|  |
| --- |
| INL/EXT-XXXXXXX  Revision: 0 |
| Implementation of Stochastic Polynomials Approach in the RAVEN Code |
|  |
| Cristian Rabiti  Paul Talbot  Andrea Alfonsi  Diego Mandelli  Joshua Cogliati |
| October 2013 |

**Disclaimer**

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the u.s. government nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness, of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trade mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. government or any agency thereof.

CONTENTS

1. INTRODUCTION 3

1.1 RAVEN for Uncertainty Quantification 3

2. Generalized Polynomial Chaos 3

2.1 Generalized Polynomial Chaos by Orthonormal Expansion 3

2.1.1 Mono-Dimensional Case 3

2.1.2 Multi-Dimensional Case 5

2.2 Numerical approximation of Generalized Polynomial Chaos by Orthonormal Expansion 7

2.3 2D Application Example 8

2.3.1 From the standard to the actual reference system 8

2.3.2 Numerical evaluation of the moment integrals 11

2.3.3 Final numerical form 13

2.3.4 Mean Values 14

3. Appendixes 15

3.1 Appendix 1: Orthonormal test of the Hermite Polynomial in the actual system 15

3.2 Appendix 2: Test of the translation rule for the Gauss Hermite quadrature 16

FIGURES

**No table of figures entries found.**  
In your document, select the words to include in the table of contents, and then on the Home tab, under Styles, click a heading style. Repeat for each heading that you want to include, and then insert the table of contents in your document. To manually create a table of contents, on the Document Elements tab, under Table of Contents, point to a style and then click the down arrow button. Click one of the styles under Manual Table of Contents, and then type the entries manually.

TABLES

**No table of figures entries found.**  
In your document, select the words to include in the table of contents, and then on the Home tab, under Styles, click a heading style. Repeat for each heading that you want to include, and then insert the table of contents in your document. To manually create a table of contents, on the Document Elements tab, under Table of Contents, point to a style and then click the down arrow button. Click one of the styles under Manual Table of Contents, and then type the entries manually.

# 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 algorithms 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 of the input parameters 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. Before deploying innovative algorithms, base capabilities need to be implemented and tested. This is the current stage of the RAVEN development project.

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

The report will cover the following subjects: introduction of the generalized Stochastic Polynomial approach, exemplification of the approach in a bi-dimensional case, results of the implementation tests and a direct comparison toward a Monte Carlo approach for the estimation of the maximum fuel temperature in an simplified Station Black Out (SBO) PWR accident scenario.

# Generalized Polynomial Chaos

## Generalized Polynomial Chaos by Orthonormal Expansion

### Mono-Dimensional Case

There is a large amount of literature on stochastic polynomials and a good starting point is given in [], here a brief introduction is reported to move later more in detail. In general any response **U** monitored of the plant (clad temperature, max pressure etc.) 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 let us consider a split of the input and parameter space such that are the initial conditions and parameters not subjected to a probabilistic distribution while are the ones showing such stochastic behavior. The dependence of from could be therefore neglected since the dependence is not relevant to the discussion:

Eq. 2‑1

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

Eq. 2‑2

with S being the support of the measure. The scalar product in such space is therefore:

Eq. 2‑3

or under the assumption that the measure admits a density function

Eq. 2‑4

Now, if is a complete function basis on , the Fourier theorem ensures that the equality

Eq. 2‑5

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

Eq. 2‑6

If is an orthonormal base in we have:

Eq. 2‑7

and in fact:

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

Eq. 2‑8

Eq. 2‑9

Clearly the orthonormal property of over translates in the orthonormal property for over . The introduction of the space found its utility when the measure is defined as:

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

Eq. 2‑10

where these properties are used:

Eq. 2‑11

With as the normalization constant for the polynomial of order 0 where S=.

In

Table 1 the most common distribution functions are paired with their respective orthonormal polynomials.

Table 1: Correspondence between density function and orthogonal polynomials

|  |  |  |  |
| --- | --- | --- | --- |
| *Distribution* | *Probability Distribution Function* | *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 Lebesgue space:

Eq. 2‑12

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

Eq. 2‑13

Eq. 2‑14

Eq. 2‑15

Eq. 2‑16

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

in the norm

in the standard norm

It is interesting to spend few words on 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, of course, 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:

Eq. 2‑17

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 whenever . 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 reduced space. For this report 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 possible and highly advantageous.

## 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 the cardinality of is and the function could be approximated by:

in the norm

in the standard norm

Eq. 2‑18

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 always achievable by a truncated development over a proper base on or a suitable variable change. The definition of the moment rests unaltered from Eq. 2‑17.

Moreover we can rewrite as follows:

Eq. 2‑19

Where:

Eq. 2‑20

Once that a proper finite polynomial representation has been chosen to represent , the main task is the calculation of . Two approaches could be followed; one relies 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 relies 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 points, 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:

Eq. 2‑21

where the integrand of highest degree is of course . This implies that to achieve an overall accuracy of degree it is necessary a minimum number of points 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 a system response mapped as a function of two random variates and, moreover let us assume it is completely multiplicative separable, so that . The corresponding probability density and density and measure of the support in the corresponding metrics are provided below:

|  |  |
| --- | --- |
|  |  |
|  |  |
|  |  |

Eq. 2‑22

### From the standard to the actual reference system

The orthonormal polynomials needed in our case are the one satisfying the following orthonormal condition:

|  |  |
| --- | --- |
|  |  |

Eq. 2‑23

Of course these are not available in the literature but generic forms are provided for standardized and support from which it is possible to derive the ones needed in the specific cases. In this specific case we need a set normal polynomials with respect to the class of weighting function represented by and constant values that respectively are given by the Hermite and Legendre polynomials. The expression of the first few term of their standard series is provided in Table 2 as well as the orthonormal conditions.

Table 2: Legendre and Hermite first term of the series

|  |  |  |
| --- | --- | --- |
| Order | Hermite | Legendre |
| 0 |  |  |
| 1 |  |  |
| 2 |  |  |
| 3 |  |  |
| Orthonormal condition |  |  |

The following coordinate change are applied to obtain the needed polynomials:

|  |  |
| --- | --- |
| Hermite | Legendre |
|  |  |
|  |  |

Eq. 2‑24

By applying this changes of coordinate in the orthonormal conditions it is possible to derive the relationship between the polynomials in the standard system and in the reference one.

*Hermite:*

First the transformation of coordinate is applied into the orthonormal condition for the standard system in Table 2:

To satisfy the relationship in Eq. 2‑23 have than to be expressed by:

.

Eq. 2‑25

is therefore orthonormal over with density function and is orthonormal over the standard norm with support are therefore defined by:

Eq. 2‑26

The derivation is tested checking the orthonormal condition for few moment integrals in appendix 1.

*Legendre:*

The standard Legendre polynomials from Table 2 re-casted following the coordinate transformation in Eq. 2‑24 leads to:

Eq. 2‑27

The normalization condition to satisfy Eq. 2‑23 is therefore met by posing:

Eq. 2‑28

is therefore orthonormal over with density function and

Eq. 2‑29

is orthonormal over with the standard measure.

It is required in this case to verify that =1:

Now that the new orthonormal polynomials have been defined by means of the polynomials in the reference system and the change of coordinates described by Eq. 2‑24 is done the expansion series becomes:

Eq. 2‑30

Where the moments are expressed by:

Eq. 2‑31

Eq. 2‑32

Table 3 reports the expression of the and for a generalized reference system.

Table 3: Expression for the first 3 orders of Hermite polynomials

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

### Numerical evaluation of the moment integrals

Collocation methods have the characteristics of not altering the solution scheme for introducing additional equations for the solution of its moments but rather reconstruct the moments from the knowledge of with to respect predetermined values of . Essentially collocation methods implements Gauss or Gauss like methodologies, with respect the polynomial basis, to compute the moment integrals. Here we will illustrate only the exact Gauss methodology that has been implemented into RAVEN.

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:

|  |  |
| --- | --- |
| Legendre | Hermite |
|  |  |

Eq. 2‑33

*Hermite:*

The first step is to recall the coordinate transformation provided by Eq. 2‑24 and the moment expression given at Eq. 2‑31

Combining the two and after few algebraic manipulation it is possible to recast the integral in a form compatible with the Gauss integration formula available.

If we assume , the quadrature formula we find is the following:

Eq. 2‑34

In Appendix 2, the analytical demonstration of the correctness of this derivation is reported, where the quadrature is used to integrate a few of the initial moments of the series.

Before moving forward there is an important remark to be made on the relationship between the number of points in the quadrature and the overall accuracy of the Fourier representation of the function. Let’s replace the expansion of in the moment integral expression:

From the last expression it could be seen that to compute accurately a moment of order the integrands needs to be of order . Given the rule that relates the number of point to the order of accuracy of any gauss rule the number of points needed are therefore:

Eq. 2‑35

This is of course a rule of general applicability for all Gauss derived quadrature rules, and therefore it will be not repeated for the Legendre based one.

*Legendre:*

Combining the transformation of coordinate (Eq. 2‑24) and the definition of the Gauss rule in Eq. 2‑33 for the Legendre polynomials we have:

Posing

Finally:

Eq. 2‑36

### Final numerical form

Replacing both expression of the numerical integration of the moments (Eq. 2‑34 and Eq. 2‑36) in the original expansion (Eq. 2‑30):

Eq. 2‑37

or using the polynomial expression in the reference system:

Eq. 2‑38

Where the coordinate mapping is of course:

### Mean Values

Starting from the definition of mean value and the definition of the orthonormal polynomials we can verify the relationship of the zero-th order moment and the mean value of the system response as computed in Eq. 2‑10.

*Hermite:*

Eq. 2‑39

*Legendre:*

Eq. 2‑40

# Appendixes

## Appendix 1: Orthonormal test of the Hermite Polynomial in the actual system

From the expression of the Hermite polynomials in the actual system given (Eq. 2‑26) as a function of the Hermite polynomials in the standard system reported in Table 2, it is possible to write:

Now the following tests will be performed:

*Test 1*

*Test 2*

*Test 3*

## Appendix 2: Test of the translation rule for the Gauss Hermite quadrature

The purpose of this test is to verify that if than its projection properly leads to and . For doing so we are going to use the Gauss-Hermite quadrature for which points and weight are given in Table 4.

Table 4: Points and Weights for the Gauss-Hermite quadrature formula

|  |  |  |
| --- | --- | --- |
| Points | Coordinate | Weight |
| 2 |  |  |
| 3 | 0 |  |
|  |  |

The problem could be formulated as follows:

Given: verify

It is convenient first to reformulate the Gaussian quadrature as follows:

The desired results follow immediately: