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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) program, has 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) [1] path. RISMC is one of the paths defined under the Light Water Reactor Sustainability (LWRS) DOE program [2].

One of the most challenging requests of the RISMC framework is a holistic estimation of margins, and therefore uncertainties, in Nuclear Power Plant (NPP) 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 [3] 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 [4] show the implementation in RAVEN of Monte Carlo sampling methodologies, and also dynamic event trees [5] . The next step of this strategy is described here and involves the implementation of the infrastructure to support the generalized Polynomial Chaos [6] methodology for uncertainty propagation.

In this report we 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

Of the large amount of literature on stochastic polynomials, a good starting point is provided by [6]. We present here a brief introduction is with focus on the implementation strategy.

In general any response **U** monitored of the plant (clad temperature, max pressure etc.) at a given point in time may 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 we 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 has already been assumed to be orthonormal. Than the expansion series is therefore similar to what found in the one-dimensional case:

in the norm,

and in the standard norm.

We find it 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 to zero whenever . If such a linear space exists then the effective dimensionality of the input space could be reduced and the study of the function could be correspondingly simplified. 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. For cases when the dimension of is rather large but strongly correlated, 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 a hierarchical system of equations with unknowns . 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 RELAP-7. Given that this second methodology relies on the knowledge of the only at selected points, it is named Collocation Generalized Polynomial Chaos [7].

Of course the choice of the points where the function is evaluated could be optimized to minimize the number of code runs needed, 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 (rounding ½ to 1 is the consequence of the number of point being an integer).

# 2D Application Example

It is useful to illustrate the methodology with a two dimensional example. Consider a system response mapped as a function of two random variates . Moreover, assume it is completely multiplicatively separable, so . The corresponding probability density, 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 conditions:

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

Eq. 2‑23

Since these are not available in the literature, 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 terms 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 changes are applied to obtain the needed polynomials:

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

Eq. 2‑24

By applying these changes of coordinate in the orthonormal conditions it is possible to derive the relationship between the polynomials in the actual 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 Eq. 2‑23 has to be expressed by:

.

Eq. 2‑25

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

Eq. 2‑26

This derivation is checked against the orthonormal condition for few moment integrals in appendix 1.

*Legendre:*

Re-casting the standard Legendre polynomials from Table 2 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 using the polynomials in the reference system using the change of coordinates described by Eq. 2‑24, 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 by introducing additional equations for the solution of its moments but rather reconstructing those moments from the knowledge of with respect to 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 is non-trivial and costly. Therefore it is useful to use existing external libraries. RAVEN makes use of numpy [8], which provides the points and weights for the standardized weighting and support functions. In this particular case numpy provides and that satisfy:

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

Eq. 2‑33

*Hermite:*

The first step is to recall the coordinate transformation (Eq. 2‑24) and the moment expression (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:

Eq. 2‑34

In Appendix 2, an analytical test 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

Substituting both expressions of the numerical integration of the moments (Eq. 2‑34 and Eq. 2‑36) into the original expansion (Eq. 2‑30) yields:

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 zeroth order moment and the mean value of the system response as computed in Eq. 2‑10.

*Hermite:*

Eq. 2‑39

*Legendre:*

Eq. 2‑40

# Application Demo

In order to test the capabilities introduced with the new Stochastic Polynomial approach, a simplified PWR PRA scenario is here presented. Figure 1 shows the scheme of the PWR model.

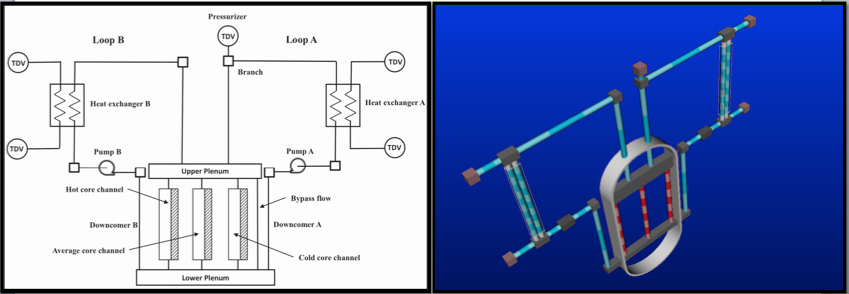


Figure 1 - PWR model scheme

The reactor vessel model consists of the Down-comers, the Lower Plenum, the Reactor Core Model and the Upper Plenum. Core channels (flow channels with heat structure attached to each of them) are used to describe the reactor core. The core model consists of three parallel core channels and one bypass flow channel. There are two primary loops, i.e., loop A and loop B. Each loop consists of the Hot Leg, a Heat Exchanger and its secondary side pipes, the Cold Leg and a primary Pump. A Pressurizer is attached to the Loop A piping system to control the system pressure. A Time Dependent Volume (pressure boundary conditions) component is used to represent the Pressurizer. Since the RELAP-7 code two-phase flow capability has not being used for this test, single-phase counter-current heat exchanger models are implemented to mimic the function of steam generators in order to transfer heat from the primary to the secondary. In the following paragraph, the PRA station black out sequence of events is reported.

