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| Implementation of Stochastic Polynomials Approach in the RAVEN Code |
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# INTRODUCTION

## RAVEN for Uncertainty Quantification

RAVEN, under the support of the Nuclear Energy Advanced Modeling and Simulation (NEAMS) [1] program, have been tasked to provide the necessary software and algorithmic tools to enable the application of the conceptual framework developed by the Risk Informed Safety Margin Characterization (RISMC) [2] path. RISMC is one of the paths defined under the Light Water Reactor Sustainability (LWRS) DOE program [3].

One of the most challenging requests of the RISMC framework is a holistic estimation of margins, and therefore uncertainties, in nuclear power plants (NPPs) system analysis. Those estimations, in conjunction with more accurate simulation tools, should enable an optimization process leading to safer and more economical competitive nuclear power plants.

The improvement of the accuracy of the simulations is tasked to other DOE projects like RELAP-7 [] while margin quantification and the generation of information suitable to perform safety margin managements is assigned to RAVEN.

How the uncertainty presents in the input parameters, used to build the mathematical representation of the NPP system, impacts the simulation results (uncertainty propagation) is clearly a fundamental step of the process. The uncertainty propagation analysis is a complex process and several methodologies are currently used. Clearly before deploying innovative algorithms base capabilities needs to be implemented and tested. This is the current stage of the RAVEN development project.

Earlier reports explain the implementation in RAVEN of Monte Carlo [] sampling methodologies, and also dynamic event trees []. Next step of this approaching strategy is here described and involves the implementation of the infrastructure to support the generalized Polynomial Chaos [] methodology for uncertainty propagation.

The report will cover the following subject, introduction of the generalized Stochastic Polynomial approach, description of the software implementation, and comparative analysis of clad failure probability between Monte Carlo and generalized Polynomial Chaos (gPC), in a Pressurized Water Reactor (PWR) following Station Black Out (SBO) condition.

# Generalized Polynomial Chaos

## Generalized Polynomial Chaos by Orthonormal Expansion

### Mono Variate expansion

In general any response monitored of the plant (clad temperature, max pressure etc.) **U** at a given point in time could be represented as a function of the initial condition of the plant and of the values of the parameters used to construct the mathematical models. For our purpose lets’ consider a split of the input and parameter space such as and are respectively the initial condition and parameters not subjected to a probabilistic distribution while are. The dependence of from could be therefore neglected since not relevant to the discussion, it will follow.

Next, we introduce the Lebesgue space equipped with measure (for simplicity for the moment we assume a one dimensional problem ),

being S the support of the measure, the scalar product in such space is therefore:

or under the assumption that the measure admit a density function

Now, if is a complete function basis on the Fourier theorem ensure that the series

is convergent in the norm, if the moment of the series are defined as it follows:

If is an orthonormal base in we have:

and verifying the coherence of the formulation is immediate by:

To reformulate the problem in space with standard measure it is sufficient to replace with , where:

Clearly the orthonormal property of over translate in the orthonormal property for over

The introduction of the space founds its utility when the measure is defined such as its density function is the square of the probability distribution function of ().

In this case the expected value of has an immediate formulation with respect the term of the Fourier series:

Where it has been used the property:

One of the most used cased and actually the first application of this methodology refers to the case where the is the normal distribution. For this special case the are the Hermite polynomials given by:

Table : Expression for the first 3 orders of Hermite polynomials

|  |  |  |
| --- | --- | --- |
| Order |  |  |
| 0 |  |  |
| 1 |  |  |
| 2 |  |  |
| 3 |  |  |

Table : Correspondence between density function and integrating orthogonal polynomials

|  |  |  |  |
| --- | --- | --- | --- |
| Distribution | pdf | Polynomials | Support |
| Uniform |  | Legendre | [−1 : 1] |
| Normal |  | Hermite | [−∞ : ∞] |
| Exponential |  | Laguerre | [0 : ∞] |
| Beta |  | Jacobi | [−1 : 1] |

### Multi Dimensional Case

The extension to the multi dimensional case has no special complication if care is used in merging the different density functions. As in the mono-dimensional case we can introduce the following Lesbeque space:

If to obtain the expansion of we define first the multi dimensional polynomial base using vector indexing: so that:

where the polynomial have been already assumed to be orthonormal. Than the expansion series is therefore similarly to what found in the one-dimensional case:

in the norm

in the standard norm

It is interesting to spend few words in the multidimensional case about the implication that the structure of the measure has on the choices for the expansion base.

