points for a total of 30 design sites based on the obtained linear model.

### (3) The 4'th Stage Design and Change of Region

The former model (with a common  $\theta$ ) in the third stage was used in searching for the next design (5 more points for a total of 35 design sites). A quadratic model (based on 35 observations) with selected  $x$ 's and  $\theta$ 's was turned out to be the best (based on the cross-validated mean squared residual), but still with 0.005 MMSE.

At this time, a numerical algorithm to solve differential equations in BALDUR code was changed to save running time. Four more experimental runs were done to check how much difference resulted in  $\tau_E$  from the previous code (up to now, we have 39 observations).

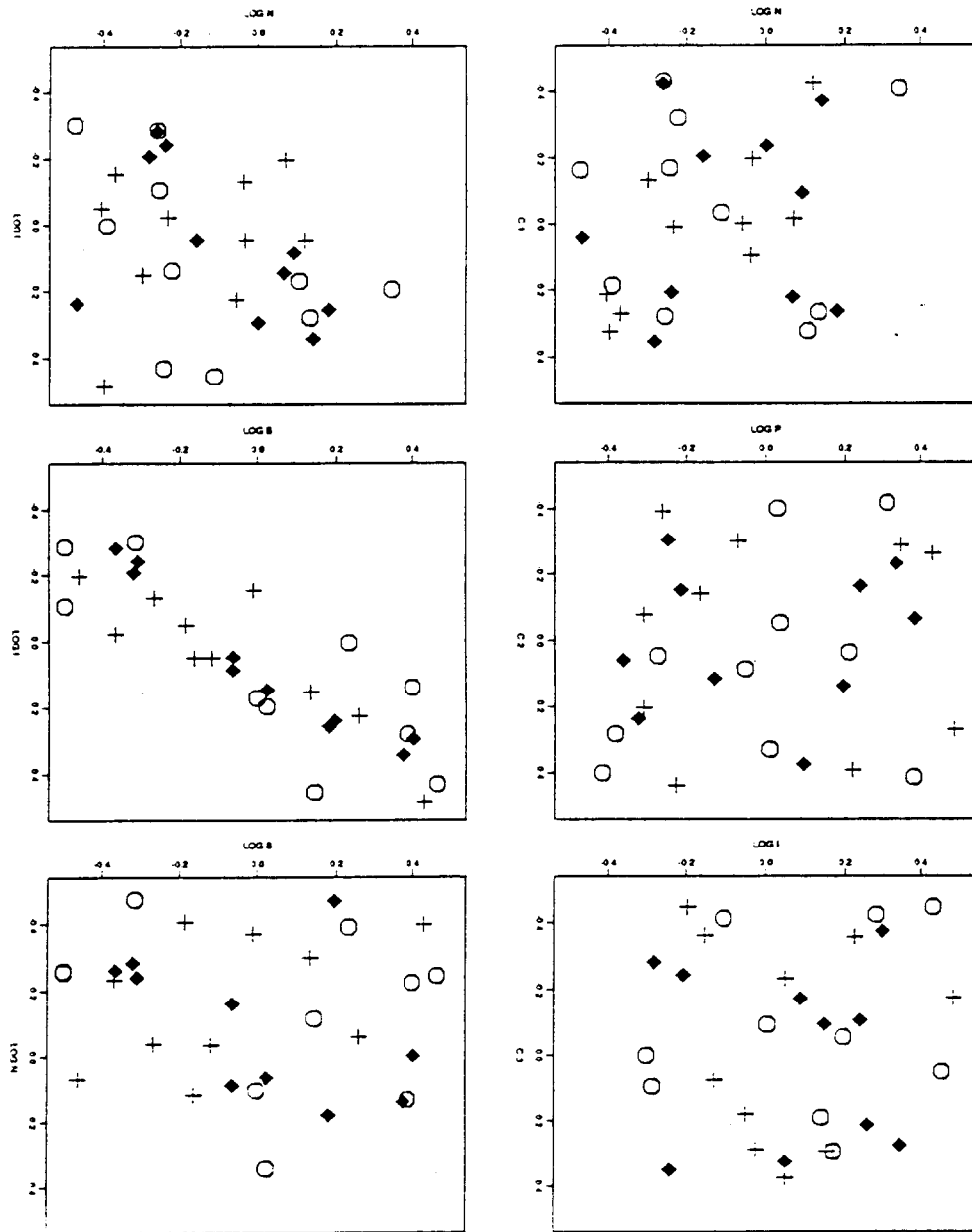


Figure 2. Two-dimensional plots of data-adaptive sequential 30 design sites for ASDEX tokamak simulator. Filled diamond -- the initial 10 points, octagon -- the second and third stage 10 points, cross -- the fourth stage 10 points.

