Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007)
Monterey, California, April 15-19, 2007, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2007)

CROSS-SECTION PARAMETERIZATION USING QUASI-REGRESSION APPROACH

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ABSTRACT

A quasi-regression approach for parameterization of multi-group neutron cross-sections is presented. This approach consists in approximation of cross-section dependencies on burnup and thermohydraulic parameters (fuel temperature, coolant temperature, coolant density, etc.) by a finite set of multidimensional orthogonal basis functions. The basis functions are constructed as a tensor product of univariate orthogonal polynomials. Expansion coefficients are estimated via calculation of multidimensional integrals using a hybrid (deterministic - Monte Carlo) quadrature formula. The calculational procedure includes three essential parts: generation of a hybrid grid which is regular in the burnup dimension and quasi-random over other dimensions; quasi-regression calculations and, finally, post-regression analysis consisting in construction of an approximate polynomial which minimizes the error. Advantages of this approach such as generality, flexibility and modularity of algorithm, as well as possibility of on-line error estimation are discussed. Applicability of such an approach is tested on a set of realistic fuel cross-sections.

Key Words: quasi-regression, parametrization, Monte Carlo, reactor physics

1. INTRODUCTION

Nuclear reactor neutronic calculations require multi-group neutron cross-sections of a cell or a fuel assembly, dependant upon material composition and thermohydraulic parameters (called *state parameters*). In practice, cross-sections resulting from reactor burnup calculations are approximated as a function of state parameters at different levels of burnup. Traditional approaches to deal with the problem of cross-section preparation are explained in Ref.[1] and the references therein. In brief, there exist two major approaches to cross-section approximation: the first one consists in multi-dimensional table interpolation and the second is an approximation by a function of several variables.

Advantages and drawbacks of these two approaches are discussed in detail in Ref. [1], where the authors propose a hybrid interpolation-approximation approach to cross-section parameterization. An interpolation of cross-sections at nominal conditions (so-called *base* dependence) as a function of burnup is carried out and subtracted from the total cross-section dependencies; the remainder is approximated by multi-dimensional polynomials by means of a stepwise regression algorithm.

In this paper, inheriting the main stages of the approach described in Ref. [1], which are mostly dictated by restrictions of a practical nature, we propose an alternative approach to the regression procedure with the intention to create an approximation (regression) algorithm satisfying the following requirements:

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- **modularity** - can be easily plugged into a neutron transport code;
- **generality** - must be able to treat cross-sections with different dependencies uniformly;
- **flexibility** - an arbitrary number of state parameters may be treated;
- **error control** - a built-in estimation of approximation error;
- **computational efficiency** - requires a reasonable number of function evaluations as input; has to be fast and numerically stable; the computational effort must not increase drastically with an increase of the number of state parameters.

The so-called *quasi-regression* technique [2, 3] seems to be particularly suitable in this context. As can be seen later, this approach fulfills the above requirements well. Moreover, as discussed by Lemieux and Owen [4] quasi-regression can be boosted even further by a powerful technique of functional analysis known as ANOVA (analysis of variance), with the result that it is not only one more fitting procedure but a flexible and "intelligent" tool for the exploration of parameter space.

Nevertheless, the applicability of the quasi-regression technique to cross-section approximation has never been demonstrated. This demonstration of applicability becomes crucial as some specific practical limitations may appear in the case of cross-section parameterization. Thus, the following limitations must be taken into account:

(a) a limited budget of cross-section evaluation is available in practice;

(b) a problem in combining a one-dimensional mesh for burnup with a multi-dimensional mesh for branch calculations;

(c) as a consequence of limitations (a) and (b), the error control has to be revised.

Each particular restriction, along with its origin and influence on the approximation procedure, will be addressed in more detail later in this paper. We will focus our attention on the case of Material Test Reactor (MTR) calculations where all the above limitations are prominent.

In general, in our paper we discuss the applicability of the quasi-regression approach to cross-section parameterization, focusing our attention on the case of MTRs. The method described here is based on ANOVA principles and it takes the above practical problems and restrictions as discussed into consideration.

2. STANDARD QUASI-REGRESSION

Before proceeding with the new method, let us first briefly describe the principles and the background of the standard quasi-regression technique.

Quasi-regression is a Monte Carlo method for constructing approximations to functions, based on observations sampled from the domain of the function to be approximated [2–4]. We consider a problem of

approximating a real valued function $F(\mathbf{x})$ defined on a multidimensional rectangular problem domain D by another function $\hat{F}(\mathbf{x})$ which is close to $F(\mathbf{x})$ in L^2-norm and possessing some advantages over $F(\mathbf{x})$. In our work we require that $\hat{F}(\mathbf{x})$ is computationally more efficient than a straightforward calculation of the initial function $F(\mathbf{x})$. As any rectangular problem region D can be easily scaled to a unit hypecube $I^d = \left\{\mathbf{u} \in \mathbb{R}^d \,:\, 0 \le u_i \le 1,\ 1 \le i \le d\right\}$, where d is the problem dimensionality, let us consider a problem of approximating the square integrable function $F(\mathbf{u}) \in L^2(I^d)$, defined over I^d.

The key idea of the quasi-regression technique is to approximate the function $F(\mathbf{u})$ by a linear combination of orthogonal basis functions $\psi_{\mathbf{r}}(\mathbf{u})$ over I^d, constructed as a tensor product of univariate orthogonal basis functions $\phi_m(u)$:

$$\psi_{\mathbf{r}}(\mathbf{u}) = \prod_{i=1}^{d} \phi_{r_i}(u_i)\,. \tag{1}$$

where u_i denote d components of $\mathbf{u}$ and $\mathbf{r} = (r_1, r_2, ..., r_d)$ is a vector of d non-negative integers ($i = 1, ..., d$). It is easy to prove that to each index vector $\mathbf{r}$ corresponds a unique tensor product function and the countably infinite set $\{\psi_{\mathbf{r}}(\mathbf{u})\}$ forms an orthonormal basis on I^d. We will denote the countable infinite set of index vectors $\mathbf{r}$ as U.

Orthogonality of basis functions is an important requirement. In principle any orthogonal functions can be employed and, moreover, different types of orthogonal functions can be used for different parameters. In our work we use rescaled (to the unit interval $I = [0, 1]$) and renormalized Legendre polynomials as a univariate orthogonormal basis $\phi_m(u)$.

In practice, only a finite number of basis functions can be used for approximations and we can write the approximation function in the form

$$\hat{F}(\mathbf{u}) = \sum_{\mathbf{r}\in\mathsf{R}} \beta_{\mathbf{r}} \psi_{\mathbf{r}}(\mathbf{u}), \tag{2}$$

where $\beta_{\mathbf{r}}$ are unknown expansion coefficients and the sum is assumed over the finite set $\mathsf{R} = \mathsf{R}_{B_0,B_1,B_\infty} \subset \mathsf{U}$:

$$\mathsf{R}_{B_0,B_1,B_\infty} = \left\{\mathbf{r} : \|\mathbf{r}\|_0 \le B_0,\ \|\mathbf{r}\|_1 \le B_1,\ \|\mathbf{r}\|_\infty \le B_\infty\right\}, \tag{3}$$

where $\|\mathbf{r}\|_0$, $\|\mathbf{r}\|_1$ and $\|\mathbf{r}\|_\infty$ (called *rank*, *degree* and *order* correspondingly) are defined in Ref. [2] in the following way

$$\|\mathbf{r}\|_0 = \sum_{i=1}^{d} 1_{r_i>0},\ \|\mathbf{r}\|_1 = \sum_{i=1}^{d} r_i \text{ and } \|\mathbf{r}\|_\infty = \max_{1\le i\le d} r_i \tag{4}$$

and limiting parameters B_0, B_1 and B_∞ are defined by the user. Once the index set U is truncated according to limiting values B_0, B_1 and B_∞, it is convenient to map the finite set $\mathsf{R}_{B_0,B_1,B_\infty}$ to a finite set T_p of univariate indices $t = 1, ..., p$ with $\mathsf{Card}\left[\mathsf{T}_p\right] = \mathsf{Card}\left[\mathsf{R}_{B_0,B_1,B_\infty}\right] = p$. A particular rule $\chi : \mathsf{R}_{B_0,B_1,B_\infty} \to \mathsf{T}_{\bar{p}}$ that makes correspondence between these two sets is not important but it is convenient that low-rank, low-order and low-degree terms correspond to small t-values and $t = 1$ corresponds to $\mathbf{r} = 0$.

Let $\Psi = \mathrm{Col}\left(\psi_1, \cdots, \psi_t, \cdots, \psi_p\right)$ and $\beta = \mathrm{Col}\left(\beta_1, \cdots, \beta_t, \cdots, \beta_p\right)$ be column vectors of multivariate base functions and of expansion coefficients, correspondingly. We can rewrite the expression above in a matrix form:

$$\hat{F}(\mathbf{u}) = \Psi^T(\mathbf{u})\,\beta. \tag{5}$$

The integrated square error

$$\mathsf{ISE} = \int_{I^d} \left(F(\mathbf{u}) - \hat{F}(\mathbf{u}) \right)^2 d\mathbf{u} = \int_{I^d} E(\mathbf{u})^2 \, d\mathbf{u}, \tag{6}$$

where $E(\mathbf{u}) = \left(F(\mathbf{u}) - \hat{F}(\mathbf{u}) \right)$, qualifies the least square (L^2-norm) approximation error, which appears due to the truncation of the infinite set U of indices $\mathbf{r}$ to a finite set R. As shown in Refs. [2, 4], the optimal coefficients β^* in this expansion, leading to the minimal ISE, are defined by

$$\beta = \int_{I^d} F(\mathbf{u}) \, \Psi(\mathbf{u}) d\mathbf{u}. \tag{7}$$

Hence, the approximation problem is reduced to the calculation of integrals of multivariate functions over the multidimensional problem domain. Within the so-called *Monte Carlo* integration approach (which is the most appropriate for multidimensional integration and for this reason usually used in quasi-regression) the estimate $\hat{\beta}^{(n)}$ of the expansion coefficients β based on n samples can be calculated via:

$$\hat{\beta}^{(n)} = \frac{1}{n} \sum_{k=1}^{n} F(\mathbf{u}_k) \Psi(\mathbf{u}_k), \tag{8}$$

where $\{\mathbf{u}_k\}$ represents a set of properly generated points uniformly distributed within the problem domain (e.g. Refs. [4–6] and the references therein). Depending on the nature of this underlaying point sequence, i.e. random (*pseudo-random*) points or low-discrepancy deterministic (*quasi-random*) points, the integration method is classified as Monte Carlo (MC) or *quasi-Monte Carlo* (QMC), correspondingly.

As discussed in the literature, in terms of the convergence rate of the integration formula, QMC usually out-performs MC, but the main drawback of the QMC technique is that it does not possess an easy way of error estimation. Indeed, in the case of the Monte Carlo approach, the error estimate of the integration formula (8) is based on the Central Limit Theorem, while relatively sophisticated techniques [2–4] are required to calculate errors of estimates $\hat{\beta}^{(n)}$ in the case of QMC. Our own experience confirmed that QMC is more efficient than MC. Hence, in our further discussions we only consider the quasi-Monte Carlo integration scheme with the so-called *Sobol' sequences* of low-discrepancy points [6]. We will return to a practical method of estimation of the approximation error in Section 4.

3 PRACTICAL LIMITATIONS

As we can see from the discussion of the quasi-regression above, its implementation requires samples of the approximated function $F(\mathbf{u})$ on a set of quasi-random points $\mathbf{u}_k \in I^d$. It becomes problematic when the quasi-regression approach is envisaged for the approximation of cross-sections $\sigma(\mathbf{u})$, namely in the case of MTRs. The reason for this is that the list of state parameters includes burnup, which is a specific state parameter: very often in practice cross-sections can not be calculated at arbitrary burnup points, as it is either calculationally inefficient or it is in contradiction with the ideology (numerical method) of the cross-section calculational code. Therefore a choice of the mesh in the burnup dimension is mostly limited to the underlaying physical code. If the QMC integration rule is foreseen for integration over non-burnup variables, it raises the problem of combining the one-dimensional burnup mesh with the QMC mesh in the other $(d-1)$ dimensions as well as an adaptation of quasi-regression for this hybrid-mesh case.

Moreover, the accuracy of the estimation of the regression parameters β can be improved, in principle, by increasing the number of samples from the integration domain. In the case of cross-section

parameterization this way of enhancement is limited, given that cross-section evaluations are numerically expensive and time consuming; only a relatively small number (to an order of a few thousand) of cross-section evaluations can be used for the approximation. It raises a problem of the optimal use of the given budget of function samples for an approximation with the smallest possible error.

Finally, in light of the remarks above, the way in which the approximation error is treated, must also be revised.

In the next section we present a modified method which makes an attempt to overcome these difficulties. The whole regression procedure includes three essential parts: generation of a hybrid grid which is regular in the burnup dimension and quasi-random over other dimensions; quasi-regression calculations and, finally, post-regression analysis consisting in construction of an approximate polynomial which minimizes the error.

4. EXTENSION OF QUASI-REGRESSION ON HYBRID MESH

4.1 Separation of variables

Fortunately, the quasi-regression method can be naturally adapted for the case of hybrid grid. Indeed, as in a crude quasi-regression approach, we construct an approximating function $\hat{F}(\mathbf{u})$ in the form $\hat{F}^{(n)}(\mathbf{u}) = \Psi^T(\mathbf{u})\,\beta$. Then Eq. (7) remains valid, and we can start developing our approach from this point. Let us denote $b \equiv u_{i_p} \in I^1$ the particular state parameter $(i = i_p)$, which requires a particular mesh (e.g. burnup); $\mathbf{v} \in I^{d-1}$ is a vector of remaining state variables: $\{u_i : i \neq i_p\}$. Therefore, in the d-dimensional hypercube axis b introduces a "particular" or *longitudinal* direction, while other dimensions (directions) form a "conventional" or *transverse* part. Therefore, we can represent the base functions $\psi_{\mathbf{r}}(\mathbf{u})$ as a tensor product of two terms:

$$\psi_{\mathbf{r}}(\mathbf{u}) = \psi_{\mathbf{r}}^{(\|)}(b)\,\psi_{\mathbf{r}}^{(\perp)}(\mathbf{v}), \tag{9}$$

