

Performing uncertainty analysis of a nonlinear Point-Kinetics/Lumped Parameters problem using Polynomial Chaos techniques

L. Gilli^{*}, D. Lathouwers, J.L. Kloosterman, T.H.J.J. van der Hagen

Department of Physics of Nuclear Reactors, Delft University of Technology, Mekelweg 15, 2629JB Delft, The Netherlands

ARTICLE INFO

Article history:

Received 3 May 2011

Received in revised form 21 September 2011

Accepted 22 September 2011

Available online 5 November 2011

Keywords:

Uncertainty analysis

Spectral methods

Polynomial Chaos Expansion

Nonlinear time-dependent problems

ABSTRACT

Uncertainty analysis methodologies represent an important tool in the field of reactor physics with applications which span from the design phase to the safety analysis, as a support to “best estimate” models. A major source of uncertainty in reactor simulations is the input data set of the problem which is propagated, throughout the model, to the final simulation output. In this paper we perform such a propagation for a nonlinear point-kinetic model coupled to a lumped parameters system using a spectral technique, based on the Polynomial Chaos Expansion (PCE). We present two different ways to implement this technique, together with an overview of standard methods, and we apply them to a positive reactivity insertion transient. We show that for low-dimensional coupled problems PCE methods achieve the precision of Monte Carlo approaches at a significantly reduced computational cost.

© 2011 Elsevier Ltd. All rights reserved.

1. Introduction

The role of uncertainty analysis in nuclear reactor simulations is becoming increasingly important and challenging as their size and precision is constantly increasing. Moreover, regulations used in reactor licensing have begun to allow the “best estimate plus uncertainty” simulations approach, increasing the need for reliable and precise uncertainty analysis methodologies (NEA, 2008). There are different kinds of uncertainties to deal with, some of which are represented by approximations introduced by the model or by the numerical scheme used to solve it, however, one of the most important challenges in Uncertainty Analysis (UA) is to handle the uncertainty present in the input data of the problem (like the material properties or the geometric descriptions).

This corresponds to estimating how the lack of knowledge in the input data set influences the simulation outputs used in design and safety analysis. Many techniques have been implemented and used in the field so far, the main methods being statistical and deterministic. The main distinction between the two is that statistical methods are exact and require a large computational effort while deterministic methods rely on model approximations which make the technique faster compared to the first approach. A common way to propagate uncertainties using a deterministic approach is the application of first order perturbation techniques based on adjoint formulations. The computational effort required

to perform this propagation is relatively small and the accuracy in the prediction of the output uncertainty for small perturbations is good even for nonlinear problems (Cacuci, 2003).

Unfortunately within a safety analysis framework we are in presence of strong nonlinearities, and large (possibly) non-Gaussian input uncertainties often in range where the linear approximation introduced by perturbation methods would not hold anymore. In this paper we present the application of spectral techniques, based on the Polynomial Chaos Expansion introduced by Wiener (1938), to a coupled time-dependent model in order to propose an alternative to standard methodologies. PCE based techniques were first proposed by Ghanem and Spanos (1991) and have been applied so far to different scientific fields, ranging from Computational Fluid Dynamics problems (Najm, 2009; Mathelin et al., 2005) to structural mechanics (Ghanem and Spanos, 1997).

Two main PCE approaches, categorized as intrusive and non-intrusive, can be used to implement these spectral techniques. As the name suggests the main difference between the approaches is that with the former it is possible to use the original code as a “black box” while the latter involves the definition of a newly coupled problem which needs to be coded and solved. Within the reactor physics field the application of an intrusive PCE approach was first presented for a neutron diffusion problem by Williams (2007) and later applied to the transport equation in two studies (Williams, 2006; Eaton and Williams, 2010) for fixed source and eigenvalue problems. This concept has been also extended to spatially random problems and to non-intrusive methods by Fichtl (2009) while Roderick et al. (2010) presented the application of a

^{*} Corresponding author.

E-mail address: l.gilli@tudelft.nl (L. Gilli).

PCE based regression technique to a coupled steady-state problem. Regarding time-dependent problems the only application in the nuclear field was proposed by Hagues et al. (2010) where an intrusive stochastic method is applied to a radionuclide dispersion model. No application to time-dependent nonlinear problems has been presented so far.

In the present work we apply two PCE techniques, the Non-intrusive Spectral Projection (NISIP) and the Stochastic Galerkin (SG) formulation, to a coupled time-dependent problem described using a Point-Kinetics/Lumped-Parameters model. The implementation and the performance of the two techniques are discussed and compared to standard methodologies. The paper is structured as follows: first the model used to simplify the coupled physical problem is introduced, then an overview of the traditional UA techniques, together with an introduction to the two main methods to implement the PCE are presented. In the final part the results of the application of these techniques to a coupled time-dependent problem, describing a reactivity insertion transient, are discussed and compared.

2. Derivation of the coupled time-dependent problem

The problem considered for the application of the Uncertainty Quantification techniques introduced in the previous section is described by a system of a coupled Ordinary Differential Equations (ODE) modeling the time-dependent behavior of a simplified reactor. The model is derived using a point-kinetic approximation for the neutron population (Duderstadt and Hamilton, 1976) together with a lumped parameter description of the reactor temperatures. These assumptions allow the elimination of the spatial dependencies and therefore focus on the time-dependent part. The point-kinetic system is

$$\begin{aligned} \frac{dP}{dt} &= \frac{\rho(T_f, T_c, t) - \beta}{\Lambda} P + \sum_{k=1}^6 \lambda_k C_k \\ \frac{dC_k}{dt} &= -\lambda_k C_k + \frac{\beta_k}{\Lambda} P \end{aligned} \quad (1)$$

where P is the reactor power, Λ the mean generation time, C_k the concentration of the k th precursor group, β_k and λ_k the delayed neutrons fraction and the decay constant for the k th precursor group and β the total delayed neutrons fraction. The thermo-kinetics/thermal-hydraulics equations, needed to describe the removal of the heat by the coolant, are approximated using a lumped parameter model, i.e. averaging the unknown values over the whole domain. Assuming the reactor is divided into a fuel and a coolant region, their time-dependent average temperatures are described by the equations

$$\begin{aligned} M_f c_{pf} \frac{dT_f}{dt} &= P + Ah(T_c - T_f) \\ M_c c_{pc} \left[\frac{dT_c}{dt} + v \frac{T_c - T_{in}}{L} \right] &= Ah(T_f - T_c) \end{aligned}$$

where M_f and M_c are the fuel and coolant mass respectively, h the heat transfer coefficient, A the heat transfer surface, v the coolant flow velocity, L the channel length and T_{in} the inlet temperature of the coolant. The coupling between these two equations is given by the presence of the power production term P and by the time-dependent reactivity $\rho(t)$ in the point kinetic equation, defined as the contribution of three different terms

$$\rho(t) = \rho_{ext} + \alpha_D [T_f - T_f(0)] + \alpha_c [T_c - T_c(0)]$$

where ρ_{ext} represents an external reactivity insertion, α_D and α_c are the Doppler and the coolant reactivity coefficients respectively, and $T_f(0)$ and $T_c(0)$ are the initial system temperatures. We assume that the system starts from the following initial conditions

$$\begin{aligned} P(0) &= P_0 \\ C_k(0) &= \frac{\beta_k}{\lambda_k \Lambda} P_0 \\ T_f(0) &= T_c(0) + \frac{P_0}{Ah} \\ T_c(0) &= T_{in} + \frac{P_0 L}{M_c c_{pc} v} \end{aligned}$$

In order to present the different techniques that can be used to perform UA of the system hitherto discussed, it is useful to reformulate it using a more generic formulation. We reformulate the model as a generic system of ODEs defined as

$$\begin{aligned} \frac{d\mathbf{u}}{dt} &= \mathbf{L}(\boldsymbol{\alpha}, \mathbf{u}) \\ \mathbf{u}(0) &= \mathbf{U}_0 \end{aligned} \quad (2)$$

where \mathbf{L} is a nonlinear operator, \mathbf{u} the unknown solution of the problem, and $\boldsymbol{\alpha}$ the set of input parameters. In general, one may not only be interested in the solution of the previous system but also in a response $\mathbf{R}(\boldsymbol{\alpha}, \mathbf{u}, t)$ which can be described as a functional of the solution and the input parameter set. The first step required to propagate uncertainties throughout the model is the introduction of a random space $\theta = [\theta_1, \dots, \theta_N]$ which can be used to describe the stochastic component of the input parameter set, $\theta_1, \dots, \theta_N$ are independent random variables used to model the random input data $\boldsymbol{\alpha}(\theta)$. The introduction of this uncertainty in the input data set turns the deterministic output of the model (represented by the unknown system parameters and by the response) into a stochastic one, with the output quantities $\mathbf{u}(\theta)$ and $\mathbf{R}(\theta)$ depending on the same random variable set.

The propagation of uncertainties involves the determination of this dependency of the system outputs on the random space θ . Many methodologies can be applied to perform the task, in the next section a brief description of the two main approaches, Monte Carlo and Sensitivity Analysis, is given together with the introduction of the two main Polynomial Chaos Expansion techniques.

2.1. Standard uncertainty analysis methodologies

In this section we briefly describe the two main methodologies used in the reactor physics domain to perform UA, in order to compare them to the alternative spectral methods, which are as follows.

2.1.1. Monte Carlo (MC) methods

The main concept behind the Monte Carlo approach is quite straightforward: the random input data set is sampled M times until the statistical moments of the simulation output converge. The unbiased definition for the mean of a response \mathbf{R} is

$$\mathbf{E}(\mathbf{R}) = \frac{1}{M} \sum_{i=1}^M \mathbf{R}(\theta^i)$$

where θ^i is a single realization of the random input set. The unbiased variance is expressed by the equation

$$\sigma^2(\mathbf{R}) = \frac{1}{M-1} \sum_{i=1}^M \left(\mathbf{R}(\theta^i) - \mathbf{E}(\mathbf{R}) \right)^2$$

the statistical error associated with these moments is proportional to $(1/M)^{1/2}$. MC methods are relatively easy to implement and they do not require any modification of the original code used to calculate the output quantities. The use of the original mathematical model to calculate the statistical moments allows the consideration of physical phenomena that would be neglected using approximated

methods, an example of this aspect can be found in the work by Rochman et al. (2009).

Since the convergence of Monte Carlo techniques is rather slow, biasing techniques such as the stratified sampling or the Latin Hypercube (Helton and Davis, 2002) are often required.

2.1.2. Adjoint Sensitivity Analysis

The other common approach for UA is the propagation of first order uncertainty components by means of a perturbation analysis. The first order variation of the response can be expressed using a sensitivity coefficient defined as

$$S_k \equiv \frac{\alpha_k}{R} \frac{\delta R}{\delta \alpha_k}$$

after the sensitivity coefficient for each of the input variables is calculated the following expression can be used to obtain a first order estimation of the statistical moments

$$E(R) = R_0$$

$$\sigma^2(R) = \mathbf{S}^T \mathbf{C} \mathbf{S}$$

where R_0 is the response computed using the expectation value of each input parameter, \mathbf{S} is a vector containing the sensitivity coefficients and \mathbf{C} is the covariance matrix for the input parameter set (in the case of independent random variables, \mathbf{C} is a diagonal matrix containing the variance of each parameter). The Adjoint Sensitivity Analysis Procedure, derived by Cacuci (2003), allows the definition of the first order perturbation of a system response as follows:

$$\delta R \approx \frac{\partial R}{\partial \boldsymbol{\alpha}}(\boldsymbol{\alpha}_0, \mathbf{u}_0) \cdot \delta \boldsymbol{\alpha} + \int_0^{t_f} \mathbf{u}^*(t) \cdot \left[\frac{\partial L}{\partial \boldsymbol{\alpha}}(\boldsymbol{\alpha}_0, \mathbf{u}_0) \delta \boldsymbol{\alpha} \right] dt + \mathbf{u}^*(0) \cdot \delta \mathbf{U}_0$$

where $\boldsymbol{\alpha}_0$ and \mathbf{u}_0 are, respectively, the expectation of the input parameter set and the corresponding solution. The operators of the equation are obtained applying the Gateaux Derivative (GD) (Cacuci, 2003) to the original nonlinear problem while \mathbf{u}^* is defined as the solution of the adjoint problem

$$-\frac{d\mathbf{u}^*}{dt} - \left[\frac{\partial L}{\partial \mathbf{u}}(\boldsymbol{\alpha}_0, \mathbf{u}_0) \right]^T \mathbf{u}^* = \frac{\partial R}{\partial \mathbf{u}} \quad (3)$$

where the inhomogeneous term is the partial GD of the required response with respect to the solution. Due to their approximation, first order adjoint methods are very fast when large input data sets are present, requiring only the nonlinear reference solution and a single linear adjoint problem to be computed. This does not happen when a large number of responses is considered, since the adjoint problem has to be solved for each of them. This also means that for time dependent problems the application of adjoint techniques has to be localized to a limited number of instants since each of them requires the solution of Eq. (3) with a different response.

2.2. Spectral techniques

Spectral techniques are based on the approximation of the stochastic processes involved in the mathematical model by means of a spectral expansion in the random space. There are many ways to implement this expansion depending on the type of functions used: in the present work we apply a generalized Polynomial Chaos (gPC) Expansion defined using multidimensional orthogonal polynomials. Xiu and Karniadakis (2002) introduced a family of orthogonal polynomials, the Wiener–Askey scheme, that can be used to represent different stochastic processes. In their work, the authors shown that some polynomial are more suitable than others to represent a particular random distribution. Hermite polynomials, for example, are the best way to represent Gaussian random variables while Legendre are better for uniform distributions.

The first step to implement the gPC is the introduction of a set of identically distributed random variables $\boldsymbol{\xi} = [\xi_1, \dots, \xi_N]$, where N is the number of independent random variables needed to describe the input data set, these variables depend on θ and their distribution is defined by the polynomial basis used to describe the random processes. The main property of any polynomial family of the Wiener–Askey scheme is its orthogonality with respect to the following definition of the inner product:

$$\langle \Psi_n, \Psi_m \rangle = \int_{-\infty}^{+\infty} \Psi_n(\boldsymbol{\xi}) \Psi_m(\boldsymbol{\xi}) w(\boldsymbol{\xi}) d\boldsymbol{\xi} = h_n^2 \delta_{mn}$$

where w is a weight function (measure) which depends on the polynomial expansion used.

Once the polynomial family is chosen, it is possible to represent any stochastic quantity using a truncated expansion. For example the random input data set can be expanded as

$$\boldsymbol{\alpha}(\boldsymbol{\xi}) = \sum_{i=0}^P \boldsymbol{\alpha}_i \Psi_i(\boldsymbol{\xi})$$

where the number of terms P of the truncated expansion is given by the equation

$$P + 1 = \frac{(N + p)!}{N! p!}$$

where p is the highest polynomial degree used and N is the number of independent random variables. The other stochastic quantities involved in the problem (solution and responses) can also be represented using the same spectral expansion

$$\begin{aligned} R(\boldsymbol{\xi}) &= \sum_{i=0}^P r_i(t) \Psi_i(\boldsymbol{\xi}) \\ \mathbf{u}(\boldsymbol{\xi}) &= \sum_{i=0}^P \mathbf{u}_i(t) \Psi_i(\boldsymbol{\xi}) \end{aligned} \quad (4)$$

Applying spectral techniques means propagating the input coefficients α_i to the output sets \mathbf{u}_i or r_i . Once these approximated solutions are known it is possible to calculate (Le Maitre and Knio, 2010) the mean and standard deviation for the expansions as follows:

$$\mathbf{E}[R] = r_0 \quad (5)$$

for the mean and

$$\sigma[R] = \sqrt{\sum_{i=1}^P \langle \Psi_i, \Psi_i \rangle r_i^2} \quad (6)$$

for the variance.

Different techniques can be used to determine the coefficients of the solution expansions, the main distinction that can be made is between intrusive and non-intrusive approaches. In the subsequent paragraphs the two different techniques will be briefly introduced.

2.2.1. Non-intrusive Spectral Projection

The i th coefficient of the gPC expansion describing a system response can be calculated by projecting it on the respective polynomial

$$r_i = \frac{\langle R, \Psi_i \rangle}{\langle \Psi_i, \Psi_i \rangle} \quad (7)$$

The problem is that the response R is unknown and determining its behavior along each random direction would be a huge effort in terms of calculations required.

One may think of solving the numerator of Eq. (7) using a Monte Carlo technique, sampling the model until a statistical convergence is reached. In this way the code could be used as a “black box” to

determine the coefficients of the Chaos expansion, but the problem is that the computational cost would be the same as for a direct Monte Carlo sampling approach.

The deterministic alternative is, on the other hand, the introduction of numerical integration techniques as quadrature formulae. In the case of a one dimensional random problem, the numerator of Eq. (7) can be computed using the numerical approximation

$$\int R(\xi_1) w_1(\xi_1) d\xi_1 = \sum_{i=1}^{nq} w_i^1 R(\xi_1^i) = Q^1 R$$

ξ_1^i and w_i^1 are, respectively, the quadrature points and weights associated with the quadrature formula used. This means that the integral can be solved by “sampling” the output in the specific quadrature random locations, thereby reducing the computational effort with respect to a standard Monte Carlo integration. In case of a multidimensional random input the quadrature formula can be easily extended using a tensor product notation

$$Q^{(N)} R = \left(Q_1^1 \otimes \dots \otimes Q_N^1 \right) R = \sum_{i_1=1}^{n_{i_1}} \dots \sum_{i_N=1}^{n_{i_N}} R(\xi_1^{i_1}, \dots, \xi_N^{i_N}) w_{i_1}^1, \dots, w_{i_N}^1$$

where we assume that the same quadrature formula is used in each direction. Fig. 1 shows the quadrature map used in the present work for a two-dimensional problem. Rules to build quadrature formulae are provided with more details in reference (Le Maitre and Knio, 2010).

In general the method offers an optimal degree of exactness in the determination of the spectral projection we are looking for, however its main issue is given by the number of quadrature points required to achieve this accuracy. For tensor product formulae this number is equal to l^N , where l is the number of quadrature points in each direction and N the dimension of the random space. It is clear that for high dimensional problems the method would have a computational cost comparable or even larger than a standard Monte Carlo technique, making the approach less appealing. The problem is usually tackled using sparse grid constructions and nested quadrature in the random space which allow the reduction of the dimensionality of the problem drastically. Although we limit the present application to a low dimensional problem solved

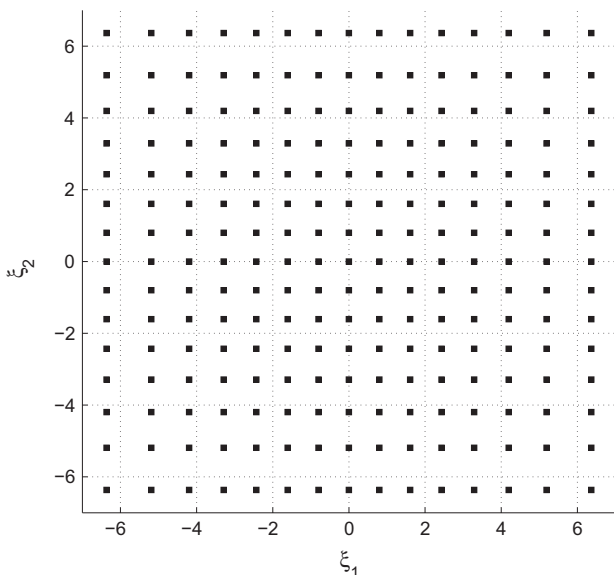


Fig. 1. Quadrature points for a two-dimensional tensor product formula, 15 quadrature points in each direction.

using a standard tensor product formula, the use of these techniques becomes necessary as soon as the random dimension increases.

2.2.2. Non-intrusive projection using first order information

As mentioned before, the first order sensitivity analysis can give accurate predictions at a very low computational cost. This happens when the dependency of the model output is linear with respect to the input parameters or when their variation is small. In these cases a first order perturbation technique would represent a very convenient way to perform uncertainty propagation.

Supposing we are in presence of a subset of input parameters for which the previous conditions are true, one may think of using a first order perturbative estimation to calculate the solution corresponding to the stochastic points required to build the spectral coefficients. In other words, we can calculate a subset of output values using a SA technique assuming that the output variation in the corresponding directions is linear. Which corresponds to using the following first order Taylor expansion, e.g. for the component ξ_2

$$R(\xi_1, \xi_2, \dots, \xi_N) \approx R(\xi_1, 0, \dots, \xi_N) + \frac{\partial R}{\partial \xi_2} \delta \xi_2 \quad (8)$$

NISP techniques define a strategy to choose the stochastic points needed to build the coefficients of the spectral expansion without specifying how these points are obtained, it is therefore possible to use a partially linearized model to reduce the number of full calculations performed.

The problem is that the behavior of the model output with respect to the input parameters is not known a priori, which means that we need a method to define the random directions that can be linearized. A preliminary criterion to decide if the influence of a random variable is linear can be based on its standard deviation magnitude, however a more detailed and deep analysis is needed. One way to deal with this issue could be derived from the definition of the Second Order Adjoint problem: as it has been shown in Williams (1986) with N further calculations one can determine the second order perturbation components of the system. This analysis has not been performed in the present work but the concept of partially linearized sampling is presented within the example section.

2.2.3. Stochastic Galerkin approach

The final approach we present, known as Stochastic Galerkin, provides an alternative way to obtain the coefficients of the spectral expansion, based on a direct projection of the model. Firstly, all the random quantities of the system described in Eq. (2) are replaced by their spectral expansion

$$\frac{d\left(\sum_{i=0}^P \mathbf{u}_i \Psi_i(\xi)\right)}{dt} = \mathbf{L} \left(\sum_{i=0}^P \alpha_i \Psi_i(\xi), \sum_{i=0}^P \mathbf{u}_i \Psi_i(\xi) \right) \quad (9)$$

In this way, taking the inner product of this system with respect to each polynomial of the expansion, it is possible to define a new system of ODEs for each unknown coefficient

$$\langle \Psi_j, \Psi_j \rangle \frac{du_j}{dt} = \left\langle \mathbf{L} \left(\sum_{i=0}^P \alpha_i \Psi_i, \sum_{i=0}^P \mathbf{u}_i \Psi_i \right), \Psi_j \right\rangle \quad (10)$$

the system of ODEs generated by this operation describes the coupling between P subsystems where each of them refers to the j th coefficient of the spectral expansion of the solution. In other words, determining the components of the spectral approximation requires the solution of a system P times larger than the original one. This dimension depends both on the number of random variables introduced and on the order of the polynomial approximation,

hence the solution may be problematic in presence of a large input data set.

Furthermore, a larger effort from the implementation point of view (compared to the other methods introduced so far) is required since a new differential problem has been defined. In general, using spectral expansions to represent the stochastic quantities in Eq. (9) introduces operations between summations: in case of linear problems these are simple products between the expansions used to approximate the random parameters and the ones representing the stochastic unknowns while for nonlinear problems more complicated forms could arise. For example, in presence of first order nonlinearities (as in Eq. (1)) the introduction of spectral expansions would generate for each nonlinear term a triple product between a stochastic input quantity and two stochastic unknowns.

The definition the Stochastic Galerkin problem of Eq. (10) means knowing how these terms are projected on each term of the polynomial basis. If we have the following double summation

$$\alpha(\xi)u(\xi) = \sum_{i=0}^P \sum_{j=0}^P \alpha_i u_j \Psi_i(\xi) \Psi_j(\xi) = f(\xi)$$

projecting it on the k th polynomial corresponds to performing the following operation:

$$f_k = \sum_{i=0}^P \sum_{j=0}^P \alpha_i u_j \mathbf{C}_{ijk} \quad (11)$$

where \mathbf{C}_{ijk} is a three dimensional tensor defined as

$$\mathbf{C}_{ijk} = \frac{\langle \Psi_i \Psi_j \Psi_k \rangle}{\langle \Psi_k \Psi_k \rangle}$$

In the same manner, it is possible to derive an expression for the triple product

$$[\alpha(\xi)u_1(\xi)u_2(\xi)]_m = \sum_{j,k,l=0}^P \mathbf{T}_{jklm} \alpha_j u_{1k} u_{2l} \quad (12)$$

where the four dimensional tensor

$$\mathbf{T}_{jklm} = \frac{\langle \Psi_j \Psi_k \Psi_l \Psi_m \rangle}{\langle \Psi_m \Psi_m \rangle}$$

is used. The tensors therefore define the coupling between the different stochastic coefficients of the PCE expansion. Using these forms, performing the projection for the system defined by Eq. (1) is relatively simpler. The detailed description about the definition of the Stochastic Galerkin problem for Eq. (1) has been included in Appendix A.

2.2.4. Comparison between the different approaches

The spectral techniques introduced so far can be regarded as one way to achieve the accuracy of Monte Carlo calculations in a deterministic fashion. But the computational cost required for the application of such methods increases rapidly with the dimension of the random problem, this drawback is usually known as the “curse of dimensionality” (Le Maitre and Knio, 2010).

The number of black box calculations required by NISP approach using a uniform tensor product quadrature is n^N , where N is the number of independent random variables used and n the number of quadrature points in each direction, on the other hand the Galerkin problem would be P times larger than the original, with P directly depending on the dimension and on the polynomial order used. This means that in the presence of 10 independent random variables a NISP would need around 1 million calculations using a 4 points quadrature rule while a fourth order Stochastic Galerkin would involve the definition and the solution of a

problem 1000 times larger than the original, in other words with the increase of the stochastic dimension both techniques become eventually computationally more expensive than Monte Carlo. The application of optimization procedures is therefore necessary to make spectral techniques attractive for more realistic models. From this point of view non-intrusive approaches offer a broader range of ways of reducing the number of calculations required. For example, the use of a sparse grid would reduce the computational requirements of the projection drastically.

3. Application to a reference transient

The techniques introduced so far have been applied to the coupled Point Kinetics/Lumped Parameters model (1) presented in the second section. The simplified model was used to analyze the time dependent behavior of a BN800 sodium fast reactor design described in the IAEA technical report (IAEA, 1994). The input data needed by the simplified model (collected in Table 1) were obtained using the ERANOS suite (Rimpault et al., 2002) for the neutronics parameters and using (Waltar and Reynolds, 1981) as a reference for the heat removal parameters.

The reference transient analyzed using the model is the response to a step reactivity insertion of 1\$. The uncertainty analysis around this reference solution has been performed considering two different stochastic problems.

- Case a: The first problem, where both reactivity coefficients (α_d and α_c) are stochastic, with a Relative Standard Deviation of 10% each.
- Case b: The second problem, where the inserted reactivity and the Doppler coefficient are stochastic (5% and 10% RSD respectively).

In both cases the random inputs are assumed to be Gaussian (using the data from Table 1 for their mean values) and independent. This kind of distribution has been chosen in order to compare the results with the outcome of the first order uncertainty propagation despite the fact that the infinite support of the distribution could in theory lead to the generation of “undesired” transients (corresponding to a change of sign of the external reactivity or feedback coefficients). However, due to the small standard deviation of the input quantities, all the realizations needed to build the quadrature formulae for the NISP and the coupling tensors for the SG were within the desired limits.

We limited the application to a two-dimensional random problem for the sake of simplicity, however the introduction of larger random spaces would be relatively easy to implement using the multidimensional polynomial derivation explained in Le Maitre and Knio (2010). The solution of the reference transient and the application of the UQ techniques has been performed using MATLAB and its built-in solvers. The Monte Carlo method has been implemented using unbiased sampling while the sensitivity coefficients have been obtained using the adjoint problem defined by Eq. (3).

Table 1
Parameter values and uncertainties used in the coupled model.

P (MW)	1800	λ (s)	4e-7
M_f (kg)	9675	M_c (kg)	1168
c_{pf} (J/kgK)	500	c_{pc} (J/kg K)	1200
Ah (kW/K)	2.5e+6	v (m/s)	7.5
α_d (pcm/K)	-0.687	%RSD(α_d)	10
α_c (pcm/K)	0.123	%RSD(α_c)	10
ρ_{ext} (\$)	1	%RSD(ρ)	5

In order to implement the NISP and the Stochastic Galerkin methods we used a gPC expansion based on two-dimensional Hermite polynomials. This expansion is the best choice in case of Gaussian processes since it can fully describe them within the first two terms. A fifth order polynomial expansion was used for both spectral techniques, this truncation order has been chosen in order to verify the convergence of the spectral expansion. The non-intrusive projection was obtained using a tensor product quadrature formula while the Galerkin problem derived for the intrusive approach is described in Appendix A.

3.1. Results and discussion

The results of the application of the different techniques introduced so far are presented in this section. The analysis was done for the transient described in the previous section considering the two different stochastic inputs *a* and *b*.

Figs. 2 and 3 show the time dependent mean values and the associated uncertainty bands (given by adding and subtracting the standard deviation) of the reactor power and the system temperatures for cases *a* and *b*. The solutions obtained using the two different spectral methods present in all cases a very small difference which can be expected since the two numerical approaches differ sensitively. The time-dependent behavior of the uncertainties associated with the system temperatures is similar for both

stochastic cases while the uncertainty on the power prediction reaches a sensitively higher maximum value for the case *b* (intuitively since there is an uncertainty on the reactivity introduced in the system which is the driving quantity of the transient). In this case the large magnitude of the standard deviation causes an irregular profile of the uncertainty band around the power peak. The first important thing to point out is that, since the probability density function of the output quantities can be nonsymmetric, the mean value does not correspond to the solution obtained using the expectation values of the input data, as we would assume while performing a first order uncertainty propagation. A second remark is that obtaining these plots with an adjoint sensitivity technique would require the solution of the adjoint problem at each instants that require the determination of the uncertainty, thus increasing the computational cost. On the contrary, this is much easier with Monte Carlo and PCE techniques since the evolution of the time-dependent behavior of the uncertainty is a direct outcome of the method. While adjoint methods should be applied to estimate the uncertainties for few time-localized responses, spectral methods can be used to determine the most sensitive points during a transient.

The choice of using a fifth order truncated spectral expansion has been made in order to perform a convergence analysis of the solution with respect to the polynomial approximation used. Fig. 4 shows the time dependent standard deviation of the power

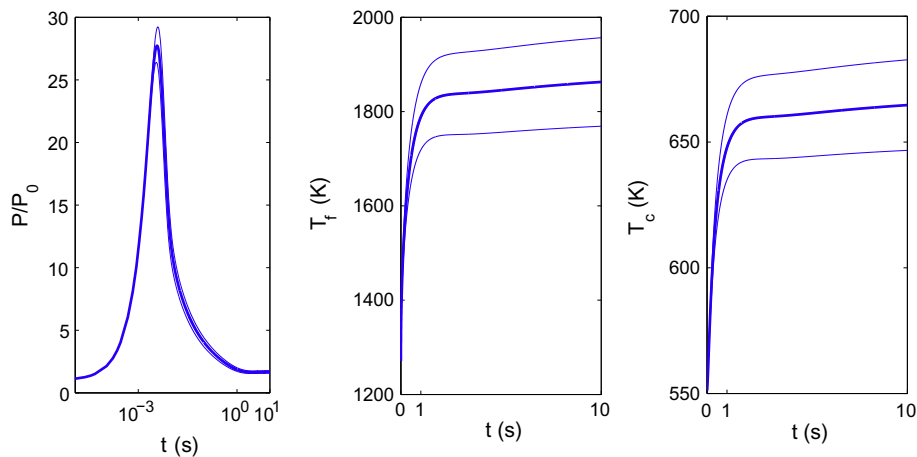


Fig. 2. Mean value and uncertainty bands caused by the uncertainty on the reactivity coefficients α_d and α_c (case *a*). Power plotted in a semi-logarithmic scale.

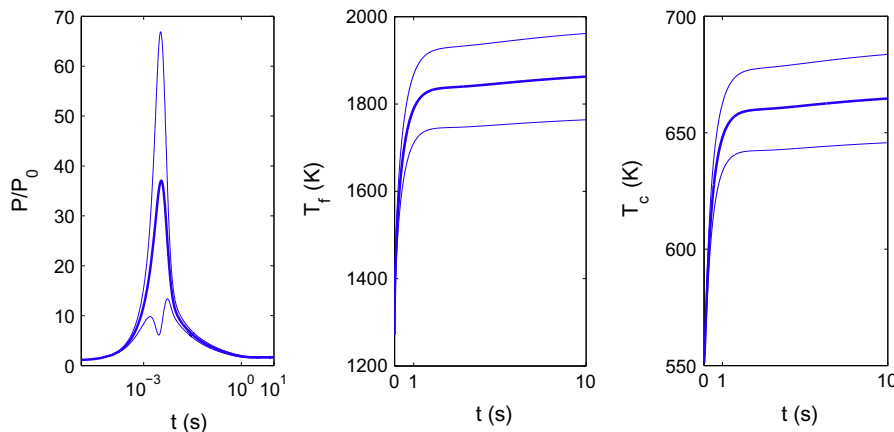


Fig. 3. Mean value and uncertainty bands caused by the uncertainty on the reactivity insertion ρ_{ext} and on the Doppler coefficient α_d (case *b*). Power plotted in a semi-logarithmic scale.

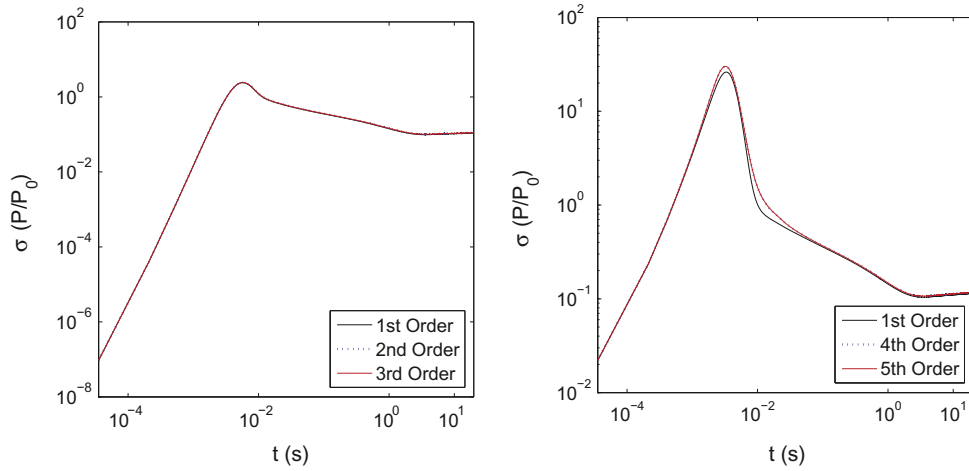


Fig. 4. Time-dependent standard deviation of the power for cases a (left) and b (right) calculated with different PCE truncation orders.

Table 2

Mean and standard deviations (obtained with different techniques) of the power and fuel temperature for the stochastic case a at two different instants ($t = 0.0034$ s and $t = 1$ s).