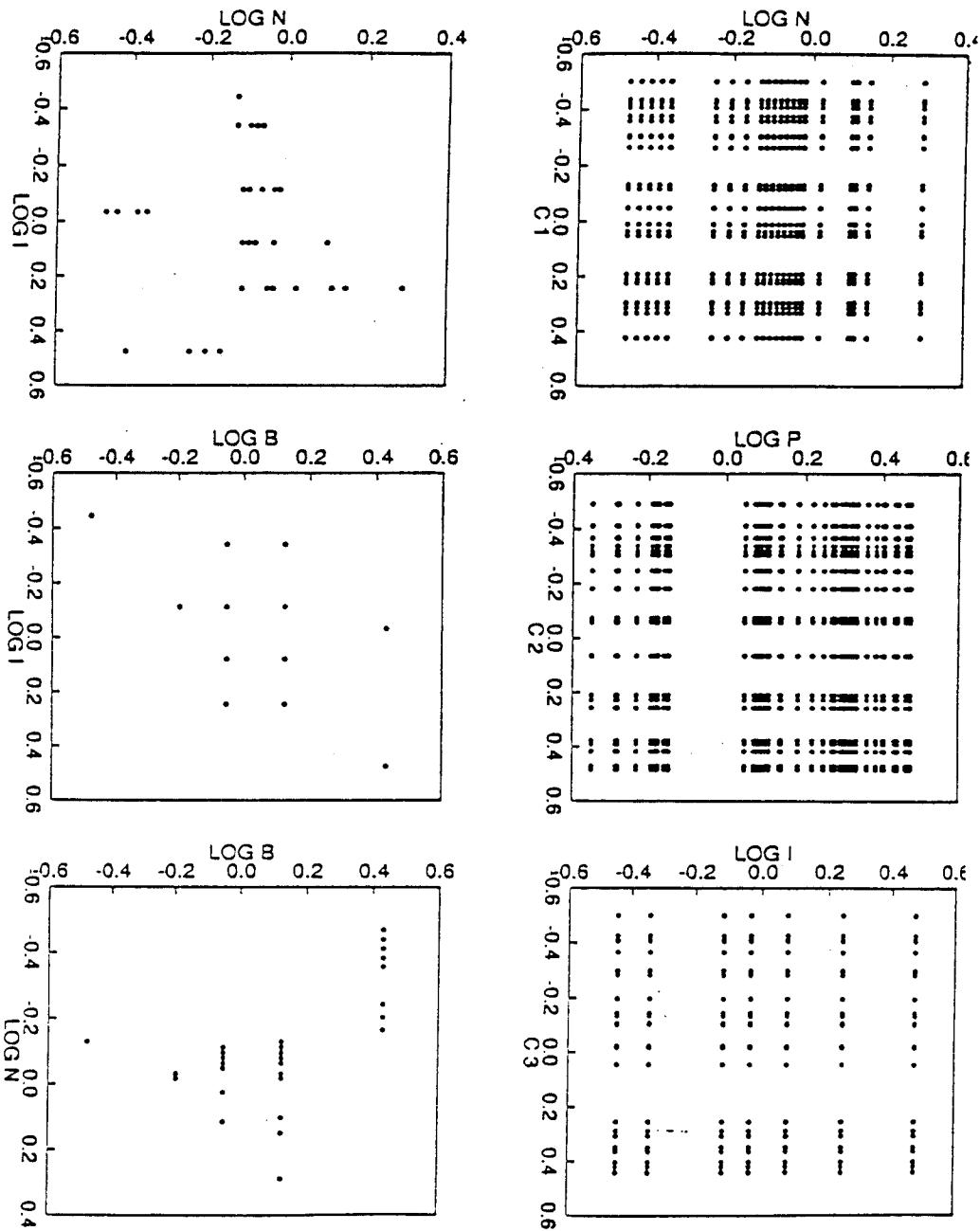


Figure 3. Two-dimensional plots of an irregular "semi-random" design region for PDX tokamak simulator, based on PDX tokamak database.

The differences (4.0 % in average) can be thought of as measurement error. A new variable  $c_4$  was introduced with range 1.0 through 1.4. Because the value of  $c_4$  was set 1.0 by default in the previous runs, two experiments were done setting the value equal to 1.4. The "semi-random" points (see Figure 3 for PDX) which are crossproduct of random vectors (corresponding to  $\underline{c}$ ) and experimental data (corresponding to  $P$ ,  $I$ ,  $N$  and  $B$ ), were used to calculate the IMSE as in (2.6).

#### (4) The 5'th Stage and Final Designs

Nine more points were obtained to make a total of 45 design sites. Because of the computational burden, a constant model with 7  $\theta$ 's was used after shifting some zero  $\theta$ 's to 0.5. Many changes at the above step lead to little improvement in MMSE (.0035) for the best prediction model selected based on 45 observations. We then obtained 10 more points to make 55 observations.