Many times the probability distributions of the input parameters are uncorrelated and therefore, if we impose that the density function of the measure is the Cumulative Distribution Function of those random variates, it follows that the density function is (completely) multiplicatively separable (completeness is true if all the input variable are uncorrelated). For completely multiplicatively separable density function the construction of the orthonormal base in the multidimensional space with respect the standard measure is straightforward:

Another interesting discriminant for approaching the construction of the orthonormal polynomial base is provided by the existence of a vector sub space such as the directional derivative of the density function is equal zero whatever . If such a linear space exists than the effective dimensionality of the input space could be reduced and the study of the function could be performed in a reduce space. For this moment this condition will not be investigated further but it could be very useful when the input space is representative of a physical field. In this case it is possible that the dimension of the is rather large but strongly correlated (large dimension of ) and therefore reducing the effort required to represent the original function is advantageous and useful.

## Numerical approximation of Generalized Polynomial Chaos by Orthonormal Expansion

The first step toward achieving a numerical approximation of the stochastic expansion of the is introducing a finite expansion approximation over the orthonormal polynomial base. If is the maximum polynomial order over the variable than, first the cardinality of is and second the function could be approximated by:

in the norm

in the standard norm

For simplicity we can assume that the density function is completely multiplicatively separable. This simplification does not affect the substance of the following derivation since this condition is achievable by an truncated development over a proper base on or a suitable variable change.

In this case:

Moreover we can rewrite as it follows:

Where:

and

Once that a proper finite polynomial representation has been chosen to represent the the main task is the calculation of the . Two approaches could be followed, one relays on a projection of the equation set representing the system of which is solution on , usually this leads to an hierarchal system of equation where the unknown are the , the second approach seeks a numerical solution of the integral representing the by the knowledge of for specific point of the input domain . The second methodology is the one currently implemented in RAVEN since it does not require the alteration of the software solving for that in our case is the RELAP-7 code. Given that this second methodology relays on the knowledge of the only on selected points is named Collocation Generalized Polynomial Chaos [].

Of course the choice of the point where the function is evaluated could be optimized to minimize the number of point while maximizing the order of the polynomial representation achievable. This is of course obtained by the Gauss integration rule pertinent to the orthonormal polynomial set under consideration. In general, using the Gauss integration ‘p’ points will integrate exactly a polynomial of order n=2p-1. It is important to recognize that the integrand that appears in the definition of is of degree , in fact:

Where the integrand of highest degree is of course . This imply that to achieve an overall accuracy of degree it is necessary a minimum number of point that satisfy .

## 2D Application Example

It is useful to illustrate an application to a 2D dimensional case to provide a hands on view of the methodology.

Lets consider

The orthonormal polynomial are not ready available but in literature are provided for standardized and support from which it is possible to derive the one needed in this case.

First we introduce the following change of coordinate

The new orthonormal polynomial sets are therefore defined by:

is therefore orthonormal over with density function or is orthonormal over with the standard measure.

is therefore orthonormal over with density function or is orthonormal over with the standard measure.

Now that the new orthonormal polynomials have been defined the development of could be written as:

where:

The last step is the implementation of the Gauss integration rule. Finding the Gauss point and weights it is a costly and not trivial task therefore it is useful to use external libraries, RAVEN uses the special function module of numpy []. This library provides the points and weights for standardized weighting function and support. In this particularly case it is provided and that satisfy:

Now we can try to recast the quadrature in a more convenient form using the following change of coordinate:

we pose

using the quadrature rule:

For the Legendre based quadrature:

Posing

from the quadrature rule:

Replacing both expression in the original expansion:

compute hat perform such task. In our caseOnce more gauss rule are provided for standard function and domain. In the case of the statistical Hermite function the known relation is provided for