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Sensitivity Analysis Technique of Non-linear Problems Based on Sobol's Sensitivity Index and Fourier Analysis

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Abstract - *This paper presents a new sensitivity analysis method which can be applied effciently to non-linear response models. It was developed and tested on the TREAT minimum critical core model, but can be easily applied to all general models of interest. The method performs model variance decomposition and captures the uncertainty effect attributable to each input factor based on the Sobol's sensitivity index and Fourier analysis. An preliminary efficiency and error analysis of this method is also described. Results obtained showed high accuracy for the application to the TREAT Minimum Critical Core.*

I. INTRODUCTION

The objective of this paper is to describe a new sensitivity analysis method which is applicable to non-linear response models. It was developed based on the Sobol's sensitivity index [1] and multivariate Fourier series. It is a variance decomposition method which can estimate the variance contribution of each parameter to the total model uncertainty.

Traditional sensitivity analysis methods in the reactor physics field are usually established based on the assumption that the model studied is linear or could be treated as a linear system within a small perturbation range. However, the uncertainty analysis of the TREAT minimum critical loading eigenvalue calculation has shown that this assumption may not be appropriate for models which include perturbations on geometry parameters. [2] Hence it is difficult to obtain an accurate estimation of the sensitivity information about parameters such as fuel block size and assembly outer radius. The method described in this paper was developed to address this problem.

The method was tested with two simple nonlinear non-monotonic models and then applied to the TREAT minimum critical core model. Results showed its accuracy and suggests that it deserves further investigation.

II. THEORY

The method discussed in this paper is based on Sobol's sensitivity index and multidimensional Fourier transform. Sobol's sensitivity index decomposes the total variance of model output into conditional variances of each factor and possible factor combinations the model contains. Multidimensional Fourier transform is then applied to estimate the conditional variances.

1. Conditional Mean and Conditional Variance

Consider two random variables X and Y. The conditional mean of Y given $X = x$ is defined as:

$$\mu_{Y|x} = E[Y|x] \tag{1}$$

Then, the conditional variance of Y given $X = x$ is defined as:

$$\sigma^2_{Y|x} = E\{[Y - \mu_{Y|x}]^2|x\} \tag{2}$$

In the case that both X and Y are continuous random variables, the conditional mean and variance of Y given $X = x$ are calculated as

$$\mu_{Y|x} = \int_{-\infty}^{\infty} yh(y|x)dy \tag{3}$$

$$\sigma^2_{Y|x} = \int_{-\infty}^{\infty} [y - \mu_{Y|x}]^2 h(y|x)dy = \int_{-\infty}^{\infty} y^2 h(y|x)dy - \mu^2_{Y|x} \tag{4}$$

The conditional variance of $Y|X = x$ depends on x, and depends on x alone. It is calculated much like a variance, except the probability distribution should be replaced with a conditional probability distribution $h(y|x)$. Consider the conditional variance of Y given $X = x$ as a random variable, its expected value is calculated as

$$\begin{aligned} E[\sigma^2_{Y|x}] &= E[\int_{-\infty}^{\infty} y^2 h(y|x)dy - \mu^2_{Y|x}] \\ &= E[\int_{-\infty}^{\infty} y^2 h(y|x)dy] - E[\mu^2_{Y|x}] \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y^2 h(y|x)dy f_X(x)dx - E[\mu^2_{Y|x}] \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y^2 f_{X,Y}(x,y)dxdy - E[\mu^2_{Y|x}] \\ &= E[Y^2] - E[\mu^2_{Y|x}] \end{aligned} \tag{5}$$

$f_{X,Y}(x, y)$ is the joint probability distribution of X and Y.

The conditional mean of Y given $X = x$ is also a random variable. Its variance is defined as:

$$\begin{aligned} Var[\mu_{Y|x}] &= E[\mu^2_{Y|x}] - E[\mu_{Y|x}]^2 \\ &= E[\mu^2_{Y|x}] - \left(\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} yh(y|x)dy f_X(x)dx\right)^2 \\ &= E[\mu^2_{Y|x}] - \left(\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} y f_{X,Y}(x,y)dxdy\right)^2 \\ &= E[\mu^2_{Y|x}] - E[Y]^2 \end{aligned} \tag{6}$$

Combining eq. (5) and (6):

$$E[\sigma^2_{Y|x}] + Var[\mu_{Y|x}] = E[Y^2] - E[Y]^2 = Var[Y] \tag{7}$$

Hence in the case if the random variable Y is the model output and X is the model input, the variance of model output is the sum of the expected value of the conditional variance and the variance of the conditional means. [3] In the case that $X = (X_1, \ldots, X_n)$ is a vector of random variables and Y is a function of X, eq. (7) can be used to evaluate Y's sensitivity with respect to components of X. Details are included in the next section.

2. Sobol's Sensitivity Index

Suppose that the mathematical model of interest in sensitivity analysis is described by a function $f(\boldsymbol{x})$, where $\boldsymbol{x} = (x_1, \ldots, x_n)$ and is defined in a unit n-dimensional cube $K^n = \{\boldsymbol{x} | 0 \le x_i \le 1,\ i = 1, \ldots, n\}$.

Consider a group of indices $i_1, \ldots, i_s$, where $1 \le i_1 < \ldots < i_s \le n$ and $s = 1, \ldots, n$, a notation for a sum over all the different groups of indices is introduced as

$$\widehat{\sum} T_{i_1,\ldots,i_s} = \sum_{t=1}^{n} T_i + \sum \sum_{1 \le i \le j \le n} T_{ij} + \cdots T_{1,2,\ldots,n} \tag{8}$$

This sum has $2^n - 1$ summands. A representation of a function $f(x_1, \ldots, x_n)$ as the sum

$$f = f_0 + \widehat{\sum} f_{i_1,\ldots,i_n}(x_{i_1,\ldots,x_{i_n}}) \tag{9}$$

is referred to as an expansion into summands of different dimensions, if f_0 is constant and the integrals of the subfunctions $f_{i_1,\ldots,i_n}$ with respect to any of their parameters are zero, i.e.

$$\int_0^1 f_{i_1,\ldots,i_s}(x_{i_1}, \ldots, x_{i_s}) dx_k = 0,\ 1 \le k \le s \tag{10}$$

By the definition, one will find:

$$\int_{K^n} f(\boldsymbol{x}) d\boldsymbol{x} = \int_{K^n} (f_0 + \widehat{\sum} f_{i_1,\ldots,i_n}(x_{i_1,\ldots,x_{i_n}})) d\boldsymbol{x} = f_0 \tag{11}$$

Also, all the summands on the right-hand side of eq. (9) are orthogonal, i.e.

$$\int_{K^n} f_I f_J d\boldsymbol{x} = 0 \tag{12}$$

$I = (i_1, \ldots, i_s)$ and $J = (j_1, \ldots, j_k)$ are two different sets of indices. Since I and J are different, at least one of the indices among I and J is not repeated. Integral with respect to this variable vanished according to the definition in eq. (10).

For any integrable function $f(\boldsymbol{x})$ in K^n, there exists a unique expansion in the form defined by eq. (9). [1] Consider the integration below, $\boldsymbol{x}/dx_i$ is the product of all the elements in $\boldsymbol{x}$, except x_i.

$$\int_{K^{n-1}} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i = f_0 + f_i(x_i) \tag{13}$$

Hence all the summands f_i with one index are calculated as:

$$f_i(x_i) = \int_{K^{n-1}} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i - f_0 \tag{14}$$

Now let $i \ne j$, consider the integration

$$\int_{K^{n-2}} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i/dx_j = f_0 + f_i(x_i) + f_j(x_j) + f_{i,j}(x_i, x_j) \tag{15}$$

Hence all the summands $f_{i,j}$ with two indices are calculated as:

$$f_{i,j}(x_i, x_j) = \int_{K^{n-2}} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i/dx_j - f_0 - f_i(x_i) - f_j(x_j) \tag{16}$$

Therefore, given a function $f(\boldsymbol{x})$ integrable in K^n, its expansion into summands of different dimensions can be calculated by integrations. First, calculate f_0 with eq. (11). Then calculate the summands with one index using eq. (13) and f_0. Summands with two indices are calculated using eq. (16). Other summands with number of indices higher than two are calculated in a similar way. A more detailed proof is provided in [1].

In the case that the given function is a function of random variables $x_1, \ldots, x_n$, (To be consistent with the notations used before, small letters are used here to represent random variables. Usually they should be noted as capital letters.) and the random variables are identical, independent uniformly distributed, i.e. the marginal distribution of each variable and the joint distribution of every possible variable combination are identical and equal to 1, the variance of function $f(\boldsymbol{x})$ is

$$\begin{aligned} Var[f(\boldsymbol{x})] &= \int_{K^n} f^2(\boldsymbol{x}) d\boldsymbol{x} - (\int_{K^n} f(\boldsymbol{x}) d\boldsymbol{x})^2 \\ &= \int_{K^n} f^2(\boldsymbol{x}) d\boldsymbol{x} - f_0^2 \end{aligned} \tag{17}$$

To find the variance of the conditional mean of $f(\boldsymbol{x})$ given $x_i = x_i^*$:

$$E[f(\boldsymbol{x})|x_i^*] = \int_{K^{n-1}} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i \Big|_{x_i = x_i^*} = f_0 + f_i(x_i^*) \tag{18}$$

$$\begin{aligned} Var[E[f(\boldsymbol{x})|x_i^*]] &= \left(\int_0^1 E[f(\boldsymbol{x})|x_i^*]^2 dx_i^*\right) - \left(\int_0^1 E[f(\boldsymbol{x})|x_i^*] dx_i^*\right)^2 \\ &= \int_0^1 (f_0^2 + f_i^2(x_i^*) + 2 f_0 f_i(x_i^*)) dx_i^* - f_0^2 \\ &= \int_0^1 f_i^2(x_i^*) dx_i^* \end{aligned} \tag{19}$$

In order to quantify the importance of an input factor x_i on the variance of $f(\boldsymbol{x})$, x_i can be "fixed" at its "preferred" value x_i^*, then the conditional mean of $f(\boldsymbol{x})$ can be calculated and expressed as a function of (x_i^*) with eq. (18). However, the true value of x_i cannot be fixed, the variance of the conditional mean over all possible x_i values gives an estimation of x_i's importance. This is essentially what is expressed in eq. (19). [4]

Consider the orthogonality between the summands, the integral of $f(\boldsymbol{x})^2$ over K^n gives

$$\int_{K^n} f(\boldsymbol{x})^2 d\boldsymbol{x} = f_0^2 + \widehat{\sum} \int_{K^s} (f_{i_1,\ldots,i_s})^2 dx_{i_1} \cdots dx_{i_s} \tag{20}$$

Combining eq. (17) and (20), normalizing the variance terms by the total variance of $f(\boldsymbol{x})$, the sensitivity indices can be defined as

$$S_{i_1,\ldots,i_s} = \frac{\int_{K^s} (f_{i_1,\ldots,i_s})^2 dx_{i_1} \cdots dx_{i_s}}{Var[f(\boldsymbol{x})]},\ 1 \le i_1, \ldots, i_s \le n \tag{21}$$

Note that $\widehat{\sum} S_{i_1,\ldots,i_s} = 1$.

This set of sensitivity indices are called the Sobol's sensitivity indices. They are used to measure the sensitivity of $f(\boldsymbol{x})$ with respect to components as well as component combinations of $\boldsymbol{x}$.

Therefore if a model can be described as a integrable function, the output variance can be decomposed into the contributions associated with each input factor of the model. In the real world, most of the models do not have a known analytical functional solution. Instead, the integrals required to calculate the sensitivity indices can be estimated by numerical methods.

To simplify the problem, consider single input factor associated sensitivity indices only, to calculate $S_1, \ldots, S_n$ for a n-dimensional model, one needs to evaluate

$$\int_0^1 f_i(x_i)^2 x_i, \text{ where } f_i = \int_{K^n} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i - \int_{K^n} f(\boldsymbol{x}) d\boldsymbol{x}$$

for n times. If a traditional method is used to calculate the numerical integrals, one needs to

- Choose a input factor, x_i.
- Generate samples of x_i.
- For each sample value of x_i, generate samples for the other input factors in the subspace K^{n-1}.
- Run the given model with all the sample sets generated.
- Evaluate S_i and repeat all steps for all input factors $x_{j,\ j\neq i}$.

The computational effort will be at $T \cdot O(nC^n)$ level. T represents the average time/computational cost for each trial of model run and C is a constant which describes the number of samples desired in each dimension. This is a considerable computational expense and not practical for most of the physical models being studied. To ease the computational pressure and simplify the sampling procedures, a Fourier series can be used to estimate the function integrals.