The target MMSE (.002) was achieved in the best model (.0019) so that we can tentatively stop the sequential design process. The final 55 design points with 2-dimensional plots of the final 55 design points is given in Figure 4.

### 3.2 Sequential designs for PDX Tokamak simulator

The design region  $Q$  for PDX was same with ASDEX region except the constraint, which was changed from (3.2) to  $4.375 \leq B/I \leq 7.0$ . After 30 observations were obtained over the above region,  $Q$  was changed, by adapting the minimum and maximum values of variables in the data base, as follows :

$$\begin{aligned} .6 \leq P \leq 5.3 , \quad .22 \leq I \leq .49 , \\ .2 \leq N \leq .98 , \quad .68 \leq B \leq 2.4 , \end{aligned}$$

with constraints

$$\frac{N}{I} \leq 2.0 , \quad 3.0 \leq \frac{B}{I} \leq 7.25 ,$$

and others are same. Then 20 more data were taken over the new design region. The construction procedure of sequential optimal designs for PDX simulator is almost same as the ASDEX procedure, so details are omitted here (see Park, 1991 for details).

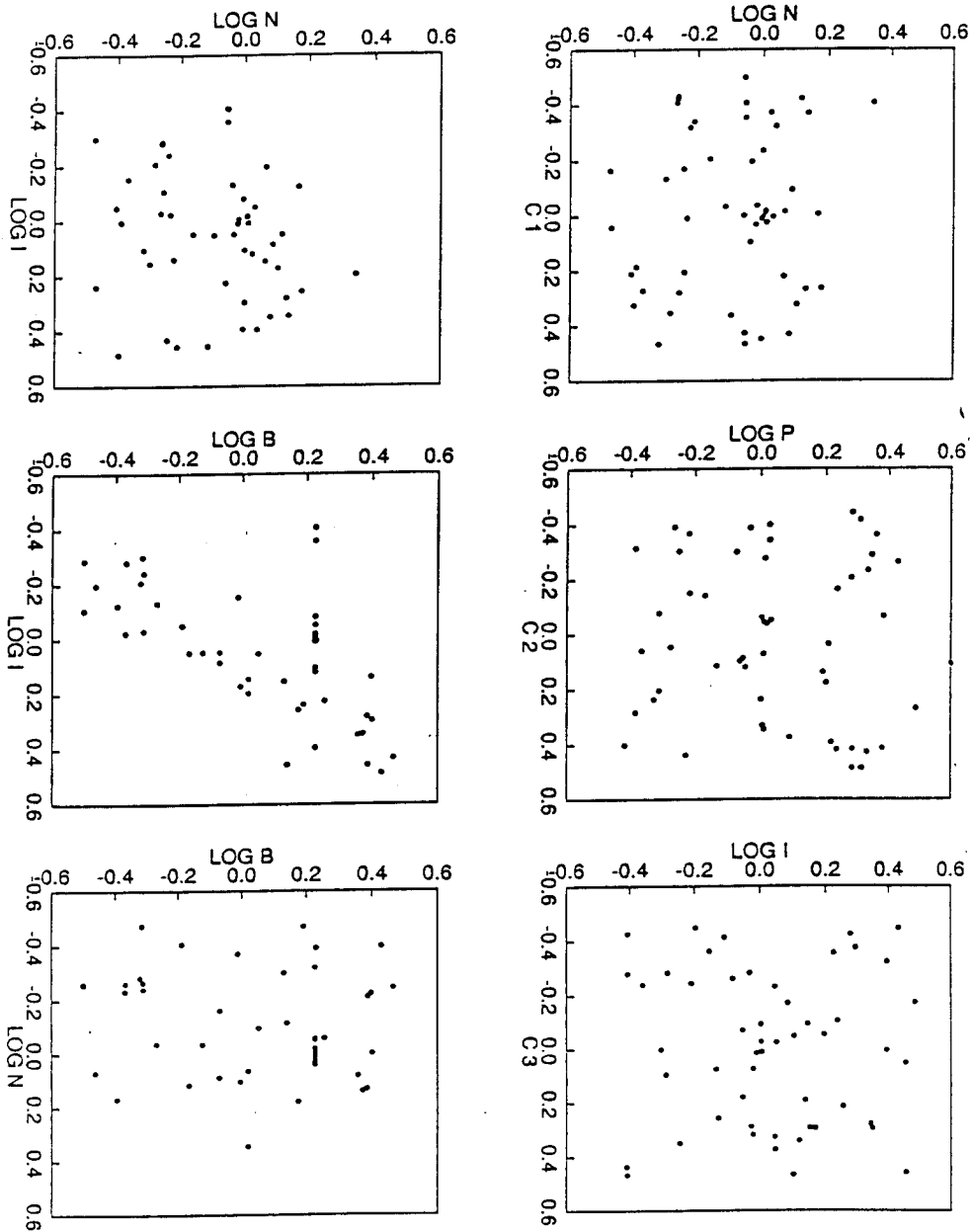


Figure 4. Two-dimensional plots of final 55 design sites for ASDEX tokamak simulator.