where the longitudinal part, according to our previous notations, is $\psi_{\mathbf{r}}^{(\|)}(b) \equiv \phi_{r_{ip}}\left(u_{i_p}\right)$ and the transverse part is $\psi_{\mathbf{r}}^{(\perp)}(\mathbf{v}) = \prod_{i=1,\, i\neq i_p}^{d} \phi_{r_i}(u_i)$. We can now rewrite the expression for $\beta_{\mathbf{r}}$ in the following way:

$$\beta_{\mathbf{r}} = \int_{I^{d-1}} d\mathbf{v}\, \psi_{\mathbf{r}}^{(\perp)}(\mathbf{v})\, F_{\mathbf{r}}^{(\perp)}(\mathbf{v}) \tag{10}$$

where $F_{\mathbf{r}}^{(\perp)}(\mathbf{v}) = \int_0^1 db\, \psi_{\mathbf{r}}^{(\|)}(b)\; F(b, \mathbf{v})$ is the "projection" of the function $F(\mathbf{u})$ to the transverse dimensions. As the order of integration commutes, then after swapping the order of integration, the formula above can be written in an alternative form

$$\beta_{\mathbf{r}} = \int_0^1 db\, \psi_{\mathbf{r}}^{(\|)}(b)\; F_{\mathbf{r}}^{(\|)}(b), \tag{11}$$

where $F_{\mathbf{r}}^{(\|)}(b) = \int_{I^{d-1}} d\mathbf{v}\, \psi_{\mathbf{r}}^{(\perp)}(\mathbf{v})\; F(b, \mathbf{v})$ is, by analogy, a projection to the longitudinal dimension.

Splitting the multidimensional integration on two commutative parts allows us to implement different and independent methods of numerical integration: in general, some deterministic one-dimensional quadrature formula can be used for integration over longitudinal direction, whereas the Monte Carlo approach can be

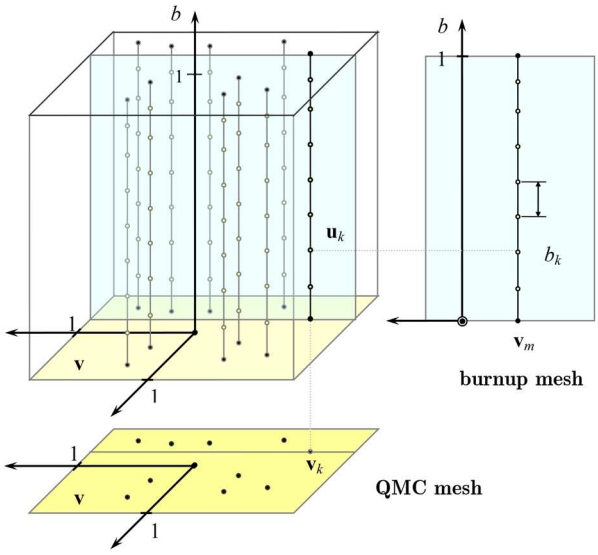

Figure 1. Hybrid calculational mesh

applied for integration over transverse dimensions, where, unlike burnup, we can freely choose mesh points. Hence, the principal result of this separation variable exercise is that the *changes are necessary only on the level of descretization of the integration operator*, while the base of the quasi-regression approach, described in the previous section (i.e. approximation with a linear combination of orthogonal basis functions, constructed as a tensor product of univariate basis functions; calculation of expansion coefficients through integration, etc.), does not require any modification.

This idea was realized via a combined deterministic-Monte Carlo integration rule over a hybrid regular-random mesh, illustrated in Fig. 1. In our work we used Simpson's rule for the burnup b integration and the QMC integration over $\mathbf{v}$, based on the Sobol' sequence of low discrepancy points [5, 6]. Note, that here are two possible ways of mesh generation in the transversal direction: the first one consists in repeating the same branch points at each burnup step (as in Fig. 1). An advantage of this approach is that it can (potentially) supply an easy and transparent way of error control. The second method consists in continuation of the Sobol' sequence on each burnup step with the goal to cover better parameter space in the transversal direction. It can (potentially) supply a more precise estimation of $\beta_{\mathbf{r}}$ for a given number of points. Our comparison of these two approaches proved that, on average, the second one does perform better.

4.2 Subtraction of base dependence

Following the recommendations of Zimin and Semenov [1], cross-section dependencies $\sigma\left(b, \mathbf{v}_0\right)$ on the burnup for the nominal values of branch state parameters (one-dimensional dependencies which can be approximated with cubic splines) were subtracted from the total dependence $\sigma\left(\mathbf{u}\right) = \sigma\left(b, \mathbf{v}\right)$ and quasi-regression approximations were carried out for the remainder

$$\Delta\sigma\left(b, \mathbf{y}\right) = \sigma\left(b, \mathbf{v}\right) - \sigma\left(b, \mathbf{v}_0\right), \tag{12}$$

where σ denotes either a microscopic or a macroscopic cross-section for some energy group and of some specific type or isotope. It allows the decreasing of the total variance of approximated functions, as the dependence on burnup is usually more prominent than dependence on the other parameters [1].

4.3 Error control

The in-line error estimation, introduced for quasi-regression in the Refs. [2, 3], can not be always used in the modified method discussed here. Hence the in-line error estimation in our approach is replaced by a *post-regression* practical error estimation. It means that the quality of approximation is verified after the regression is accomplished on the data set, used for regression. Obviously it is a drawback when compared with the case of convenient quasi-regression but, probably it is the price to pay for the complications we have introduced.

The Lack of Fit

$$\mathsf{LOF} = \frac{\mathsf{ISE}}{\mathsf{Var}\left[F(\mathbf{u})\right]} \tag{13}$$

describes the fraction of the function variance

$$\mathsf{Var}\left[F(\mathbf{u})\right] = \int_I \left(F\left(\mathbf{u}\right) - \int_I F\left(\mathbf{u}\right) d\mathbf{u} \right)^2 d\mathbf{u}$$

not explained by the regression model. In practice the LOF value can be estimated via the following formula:

$$\widehat{\mathsf{LOF}}^{(n)} = \frac{\widehat{\mathsf{MSE}}^{(n)}}{\hat{S}^{(n)}}, \tag{14}$$

where $\hat{S}^{(n)}$ is the sample variance of the function $F(\mathbf{u})$ and

$$\widehat{\mathsf{MSE}}^{(n)} = \frac{1}{n} \sum_{k=1}^{n} \left(F\left(\mathbf{u}_k\right) - \hat{F}^{(n)}\left(\mathbf{u}_k\right) \right)^2 \tag{15}$$

is a Mean Squared Error of approximation after of quasi-regression. Note, that this value includes both the truncation error and the integration error. Here the approximation function $\hat{F}^{(n)}\left(\mathbf{u}_k\right)$ is defined in the following way:

$$\hat{F}^{(n)}\left(\mathbf{u}_k\right) = \sum_{t \in \mathsf{T}^*} \hat{\beta}_t^{(n)} \psi_t\left(\mathbf{u}_k\right), \tag{16}$$

where symbol T^* denotes a set of expansion terms used in the approximation. We assume that for some reason (the complete discussion will be carried out in the next section) only subset $\mathsf{T}^* \subseteq \mathsf{T}_p$ of terms is included into the approximation polynomial.

The obvious drawback of the Lack of Fit is that it supplies a *mean* measure of discrepancy between two functions. In our case of multidimensional interpolation it is of interest to estimate a local error, as we are intended to build an approximation function with not only a small *average* error but also small *maximal local* errors. The estimator, that we will denote $\widehat{\mathsf{MaxSE}}$, is introduced in the following way

$$\widehat{\mathsf{MaxSE}} = \max_{1 \le k \le n} \left(F\left(\mathbf{u}_k\right) - \hat{F}^{(n)}\left(\mathbf{u}_k\right) \right)^2. \tag{17}$$

is a practical estimator of the maximal local error. Normalised to function sample varience it gives a relative (similarly to $\widehat{\mathsf{LOF}}$) measure of the local error. If necessary the two indicators above of error can be combined in the one efficient squared error, which can be a subject of minimization:

$$\mathsf{ESE} = (1-\gamma)\widehat{\mathsf{MaxSE}} + \gamma\widehat{\mathsf{MSE}}, \tag{18}$$

where $0 \leq \gamma \leq 1$ is the weight attributed to the Mean Squared Error.

4.4 Construction of an approximate polynomial. Post-regression treatment

Once the quasi-regression run is accomplished, we obtain estimators $\hat{\beta}_t^{(n)}$ of expansion coefficients β_t, where $t = 1, .., p$. These estimators require a further post-regression treatment for the following two reasons (and, correspondingly, for two goals):

1. Given that these estimations are not always equal to the correct values of β_t, it is important to choose the subset $\mathsf{T}^+ \subseteq \mathsf{T}_p$ of coefficients $\hat{\beta}_t^{(n)}$ that does reduce the error of the approximation.
2. In order to decrease the memory necessary to keep the approximation polynomial coefficients and the time of calculation of these polynomials, it is preferable to omit all non-pertinent (small) terms.

Both goals 1 and 2 may be achieved within one simple, but mathematically consistent, approach based on ANOVA principles, briefly described below.