	P				T_f				N. Calc.
	$t = 0.0034$		$t = 1$		$t = 0.0034$		$t = 1$		
	E	σ	E	σ	E	σ	E	σ	
NISP(7)	26.4975	0.7948	1.8612	0.1458	1287.2526	0.2035	1788.8997	70.1142	49
NISP(15)	26.4975	0.7948	1.8612	0.1458	1287.2526	0.2035	1788.8997	70.1155	225
ASAP	26.4778	0.7931	1.8405	0.1134	1287.2400	0.2033	1779.5600	64.3146	1 + 2l
NISP + ASAP	26.4975	0.7948	1.8612	0.1457	1287.2526	0.2035	1788.8912	70.1150	7 + 2l
SG	26.4975	0.7948	1.8612	0.1457	1287.2526	0.2035	1788.8997	70.1156	1*
MC	26.4975	0.7948	1.8612	0.1458	1287.2532	0.2031	1788.8854	70.1163	10,000
	$\pm 5e-5$	$\pm 6e-5$	$\pm 2.5e-5$	$\pm 3.5e-5$	± 0.01	± 0.002	± 0.016	± 0.002	

for the stochastic cases a and b obtained using different expansion orders. As it can be observed from the figure, a second order expansion is enough to represent case a while a fourth order one is required to represent case b. It is also possible to see how a higher order expansion is necessary to calculate the standard deviation during the power peak, while when the solution relaxes due to the feedback mechanisms the discrepancy with respect to the first order approximation reduces considerably. This suggests that, for the problem analyzed, a lower order chaos expansion is suitable to represent random processes during the transient. It is known that spectral representations of time-dependent stochastic processes may be afflicted by convergence issues (Wan and Karniadakis, 2006) requiring an increasing number of polynomial terms for their accurate representation during the time-evolution. Different techniques to overcome this problem have been proposed and they generally require a more complicated implementation (Geritsma et al., 2010; Wan and Karniadakis, 2005).

However, in this particular example, the presence of feedback mechanisms causes the solution to grow relatively slowly during

the time interval following the power peak. For time-dependent problems reaching a steady state PCE techniques have been proved to converge even for long transient behaviors (Hagues et al., 2010) in this case the feedback nature of the problem and the relatively short time interval make the PCE to converge to an accurate solution. In general, this convergence needs to be confirmed for longer transients or for large scale system because it could represent one of the main obstacles for the application of PCE techniques to time-dependent problems.

Tables 2 and 3 contain the mean value and the uncertainty in the prediction of the power and the fuel temperature at two different instants: in the proximity of the power peak ($t = 0.0034$ s) and at $t = 1$ s, when the standard deviation of the fuel and the coolant temperatures starts to increase. Each table includes the results obtained with the two PCE techniques (NISP and SG) together with the values calculated using a standard Monte Carlo sampling and the ASAP method. The NISP technique has been applied using two different quadrature grids (7×7 and 15×15) while the row NISP + ASAP means that a partially linearized model has been used

Table 3

Mean and standard deviations (obtained with different techniques) of the power and fuel temperature for the stochastic case b at two different instants ($t = 0.0034$ s and $t = 1$ s).

	P				T_f				N. Calc.
	$t = 0.0034$		$t = 1$		$t = 0.0034$		$t = 1$		
	E	σ	E	σ	E	σ	E	σ	
NISP(7)	35.6535	29.5391	1.8603	0.1477	1290.6895	12.5270	1789.0554	78.6719	49
NISP(15)	35.6529	29.5293	1.8603	0.1477	1290.6895	12.5276	1789.0554	78.6731	225
ASAP	26.4778	18.0783	1.8405	0.1357	1287.2495	8.4011	1779.5634	72.7214	1 + 2l
NISP + ASAP	35.5562	29.0222	1.8396	0.1357	1290.6762	12.4670	1779.7154	72.7067	7 + 2l
SG	35.6531	29.5395	1.8603	0.1477	1290.6895	12.5271	1789.0553	78.6735	1*
MC	35.6571	29.5212	1.8603	0.1477	1290.6895	12.5276	1789.0501	78.6811	10,000
	± 0.004	± 0.01	$\pm 5e-5$	$\pm 4e-5$	$\pm 9e-2$	± 0.0025	± 0.018	± 0.015	

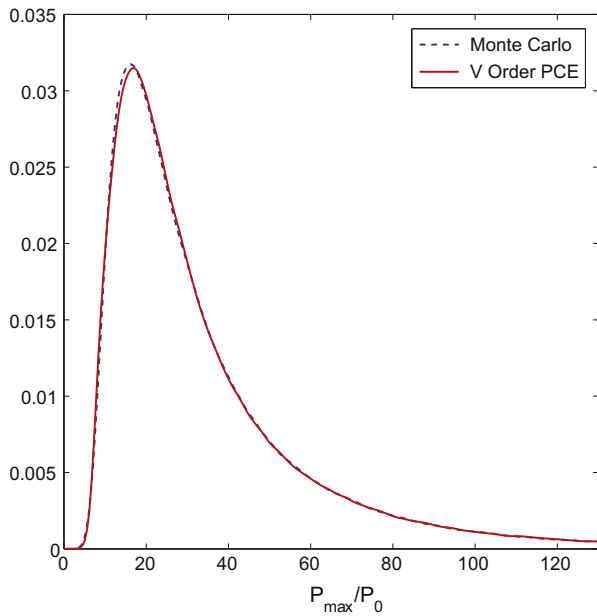


Fig. 5. Pdf for the peak power of case *b* between PCE (continuous) and Monte Carlo (dashed).

to calculate the output value on the quadrature points of the NISP (the linearized direction is α_c for the first case and α_D for the second). The right column contains the number of calculations needed to apply the method, the letter *l* means that the calculation is linear (2 linear calculations are needed to apply the ASAP technique, 1 for each of the responses considered) while the star (*) means that a system 20 times larger than the original one has been solved in order to apply the SG approach. The calculation of the standard deviation at $t = 1$ s needed approximately 10 s using the ASAP

technique, 29 s using the 7×7 NISP approach, 180s using the SG and 1.5 h using the unbiased Monte Carlo sampling.

As the results show, implementing the NISP using a 7 points quadrature instead of a 15 points leads to no numerical difference in the uncertainty for case *a* while a small error is present in case *b*. In presence of Gaussian profiles, quadrature rules need few points to approximate integrals with a larger accuracy. If a large number of points is needed to reduce the projection error (as for case *b*) it means that the probability distributions are nonregular.

The values obtained with both spectral techniques compare very well to the Monte Carlo estimations, the first methods being much faster due to the small number of random parameters. This agreement can be also verified for the probability density functions of the problem, for example Fig. 5 shows the pdf associated to the power at $t = 0.0034$ s, obtained with the PCE approach and with a standard Monte Carlo sampling. It is apparent to see how the shape of this pdf is far from the Gaussian distribution (in other words it requires more terms for its spectral representation) which is the shape assumed by first order propagation techniques. The tables show how, in fact, the first order approximation gives a considerable error in the prediction of many of the responses considered. The main reason for this is the large input uncertainty which places the problem in the region where the linear assumption ceases to be valid. Nevertheless, for case *a* many results present, compared to the other techniques, a good degree of accuracy. In these cases the adjoint technique would be the best choice from a computational point of view, being the fastest of the group. However, as it can be seen in Table 3, the method largely fails to predict some values for the second case, in particular the uncertainty on the peak power. This discrepancy is shown in Fig. 6 where the probability density functions (for case *b*) obtained using the NISP approach are compared with the Gaussian prediction resulting from the adjoint method. This example clearly shows how in some cases the first order approximation is not suitable to perform UA and how PCE techniques are able to rebuild this stochastic information

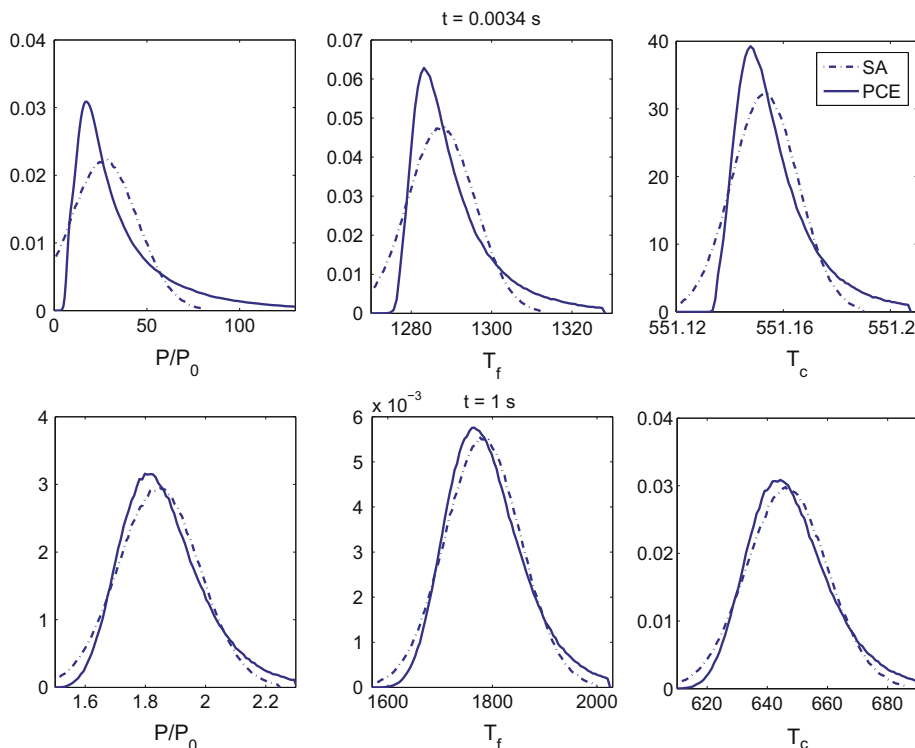


Fig. 6. Comparison of the pdfs associated to the system unknowns for the case *b* obtained with a PCE expansion (continuous line) and with a first order adjoint technique (dashed line).

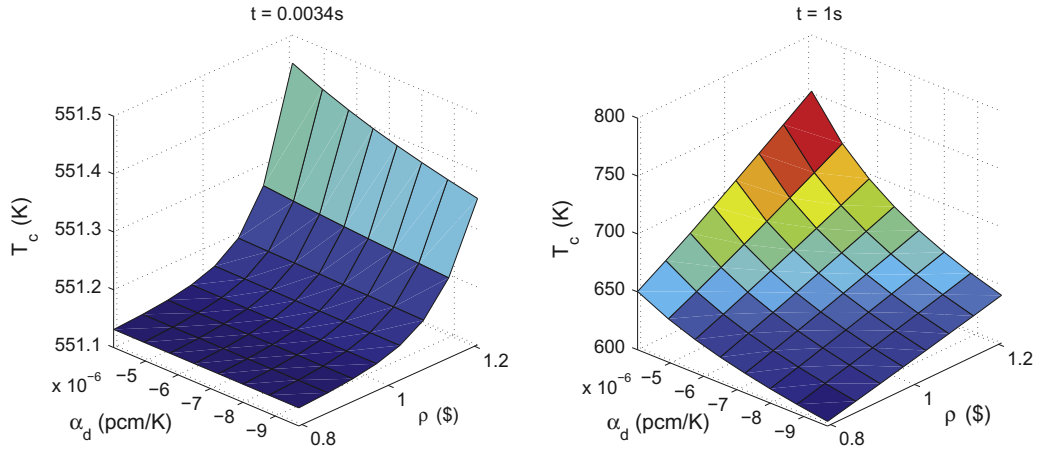


Fig. 7. System response (Coolant temperature at $t = 0.0034$ s and $t = 1$ s, case b) in the two-dimensional random space.

in a deterministic way. This type of probability density profile could have important consequences from a probabilistic risk assessment point of view. In our example the probability density function for the fuel temperature has a tail toward higher values which means that the probability of it being higher than a safety limit we may be interested in (ex. melt down temperature) is larger than the one calculated using a Gaussian distribution.

One last remark is about the results obtained using a NISP method with a partially linearized model. The row NISP + ASAP in the tables shows that if a partially linearized model is used to linearize the dependency with respect to the coolant coefficient for case a and the Doppler coefficient for case b , the results obtained are, in most of the cases, very similar to the results of the two-dimensional projection. The only case where the prediction suffers from the partial linearization is for case b at $t = 1$ s, where the statistical moments are closer to the ones obtained with the ASAP technique. The reason can be understood from Fig. 7 where the response surface for the coolant temperature has been plotted for case b at the two different instants considered: at $t = 0.0034$ s the behavior along the Doppler direction is almost linear and we can therefore approximate it by using the first order information obtained from sensitivity analysis while at $t = 1$ s the first order approximation is not good enough to approximate the model without losing important information.

In theory, first order techniques could be carefully used to apply the NISP in presence of high dimensional random problems, reducing the number of sampled points and therefore the computational cost. That would require an “a priori” knowledge of the time dependent response behavior with respect to the input parameters, an aspect which would need further investigation.

4. Conclusion and future work

In this paper we propose the application of spectral techniques as an alternative method for Uncertainty Quantification of time-dependent multi-physics problems. Two different approaches have been introduced: the Non-intrusive Spectral Projection and the Stochastic Galerkin, which are both based on the definition of the Polynomial Chaos Expansion. The methods have been applied to a simplified coupled problem, a Point-Kinetics/Lumped Parameters system, and their outcomes have been analyzed and compared to the values obtained with an exact Monte Carlo sampling and with a first order adjoint technique.

For the example considered, Polynomial Chaos techniques proved to converge to an accurate solution during the whole transient, achieving the precision of direct sampling at a reduced

computational effort. Although in many cases the prediction provided by first order approximations is rather good, there are situations in which the linearization neglects important phenomena that can lead to nonconservative estimations in safety analysis. However, in presence of a large set of random input variables the number of computations needed by spectral methods increases, becoming even larger than Monte Carlo techniques: hence optimization techniques have to be used.

Intrusive and non-intrusive projections lead to the same results but require a completely different implementation: the main difficulty for intrusive methods is that a large coding effort is required when Non-intrusive Spectral Projection techniques rely only on the definition of the sampling points in the random space. The immediate consequence is that, unlike the Stochastic Galerkin formulation, the extension of Non-intrusive Spectral Projection to large scale problems is straightforward, i.e. once the quadrature points are chosen we can use any “black box” code for the calculation of their values. The relative simplicity and the potential improvability of Non-intrusive Spectral Projection methods prompts us to continue our work in this direction, with the implementation of adaptive sparse grid quadratures techniques and the development of a partially linearized scheme in order to reduce the overall computational requirements.

Acknowledgements

The authors acknowledge the Nuclear Research and consultancy Group (Petten, the Netherlands) for their financial support.

Appendix A. Stochastic Galerkin problem for the nonlinear point-kinetic model

First we approximate the stochastic input quantities using the following spectral expansions:

$$\rho_{ext} = \sum_{i=0}^1 \rho_{ext}^i \Psi_i(\xi)$$

$$\alpha_D = \sum_{i=0}^1 \alpha_D^i \Psi_i(\xi)$$

$$\alpha_C = \sum_{i=0}^1 \alpha_C^i \Psi_i(\xi)$$

where the sum is truncated to 1 assuming that the quantities are Gaussian and that we are using Hermite polynomials. The same is done for the stochastic unknowns

$$P = \sum_{i=0}^P P_i \Psi_i(\xi)$$

$$C_k = \sum_{i=0}^P C_{k,i} \Psi_i(\xi)$$

$$T_f = \sum_{i=0}^P T_{f,i} \Psi_i(\xi)$$

$$T_c = \sum_{i=0}^P T_{c,i} \Psi_i(\xi)$$

the implementation of the Stochastic Galerkin formulation is done by substituting these expansions in Eq. (1) and projecting the resulting system on the p th polynomial of the basis. The first complication arises from the product between the stochastic external reactivity and the power

$$\rho_{\text{ext}} P = \sum_{i=0}^1 \sum_{j=0}^P \rho_{\text{ext}}^i P_j \Psi_i(\xi) \Psi_j(\xi)$$

the projection on the p th polynomial of this expression is, using Eq. (11),

$$(\rho_{\text{ext}} P)_p = \sum_{i=1}^P \sum_{j=0}^P \rho_{\text{ext}}^i P_j \mathbf{C}_{ijp}$$

where we used the three dimensional tensor \mathbf{C}_{jlp} introduced before. Similarly we can project the nonlinear reactivity feedback term using the four dimensional tensor \mathbf{T}_{jklp} as

$$(\alpha_d T_f P)_p = \sum_{j=0}^1 \sum_{k,l=0}^P T_{jklp} \alpha_d^j T_{fk} P_l$$

the tensors \mathbf{C}_{jlp} and \mathbf{T}_{jklp} define the coupling between each of the coefficients of the spectral expansion. After some small manipulation, the final stochastic system can be written as

$$\frac{dP_p}{dt} = \sum_{j=0}^1 \sum_{l=0}^P \mathbf{C}_{jlp} \left[\frac{\rho_{\text{ext}}^j - \alpha_d^j T_f(0) - \alpha_c^j T_c(0)}{\Lambda} \right] P_p + \sum_{k=1}^6 \left[\frac{\beta}{\Lambda} P_p + \lambda_k C_{k,p} \right]$$

$$+ \sum_{j=0}^1 \sum_{l=0}^P \sum_{k=0}^P \mathbf{T}_{jklp} \left[\frac{\alpha_d^j}{\Lambda} T_{f,l} P_k + \frac{\alpha_c^j}{\Lambda} T_{c,l} P_k \right]$$

$$\frac{dC_{k,p}}{dt} = \left[\frac{\beta_k}{\Lambda} P_p - \lambda_k C_{k,p} \right]$$

$$M_f C_{pf} \frac{dT_{f,p}}{dt} = P + Ah(T_{c,p} - T_{f,p})$$

$$M_c C_{pc} \left[\frac{dT_{c,p}}{dt} + \nu \frac{T_c - T_{in}}{L} \right] = Ah(T_{f,p} - T_{c,p})$$

If we assume the initial conditions to be deterministic we will have the same initial value as (1) for $p = 0$ and zero initial amplitude for

the rest of the coefficients. On the other side, in case of stochastic initial conditions the initial value for each coefficient p needs to be evaluated by performing the usual projection.

References

- Cacuci, D.G., 2003. Sensitivity and Uncertainty Analysis, Theory, vol. 1. Chapman and Hall, CRC.
- Duderstadt, J.J., Hamilton, L.J., 1976. Nuclear Reactor Analysis. John Wiley and Sons.
- Eaton, M.D., Williams, M.M.R., 2010. A probabilistic study of the influence of parameter uncertainty on solutions of the neutron transport equation. Progress in Nuclear Energy 52, 580–588.
- Fichtl, E.D., 2009. Stochastic Methods for Uncertainty Quantification in Radiation Transport. PhD Thesis, University of New Mexico.
- Geritsma, M., van der Steen, J.B., Vos, P., Karniadakis, G., 2010. Time dependent generalized polynomial chaos. Journal of Computational Physics 229 (22), 8333–8363.
- Ghanem, R.G., Spanos, P.D., 1991. Stochastic Finite Elements: a Spectral Approach. Dover Publications.
- Ghanem, R.G., Spanos, P.D., 1997. Spectral techniques for stochastic finite elements. Archives of Computational Methods in Engineering 4, 63–100.
- Hagues, A.W., Williams, M.M.R., Eaton, M.D., 2010. A probabilistic study of the effect of retardation factor uncertainty using a compartment model for radionuclide release into the biosphere. Annals of Nuclear Energy 37, 1197–1207.
- Helton, J.C., Davis, F.J., 2002. Latin Hypercube Sampling and the Propagation of Uncertainty in Analyses of Complex Systems. Technical Report SAND2001-0417, Sandia National Laboratories.
- IAEA, 1994. Evaluation of Benchmark Calculations on a Fast Power Reactor Core with Near Zero Sodium Void Effect. Technical Report IAEA-TECDOC-731, IAEA.
- Le Maitre, O.P., Knio, O.M., 2010. Spectral Methods for Uncertainty Quantification. Springer.
- Mathelin, L., Hussaini, M., Zang, T., 2005. Stochastic approaches to uncertainty quantification in CFD simulations. Numerical Algorithms 38, 209–236.
- Najm, H.N., 2009. Uncertainty quantification and polynomial chaos techniques in computational fluid dynamics. Annual Review of Fluid Mechanics 41, 35–52.
- NEA, 2008. Uncertainty and target accuracy assessment for innovative systems using recent covariance data evaluations. OECD-NEA.
- Rimpault, G., Plisson, D., Tommasi, J., Jacqmin, R., 2002. The eranos code and data system for fast reactor neutronic analyses. In: Proceedings of the 2002 PHYSOR conference.
- Rochman, D., Koning, A., van der Marck, S., 2009. Uncertainties for criticality-safety benchmarks and keff distributions. Annals of Nuclear Energy 36, 810–831.
- Roderick, O., Animescu, M., Fischer, P., 2010. Polynomial regression approaches using derivative information for uncertainty quantification. Nuclear Science and Engineering 164, 122–139.
- Waltar, A., Reynolds, A., 1981. Fast Breeder Reactors. Pergamon Press.
- Wan, X., Karniadakis, G.E., 2005. An adaptive multi-element generalized polynomial chaos method for stochastic differential equations. Journal of Computational Physics 209 (2), 617–642.
- Wan, X., Karniadakis, G.E., 2006. Long term behavior of polynomial chaos in stochastic flow simulations. Computational Methods in Applied Mechanical Engineering 195 (41–43), 5582–5596.
- Wiener, N., 1938. The homogeneous chaos. American Journal of Mathematics 60, 897–936.
- Williams, M.L., 1986. CRC Handbook for Nuclear Reactors Calculations, Perturbation Theory for Nuclear Reactor Analysis, vol. III. CRC Press.
- Williams, M.M.R., 2006. Polynomial chaos functions and stochastic differential equations. Annals of Nuclear Energy 33, 774–785.
- Williams, M.M.R., 2007. Polynomial chaos functions and neutron diffusion. Nuclear Science and Engineering 155, 109–118.
- Xiu, D., Karniadakis, G.E., 2002. The Wiener–Askey polynomial chaos for stochastic differential equations. SIAM Journal on Scientific Computing 24, 619–644.