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Uncertainty quantification in nuclear criticality modelling using a high dimensional model representation

D. Ayres *, M.D. Eaton

Nuclear Engineering Group, Department of Mechanical Engineering, Imperial College of Science, Technology and Medicine, Prince Consort Road, London SW7 2AZ, UK

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ABSTRACT

An adaptive high dimensional model representation (HDMR) is used to decompose the response parameter k_{eff} into a superposition of lower dimensional subspaces which are in-turn projected on to a polynomial basis. These projections are evaluated using an adaptive quadrature scheme which is used to infer the polynomial orders of the basis. The combination of adaptive HDMR and adaptive quadrature techniques results in a sparse polynomial expansion which has been optimised to represent the variance of the response with the minimum number of polynomials. The combined application of these techniques is illustrated using UOX and MOX pin cell problems with evaluated nuclear covariance data. We show that this approach to calculating the variance in k_{eff} is an order of magnitude more efficient when compared to Latin Hypercube sampling with the same number of samples for problems involving up to 988 random dimensions.

1. Introduction

In recent years there has been significant interest in developing computationally accurate, yet efficient, uncertainty quantification methods that can model both small and large parametric uncertainties. The polynomial chaos method has attracted significant interest as it can model both small and large parametric errors whilst also being computationally efficient, accurate and able to be applied to a very wide range of physical problems. This technique has been used for a variety of applications including reactor physics (Perkó et al., 2014; Cooling et al., 2013; Williams, 2012) and neutron transport (Fichtl, 2009; Fichtl and Prinja, 2011; Ayres et al., 2012; Williams and Eaton, 2010). This paper aims to determine the computational accuracy and efficiency of polynomial chaos methods when applied to uncertainty quantification in nuclear criticality problems. More specifically, this paper focusses on the determination of the uncertainty of the effective multiplication factor (k_{eff}) due to uncertainties in the microscopic neutron cross-sections.

The technique known as polynomial chaos was originally proposed by Wiener (1938). In this approach, a random process is expanded using Hermite polynomials in terms of Gaussian random variables. This work was later generalised by Xiu and Karniadakis (2002) who associated an optimal polynomial basis from the Askey scheme to the probability weight of the underlying random process. The statistics of the random process are calculated directly from the coefficients in the polynomial chaos expansion (PCE). The PCE coefficients can be determined using one of two ways. The first is the intrusive approach. Here the random process is replaced explicitly in the governing equations with a PCE. A Bubnov–Galerkin projection is then performed yielding a set of coupled equations for the coefficients, see Ghanem (1999) for a complete description. The second is the non-intrusive approach which is performed either by projection (Xiu, 2010) or regression (Berveiller et al., 2006). The non-intrusive approach is the method we adopt here since it requires no modification to existing modelling codes. In the non-intrusive approach the PCE is computed by strategically sampling the space of all the uncertain inputs in a similar manner to Monte Carlo approaches but at prescribed collocation points in stochastic space.

The number of polynomials, N_p, in a PCE depends upon the number of random dimensions, M, and the order of the polynomial expansion, p, as follows:

$$N_p + 1 = \frac{(M+p)!}{M!p!} \tag{1}$$

As we can see from Eq. (1), the number of terms increases rapidly with M and p. There are some techniques which *a-priori* reduce the number of terms N_p. One such method, known as a low rank set (Blatman, 2009), limits the number of multivariate polynomials in the expansion. i.e. only bi-variate or tri-variate polynomials

* Corresponding author.
E-mail address: d.ayres10@imperial.ac.uk (D. Ayres).

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would be admissible. This approach does not converge to the true model response as $p \to \infty$. For example, considering only bi-variate terms would exclude all tri-variate and higher interactions. Another method computes a so called hyperbolic set (Blatman, 2009). This approach restricts the polynomial order p to below a hyperbola which reduces the growth rate of N_p. As $p \to \infty$ the hyperbolic set converges to the true response. The success of both of these PCE construction methods relies upon prior knowledge of the random process. If the structure of the process is unknown, then these constructions may be inefficient.

As we have mentioned, it is the non-intrusive approach that we adopt in this work. More specifically, we will be using the projection based approach. Here the random process is projected onto each polynomial basis in order to calculate the expansion coefficients. This projection involves an M dimensional integral which is most commonly performed using a quadrature scheme. The immediate approach to building a multidimensional quadrature is to use a tensor product of one dimensional quadrature rules. However, this results in the computational effort increasing exponentially with M. This exponential dependence was alleviated to some extent by using a sparse grid construction method (Smolyak, 1963). However, this approach has no knowledge of the structure of the function being integrated and may ultimately be inefficient and/or inaccurate. The sparse grid construction was later generalised by Gerstner and Griebel (1998, 2003) and combined with an adaptive strategy which iteratively builds a set of integration points in multi-dimensions. This generalised construction optimally integrates a function and can be used to infer its structure. As such, it has been used by Gilli et al. (2013) to build a sparse polynomial chaos expansion. In this approach the structure of the function inferred by the adaptive quadrature scheme has been used to calculate the polynomial basis required for each dimension and between combinations of dimensions.

In the work by Gilli et al. (2013), the number of dimensions of each sub-grid in the sparse grid construction was increased iteratively until an error threshold was met. In this work we use an alternative but analogous procedure known as high dimensional model representation (HDMR) (Rahman and Xu, 2004; Xu and Rahman, 2004, 2005; Rabitz et al., 1999; Rabitz and Aliş, 1999; Chowdhury et al., 2009) to describe the multivariate interactions in the integrand. The HDMR method is used to capture high dimensional relationships between input and output model parameters using a hierarchical expansion of increasing dimension. If the cooperative effect of many input parameters upon the output is weak then the HDMR provides a very efficient representation of the system response allowing the integrand to be expressed using only low order component functions.

For some engineering applications (Rabitz and Aliş, 1999) it is stated that component functions of order 3 or greater are negligible but this is obviously problem dependent. To tailor the truncation of the HDMR expansion to specific problems, adaptive strategies have been used (Yang et al., 2012). The adaptive cut-HDMR expansion has also been used for problems with a discontinuous response function (Ma and Zabaras, 2010) where an adaptive sparse-grid quadrature method was used to compute the HDMR component functions. The adaptive quadrature method used a local hierarchical basis combined with the Smolyak algorithm. The statistical moments were calculated directly from quadrature hence the solution was not projected onto a polynomial chaos basis.

In summary, the objectives of this work are to use an adaptive HDMR technique to identify all of the important dimensions and interactions that contribute to the uncertainty in k_{eff}. The component functions in the HDMR expansion will be evaluated using an adaptive quadrature rule. This will in turn be used to indicate the order of polynomial basis required in the construction of a PCE. The aim of combining these three techniques is to build a sparse PCE in M dimensions that accurately represents the uncertainty in k_{eff} whilst minimising the number of model evaluations in the non-intrusive approach.

2. Description of the problem

In this work we are concerned with determining the uncertainty in the calculation of k_{eff} due to the presence of uncertainties in the input nuclear data. The calculation of k_{eff} involves the solution of an eigenvalue problem; the eigenvector in this case describes the distribution of neutrons in space, angle and energy. As such, appropriate discretisations of the space, angle and energy variables must be performed for the problem to be amenable to numerical solution. The energy variable is discretised using the multi-group technique (Lewis, 1993) and upon application of this, the eigenvalue problem for k_{eff} is written as (Hébert, 2009)

$$\begin{aligned}\boldsymbol{\Omega}\cdot\nabla\psi_g(\boldsymbol{r},\boldsymbol{\Omega})+\Sigma_{tg}(\boldsymbol{r})\psi_g(\boldsymbol{r},\boldsymbol{\Omega}) &= \int_{4\pi} d\boldsymbol{\Omega}'\sum_{h=1}^{N_G}\Sigma_{s;h\to g}(\boldsymbol{r},\boldsymbol{\Omega}'\to\boldsymbol{\Omega})\psi_h(\boldsymbol{r},\boldsymbol{\Omega}') \\ &+\frac{\chi_g}{4\pi k_{\text{eff}}}\int_{4\pi} d\boldsymbol{\Omega}'\sum_{h=1}^{N_G}\overline{\nu}\Sigma_{f,h}(\boldsymbol{r})\psi_h(\boldsymbol{r},\boldsymbol{\Omega}') \\ & g=1,N_G \end{aligned} \tag{2}$$

where

- $\boldsymbol{\Omega}$ is the direction of neutron travel.
- $\boldsymbol{r}$ the spatial position of the neutron.
- ψ_g is the angular neutron flux in group g.
- $\Sigma_{t,g}$ and $\Sigma_{f,g}$ are the total and fission macroscopic cross sections in group g respectively. $\Sigma_{s,h\to g}$ is the differential macroscopic scattering neutron cross section from group h into group g.
- $\overline{\nu}$ is the average number of neutrons produced per fission and is expressed by

$$\overline{\nu} = \overline{\nu}_p + \sum_i \overline{\nu}_{i,d}$$

  where $\overline{\nu}_p$ is the average number of prompt neutrons produced per fission and $\overline{\nu}_{i,d}$ is the average number of delayed neutrons from delayed precursor group i produced per fission.
- χ is the steady state fission spectrum and is expressed as

$$\chi = \left[1-\sum_i \beta_i\right]\chi_p + \sum_i \beta_i \chi_{i,d}$$

  where β_i is the fraction of fission neutrons emanating from delayed precursor group i, χ_p is the prompt neutron fission spectrum and $\chi_{i,d}$ is the delayed fission spectrum from precursor group i.

The deterministic nuclear criticality (k_{eff}) calculations have been performed using a code based upon the second-order even-parity form of the neutron transport equation. This code is called EVENT and employs a geometry conforming finite element discretisation of the spatial domain and rotationally invariant spherical harmonic basis for discretising the angular domain (de Oliveira, 1986).

To model the uncertainties present in the nuclear data, the variation is represented parametrically using a set of independent, identically distributed (IID) random variables $\boldsymbol{\xi}(\theta) = \{\xi_1(\theta), \xi_2(\theta), \ldots, \xi_M(\theta)\}$. Here θ is a random event belonging to the probability space of $\boldsymbol{\xi}$ and M is the total number of stochastic/random dimensions in the problem. In this work it is assumed that the uncertainties are in the microscopic neutron cross-section