3. Multidimensional Fourier Series

Consider the integrable function $f(\boldsymbol{x})$ defined on K^n in the previous section, assuming that the function is periodic outside K^n, (i.e. take K^n as its period and repeat the segment of function values outside K^n) then it can be expressed as a Fourier series using multidimensional complex exponential.

$$f(\boldsymbol{x}) = \sum_{\hat{\omega}} c_{\hat{\omega}} e^{2\pi i \hat{\omega}\cdot\boldsymbol{x}} \tag{22}$$

$$c_{\hat{\omega}} = \int_{K^n} e^{-2\pi i \hat{\omega}\cdot\boldsymbol{x}} f(\boldsymbol{x}) d\boldsymbol{x},\ \hat{\omega} = (\omega_1, \ldots, \omega_n) \in \mathbb{Z}^n \tag{23}$$

With the Fourier series expansion, the summands can be rewritten as

$$\begin{aligned} f_i &= \int_{K^n} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i - \int_{K^n} f(\boldsymbol{x}) d\boldsymbol{x} \\ &= \int_{K^n} \sum_{\hat{\omega}} c_{\hat{\omega}} e^{2\pi i \hat{\omega}\cdot\boldsymbol{x}} d\boldsymbol{x}/dx_i - \int_{K^n} \sum_{\hat{\omega}} c_{\hat{\omega}} e^{2\pi i \hat{\omega}\cdot\boldsymbol{x}} d\boldsymbol{x} \\ &= \sum_{\hat{\omega}} \int_{K^n} c_{\hat{\omega}} e^{2\pi i \hat{\omega}\cdot\boldsymbol{x}} d\boldsymbol{x}/dx_i - \sum_{\hat{\omega}} \int_{K^n} c_{\hat{\omega}} e^{2\pi i \hat{\omega}\cdot\boldsymbol{x}} d\boldsymbol{x} \\ &= \sum_{\hat{\omega}_i} c_{\hat{\omega}_i} e^{2\pi i \omega_i x_i} \end{aligned} \tag{24}$$

$$\hat{\omega}_i = (0 \ldots, \omega_i, \ldots 0),\ \omega_i \text{ is the } i^{th} \text{ component of } \hat{\omega}_i,\ \omega_i \neq 0.$$

This is based on the fact that $\int_0^1 e^{2\pi i k x} dx = 0$ for $k \in \mathbb{Z},\ k \neq 0$.

Therefore, the sensitivity indices are calculated as

$$\begin{aligned} S_i &= \int_0^1 f_i^2(x_i) dx_i / Var[f(\boldsymbol{x})] \\ &= \int_0^1 \left(\sum_{\hat{\omega}_i} c_{\hat{\omega}_i} e^{2\pi i \omega_i x_i} \right)^2 dx_i / Var[f(\boldsymbol{x})] \\ &= \left(\sum_{\hat{\omega}_i} |c_{\hat{\omega}_i}|^2 \right) / Var[f(\boldsymbol{x})] \end{aligned} \tag{25}$$

based on Parseval's theorem. [5]

Hence, the calculation of sensitivity indices is transformed into calculations of the Fourier amplitudes.

$$c_{\hat{\omega}_i} = \int_{K^n} e^{-2\pi i \omega_i \cdot x_i} f(\boldsymbol{x}) d\boldsymbol{x} \tag{26}$$

Note that the evaluation of Fourier amplitudes does not include the $\int_{K^n} f(\boldsymbol{x}) d\boldsymbol{x}/dx_i$ term, the computational cost of running the samples necessary for sensitivity evaluation is therefore decreased to $T \cdot O(C^n)$.

In the case that all the input factors follow identical, independent uniform distributions, eq. (26) describes the expectation of the integrated term. Hence the Fourier coefficients can be estimated as

$$c_{\hat{\omega}_i} \approx \frac{1}{N} \sum_{j=1}^{N} e^{-2\pi i \omega_i \cdot x_i^{(j)}} f^{(j)} \tag{27}$$

N is the number of samples generated in K^n space. $x_i^{(j)}$ is the value of x_i in the j^{th} sample set of $\boldsymbol{x}$. $f^{(j)}$ is the j^{th} model output.

4. Method Description and Error Analysis

In the previous discussion, the input factors of the studied models are always assumed to be independent and uniformly distributed. This section completes the theory introduced and describes a method which has no assumptions on input factor distributions. A weighted average is used in this method to evaluate eq. (27).

Given the model of interest, assume that it can be described by a integrable function within its sample space, one can then evaluate its single factor associated sensitivity indices following the steps listed below.

- Draw random samples in the sample space of the given model based on the desired distribution type for each input factor $x_1, \ldots, x_n$.

- Run the model based on the sampled values of parameters.

- Define a new set of variables $s_1, \ldots, s_n$ which satisfies

$$s_i = F_i^{-1}(x_i) \tag{28}$$

Where F_i^{-1} is the inverse function of x_i's cumulative probability distribution function.

In the case that all the random variables are independent, the s variables are guaranteed to follow independent uniform distributions. In cases that correlation exists between input factors, extra effort is required during this step. An example is the sensitivity analysis of neutronics calculations with respect to nuclear data uncertainties. When one generates nuclear data samples, the correlation between data is usually added upon a random vector of independent random variables. Hence the method presented in this paper can be applied to the analysis of the sensitivity indices of the initially uncorrelated samples. Furthermore, reference [6] describes the method of transferring correlated random variables into uncorrelated ones. It provides possibilities of using the sensitivity analysis method in this paper on models which contain correlated random variables.

After this step, the model being studied is transferred into s-space. This transformation does not change the variable sensitivity indices in the x-space because

$$\begin{aligned}
f_X(x)dx &= f_S(s)ds \\
f_{X,Y}(x,y)dx &= f_{S,Y}(s,y)ds \\
h(y|x)dy &= \frac{f_{X,Y}(x,y)dxdy}{f_X(x)dx} = \frac{f_{S,Y}(s,y)dsdy}{f_S(s)ds} \\
Var[E[Y|x]] &= E[Y^2] - E[\mu^2_{Y|x}] \\
&= E[Y^2] - \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} yh(y|x)dy\right)^2 f_X(x)dx \\
&= E[Y^2] - \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} yh(y|x)dy\right)^2 f_X(x)dx \\
&= E[Y^2] - \int_{-\infty}^{\infty}\left(\int_{-\infty}^{\infty} yh(y|s)dy\right)^2 f_S(s)ds \\
&= Var[E[Y|s]]
\end{aligned}$$

X, Y and S are random variables.

- Choose the maximum harmonic order M. For the work shown in this paper, M was chosen to be 20. This is the value used in one of the references [5]. Test results of simple models also showed that this choice provides acceptable estimations.

- For each input factor x_i, take $\omega_i = 1, 2, \ldots, 20$, compute the weighted average in $s - space$:

$$c_{\hat{\omega}_i} \approx \frac{\sum_{j=1}^{N} e^{-2\pi i\omega_i \cdot s_i^{(j)}} f^{(j)} \cdot w_j}{\sum w_j} \tag{29}$$

The reason of estimating the function expectation with weighted average is to overcome errors caused by uneven sampling. Notice that Latin hypercube sampling can be used to decrease the error. The weighted average method introduced below is applied only when no specific care was taken at the sampling stage.

By definition, the sample points of $\boldsymbol{s}$ are uniformly distributed in the n-dimensional cube. However, since the samples of $\boldsymbol{s}$ are transferred from randomly taken samples of $\boldsymbol{x}$ and the sample size is limited, the real histogram of the N sample points will never have same counts for each sub-region in the s-space. Segments of the sample space which contain more sample points may have fake higher significances in the function expectation estimation.

The weighting factors w_j are chosen with the following steps:

  - Divide the n-dimensional cube (s-space) evenly into L sub-regions. The boundaries of the sub-regions are user defined.
  - Check each variable vector $\boldsymbol{s}^{(j)} = (s_1^{(j)}, \ldots, s_n^{(j)})$ to decide which sub-region the sample point falls into. Keep counts for all the sub-regions $(C_1, \ldots, C_L)$.
  - Use $\frac{1}{C_l}$ as the weight w_j for all sample points $\boldsymbol{s}^{(j)}$ that falls into the l^{th} sub-region.

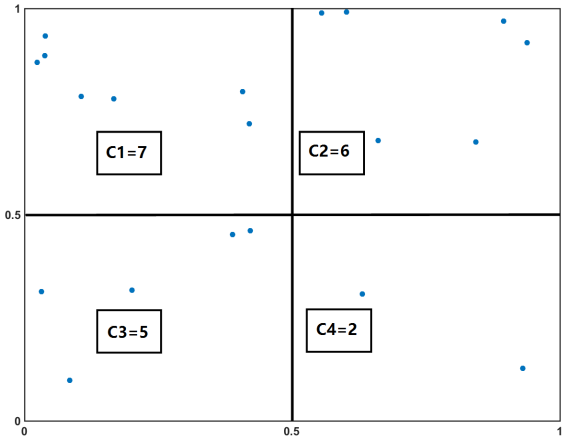

Fig. 1. Example of weighting factor generation

  - Figure 1 shows an example with a 2-D sample space. For a model which has two input factors, 20 sample points were generated and transferred into the s-space. The 2D sample space is cut into four sub-regions. For the seven sample points falling in region one, they have the same weight factor $w = \frac{1}{7}$.

Note that when all the user defined sub-regions contain the same number of sample points, eq. 29 becomes eq. 27

- Since the counts of sample points falling in each sub-region is used as the denominator of the weight factor, it is important that user should define the sub-region grid carefully so that each defined sub-region contains at least one sample point. If this condition is not satisfied, the sub-regions should be redefined into "larger" segments.

- Clean up the high frequency terms. It has been mentioned that the maximum harmonic order M was chosen to be 20, i.e the sensitivity index given in eq. (25) is estimated as

$$S_i = \frac{\sum_{|\omega_i|=1}^{|\omega_i|=20} |c_{\hat{\omega}_i}|^2}{\frac{1}{N-1}\sum_{j=1}^{N}(f^{(j)} - \bar{f})^2} \tag{30}$$

For most of the physical models being studied, the Fourier coefficients of high order harmonics decays away fast. [5] $M = 20$ is a relatively large choice. However, since the Fourier series coefficients are estimated, each of the coefficients contains some random error:

$$\tau_{\omega_i} = \left| \int_{K^n} e^{-2\pi i \omega_i \cdot s_i} f(\boldsymbol{s}) d\boldsymbol{s} \right|^2 - \left| \frac{\sum_{j=1}^{N} e^{-2\pi i \omega_i \cdot s_i^{(j)}} f^{(j)} \cdot w_j}{\sum w_j} \right|^2 \tag{31}$$

Note that the Fourier coefficient $c_{\hat{\omega}_i}$ is a complex number. The square of its absolute value is used in the estimation of the sensitivity indices. Hence the error τ is defined by the square of the modulus values.

Use the sum expansion of function $f(\boldsymbol{s})$ and the orthogonality between summands:

$$\tau_{\omega_i} = \left| \int_0^1 e^{-2\pi i \omega_i \cdot s_i} f_i(s_i) ds_i \right|^2 - \left| \frac{\sum_{j=1}^{N} e^{-2\pi i \omega_i \cdot s_i^{(j)}} (f_i^{(j)} + \widehat{\sum} f_{i_0,\ldots,i_n/i}^{(j)}) \cdot w_j}{\sum w_j} \right|^2$$

The term $\widehat{\sum} f_{i_0,\ldots,i_n/i}$ denotes the sum of all the sub-functions of $f(\boldsymbol{s})$ (include f_0) except $f_i(s_i)$.

Therefore, the error τ_{ω_i} can be divided into two parts:

$$\tau_{\omega_i} = \tau_i + \tau_0 \tag{32}$$

$$\tau_i = \left| \int_0^1 e^{-2\pi i \omega_i \cdot s_i} f_i(s_i) ds_i \right|^2 - \left| \frac{\sum_{j=1}^{N} e^{-2\pi i \omega_i \cdot s_i^{(j)}} f_i^{(j)} \cdot w_j}{\sum w_j} \right|^2$$

$$\tau_0 = - \left| \frac{\sum_{j=1}^{N} e^{-2\pi i \omega_i \cdot s_i^{(j)}} \widehat{\sum} f_{i_0,\ldots,i_n/i}^{(j)} \cdot w_j}{\sum w_j} \right|^2$$

Proof of eq. (32) used the theorem: define a set of nonzero complex numbers $z_k = r_k \exp(i\theta_k)$, then

$$\left| \sum_{k=1}^{N} z_k \right|^2 = \sum_{k=1}^{N} r_k^2 + \sum_{j \neq k} r_j r_k \exp(i(\theta_j - \theta_k)) = \sum_{k=1}^{N} r_k^2, \text{ in the case that } \theta_k \text{ is a constant.}$$

τ_i is the error from 1-D numerical integration with respect to s_i. It can be decreased by modifying the weight factors w_j. For example, if the sub-regions of the sample space are defined in a way that any two sample points falling in the same region have different s_i values, the weight factors calculated using the sub-region method should provide a better estimate. Other algorithms of numerical integration may also be modified and used to give better estimations.

τ_0 is the random error resulted from sampling. Unlike τ_i which is related to the numerical integration algorithm, τ_0 cannot be effectively decreased by the weight factors w_j without knowing the analytical function format of the model. The only certain way of decreasing τ_0 is to increase the sample size.

Hence, the value of τ_{ω_i} depends mostly on the numerical integration algorithm and the sample size. It is acceptable to assume that the error τ_{ω_i} is independent of ω_i. With the maximum harmonic order M fixed, Fourier coefficients of $\omega > M$ terms can be used to estimate the average error $\bar{\tau}$. Assume that the real Fourier coefficients of the model vanishes at harmonic orders higher than M, $\bar{\tau}$ can be approximated as

$$\bar{\tau} \approx \frac{1}{M' - M} \sum_{\omega_i = M+1}^{\omega_i = M'} |c_{\hat{\omega}_i}|^2. \tag{33}$$

Again, $|c_{\hat{\omega}_i}|^2$ are estimated with eq. (29). For the results included in this paper, M' was chosen as 60.

- Subtract the average error from the numerator of eq. (30) to avoid overestimation of the sensitivity indices, the final result is given as:

$$S_i = \frac{\sum_{|\omega_i|=1}^{|\omega_i|=20} (|c_{\hat{\omega}_i}|^2 - \bar{\tau})}{\frac{1}{N-1}\sum_{j=1}^{N}(f^{(j)} - \bar{f})^2} \tag{34}$$

5. Simple Test Models Description

The method was tested with two simple test models before it was applied to TREAT. The analytical solutions of these two models are known.

The first simple test problem contains three independent random variables which all follow standard uniform distribution. The function of the model is given as

$$y = x_1^2 + 2x_2^2 + 3x_3^2 + x_1x_2 2x_2x_3 + 3x_1x_3 + x_1x_2x_3. \quad (35)$$

The second test problem contains three independent random variables which follow different distribution types. The function of the model is given as

$$y = x_1^3 + x_2^3 + x_3^3 + x_1x_2x_3 + x_1x_2^2 + x_2x_3^2 + x_3x_1^2. \quad (36)$$

Both models are nonlinear and non-monotonic. Detailed distribution information of the variables are listed in Table II and Table III.

For each test, 1000 sample points were generated and the corresponding y values (model output) were calculated.

Since these two models are very simple, the numerical cost of model output evaluation for a large sample size is almost negligible. 1000 seems to be a relatively small sample size. However, for most of the high-fidelity models of interest, 1000 is already at the upper bound of the affordable sample size. In these two simple tests, it is necessary to prove that the method can provide acceptable predictions with (at most) 1000 samples.

6. TREAT Model Description

The method presented in this paper was motivated by the uncertainty analysis of the TREAT reactor which is an air-cooled, graphite moderated, thermal test facility designed to evaluate reactor fuels and structural materials under severe reactor-accident conditions. [7] The reactor has not operated since 1994, but recently the DOE decide to restart TREAT.

To prepare for its resumption of testing, a baseline assessment report ([7]) was prepared by the Idaho National Laboratory. An example uncertainty evaluation of infinite lattice fuel assembly model was given in [7]. In this analysis, the uncertainty of eigenvalue calculation related to material composition and geometry factors was studied. Results pointed out that the following five factors are the most significant "contributors" of the uncertainties in the TREAT eigenvalue calculation.

- Boron contamination in the fuel graphite.
- Flat to flat distance of the fuel block.
- Al-6063 can thickness.
- Standard fuel assembly outer radius.
- Zr can thickness.

Based on the results obtained with infinite lattice fuel assembly model in [7], the uncertainties in the prediction of TREAT minimum critical core loading k_{eff} attributable to uncertainties in the fuel material composition and geometry parameters was studied. Results showed that TREAT minimum critical core has non-linear response to the geometry factors studied, such as the Al can thickness and the flat-to-flat distance of fuel block. [2] Hence a sensitivity analysis method applicable to nonlinear problems is necessary for this model. Also, the boron contamination in the TREAT minimum critical core model contained large uncertainty ([2], [7]) and was assumed to follow a normal distribution with $\mu = 7.53ppm$, $\sigma^2 = 1.16ppm^2$. This caused large deviation among the parameter samples and difficulties in applying general perturbation theory to the TREAT model.

The uncertainty results presented in [2] used 1200 random sample sets of TREAT minimum critical core model input factors which were simulated using the SERPENT Monte Carlo code. Each sample contained perturbations on all of the five significant parameters listed.

In this case, traditional sensitivity analysis methods usually require running the given model with single parameter perturbations. When the model sensitivity with respect to one input factor is being studied, the other factors are fixed at their "preferred" values. This means generating a new set of samples and re-test them through the TREAT minimum critical core model. Because the numerical cost for this is expensive, it was advantageous to have a sensitivity analysis method which makes use of the existing tested samples instead of generating new specific samples.

Applicable to non-linear response model and requires no extra sample generation, these two requirements together motivated the sensitivity method introduced in this paper.

Figure 2 shows the minimum critical core configuration of TREAT. It consists 133 standard fuel assemblies, 8 control rod fuel assemblies and 16 Zircaloy-clad dummy fuel assemblies. A more detailed description of the geometry of the configuration is given in [7]. The SERPENT model of TREAT standard fuel assembly is shown in Figure 3. The left most part in Figure 3 is the side view of the assembly, followed by the partial enlarged views of the fuel can outgas tube and the spacer. The right most part provides cross views of different sections of the fuel assembly. The geometry factor mentioned are marked in Figure 3.

Table I summarises the detailed information of the TREAT uncertainty analysis in [2]. The sensitivity analysis is based on the same samples.

III. RESULTS AND ANALYSIS

Results from three models are presented in this paper. Two models are the simple tests and the last one is TREAT minimum critical core SERPENT model. Theoretically this method allows user to evaluate partial variance attributable to combinations of variables of the given model. However, to simplify the calculation and validate the method, only the single parameter effects were calculated. i.e. sensitivity indices $S_i,\ i = 1, 2, \ldots, n$ were evaluated. The other terms in the sum expansion $\widehat{\sum} S_{i_1,\ldots,i_s}$ are beyond the scope of this paper.

Factor	Distribution	Distribution parameters
Graphite fuel B content (wt.%)	Normal	$\mu = 7.53,\ \sigma = 1.1619$
Flat-to-flat distance of graphite fuel (in.)	Triangular	a=3.795, b=3.82, c=3.8
Standard fuel assembly outer radius (in.)	Triangular	a=3.935, b=3.985, c=3.96
Al 6063 can thickness (in.)	Triangular	a=0.05-1/64, b=0.05+1/64, c=0.05
Zr-3 can thickness (in.)	Triangular	a=0.025-1/64, b=0.025+1/64, c=0.025
Summary: Sample size=1200, Mean k_{eff}: $1.0069 \pm 3.4053E-4$, Relative uncertainty: $1171.6 \pm 23.9 pcm$		

TABLE I. Variable and distribution information summary for minimum critical core model uncertainty analysis

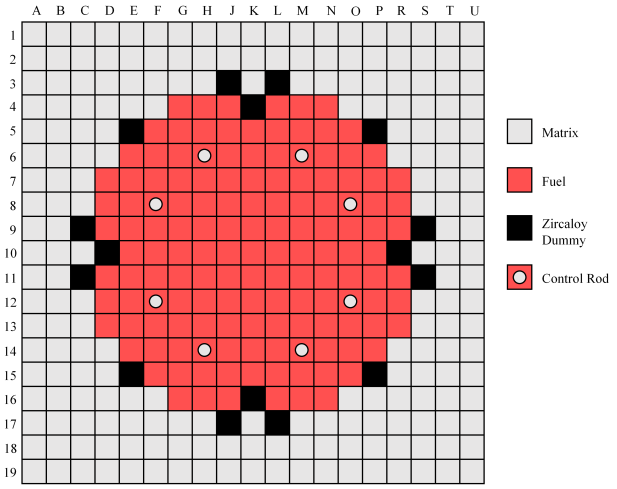

Fig. 2. TREAT minimum critical core configuration.

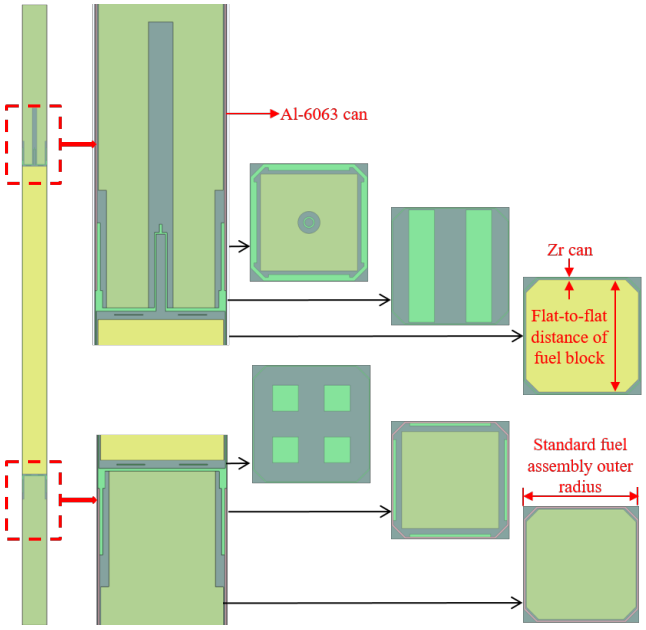

Fig. 3. TREAT standard fuel assembly SERPENT model.

1. Results of The Two Simple Test Models

Table II and Table III lists the single parameter sensitivity indices results. The last column in the two tables contains the results obtained from the sensitivity analysis method presented in this paper. Compared to the analytical solutions, estimation results of test model 1 are very accurate. For test model two, sensitivity index estimations of the first two variables have high accuracy. Sensitivity index of the last parameter was underestimated by about 10%.

Both tests were designed to verify the applicability of this method to non-linear models. Based on the results, it is clear that the method is applicable to non-linear models. It is able to perform a variance decomposition and capture the effects brought by each input factor with 1000 samples for the two simple models.

The first test contains only standard normal distributed variables while the second model contains a mixture of different distribution types. It is expected that the estimations of the second model have a lower accuracy. Note that due to the complexity of the steps in this method, there was no standard error propagation procedures available for the sensitivity index estimations listed in Table II and Table III. Hence there is no standard errors added for the values in the tables. This problem should be addressed in the future work.

Figure 4 and Figure 6 plot the Fourier coefficient estimations and the analytical values of the Fourier coefficients for each single parameter sub-function $f_i,\ i = 1, 2, 3$. The error bar for each Fourier coefficient estimation plotted in Figure 4 and Figure 6 is the standard error of mean estimation. It depends only on the sample size and the standard deviation of the sampled distribution.

For the first input factor in test model 1, the Fourier coefficient estimations contain relatively large errors. The coefficients were overestimated at some harmonic orders and underestimated at the other harmonic orders. It has been analysed in section II.5 that the errors in the Fourier spectrum are independent of their harmonic order. This observation proved the statement. Since the sensitivity index was estimated by the sum of all the coefficient modulus squares, errors over the spectrum were canceled out. An "accurate" estimation was given. For the other two factors, the errors in the Fourier coefficient estimations were much smaller.

Similar conclusions were obtained from the spectrum plots of test model 2. An error analysis in the previous section

has shown that the errors contained in the Fourier spectrum can be divided into two parts. One part is related to the numerical integration algorithm chosen for the factor of interest and the other is caused by the sampling process. For this two test models, the samples were generated using the random number generator provided by MATLAB. No specific sampling techniques were utilised. Latin hypercube sampling may be a better choice in case of decreasing the sampling related error.

For these two models the weighting factors used to estimate the Fourier coefficients were decided by cutting the s-space evenly into $5^3 = 125$ sub-regions. Other weight factors may also be tested to track the tendency of the spectrum errors.

Figure 5 and Figure 7 plot the subfunctions $f_i(s_i)$ reconstructed from the Fourier coefficients. It is clear that the maximum harmonic order $M = 20$ used is a relatively large value, as all of the functions re-constructed were oscillating around the analytical solutions. This would not affect partial variance estimation because the partial variance were defined as integrals over the whole sample space. However, if the re-constructed functions are used to estimate the sensitivity response of the model with respect to a specific sample point defined as,

$$S_{\alpha_0} = \frac{\partial R}{\partial \alpha} \frac{\alpha_0}{R_0}, \tag{37}$$

This oscillation may cause errors.

2. Results of TREAT Minimum Critical Core k_{eff}

The sensitivity indices obtained for TREAT minumum critical core is summarised in Table IV. The second column in table IV gives the ratio between two variances. The numerator of the ratio is the variances calculated from the model outputs of 300 samples which contain single factor perturbations. (These tests were run through the model to give a comparison to the sensitivity method presented in this paper.) The denominator is the variance of k_{eff} estimated from the 1200 sets of samples mentioned in [2]. This ratio represents a value similar to the sensitivity indices defined in this paper. However, the sensitivity indices defined in this paper is estimating the term

$$S_i = Var[E[f|x_i]]/Var[f] \tag{38}$$

while the ratio is estimating

$$R_i = Var[E[f|x_j^*, j \neq i]]/Var[f] \tag{39}$$

i.e. R_i calculates the variance of the model's conditional mean given that all the other factors except x_i are fixed at their user preferred values.

Hence R_i and S_i values are supposed to be different from each other. The purpose of presenting both results in Table IV is to provide the readers with comparison between different methodologies and definition of sensitivity measures.

Notice that there is no errors estimated for the S_i values. Because of the complexity of the steps used in this method to estimate S_i, it is hard to find a standard way to define the

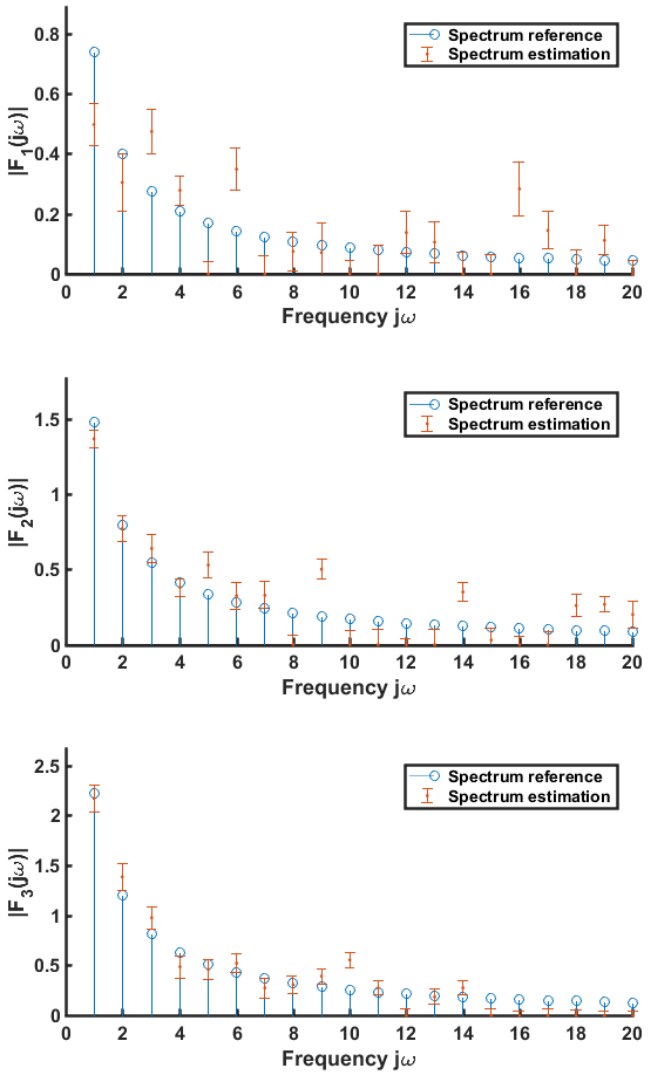

Fig. 4. Simple test model 1 results, comparison between the analytical frequency spectrum of $f_i(s_i)$ and the estimation. $i = 1, 2, 3$

Effect	Parameter distribution information	Partial variance	Analytical sensitivity	Sensitivity estimation
V_{x_1}	Normal distribution $\mu = 0,\ \sigma = 1$	2	0.047	0.043
V_{x_2}	Normal distribution $\mu = 0,\ \sigma = 1$	8	0.186	0.189
V_{x_3}	Normal distribution $\mu = 0,\ \sigma = 1$	18	0.419	0.423

TABLE II. Summary of simple test case one.

Effect	Parameter distribution information	Partial variance	Analytical sensitivity	Sensitivity estimation
V_{x_1}	Normal distribution $\mu = 0,\ \sigma = 0.5$	2.0211	0.211	0.209
V_{x_2}	Uniform distribution a=0.2, b=0.6	0.8505	0.089	0.088
V_{x_3}	Triangular distribution a=2.5, b=3, c=2.7	6.6297	0.694	0.638

TABLE III. Summary of simple test case two.

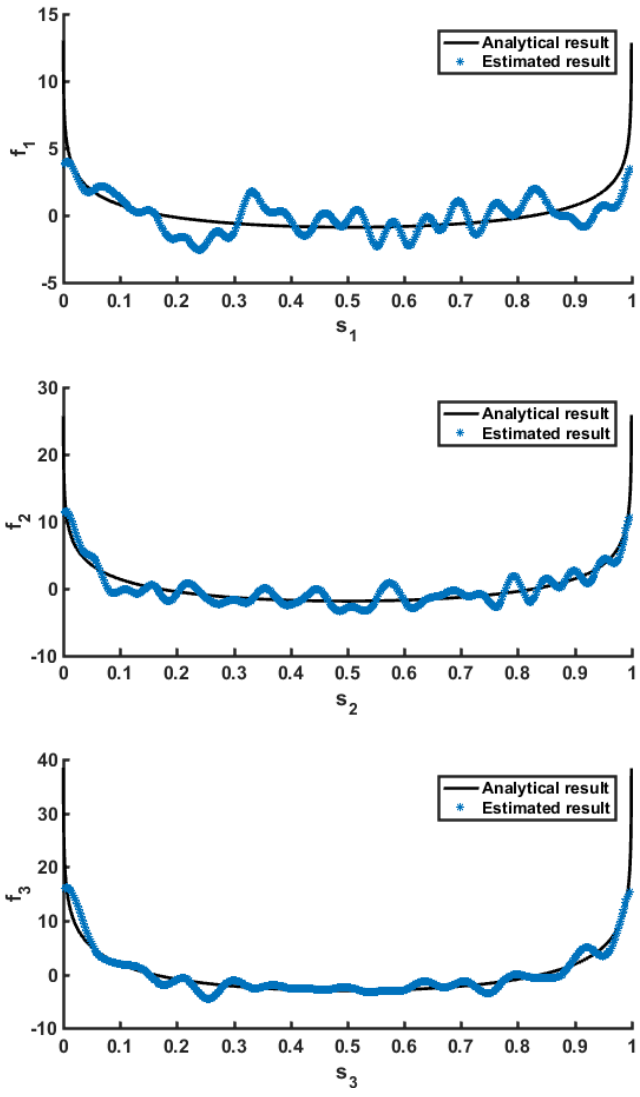

Fig. 5. Simple test model 1 results, comparison between the analytical solution of $f_i(s_i)$ and its estimation. $i = 1,\ 2,\ 3$

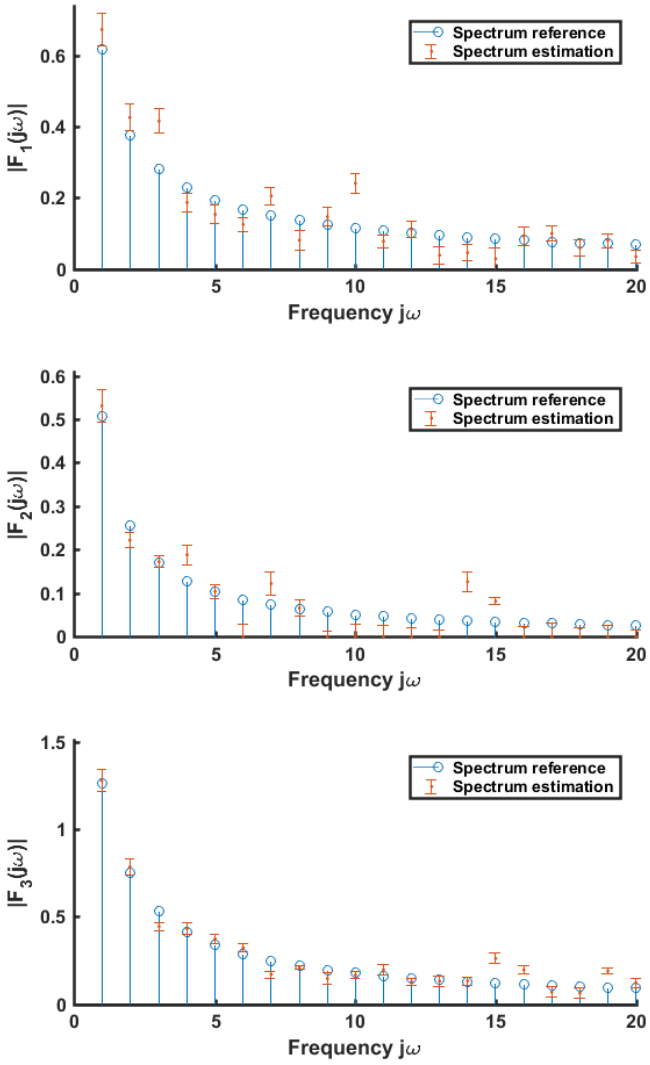

Fig. 6. Simple test model 2 results, comparison between the analytical frequency spectrum of $f_i(s_i)$ and the estimation. $i = 1,\ 2,\ 3$

Factor	$R_i = \frac{Var[K_{eff_{\text{Single factor perturbation}}}]}{Var[k_eff]}$	S_i estimations
Boron contamination	0.8675 ± 0.0501	0.7444
Flat to flat distance of fuel block	0.0361 ± 0.0021	0.0310
Standard fuel assembly outer radius	$6.7784E-4 \pm 3.9151E-5$	5.6169E-4
Al-6063 can thickness	0.0817 ± 0.0047	0.0701
Zr-3 can thickness	0.5793 ± 0.0335	0.4974

TABLE IV. TREAT minimum critical core sensitivity analysis summary

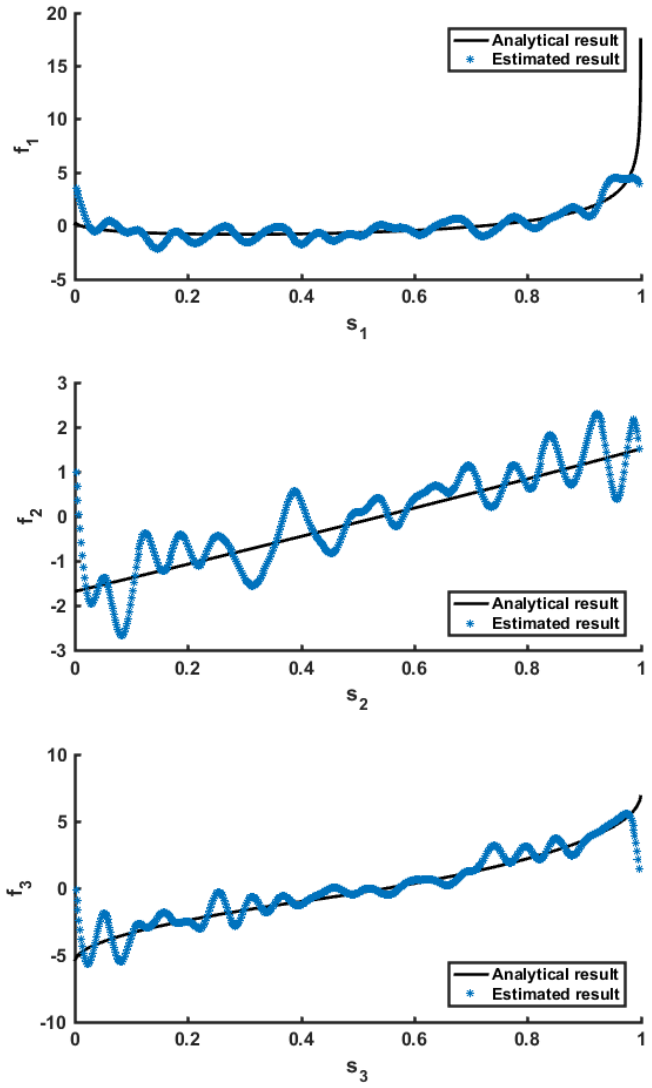

Fig. 7. Simple test model 2 results, comparison between the analytical solution of $f_i(s_i)$ and its estimation. $i = 1,\ 2,\ 3$

error of the estimations. This should be addressed in the future work.

The weight factors used to estimate the S_i results were calculated by dividing the s-space evenly into 2^5 sub-regions. Comparison between column 2 and 3 in Table IV shows that the sensitivity indices defined in this paper captures the correct model response with respect to different input factors. Note that the sum of the sensitivity indices listed here is larger than 1. This showed that the current method is slightly overestimating the sensitivity indices. Possible reason for this is the maximum harmonic order used was too large. When the Fourier coefficients of the $f_i(s_i)$ function are being summed up, noise from other sub-functions may get counted. The simple 2D example below may explain this better.

Consider a given integrable model which contains two independent, uniformly distributed random variables X_1 and X_2. As discussed before, the model can be written into the sum expansion:

$$f(x_1, x_2) = f_0 + f_1(x_1) + f_2(x_2) + f_{1,2}(x_1, x_2)$$

Consider only the variable X_1, by definition, the sensitivity index is calculated by $S_1 = \int_0^1 f_1(x_1)^2 dx_1$. Although the $f_{1,2}$ term also contains the x_1 factor, it should not be counted in the estimation of S_1. (It is counted by its own sensitivity index: $S_{1,2} = \int_0^1 \int_0^1 f_{1,2}(x_1, x_2)^2 dx_1 dx_2$)

During the estimation of the Fourier coefficients, the $f_{1,2}(x_1, x_2)$ term may get partially mixed up with the f_1 term. This explains the observed overestimation. Note that the R_i values listed of all input factors are always larger than the estimations of S_i. This is totally expected because the R_i is actually counting for all sub-functions which contain the x_i term by definition. It makes perfect sense that the S_i values obtained are slightly larger than their expectations and at the same time slightly smaller than the R_i values.

In the test with the TREAT model, the estimation of R_i took $300 \times 5 + 1200 = 2700$ trials of SERPENT model run while the estimation of S_i took 1200 trials. The new method showed its advantage.

IV. CONCLUSIONS

This paper presented a new sensitivity analysis method which can be applied efficiently to non-linear response models. It was tested on the TREAT minimum critical core model, but can be easily applied to all general models of interest. Results

presented for the two simple test models provided verification of the methods developed. A preliminary efficiency and error analysis of this method was also presented. Compared to traditional sensitivity analysis method, the method developed here can provide predictions at same level of accuracy with fewer sample tests. Future work includes further developing of the algorithms and expanding the range of applications.

V. ACKNOWLEDGMENTS

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