4.4.1 Goal 1

Consider a set of estimators $\left\{\hat{\beta}_t^{(n)} : t = 1, .., p\right\}$. Given the estimated parameters $\hat{\beta}_t^{(n)}$ are not necessary equal to correct parameters β_t, let ε_t be the error of estimation (unknown) of the corresponding coefficient β_t, i.e. $\hat{\beta}_t^{(n)} = \beta_t + \varepsilon_t$. It can be demonstrated, that the total L^2-error of approximation has the following structure

$$\mathsf{ISE} = \sum_{t \in \mathsf{T}^*} \varepsilon_t^2 + \sum_{t \notin \mathsf{T}^*} \beta_t^2, \tag{19}$$

where $\mathsf{T}^* \subseteq \mathsf{U}$ is a subset of the expansion terms included in the approximation sum, where $* = \{+, \#\}$. (For the explanation of the hierarchy of different subsets used in our discussion, see Fig. 2).

It follows from the above formula, that including a particular term $\hat{\beta}_t^{(n)}\psi_t(\mathbf{u})$ to the approximation gives a contribution to ISE equal to ε_t^2, while excluding this term yields an error of β_t^2. In other words, if $\varepsilon_t^2 < \beta_t^2$, then including the t-th term will improve the approximation, i.e. reduce ISE. Unfortunately, both ε_t^2 and β_t^2 are unknown. Nevertheless, in practice we can use $\widehat{\mathsf{MSE}}^{(n)}$ as an estimator for ISE and carry out the following test: compare $\widehat{\mathsf{MSE}}^{(n|t^+)}$ and $\widehat{\mathsf{MSE}}^{(n|t^-)}$, i.e. Mean Squared Error with t-th term retained or rejected correspondingly. The criterion which specifies a rejection or holding a particular term can be formulated as follows:

Criterion I: *If* $\widehat{\mathsf{MSE}}^{(n|t^+)} < \widehat{\mathsf{MSE}}^{(n|t^-)}$*, then the corresponding term* $\hat{\beta}_t^{(n)}\psi_t(\mathbf{u})$ *should be retained, otherwise it should be discarded.*

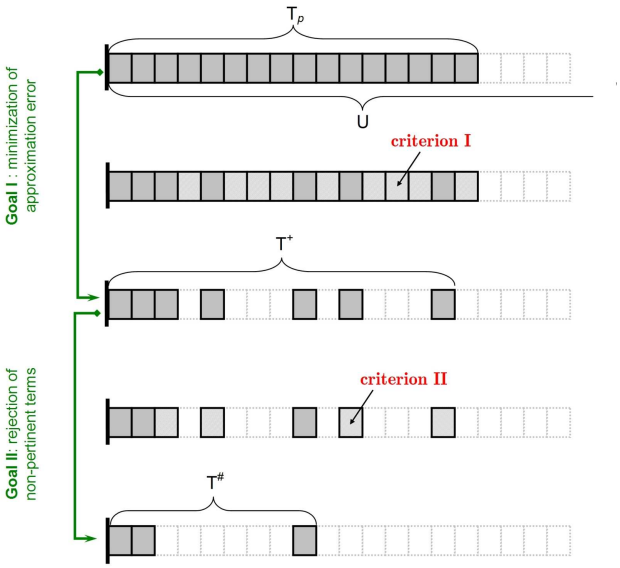

Figure 2. The initial infinite set U is truncated by a finite subset $\mathsf{R} \subset \mathsf{U}$ of multidimensional indices and the corresponding set T_p of one-dimensional indices (dark gray rectangles). Application of the first rejection criterion reduces the set T_p to its subset $\mathsf{T}^+ \subseteq \mathsf{T}_p$ (rejected terms are shown in light gray). After application of the second criterion (rejection of non-pertinent terms) one gets $\mathsf{T}^\# \subseteq \mathsf{T}^+$.

Due to orthogonality of terms in the expansion, the order in which different terms are added to the expansion is not important. Thus, in our work we test all terms consecutively, starting from the low-order ones. Note, that this *practical* approach can fail given that ISE is estimated with some error, as the estimations $\widehat{\mathsf{MSE}}^{(n)}$ are based on a finite number n of points.

4.4.2 Goal 2

The cardinality $p = \mathsf{Card}\left[\mathsf{R}_{B_0,B_1,B_\infty}\right]$ of the index set grows drastically with the number of dimensions d and with increasing values of the truncation parameters B_0, B_1 and B_∞. Nevertheless, the contribution of the majority of these terms is, in fact, negligibly small. So, discarding these small terms would not essentially affect the quality of approximation, but would allow a radical decrease in the number of terms used for approximation, and consequently the volume of memory allocated for storage of expansion coefficients. Moreover, it will drastically improve the speed of the calculation of the approximation function. This improvement is expected to appear not only due to a reduced number of terms, but because it will most likely reject an overwhelming majority of high-order terms, these latters being the most expensive numerically .

In order to carry out this selection of pertinent terms, we have to establish an appropriate criterion. This criterion can be formulated and endorsed mathematically, using the ANOVA approach. This is briefly explained below.

Taking Parseval's theorem into account we can express the variance of the function $F\left(\mathbf{u}\right)$ in terms of

expansion coefficients:

$$\mathsf{Var}\left[F\left(\mathbf{u}\right)\right]=\sum_{t=2}^{\infty}\beta_t^2, \tag{20}$$

where the term $\beta_1=\int_{\mathbb{I}}F\left(\mathbf{u}\right)d\mathbf{u}$ corresponding to the first term of the basis expansion (average of function), is not included. This formula demonstrates that a contribution of t-th term of basis expansion is proportional to the square of its expansion coefficient. In other words, ratio $\beta_t^2/\mathsf{Var}\left[F\left(\mathbf{u}\right)\right]$ characterizes the part of function variance explained by this particular term.

The value $\left(\hat{\beta}_t^{(n)}\right)^2$ can be used as a biased (see Ref. [4] for details) estimator of β_t^2. Now let us reject all coefficients smaller than some threshold value β_{min}. The remaining coefficients form subset $\mathsf{T}^{\#}=\left\{t\in\mathsf{T}^{+}\,:\,\hat{\beta}_t^{(n)}\geq\beta_{min}\right\}$. Let us denote $\mathsf{T}^{x}\equiv\mathsf{T}^{+}\setminus\mathsf{T}^{\#}$ the subset of rejected coefficients. Rejection of coefficients, corresponding to $t\in\mathsf{T}^{x}$ will lead to an integrated squared error with the upper bound given as follows:

$$\sum_{t\in\mathsf{T}^x}\left(\hat{\beta}_t^{(n)}\right)^2\leq\beta_{min}^2\mathsf{Card}\left(\mathsf{T}^x\right)\leq\beta_{min}^2 p. \tag{21}$$

We can require that this error does not exceed some small fraction α of the total function variance $\mathsf{Var}\left[F\left(\mathbf{u}\right)\right]$. As this former can be estimated via $\hat{S}^{(n)}$, we can write $\beta_{min}^2 p\leq\alpha\hat{S}^{(n)}$. Under this condition the threshold value β_{min}, which can be used for rejection of insignificant terms given that the resulting error does not exceed $\alpha\times 100$ per cent, is:

$$\beta_{min}=\sqrt{\alpha\hat{S}^{(n)}/p}. \tag{22}$$

Note that the above rule can be too conservative and the actual error, which may be easily estimated as $\sum_{t\in\mathsf{T}^x}\left(\hat{\beta}_t^{(n)}\right)^2$, can be much smaller than $\alpha\hat{S}^{(n)}$. The drawback of this conservatism is that the threshold is very low and, as a consequence, too many insignificant terms are retained. In this case the iterations can be organized and the value of β_{min} can be readjusted based on results of previous iterations (e.g., taking in Eq. (22) instead of p the value $p^{(x)}=\mathsf{Card}\left(\mathsf{T}^x\right)$ from the previous iteration). Summarizing the considerations above, we can formulate Criterion II for the rejection of coefficients:

Criterion II: *Coefficient $\hat{\beta}_t^{(n)}$, where $t\in\mathsf{T}^{+}$, is considered to be not pertinent and consequently rejected if $\hat{\beta}_t^{(n)}<\beta_{min}$, where β_{min} is defined by Eq. (22)*

Note, that the order in which Criteria I and II are applied can be swapped: this is possible due to orthogonality of different terms in the expansion.

5. DISCUSSION AND RESULTS

The quasi-regression approximation, together with the ANOVA technique, form a powerful tool for cross-section approximation that has flexibility and generality as two of its most attractive features. It is, however, important to mention that quasi-regresssion is a *global* approximation and is most efficient for continious, smooth functions. This approach could prove less effective for functions exhibiting large local variations.

Nevertheless, this approach provides not only a quantitative analysis of the approximation error, but further supplies a qualitative perspective on the cross-section behaviour. The latter occurs via the selection of

relevant basis functions and cross-terms for a given set of state parameters (as described in Ref. [4] and Section 4). This methodology may, as such, be applied to identify the set of important state parameters needed to accurately describe cross-section dependencies.

In order to demonstrate these potential applications, we apply the methodology described above to the generation of 6-group cross-sections for a MTR fuel assembly. The assembly represents is an HEU (90% enriched U-235) plate type fuel element with an initial U-235 load of 300 g. The generation of few group cross-sections for this configuration is performed with the HEADE code, which is a part of the OSCAR reactor calculational system [7] developed at Necsa, South Africa. HEADE is a collision probability transport code utilizing a low-order response matrix formalism.

The calculational procedure is as follows:

- Identification of the initial list of state parameters for cross-section calculation. For this calculation we choose burnup, moderator density, fuel temperature, moderator temperature, and boron concentration as dummy parameter. These state parameters represent a five-dimensional problem.

- We define ranges for the above state parameters. These ranges are listed in Table I below and represent typical operational conditions for the SAFARI-1 reactor.

- We generate a set of $(M \times N)$ quasi-random points to span the 5-dimensional cross-section parameter space, where M represents the number of burn-up points and N the number of points which spans the remaining 4-dimensional off-base space. Due to the current limitations in the HEADE code the burn-up dimension is spanned with a regular distribution of points and the same set of 4-dimensional state parameter points are utilized at each burnup step, as illustrated in Fig. 1. This practical restriction creates some limitations regarding the optimal efficiency of the methodology and the impact hereof will be addressed in future work when these limitations are removed. For the sake of this paper, we perform three sets of $(M \times N)$ calculations: COARSE (33×128), MEDIUM (65×256) and FINE (65×512). These numbers relate directly to the number of transport calculations to be performed, and hence, for the MEDIUM mesh, 16640 calculations are required.

- We perform the HEADE calculation to produce microscopic cross-sections at each 5-dimensional state parameter vector, for each isotope and reaction. In this paper we present specifically the U-235 capture cross-section for energy group 6 (thermal group).

- In the final step we perform the quasi-regression procedure and estimate the values of coefficients for all chosen combinations of basis functions. For this 5-dimensional calculation, utilizing values $B_0 = B_1 = B_\infty = 6$ for limiting parameters, we evaluate 461 coefficients (see Eq. (3)). In order to reduce this large number of coefficients, we apply the post regression treatment as described in Section 4 and obtain the final set of important and well approximated basis functions and their accompanying coefficients. We also obtain maximum and mean reconstruction errors, as well as a global variance for the fit and an estimate for the variances of each coefficient.

Results for this procedure are illustrated in Tables II and III below. Table II lists maximum and average errors for each calculational case, as well as the number of remaining coefficients after the post regression treatment is complete. The criterion for the rejection of non-pertinent coefficients is set to 0.05%.

Table I. Ranges for state parameters

State Parameter	Minimum	Nominal	Maximum
Burnup (0.68 MW / element)	0 Days	—	120 Days
Moderator Density	0.97738 g/cm^3	0.99800 g/cm^3	1.00000 g/cm^3
Fuel Temperature	283 K	333 K	383 K
Moderator Temperature	288 K	318 K	380 K
Boron Concentration	0	0	0

Table II. Final results for the U-235 capture cross-section for group 6 (parameter estimation)

Mesh	Final number of coefficients	Maximum local error	Average error
COARSE	5	2.34%	0.27%
MEDIUM	5	1.25%	0.12%
FINE	4	0.89%	0.11%

It is important to note that the number of coefficients utilized in the final fit have been reduced from 461 to 4 without any significant reduction in accuracy (in the FINE case). In order to provide some further insight into the advantage of the ANOVA technique, we present, in Table III, further details regarding the structure and importance of the final four basis functions and accompanying coefficient values. We reiterate that, as described in Section 4, these coefficient values relate to their relative importance.

Table III. Structure of FINE parameters

FINE case: POLYNOMIAL ORDER of					$\mathsf{Var}\left[F\left(\mathbf{u}\right)\right]$ =5.43
Burnup	Boron	Mod. density	Fuel temp.	Mod. temp.	Coefficient
0	0	0	0	0	-1.1771
0	0	0	1	0	-1.9582
1	0	0	1	0	-0.1247
0	0	0	2	0	0.1136

Table III allows us to draw important conclusions regarding the dependencies on various state parameters, and, as such, to learn from this methodology which state parameter dependencies exist. We see from Table III that the U-235 **microscopic** cross-section shows no dependence on either moderator density or moderator temperature (or the dummy Boron parameter). This may be understood in the light of the small operational range of these parameters as listed in Table I. Futhermore we notice a strong linear and weak quadratic dependency on fuel temperature, as well as a weak bi-linear cross term between burnup and fuel temperature.

6. CONCLUSIONS

In this work we have adapted the quasi-regression technique for use in cross-section parameterization. Combining this approach with the ANOVA methodology, we have extended the parameterization tool to an intelligent and flexible system which not only provides a measure of error control, but identifies relevant state parameters and the nature of their dependencies. The methodology was applied to a realistic MTR problem under operational conditions, and thermal U-235 microscopic cross-sections were investigated as a function of five state-parameters. For the reference calculational case the global fit was done to a mean accuracy of 0.1%, utilizing four automatically identified relevant basis functions.

The next natural steps in this development include further development of error estimation, post-regression treatment, and production level tests on cross-section data. These efforts should culminate in an automation tool for the complete cross-section library generation process. In this regard, we plan to investigate and implement a two-step parameterization approach. The first aims to utilize quasi-regression to efficiently identify relevant basis functions, and the second to use regular regression in order to estimate the value of the coefficients with greater precision.

ACKNOWLEDGEMENTS

The authors would like to acknowledge various members of the Radiation and Reactor Theory group at Necsa for their support in this work, and thank especially Dr. Wessel Joubert and Dr. Djordje Tomašević for their contribution.

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