## 4. Discussion and future research

In this section, we describe some problems arising in the previous work and give suggestions to overcome those difficulties. Future studies are also described.

### 4.1 Time saving with IMSE criterion

As mentioned in section 2.1, an efficient strategy for optimal design is needed, because running an optimizer with the IMSE function evaluated by Eq. (2.6) with 1000 random points is expensive. This problem is more serious when number of input variables are large and/or the model used in the design stage is complicated. Actually, it took about 500 seconds CPU time in a super-computer CRAY-Y/MP to find a 10-point (locally) optimal design with  $d = 8$  under the constant model with several  $\theta$ 's. (Note that it was a  $10 \times 8$  dimensional optimization problem with a computationally expensive objective function.)

To overcome this difficulty, first of all, we have to understand the algorithm of the optimizer very well to use it effectively, for example, by scaling variables appropriately and by setting some initial parameters and stopping rules appropriately. Practical experience with a high-dimensional numerical optimizer is helpful.

Even though the nature of the problem is constrained minimization, at first the unconstrained routine (E04JBF in NAGLIB, 1984) was used, because it was expected that the optimal design points must be in the region. In second stage design for the ASDEX tokamak, however, optimal design with a distant out-of-region point was observed. This unexpected phenomenon can be, by experience but not rigorously, explained by the existence of measurement error and/or linear model terms in the model. More study is needed to clarify this observation. Because of the convenience of implementation, an unconstrained routine with penalty was used instead of a constrained one. However constrained optimizer should be considered for the next tokamak if time savings can be realized from using it.

When the model used in the design stage is complicated, an alternative model which is simple, but does not lose so much information compared to the original one, can be considered. Actually, in some of our sequential design stages we used a constant model instead of the best linear model with several  $\theta$ 's. We propose to investigate the effect of linear terms in the model to the IMSE based design.

### 4.2 Approximated optimal design

The most time consuming part is the evaluation of IMSE, because  $m$  (say 1000) times calculations of MSE are needed for one evaluation of IMSE. Therefore fewer (say  $l = 300$ )

random numbers can be used to calculate IMSE (or MMSE) in (2.6) if more error due to poor approximation can be tolerated. Now our suggested plan to achieve both time saving and globality is as follows :

**Step 1.** Choose  $k$  (say 4 or 5) different initial designs and run the optimizer (until converge) with IMSE calculated based on  $l(=300)$  random points.

**Step 2.** Choose a design which has a minimum among the  $k$  (sub-optimal) designs obtained in the above manner and use it as a starting point to run the optimizer with IMSE based on  $m(=1000)$  random points.

For using the above procedure and the approximation (2.6), a simulation study as well as the following theoretical support are needed : suppose that  $f_n(S)$  converge to  $f(S)$  at a design  $S$  in a region  $D$ , and that

$$S_n^* = \arg \min_{S \in D} f_n(S) ,$$

$$S^* = \arg \min_{S \in D} f(S) ,$$

then does the design sequences  $S_n^*$  converge (in some sense) to  $S^*$ ? In our example,  $f_n(S)$  is an IMSE calculated by  $n$  random points as in (2.6),  $f(S)$  is the exact IMSE in (2.5) and  $\{S_n^*\}$  is a sequence of the "sub-optimal" designs. Alternatively, one may be more interested in how far  $f(S_n^*)$  is from  $f(S^*)$ .

Instead of constructing  $n$ -point designs all at once,  $n$  times sequential design by updating one point at a time based on IMSE (or MMSE or others) can save lots of computing time. A trade-off, however, between time savings and efficiency of the one-point sequential design compared to non-sequential design should be considered.

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## 복잡한 전산실험을 위한 축차적 계획법과 핵 융합모형에의 응용<sup>3)</sup>

박 정 수 4)

### 요 약

매우 복잡한 컴퓨터 시뮬레이션 실험을 이용한 제반 연구의 효율성을 높이기 위하여 공간적 예측모형에 기초한, 자료참조의 축차적 부최적 실험계획법을 고려했다. 이 실험계획법들은 실제로 핵융합기기의 반응모형 시뮬레이터에 적용되었으며, 적용상의 효과적 방법과 경험이 기술되었다. 또한 비정상적으로 주어진 실험영역과 최적 기준의 계산상의 복잡함으로 인하여 실제의 최적 실험계획을 구축하는데 어려움이 많았고, 따라서 이에 대한 대안들이 컴퓨터 알고리즘과 함께 제안되었다.

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