## Station Black Out (SBO) scenario

The simulation of a SBO initiating event required the introduction, in the control logic, of several components (see Fig. 2):

* Set of 3 diesel generators (DGs) and associated emergency buses
* Primary power grid line 138 KV (connected to the NSST switchyard)
* Auxiliary power grid line 69 KV (connected to the RSST switchyard)
* Electrical buses: 4160 V (step down voltage from the power grid and voltage of the electric converter connected to the DGs) and 480 V for actual reactor components (e.g., reactor cooling system)

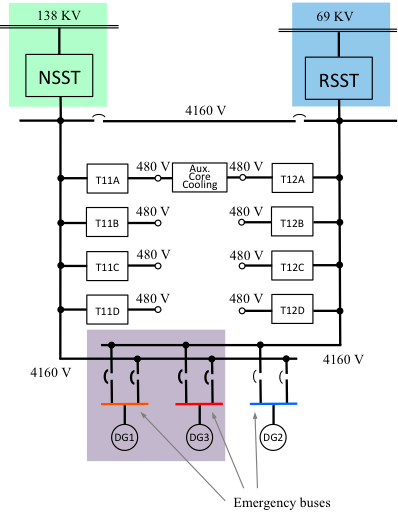


Figure 2 - Scheme of the electrical system of the PWR model

The scenario is the following:

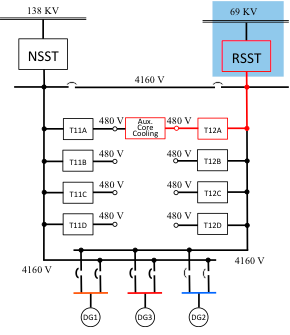
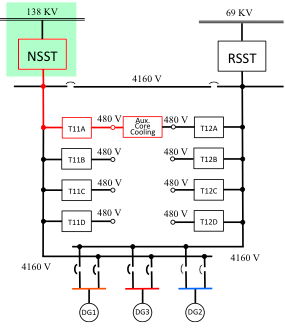
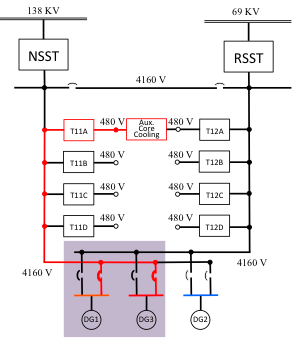
* An external event causes a loss of off-site power (LOOP) due to damage of the 138 kV line and RSST switchyard; the reactor successfully scrams and, thus, power generated in the core follows the characteristic exponentially decay curve
* The set of DGs fails to start and, hence, conditions of SBO are reached (4160 V and 480 V buses are not energized); all cooling systems are subsequently off-line
* Without the ability to cool the reactor core, its temperature starts to rise
* In order to recover AC electric power on the 4160 V and 480 V buses, two recovery teams  are assembled with the following strategy:
* Recovery Team 1 focuses on the recovery of the DGs: due to internal damage at the DG building, two DGs (i.e., DG1 and DG3) need to be repaired (see Fig. 3 (a))
* Recovery Team 2 focuses on the recovery of the RSST switchyard; 69KV line is energized but the RSST switchyard needs to be recovered (see Fig. 3 (b))
* Meanwhile the owning company is working on the restoration of the primary 138 KV line (see Fig. 3 (c))
* When the 4160 V buses are energized (through the recovery of the DGs, RSST or 138KV line), the auxiliary cooling system is able to cool the reactor core and, thus, core temperature decreases.

Given the uncertainties associated to the recovery of both DGs, RSST and 138KV line, a stochastic model has been used to represent these events. Given the time scale associated to the dynamics of the RELAP-7 PWR model the corresponding probability distribution functions were as follows:

* DGs: a dead time of 100s is required by Team 1 to gather at the DGs building and DG1 repair time *T DG1* has a normal distribution having mu = 800 and sigma = 200. This distribution is also truncated such that 0 < *T DG1* < 2500. The recovery time of DG3, TDG3 , is proportional to *T DG1.* Such relation has modeled using a multiplication factor T12, i.e., *T DG3* = *T DG1* × *T* 12. T12 is uniformly distributed between [0.5 1]
* RSST: a dead time of 400s is needed to assess the damage at the RSST switchyard and to plan its recovery. Recovery time for RSST, TRSST, is normally distributed with mu = 1400 and sigma = 400
* 138KV line: the recovery of the main AC line T138 is normally distributed with mu = 2000 and sigma = 500

(a) (b) (c)

Figure 3 - AC power recovery paths through: DGs (a), RSST (b) and 138 kV line (c). Red lines indicate electrical path to power Aux cooling system



## Analysis specifications

The set up of the methodology has been performed using uniform distributions (characterized by the same mean of previously mentioned one), associating third order polynomials to them. This choice has been taken in order to guarantee that the min

Based on the eq. 2.35, the histories (RAVEN/RELAP-7 simulations) that have been needed to run, in order to set the stochastic polynomial method up, are 256. In this analysis, the outcome of interest is the maximum temperature of the CLAD. In order to assess the accuracy of the method, two sets of Monte-Carlo simulations have been performed, one using the system code (RAVEN/RELAP-7) and the other one using the Reduced Order Model (ROM), based on the stochastic polynomial method previously set up. The results of this comparative analysis are reported in the following paragraph.

## Results

# Reference:

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# 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: