PCT Uncertainty Analysis Using Unscented Transform with Random Orthogonal Matrix

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1. Introduction

Most Best Estimate Plus Uncertainty (BEPU) methods employ nonparametric order statistics through Wilks' formula to quantify uncertainties of best estimate simulations of nuclear power plant (NPP) transients. 95%/95% limits, the 95th percentile at a 95% confidence level, are obtained by randomly sampling all uncertainty contributors through conventional Monte Carlo (MC). Advantages are simple implementation of MC sampling of input probability density functions (pdfs) and limited computational expense of 1^{st} , 2^{nd} , and 3rd order Wilks' formula requiring only 59, 93, or 124 simulations, respectively. A disadvantage of small sample size is large sample to sample variation of statistical estimators. The statistical fluctuation of 1st order Wilks' limits can be as large as the uncertainty value itself in BEPU applications [1]. Wilks' 95%/95% limits may be satisfactory for meeting regulatory requirements but do not accurately characterize the true safety margin.

This paper presents a new efficient sampling based algorithm for accurate estimation of mean and variance of the output parameter pdf. The algorithm combines a deterministic sampling method, the unscented transform (UT), with random sampling through the generation of a random orthogonal matrix (ROM). The UT guarantees the mean, covariance, and 3rd order moments of the multivariate input parameter distributions are exactly preserved by the sampled input points and the orthogonal transformation of the points by a ROM guarantees the sample error of all 4th order and higher moments are unbiased. The UT with ROM algorithm is applied to the uncertainty quantification of the peak clad temperature (PCT) during a large break loss-ofcoolant accident (LBLOCA) in an OPR1000 NPP to demonstrate the applicability of the new algorithm to BEPU.

2. UT and ROM Algorithm

2.1 Unscented Transform

The UT was developed in the context of extending the Kalman Filter (KF) to nonlinear system dynamics [2]. The KF is one of the most widely used predictorcorrector algorithms used to estimate the mean and covariance of system states of dynamic systems defined by linear process and observation models subject to noise. The KF would break down when applied to nonlinear systems so the UT was developed as a computationally efficient method to predict statistical properties of random variables transformed through nonlinear functions. The UT only requires sample sizes on the order of two times the number of input variables.

The UT generates input samples referred to as sigma points from the *n*-dimensional input joint pdf defined by the mean vector $\overline{\mathbf{x}} = [\mu_1, \mu_2, ..., \mu_n]^T$ and covariance matrix **P**. The sigma point set is symmetric with a central point for a total of 2n+1 points

$$\boldsymbol{x}^{(0)} = \overline{\boldsymbol{x}} \tag{1}$$

$$\boldsymbol{x}^{(i)} = \overline{\boldsymbol{x}} + \left(\sqrt{(n+k)\boldsymbol{P}}\right)_{i} \tag{2}$$

$$\boldsymbol{x}^{(i+n)} = \overline{\boldsymbol{x}} - \left(\sqrt{(n+k)\boldsymbol{P}}\right)_i.$$
(3)

To obtain estimates of mean and variance of the output y, the sigma points are propagated through the nonlinear function $h(\mathbf{x})$ representing a computer code or model

$$y^{(i)} = h(\boldsymbol{x}^{(i)}). \tag{4}$$

Sample mean and variance are calculated

$$\bar{y}_u = \sum_{i=0}^{2n} W_i y^{(i)}$$
(5)

$$P_{u} = \sum_{i=0}^{2n} W_{i} (y^{(i)} - \bar{y}_{u}) (y^{(i)} - \bar{y}_{u})^{T} .$$
 (6)

The UT weighting coefficients are

$$W_0 = k/(n+k) \tag{7}$$

$$W_i = 1/[2(n+k)]$$
 $i = 1, ..., 2n$. (8)

The variable k appearing in the sigma point and weight equations is a free scaling parameter.

In Eqs. 2 and 3, the i^{th} and $(i+n)^{th}$ sigma points are obtained from the i^{th} column of a matrix square root of the covariance matrix. All covariance matrices are square, positive semi-definite, and symmetric so P can be diagonalized through eigen decomposition

$$\boldsymbol{P} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^{-1} \ . \tag{9}$$

U is an (nxn) orthogonal matrix and the columns u_i are the eigenvectors of *P*. An orthogonal matrix is defined as a square matrix whose columns and rows are orthonormal vectors such that $UU^T = U^T U = I_n$ where I_n is the (nxn) identity matrix. The columns of *U* are an orthonormal basis of \mathbb{R}^n . The transpose of an orthogonal matrix is equal to its inverse $U^T = U^{-1}$. *A* is a (nxn) diagonal matrix with elements $\Lambda_{ii} = \lambda_i$, the eigenvalues of *P*. The eigenvectors and eigenvalues satisfy $Pu_i = \lambda_i u_i$. The matrix square root of Λ is the diagonal matrix $\sqrt{\Lambda}$ with nonzero entries $\sqrt{\Lambda}_{ii} = \sqrt{\lambda_i}$ which satisfies $\Lambda = \sqrt{\Lambda}\sqrt{\Lambda}^T$ and $\sqrt{\Lambda} = \sqrt{\Lambda}^T$.

Equation 9 is recast as

$$\boldsymbol{P} = \boldsymbol{U}\sqrt{\boldsymbol{\Lambda}}\sqrt{\boldsymbol{\Lambda}}\boldsymbol{U}^{-1} , \qquad (10)$$

and the matrix square root of \boldsymbol{P} is readily obtained as

$$\sqrt{P} = U\sqrt{\Lambda} . \tag{11}$$

The eigenvectors from \boldsymbol{U} define the principal axes of the covariance matrix so the UT selects the scaled principal axes as sigma points. The sample covariance of the sigma points exactly matches P because the scaled principal axes correctly encode all of the covariance information. If the input pdfs are symmetric such as Gaussian or uniform distributions, the 3rd order moments will also be matched exactly because the sigma point set is symmetric. Error is introduced in the 4^{th} order sample moments and the parameter k can be selected to reduce the error based on pdf type. The UT is a deterministic sampling algorithm due to Eqs. 1 - 8and deterministic nature of matrix eigen decomposition methods such as singular value decomposition (SVD) or Cholesky decomposition used to calculate the matrix square root.

2.2 Orthogonal Transform of Matrix Square Root

The matrix square root of Eq. 11 obtained through a deterministic eigen decomposition method is only one particular square root of P. Next we show that an infinite number of matrix square roots exist for a covariance matrix by multiplying the right hand side of Eq. 11 by any arbitrary orthogonal matrix Q that is the same size as P

$$\sqrt{P} = U\sqrt{\Lambda}Q . \tag{12}$$

Substituting Eq. 12 into Eq. 10 and applying some matrix multiplication properties

$$P = U\sqrt{\Lambda}Q(U\sqrt{\Lambda}Q)^{T} = U\sqrt{\Lambda}QQ^{T}\sqrt{\Lambda}^{T}U^{T}$$
$$= U\sqrt{\Lambda}I\sqrt{\Lambda}^{T}U^{T} = U\Lambda U^{-1} = P.$$
(13)

Equation 12 is the general form of the matrix square root and is acceptable for use in Eqs. 2 and 3. The orthogonal transformation of the matrix square root does not change the 2^{nd} order properties of the sigma point set but can have profound effects on the 4^{th} moment error terms. The accuracy of the UT using various orthogonal transforms and parameter *k* was studied in [3].

2.3 Random Orthogonal Matrix

ROMs arise from random matrix theory, a large topic in theoretical mathematics with applications in quantum mechanics, statistics, encryption, and computer science [4]. A ROM is a random matrix from the orthogonal group O_n and is Haar distributed. Specifically, the matrix entries of a ROM are jointly distributed as Gaussian variables with variance n^{-1} as the dimension of the matrix becomes large. Because ROMs are orthogonal matrices, the columns of a ROM are an orthonormal basis of \mathbb{R}^n . The individual matrix entries behaving statistically as random samples from the joint Gaussian coupled to the orthogonal structure of the matrix columns results in a powerful mathematical tool that is simultaneously random and structured with orthogonal properties. As a linear transformation, a ROM can be interpreted multi-dimensional rotation to a new coordinate system that is at a random orientation to the original frame of reference. Alternatively, the ROM is *n* random data samples drawn from an *n*-dimensional Gaussian with variance n^{-1} .

ROMs can be easily generated by performing SVD on any (nxn) matrix A that has matrix entries generated from random sampling of the standard normal distribution. The SVD of A is

$$\boldsymbol{A} = \boldsymbol{S}\boldsymbol{\Sigma}\boldsymbol{V}^T \ . \tag{14}$$

S and **V** are both (nxn) ROMs and **\Sigma** is diagonal. Recognizing Gaussian distributions are invariant under linear transformations, the Gaussian property is demonstrated by rearranging Eq. 14

$$\boldsymbol{S} = \boldsymbol{A} \boldsymbol{V} \boldsymbol{\Sigma}^{-1} \ . \tag{15}$$

The matrix **A** is distributed according to the standard normal distribution and undergoes two linear transformations **V** and Σ^{-1} so the resulting matrix **S** must also be Gaussian distributed. If SVD is applied to a symmetric matrix such as a covariance matrix, Eq. 14 is equivalent to Eq. 9 with S = V defining the principal axes and Σ are the eigenvalues.

2.4 Incorporating ROM into UT

If a ROM is used as Q, Eq. 12 can be interpreted as a random multi-dimensional linear transformation of principal axes. Alternatively, Eq. 12 can be viewed as random data points from a Gaussian with variance n^{-1} undergoing linear transformations to become aligned with the principal axes of the target covariance matrix. The latter interpretation when considered in the context of Eqs. 2 and 3 with k = 0 involves the scaling of the random points such that they become white Gaussian points. Thus the sigma points are random points that are guaranteed to match the target covariance matrix exactly. Since the sigma points are random, the sample 4th order moment including the cross product terms will be unbiased estimates of the moments from a Gaussian.

The Gaussian property of ROMs is an asymptotic property so for small n the dimension of the problem may need to be increased by augmenting the input vector by hidden noise variables v

$$\boldsymbol{x}_* = \begin{bmatrix} \boldsymbol{x} \\ \boldsymbol{v} \end{bmatrix}. \tag{16}$$

The input covariance matrix must also be augmented

(1)	Р	Construct $n \times n$ covariance matrix P from <i>n</i> input PDFs		
(2)	$\boldsymbol{P}_* = \begin{bmatrix} \boldsymbol{P} & \boldsymbol{0}_{n \times m} \\ \boldsymbol{0}_{m \times n} & \boldsymbol{I}_m \end{bmatrix}$	Augment input vector and covariance matrix with <i>m</i> white Gaussian noise variables $v \sim N(0,1)$: $\mathbf{x}_* = [\mathbf{x}^T v^T]^T$, $n_* = n + m$		
(3)	$P_* = U\sqrt{\Lambda}\sqrt{\Lambda}U^{-1} \sqrt{P_*} = U\sqrt{\Lambda}$	Perform eigen decomposition on P_* to obtain the matrix square root $\sqrt{P_*}$ from eigenvectors and eigenvalues of P_*		
(4)	$\sqrt{(n_*+k)\boldsymbol{P}_*}\boldsymbol{Q}$	Scale matrix square root by factor $\sqrt{(n_* + k)}$ and multiply by a randomly generated $n_* \times n_*$ orthogonal matrix Q		
(5)	$\boldsymbol{x}^{(0)} = \overline{\boldsymbol{x}}, \ \boldsymbol{x}^{(i)} = \overline{\boldsymbol{x}} \pm \widetilde{\boldsymbol{x}}^{(i)}$ $\widetilde{\boldsymbol{x}}^{(i)} = \left(\sqrt{(n_* + k)\boldsymbol{P}_*}\boldsymbol{Q}\right)_{1:n,i}$	Generate $(2n_* + 1)$ sigma points from columns and first <i>n</i> rows of $\sqrt{(n_* + k)P_*}Q$		
(6)	$\{y^{(0)}, y^{(1)}, \dots, y^{(2n_*)}\}$	Perform code simulations at sigma point inputs: $y^{(i)} = h(\mathbf{x}^{(i)})$		
(7)	$\overline{y}_{u} = \sum_{i} W_{i} y^{(i)}, P_{u} = \sum_{i} W_{i} (y^{(i)} - \overline{y}_{u}) (y^{(i)} - \overline{y}_{u})^{T}$	Calculate UT estimates of mean and variance using UT weights		

Table I.	Improved	Unscented	Transform	using Input	Vector Augmenta	ation and Random	Orthogonal Matrix
	1			01	U		0

$$\boldsymbol{P}_* = \begin{bmatrix} \boldsymbol{P} & \boldsymbol{0}_{n \times m} \\ \boldsymbol{0}_{m \times n} & \boldsymbol{I}_m \end{bmatrix}.$$
(17)

When sigma points are generated using the matrix square root of P_* , rows n+1 through n+m of the matrix square root are suppressed because the noise variables are not actual model inputs. The ROM generated is increased in size to (n+m)x(n+m). For approximately n < 25, a ROM will systematically underestimate the kurtosis of the Gaussian distribution so we recommend augmenting such that the total dimension n_* is at least 25 to 50 variables and the number of sigma points is 50 to 100 which is the same order of magnitude computational expense as lower order Wilks' formula. The UT with ROM algorithm is summarized in Table I.

Input augmentation was first suggested in [5] as a method to improve accuracy of the UT for low dimensional problems with highly nonlinear functions. By adding additional sigma points, the higher order terms are better characterized. The practical advantage of using a ROM with the UT is all input dimensions are simultaneously and randomly varied for every sigma point. When combined with input vector augmentation, all 4th order moment errors can be guaranteed to be unbiased improving performance for any arbitrary nonlinear function whereas some deterministic orthogonal transforms presented in [3] will introduce systematic error in some 4th order terms of the function are important.

3. PCT Uncertainty Analysis

In this section we evaluate the uncertainty of the blowdown PCT during a LBLOCA in a pressurized water reactor using the UT with ROM algorithm. The LBLOCA is an extensively studied design basis accident in the context of BEPU and provides a benchmark for the new algorithm in best estimate reactor safety simulation applications.

3.1 MARS Model for LBLOCA and Input Parameters

The MARS code version KS1.3 [6] is used to simulate the cold leg 200% doubled ended guillotine break with the Ulchin Units 3&4 (UCN3&4) input model [7] as a representative OPR1000. The reactor core is modeled with two coolant channels representing the hot rod channel and a core-averaged rod channel. Each channel has 12 axial nodes and the power distribution is set as the top-skewed cosine shape specified for the LBLOCA analysis in the Final Safety Analysis Report [8]. For the hot rod channel, the linear heat generation rate in node 8, the power peak location, is set to the limiting condition of operation of 13.9 kW/ft.

Relevant thermal hydraulic phenomena, processes, and input parameter uncertainties are identified in the phenomena identification ranking table and assessment and ranging of parameters steps of BEPU methods. For the blowdown PCT, the stored energy in the fuel rod, heat transfer coefficients, counter current flow limitation (CCFL) and reactor coolant pump two phase flow performance are important phenomena. Table II list 22 input parameters and associated pdfs to be sampled by the UT with ROM for uncertainty quantification of the blowdown PCT. The parameters and uncertainty information were adapted from other LBLOCA studies related to the OPR1000 and the MARS code [9].

3.2 UT PCT Results and Comparison to MC Sampling

With 22 input parameters, the UT with ROM algorithm should be able to accurately estimate the mean and variance of the blowdown PCT using a

minimum of 44 MARS simulations. To minimize systematic error in the 4th central moments of the input pdfs, the sigma point set should contain at least 50 to 100 data points requiring the augmentation of the input vector with at least 3 noise variables. Ten sigma point sets are generated using different ROMs. Eight sets are augmented with 3 noise variables and two sets augmented with 16 and 28 noise variables for sample sizes of 50, 76, and 100 simulations. An additional 2500 MC simulations are performed to provide a numerical benchmark for the UT PCT mean and variance estimates. All simulations are run in batches with scheduling arranged by the MOSAIQUE software [10].

Table II lists 9 variables that are uniform distributions. A complication arises with the sample 4th order moments of the uniform variables becomes the statistical properties of the ROM guarantees all variables are Gaussian distributed. The kurtosis of the uniform variables would be systematically overestimated because kurtosis of uniform distribution is 9/5 compared to 3 for Gaussian distribution. The inverse cumulative distribution function (cdf) transform is applied to the rows of the ROM corresponding to the uniform variables as a convenient way to ensure the these sigma points are statistically distributed as uniform. The Gaussian to uniform cdf transform is nonlinear so there is a slight loss of orthogonality introducing small error in the variance of the uniform variables.

Figure 1 shows the PCT pdf generated from the 2500 MC simulations. The sample mean is 1167.1 K and the variance is 2900 K^2 corresponding to a standard deviation of 53.8 K. The 95th percentile is 1264.8 K. Table III presents the UT with ROM estimates of the

PCT mean and variance from the 10 sigma point sets. The variances are reported as standard deviations. UT sample 9 is the 100 sigma point sample generated from a 50x50 ROM and sample 10 is the 76 sigma point sample generated from a 38x38 ROM. For comparison, 9 MC samples of 50 simulations each are included in Table III. The MC samples are subsets of the 2500 MC sample drawn at random.

All 10 UT estimates of the PCT mean are very close to the MC benchmark estimate. All UT estimates of the PCT standard deviations are also very close to the MC estimate. The UT with ROM samples show very little sample to sample variation of mean and variance estimates indicating the improved UT algorithm is statistically robust despite relatively small sample size with a large number of input variables. On the other hand, the 50 sample MC subsets estimators show large sample to sample variation which is expected of MC samples of limited size.

With regard to the 95th percentile and 1477 K PCT limit from 10CFR50.46 commonly regulatory considered in BEPU, the UT mean and variance estimates do not conclusively determine whether the regulatory acceptance criteria are met. Considering the data from UT sample 1, the 1477 K limit is 5.7 standard deviations from the mean. Exceeding the safety limit could be viewed as a "six sigma event" with very low probability for this example. Since the two methods require the same magnitude of computational cost, UT with ROM could be incorporated into BEPU as a complimentary approach to Wilks' formula providing additional reliable uncertainty information, mean and variance, to supplement 95%/95% limits providing a more definite statement of safety margin.

Code	Independent parameter	Distribution	me an/min	σ/max	
Input <i>x</i> _i	independent parameter	Distribution	ine an/inin		
1	Gap Width	uniform	0.05 mm	0.134 mm	
2	Cladding Roughness	normal	0.5 µm	0.3 µm	
3	Pellet Roughness	normal	2 µm	0.5 µm	
4	Rod Internal Pressure	uniform	2 Mpa	15 Mpa	
5	Fuel Thermal Conductivity	normal	1	10%	
6	Fuel Heat Capacity	normal	1	10%	
7	Cladding Thermal Conductivity	normal	1	12%	
8	Cladding Heat Capacity	uniform	90%	110%	
9	D-B Liquid HT Multiplier	normal	1	10%	
10	Chen's Nucleate Boiling HT Multiplier	normal	1	11.6%	
11	AECL lookup CHF Multiplier	normal	1	37%	
12	Transition Boiling Multiplier	normal	1	16%	
13	Film Boiling HT Multiplier	normal	1	18%	
14	D-B Vapor HT Multiplier	normal	1	10%	
15	Pump 2-1 Phase Head Multiplier	uniform	0	1	
16	Pump Torque Multiplier	uniform	0	1	
17	Pump Inlet K-factor	uniform	0.02	0.8	
18	Pump Momentum of Inertia	uniform	4487.2 kg/m2	5484.4 kg/m2	
19	CCFL Model	uniform	0	1	
20	Operating Plant Power	normal	2815 MWt	2%	
21	Power Peaking Factor Fq	uniform	1.5054	1.7147	
22	Decay Heat Multiplier	normal	1.02	3%	

Table II. MARS Input Parameters and Distributions for Blowdown PCT Analysis



Fig. 1. PCT pdf from 2500 MC MARS simulations.

Sample #	Mean (K)	STD (K)	Sample #	Mean (K)	STD (K)
UT 1 (50)	1168.1	53.8	MC 1 (2500)	1167.1	53.8
UT 2 (50)	1168.2	51.2	MC 2 (50)	1174.0	50.2
UT 3 (50)	1167.1	56.1	MC 3 (50)	1170.4	50.6
UT 4 (50)	1168.2	55.2	MC 4 (50)	1165.9	63.0
UT 5 (50)	1168.4	54.3	MC 5 (50)	1162.7	52.3
UT 6 (50)	1166.8	52.8	MC 6 (50)	1165.6	51.4
UT 7 (50)	1167.8	53.2	MC 7 (50)	1176.6	53.9
UT 8 (50)	1168.5	53.3	MC 8 (50)	1167.9	36.6
UT 9 (100)	1168.2	54.7	MC 9 (50)	1167.8	44.7
UT 10 (76)	1167.4	52.6	MC 10 (50)	1162.5	49.2

Table III. PCT Mean and Variance Estimates

4. Conclusions

This paper presented a new algorithm combining the UT with ROM for efficient multivariate parameter sampling that ensures sample input covariance and 3^{rd} order moments are exactly preserved and 4^{th} moment errors are small and unbiased. The advantageous sample properties guarantee higher order accuracy and less statistical variation of mean and variance estimates of the output pdf. For BEPU applications where on the order of 20 to 50 input parameter uncertainties are usually sampled, the UT with ROM requires the same order of magnitude of best estimate code simulations as the widely used Wilks' formula.

In addition to BEPU, the UT with ROM may be a useful sampling algorithm in other nuclear applications involving computer codes and uncertainties. One future area of research is nuclear data uncertainty propagation in neutronics calculations. Cross section uncertainties are conveniently available as covariance data in the evaluated nuclear data files so the UT only requiring covariance information appears to be an appropriate method. With many isotopes, reaction types, and fine and ultra-fine energy group libraries, application of the UT with ROM to cross section uncertainties could involve interesting computer science aspects involving matrix decomposition of very large covariance matrices and generation of very large ROMs.

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